Large deformations, rheology, plasticity

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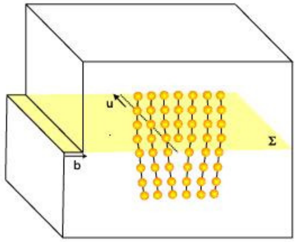
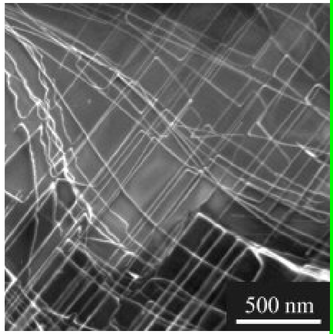
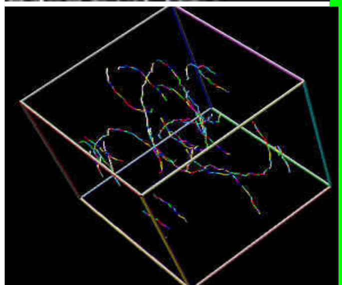
Overview

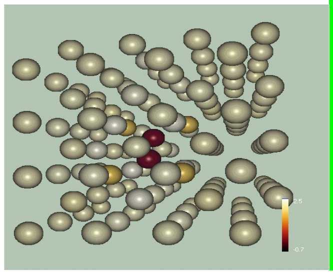
- **Introduction: soft and hard amorphous systems, rheology, elasticity, plasticity**
- Models : mean field models, discrete elements
- Atomic scale simulations

Multiscale approach ?









Flow of crystalline solids:

- **flow defects identified (dislocations, Volterra 1930), seen by TEM (1960)**
- **interaction and motion understood (Peierls, Nabarro, Friedel, 1950)**
- **dislocation dynamics in computer codes (1980)**

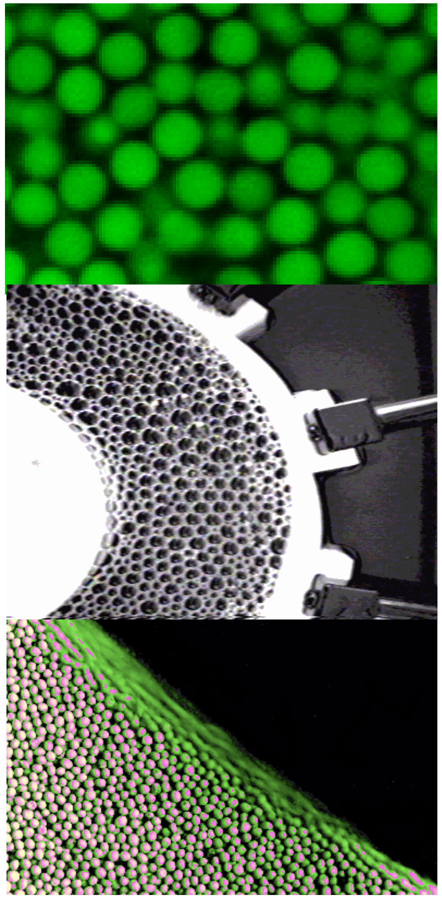
Flow of amorphous solids:

•Flow defects ?

•Interaction and Motion??

•Mesoscale codes ???

Soft amorphous systems

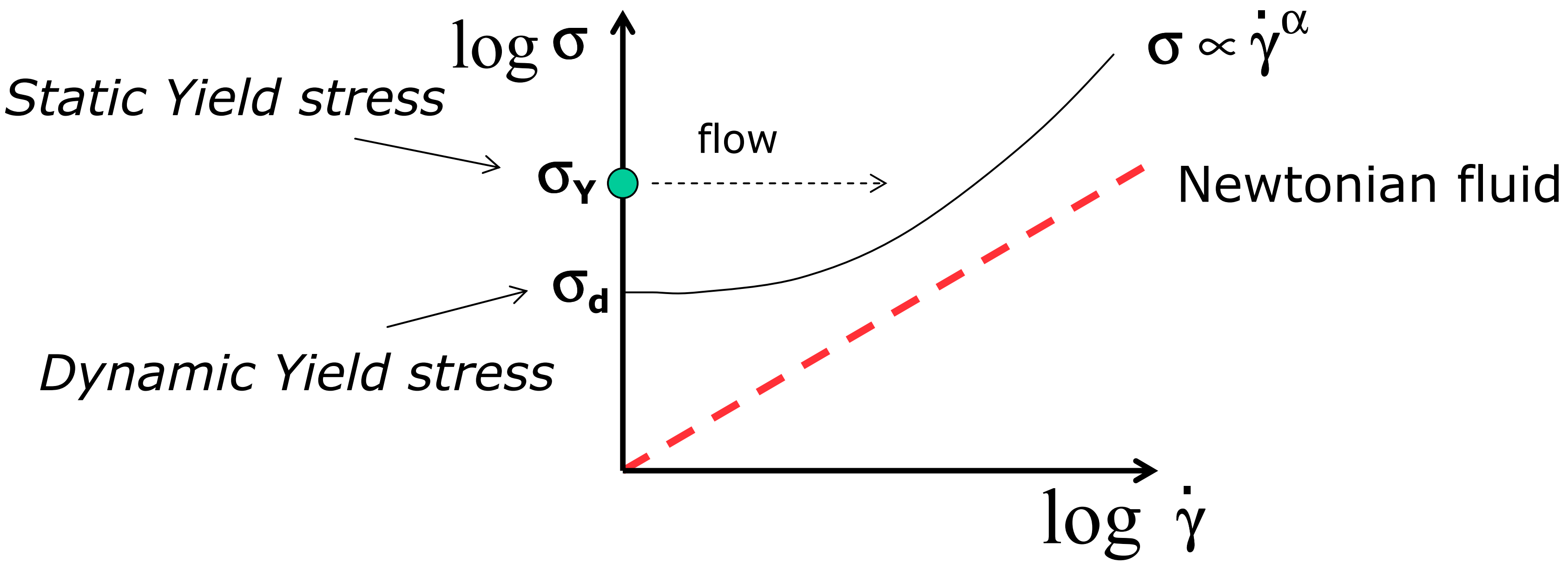


- Colloidal pastes, complex fluids
- Foams
- Granular systems

- Structurally disordered materials
- Solid like behavior until yield stress/strain is reached
- Flow easily under moderate stresses (Pa to kPa)

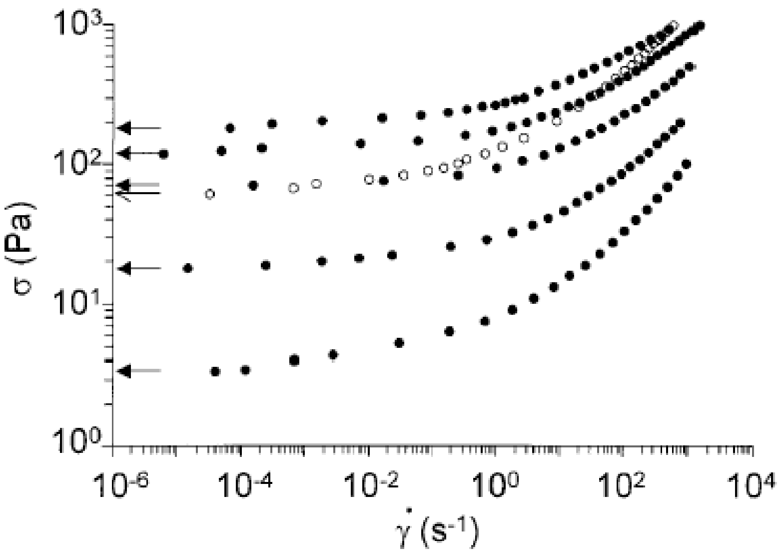
Characterized by flow curve: (shear) stress vs strain rate in steady shear

Non-linear rheology and yield stress(es):



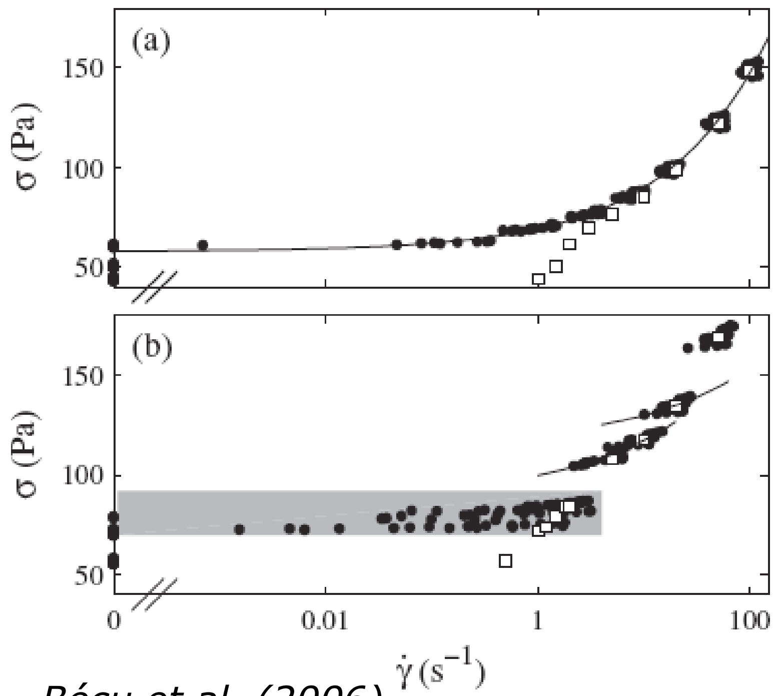
Some examples

Polyelectrolyte gels



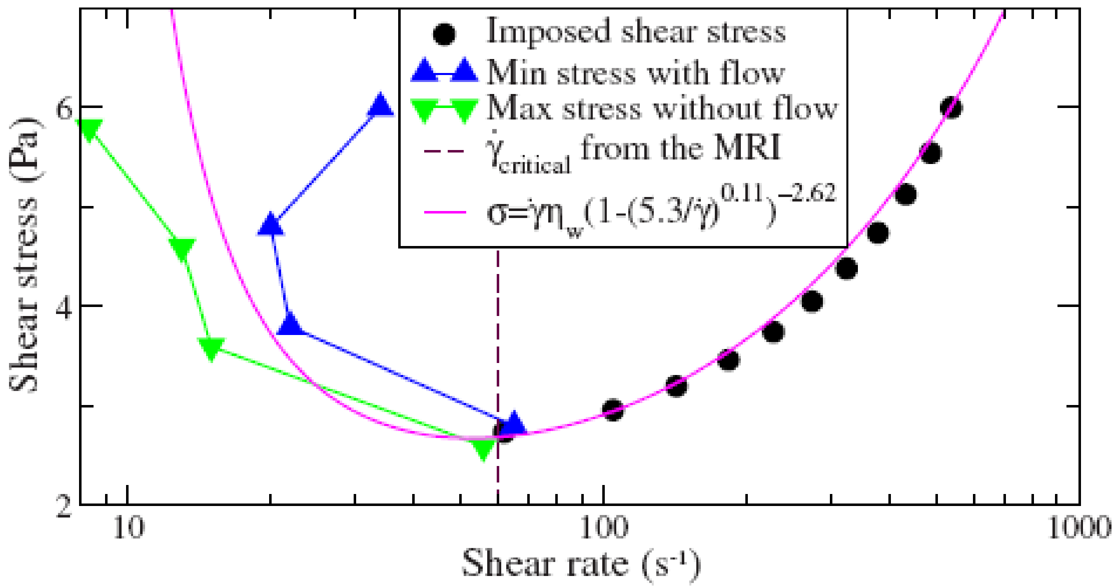
Cloitre et al. (2003)

Emulsions



Bécu et al. (2006)

Possibility of an unstable branch on the flow curve (carbopol)

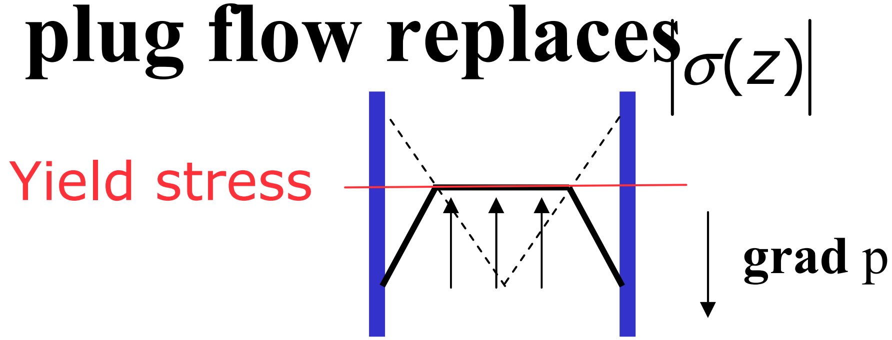


PHYSICAL REVIEW E 77, 041507 (2008)

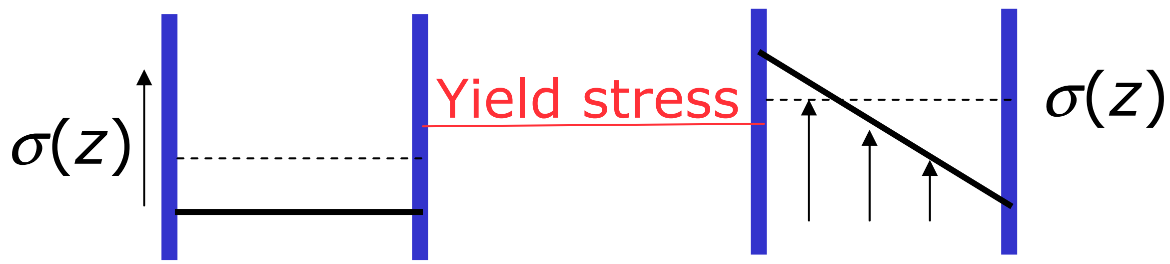
P. C. F. Møller,[1] S. Rodts,[2] M. A. J. Michels,[3] and Daniel Bonn[1,4]

Flow behavior for yield stress fluids (velocity profiles)

- **Pressure driven flow: plug flow replaces parabolic profile**



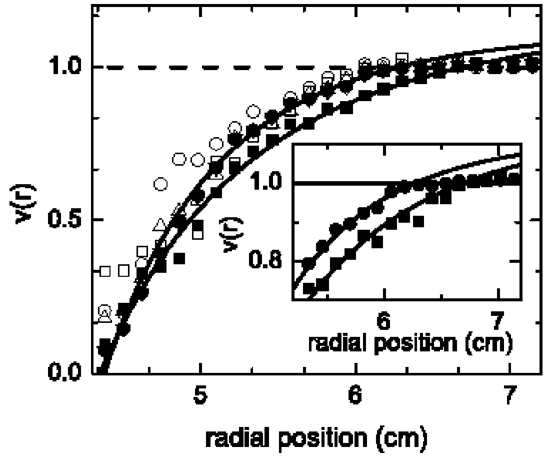
- **Simple shear flow**



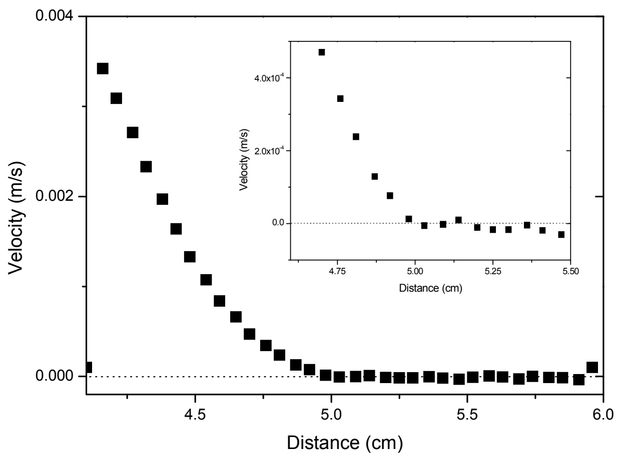
$\sigma(z) < Yield\ stress$ $\sigma(z) > Yield\ stress$

Very often flow is heterogeneous even in simple shear (*shear banding* or *strain localisation*)

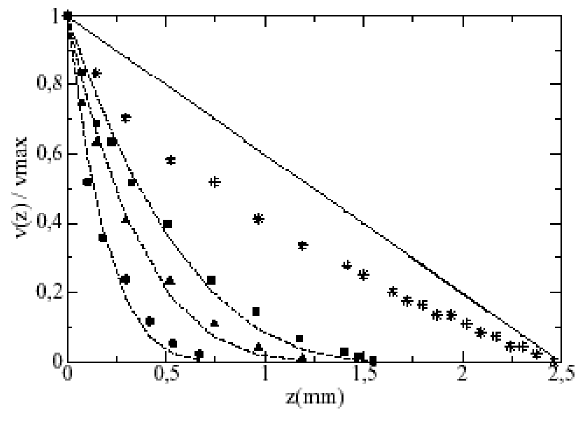
Bubble Rafts
(Dennin *et al.*, 2004)



Chocolate
(Coussot *et al.*)

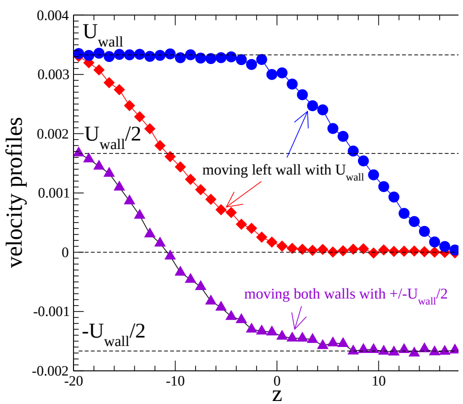


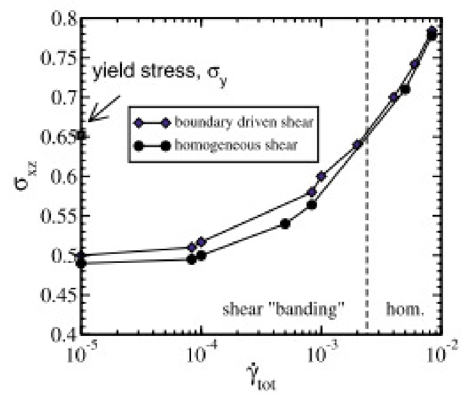
Granular pastes
(Barentin et al., 2003)



Lennard-Jones glass
(Simulation, Varnik, Bocquet, JLB, 2004)

« Explained » by static vs dynamic yield stress





« Hard » amorphous systems

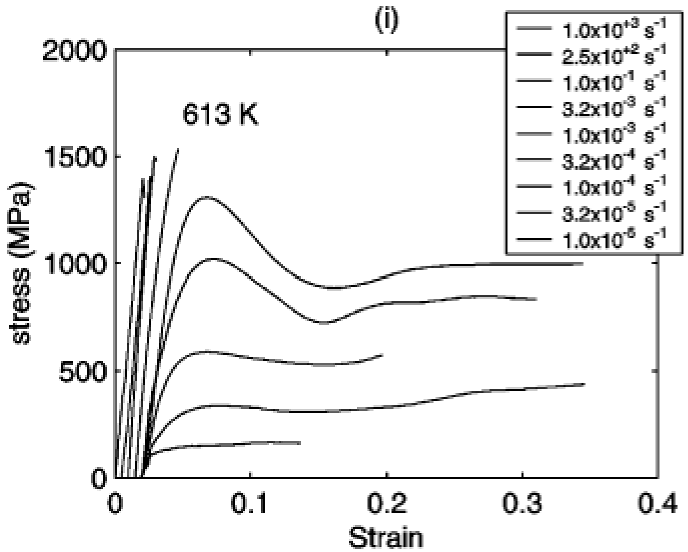
- Metallic glasses
- Polymer glasses
- Oxide glasses

Stress-Strain curves rather than flow curves (tensile, compressive, uni/tri-axial..)

Elastic, solid like behavior until yield stress/strain is reached

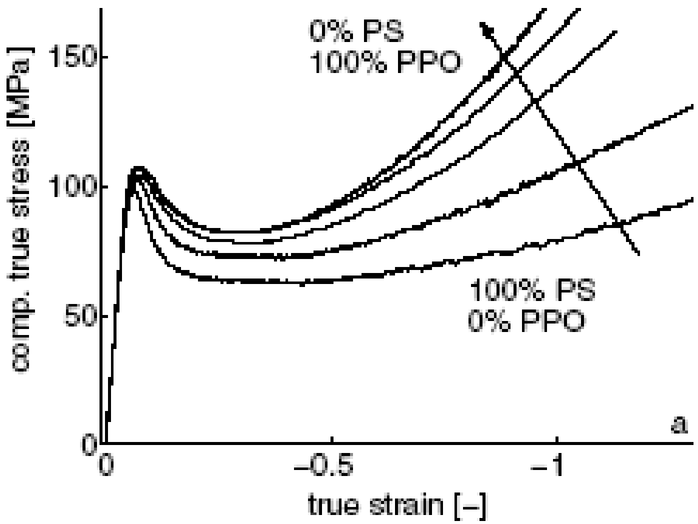
Plastic flow observed before breaking

Stress strain curves at imposed strain rate



Bulk metallic glass

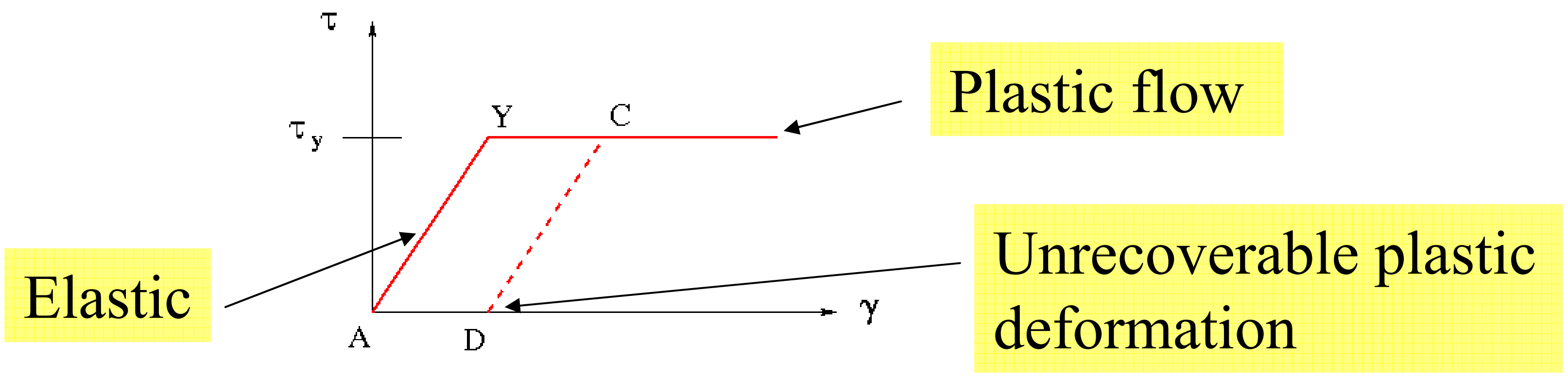
(Johnson, UCLA)



Polymers (VanMelick, Eindhoven)

Rate and temperature effects are important

Ideal elastoplastic behaviour



To observe plastic flow, it is necessary

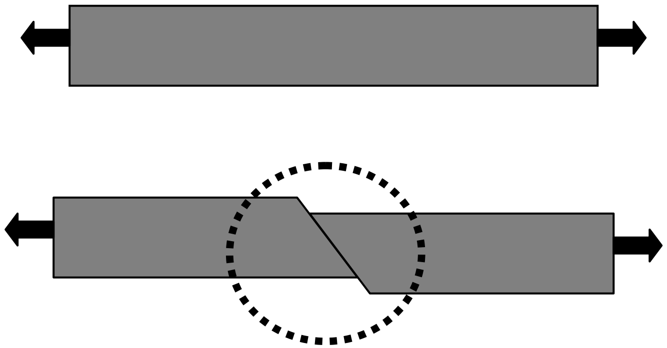
- to avoid fracture
- to avoid shear banding or strain localisation (or to have access to the strained region)

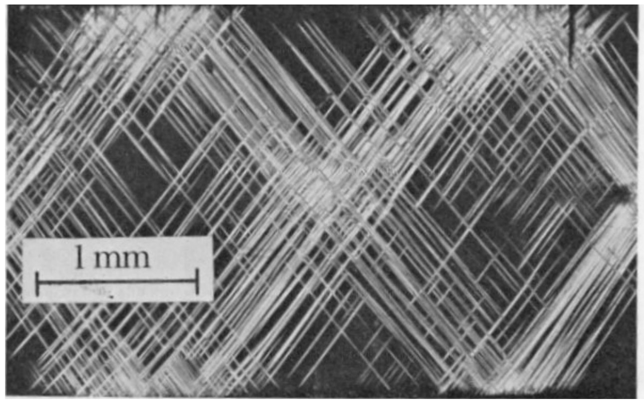
This is possible in practice in:

- Polymer glasses (close to T_g)
- Metallic glasses (close to T_g)
- **simulation**

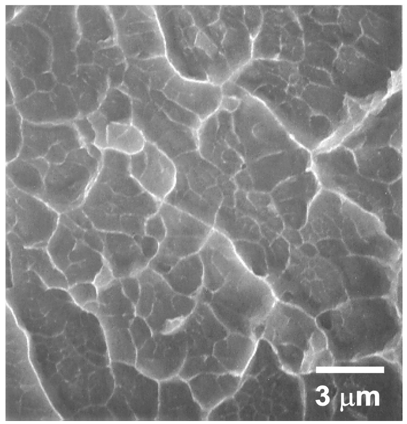
Strain localisation in hard materials

glassy polymers (Jukes, 1969)





Metallic glass



Stress-strain curves can also be monitored in « soft » systems (shear deformation)

=> models for « hard » systems (Bragg 1930, Argon 1975)

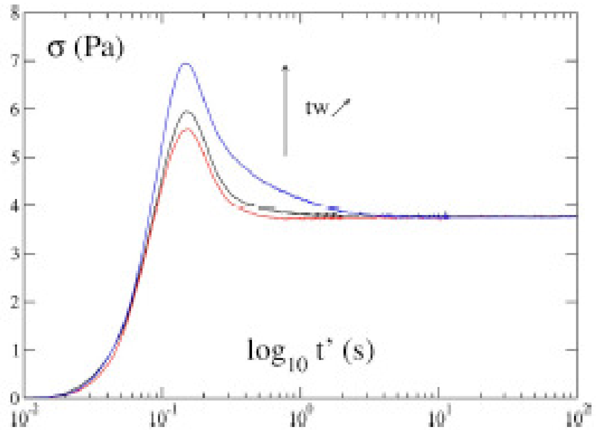
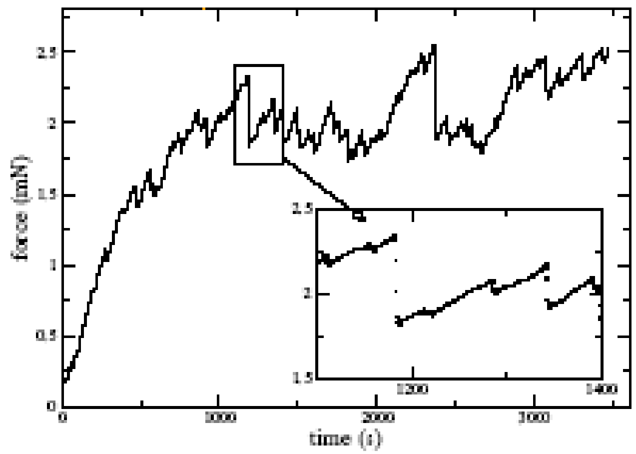


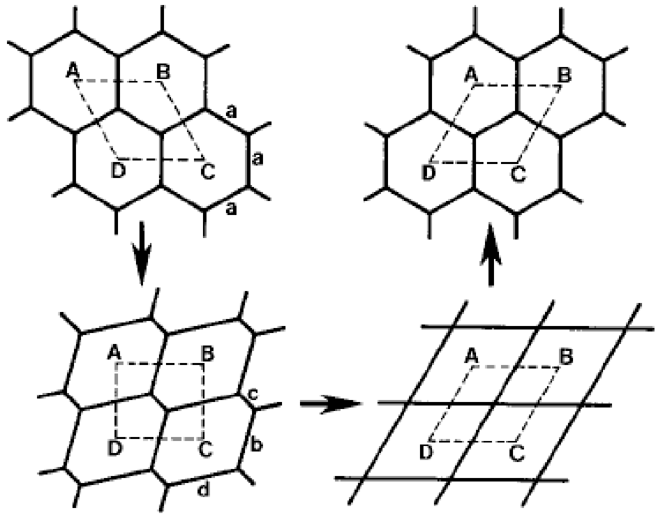
FIG. 8. Semilogarithmic plot of the stress versus t' under constant shear rate $\dot{\gamma}=1s^{-1}$, after various values of the elapsed waiting time: $t_w=100$, 1000, 10 000 s. This sample has a yield stress $\sigma_y^{app}=1.5$ Pa.

Colloids (Lequeux)

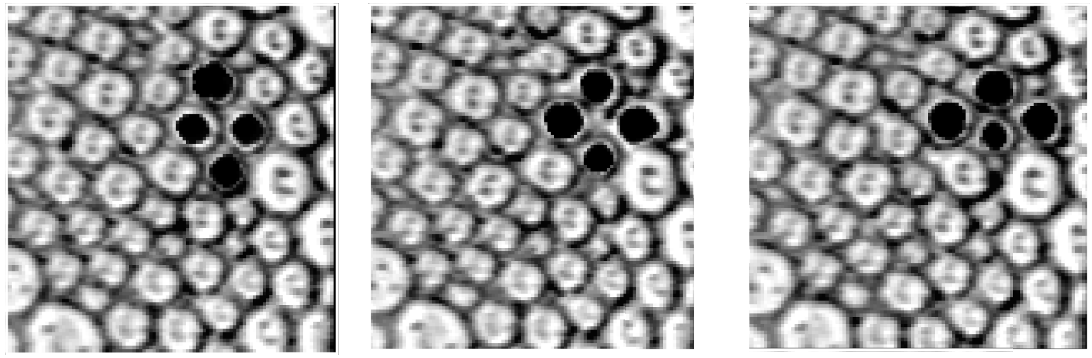


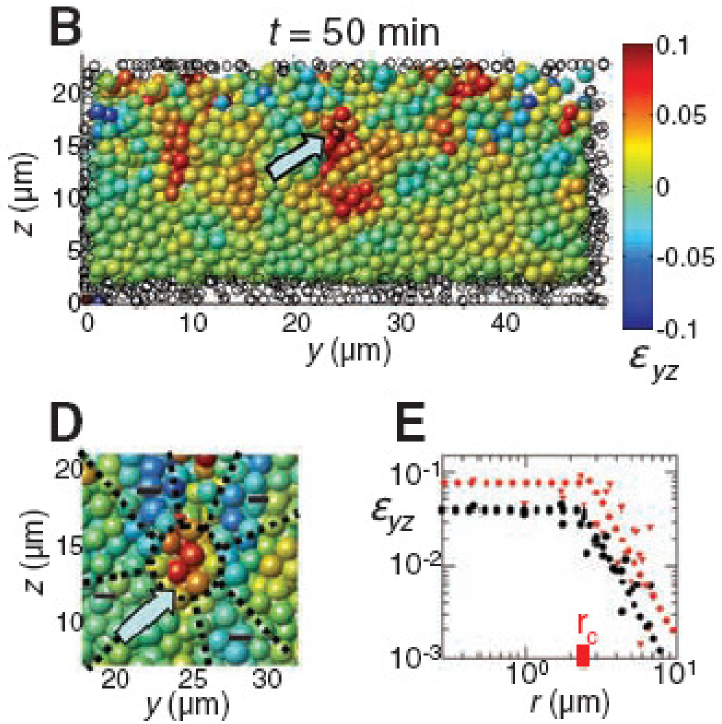
Plastic response of a foam ; I. Cantat, O. Pitois, Phys. of fluids 2006

Note the jerky aspect of the response in the « athermal » system (foam) => **well identified, localized plastic events**



« T1 » events in foams (Princen, 1981) (Dennin 2006)





Structural Rearrangements That Govern Flow in Colloidal Glasses

Peter Schall,[1,2*] David A. Weitz,[2,3] Frans Spaepen[2]

Colloidal glass, confocal microscopy

Science 318 (2007)

« Shear transformation zones » (Argon, Langer)

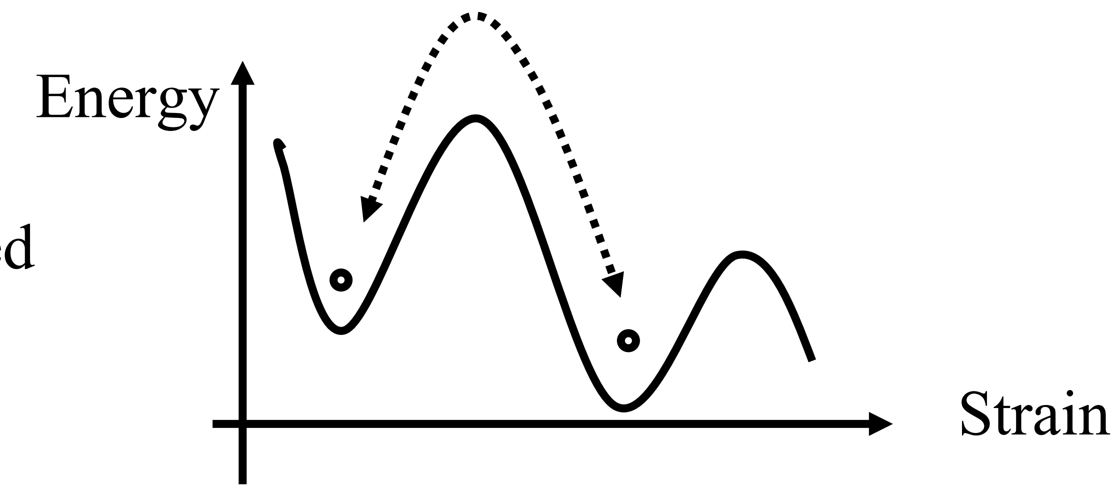
Overview

- Introduction
- **Models: Eyring, SGR et al, elasto-plastic discrete elements models**

  Also: STZ (shear transformation zone) [Falk and Langer], MCT (Mode coupling theory) [Brader,Fuchs, Cates, Voigtmann, PRL 2007]
- Atomic scale simulations

Eyring's model (1930)

Stress biased energy landscape



jump + $\tau_+ = \tau_0 e^{\frac{E-\sigma.v}{kT}}$

jump - $\tau_- = \tau_0 e^{\frac{E+\sigma.v}{kT}}$

shear rate :

$$\dot{\gamma} = \frac{1}{\tau_+} - \frac{1}{\tau_-} = \frac{1}{\tau_0}.e^{-\frac{E}{kT}}\left(e^{\frac{\sigma.v}{kT}} - e^{-\frac{\sigma.v}{kT}}\right) \approx e^{-\frac{E}{kT}}.\frac{v}{\tau_0.kT}.\sigma$$

High temperature/low shear : linear regime

Viscous fluid :

$$\eta = \tau_0 . e^{\frac{E}{kT}} . \frac{kT}{v}$$

Low temperature/high shear : non-linear regime

Nonlinear flow curve

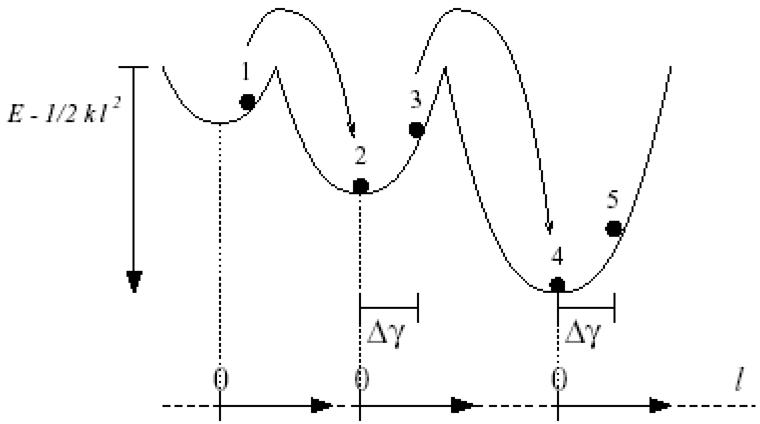
$$\sigma = \frac{kT}{v}\left[\ln(\dot{\gamma}) + \log(\tau_0 . e^{E/kT}) \right]$$

Does not account for all the complexity observed (single time scale, no yield stress)

Introduce « Rate and state » ideas: additional internal variables, effective T *(Rice Ruina for friction ; STZ model ; SGR model)*

A breaktrough: **Soft Glassy Rheology** (Sollich, Cates, Lequeux, Hébraud, Fielding)

Sollich P., Lequeux, F., Hebraud P. and Cates M. E., "Rheology of Soft Glassy Materials", Phys. Rev. Lett. 78 (1987) 2020–2023.



- distribution of energy barriers
- glass transition (trap model)
- *l* strain variable, increases linearly with time

$$E \to E - kl^2/2$$

P(L,E,t) distribution of systems in different « traps » and at different strains is the internal variable

Fixed strain rate evolution $\quad l = \dot{\gamma} t \qquad \sigma = k\langle l \rangle$

Activated escape from traps due to « mechanical noise »

Dynamical equation for the strain distribution function P(E,l,t) similar in spirit to the trap model of glasses (Bouchaud) – Trap depths are distributed

$$\frac{\partial}{\partial t}P = -\dot{\gamma}\frac{\partial}{\partial l}P - \Gamma_0 e^{-(E-\frac{1}{2}kl^2)/x}P + \Gamma(t)\rho(E)\delta(l)$$

X= mechanical noise temperature

Very successful model, describes many features of the flow of glassy systems

- a glass transition at $x=x_g=1$
- for $x< x_g$: aging, yield stress σ_Y, $\sigma=\sigma_Y+A\,\gamma^{1-x}$

But..

- **mechanical temperature X is not defined self consistently**
- **the model is « mean-field » (lacks spatial information)**

An attempt to self consistency: Hébraud Lequeux fluidity model: focuses on stress distribution on sites

$$\partial_t P(\sigma,t) = -G_0\dot{\gamma}\partial_\sigma P(\sigma,t) - \frac{1}{\tau}H(|\sigma|-\sigma_c)P(\sigma,t)$$

$$+\frac{1}{\tau}\delta(\sigma)\int_{|\sigma'|>\sigma_c} P(\sigma',t)d\sigma' + D\partial^2_{\sigma^2}P(\sigma,t)$$

where the "stress diffusion term" D (fluidity) is given self consistently by

$$D = \frac{\alpha}{\tau}\int_{|\sigma'|>\sigma_c} P(\sigma',t)d\sigma'$$

(rate of plastic events)

Can be solved exactly

Displays a jamming transition

$$\alpha_c = \frac{1}{2} : \text{jamming point}$$

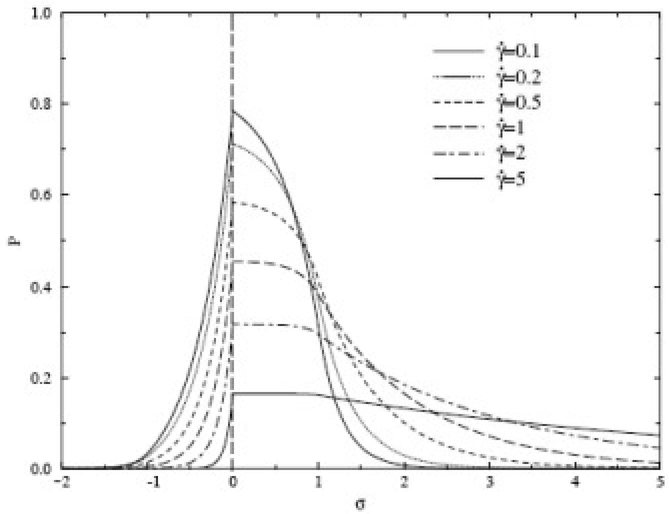


FIG. 1. Distribution probability $P(\sigma)$ of the stress, for different values of $\dot{\gamma}$.

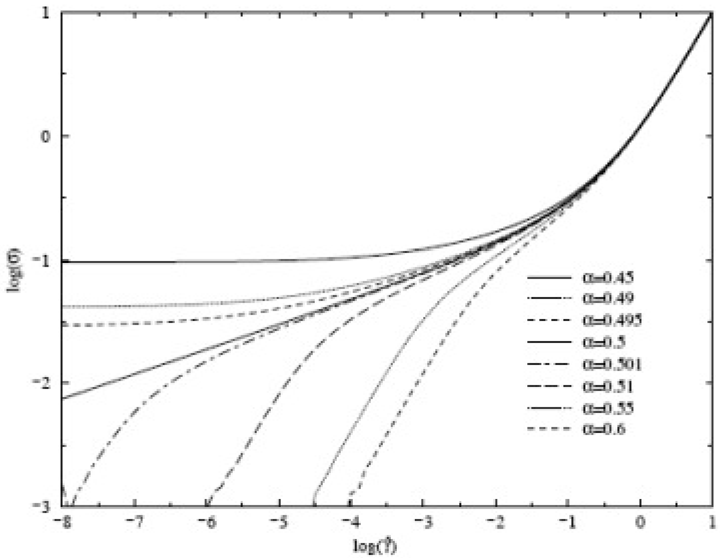
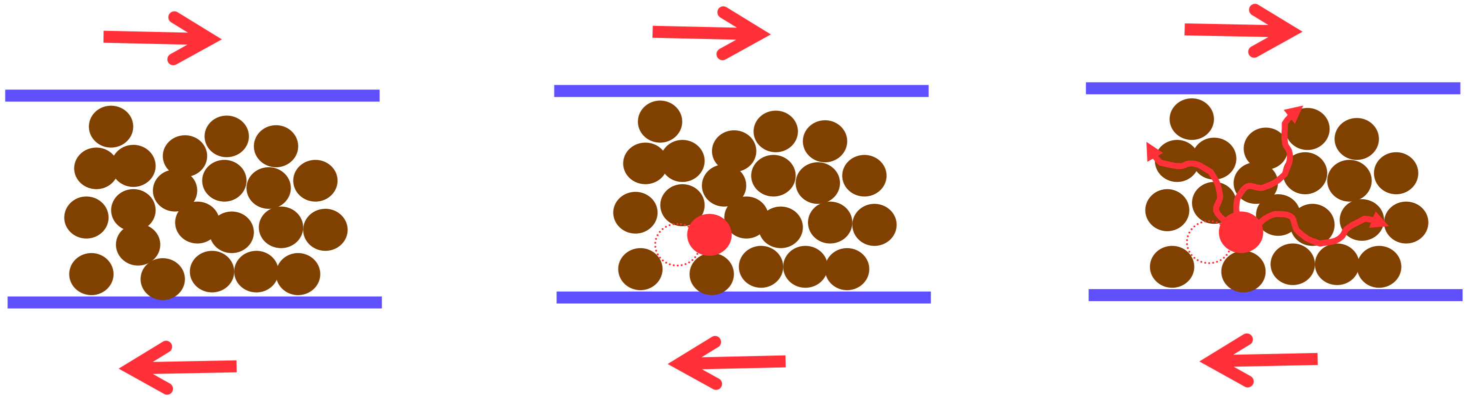


FIG. 2. Stress σ vs shear rate $\dot{\gamma}$ for different values of α.

Elasto-Plastic discrete element models

Argon Bulatov 1994, Picard Bocquet *et al* 2002

- Try to capture the generic scenario …



Elastic resistance | Localized yield event | Stress redistribution

- … but keep non-local effects to study collective behavior

Picard et al. PRE (2005); earlier models by Argon Bulatov, Roux…

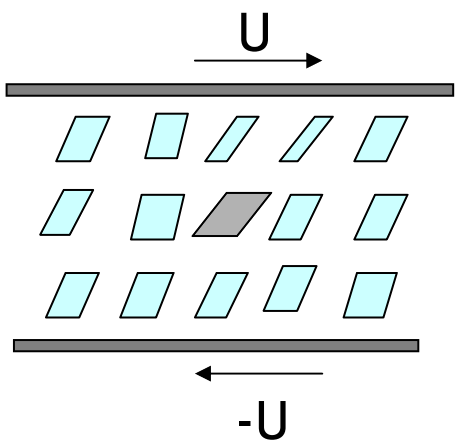
Stress dynamics in the model of Picard *et al*

$$\partial_t \sigma(\vec{r},t) = \mu\dot{\gamma} + \int d\vec{r}'\, G(\vec{r}-\vec{r}')\, \dot{\varepsilon}^{plast}(\vec{r}',t)$$

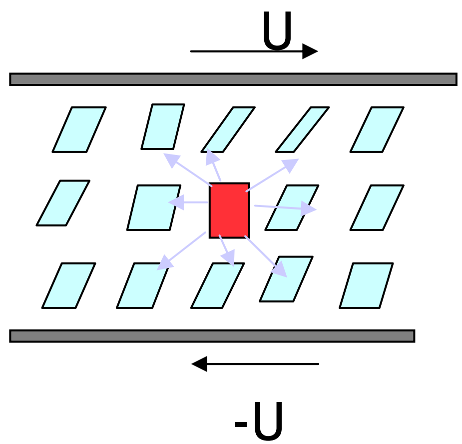
$G(r,\theta) \sim \frac{\cos 4\theta}{r^2}$
elastic propagator

Plastic activity (number of sites that reach yield point)

Global elastic forcing

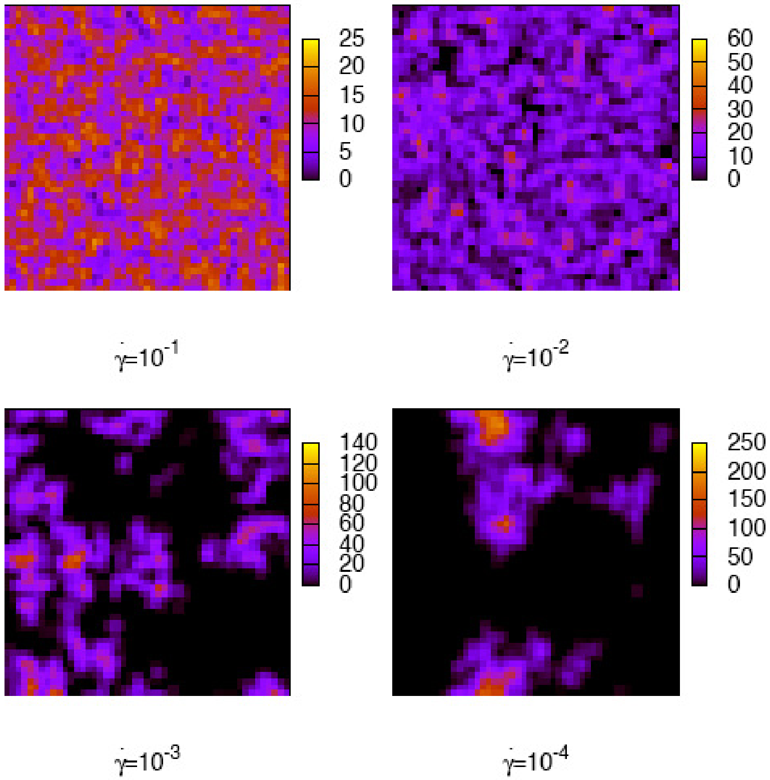


Plastic relaxations



Models exhibit dynamical heterogeneities at low strain rates (numerical results)

Cumulated plastic activity (+1 if plastic)



Low shear rate behavior :

localized plastic bursts

- « always » crack in the same region
- « fragile » zones

Heterogeneous behavior at low shear rates

To be quantified for large systems, long times (scaling of 4-points correlations, work in progress…)

Overview

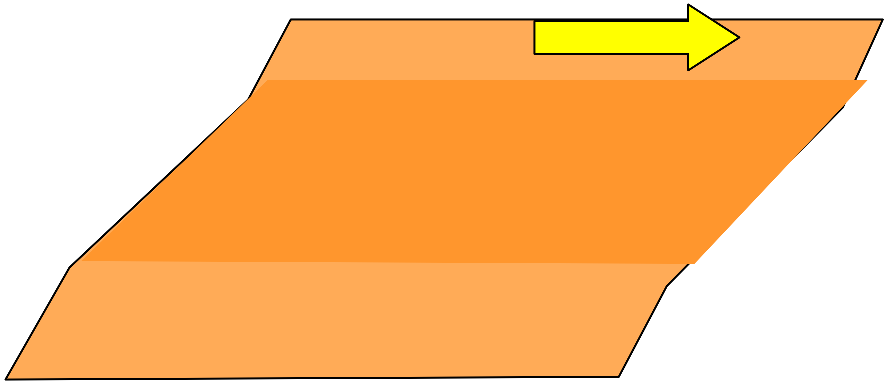
- Introduction
- Models
- **Atomic scale simulations: probe assumptions in models, mapping onto mesoscale models, measure new quantities…**

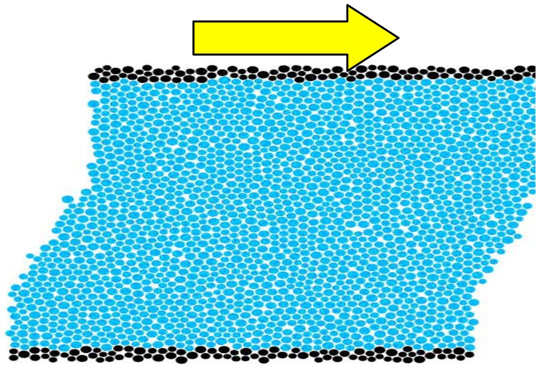
-investigation of elementary plastic events

-mechanical activation idea

-strain localisation, local vs dynamical yield stress

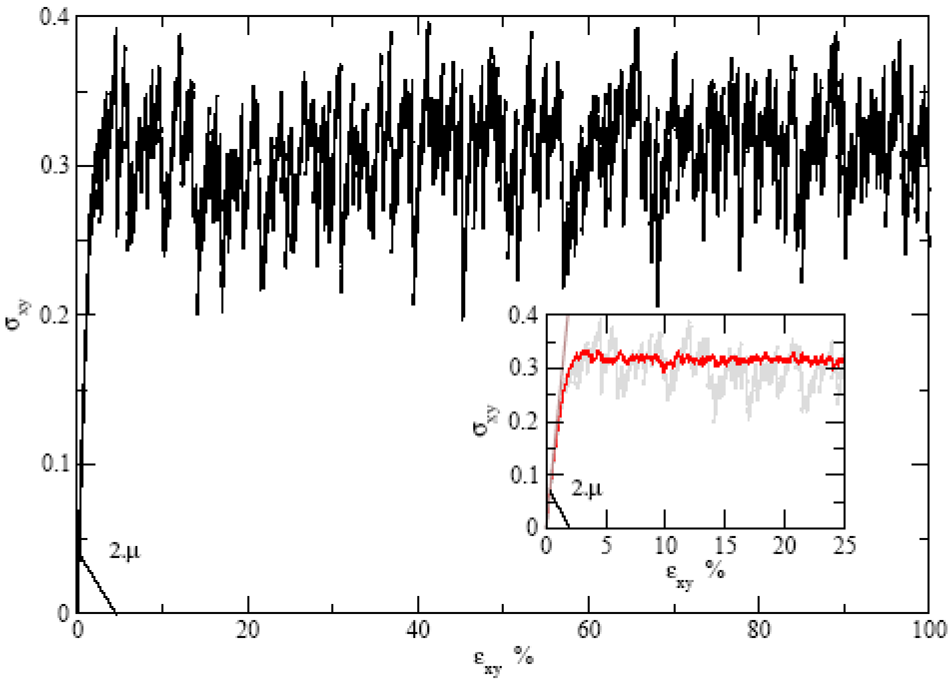
QUASI STATIC DEFORMATION IN A 2D SYSTEM





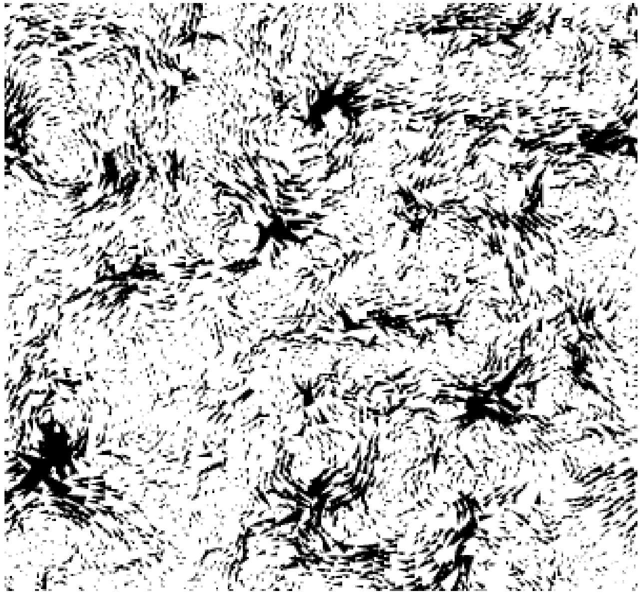
Polydisperse Lennard-Jones system, quench to T=0 from liquid state; quasistatic shear (minimization after each deformation step 0.00001 strain increments)

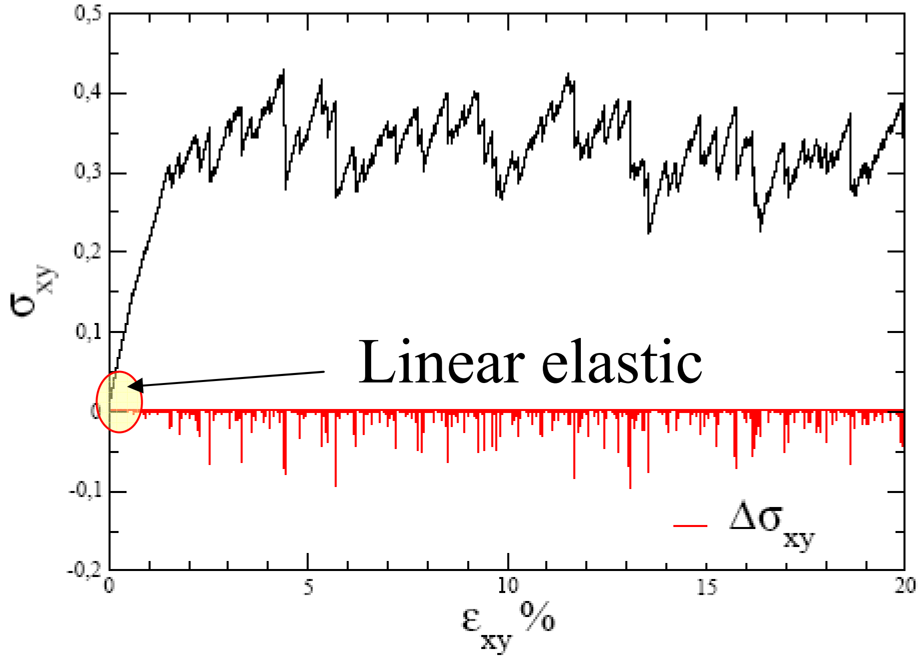
Stress strain curve

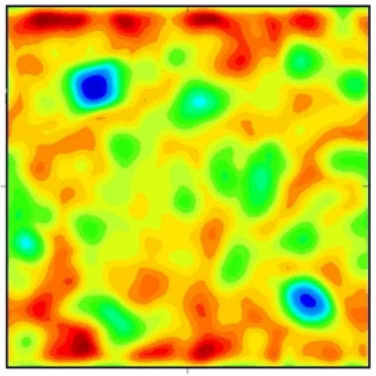


(see also similar work by C. Maloney, A. Lemaitre)

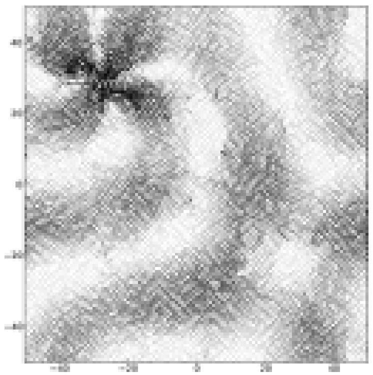
Very small strain : elastic deformation **(heterogeneous, non affine part is important!)**



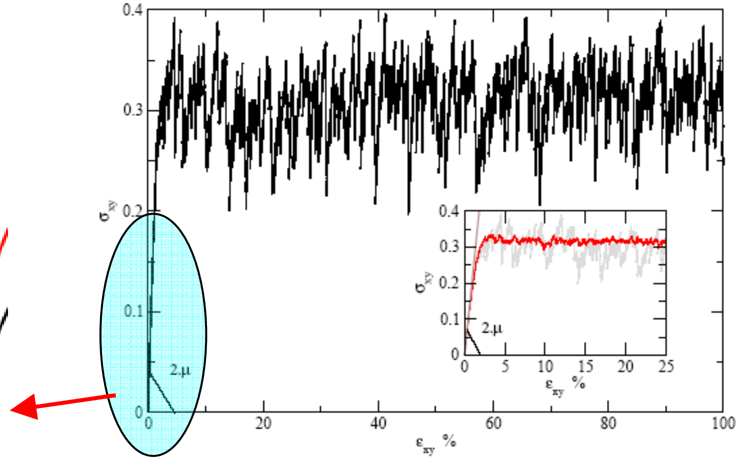




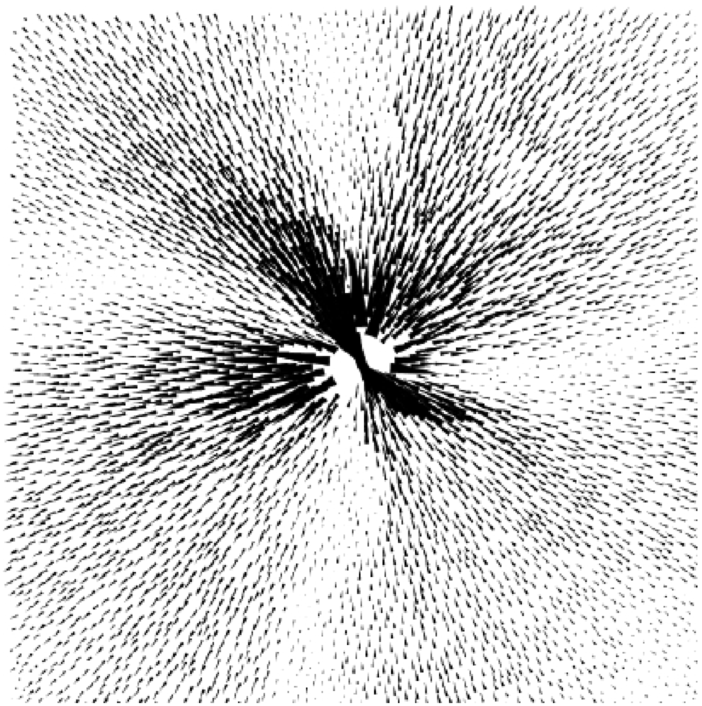
Map of local shear modulus (*Tsamados, Tanguy, JLB PRE 2009*) and a low frequency vibrational mode



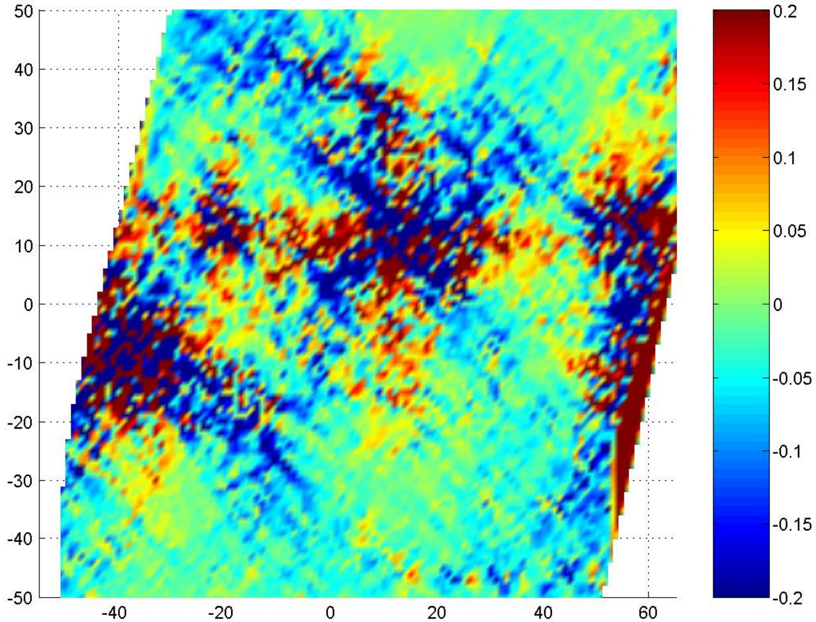
Onset of plastic deformation



Localized, quadrupolar events
(shear transformation zones!)

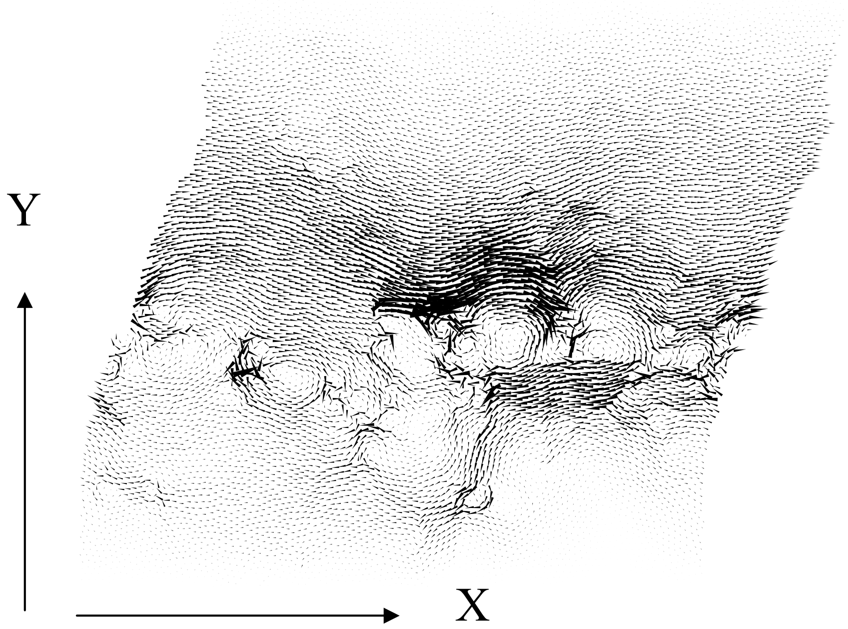


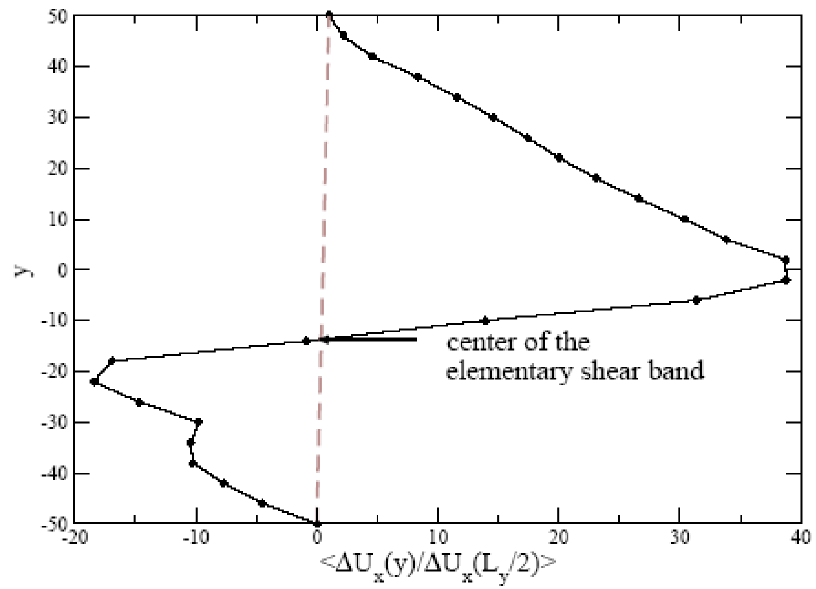
Irreversible displacement



Stress drop $\Delta\sigma_{xy}$

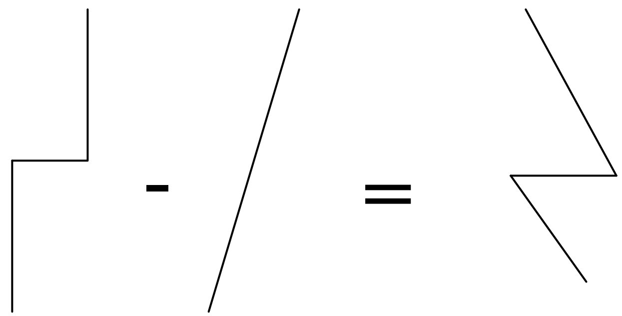
Plastic flow regime – Larger stress drops





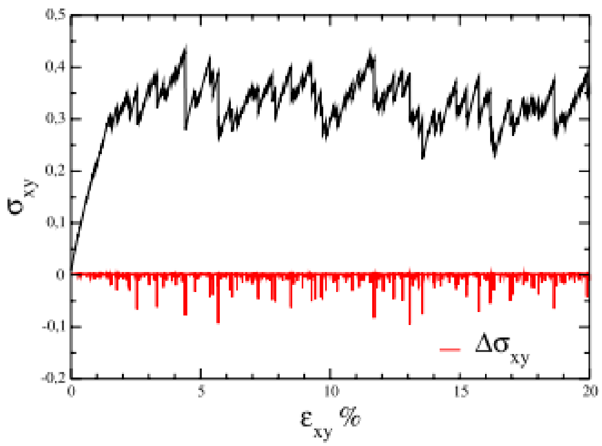
Simultaneous alignement of events to form a system spanning « mini shear band » or « crack »

True velocity profile – linear profile =



In this plastic flow regime :

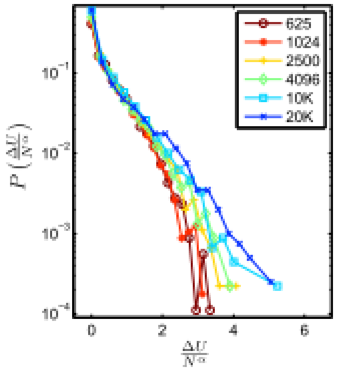
stress/energy drops of all amplitudes (from simulations with continuous potentials: Tanguy *et al*, Procaccia *et al*, Lemaître *et al*)



$$\Delta U \sim L^{\alpha}$$

$$\Delta\sigma \sim L^{-\beta}$$

Scaling of stress drop distributions (not very good)



$$\Delta U \sim \Delta\sigma L^{d} \Rightarrow \alpha + \beta = d$$

α may be system dependent ; large events may be cut off by finite shear rate (Caroli, Lemaître) or thermal effects (Procaccia), work in progress to quantify these aspects

Qualitative elements common to models, simulations and experiments

-elementary plastic events can be identified (size, intensity)

-interaction between these events, stress redistribution

-organisation at intermediate scale (strain localisation)

-Mapping microscopic dynamics onto the models ?

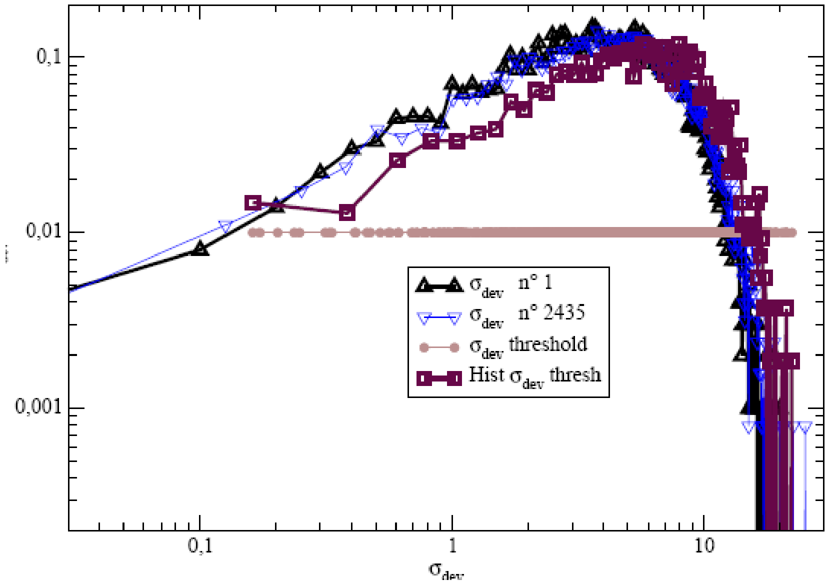
-**local yield stress ??** [problematic: many events take place at low local stress see Tanguy et al, EPJE 2008]

-**identication of elementary yield events prior to yielding** ? Weak local elastic constants

-**quantify interaction between events?** Elastic quadrupoles OK

-quantification of collective behaviour: correlation lengths ?

Local Yield Stress idea ? Yes and No



Histogram of local deviatoric stress

-at yield points

-for the entire system

Difference is small; probability of yielding is higher above some « threshold » value, but nonzero below
=> **Most yield events take place below threshold**

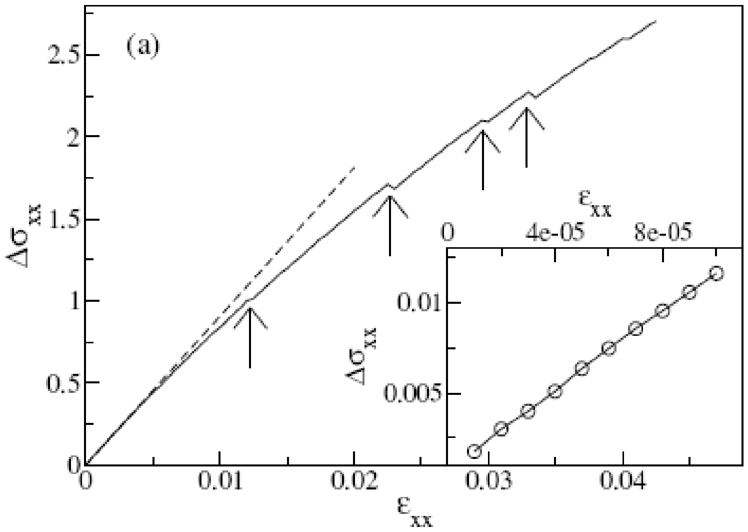
⇒Build mesoscopic models with less strict « threshold » conditions

Identifying plastic events prior to yielding ?

Example: polymer model, elongational strain

(G. Papakonstantopoulos, JJ. De Pablo, JLB, PRE 2007)

(M. Tsamados , A. Tanguy, JLB, PRE 2009 for LJ systems)



Sites that fail have typically

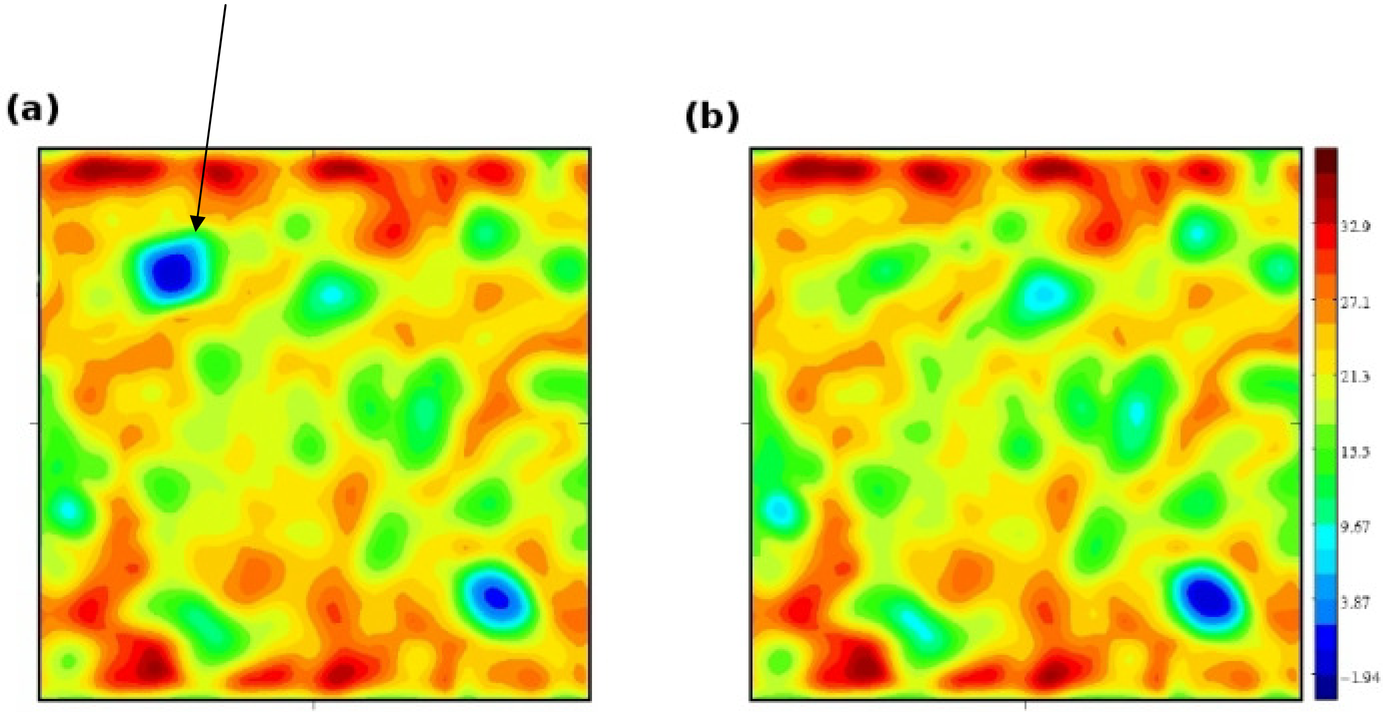
-smaller local elastic constants

-less spherical Voronoi cells

-are not under high stress

=> Introduce disorder in the local moduli in mesoscopic models

Position of plastic event



Perspectives

- Quantify dynamical heterogeneities (dynamical correlation length)
- Better characterization of stress drops in quasistatic simulations, 2d and 3d
- Influence of strain rate and finite T

Mechanical activation

Question: could « mechanical noise » induce activated processes in the same way thermal noise does ?

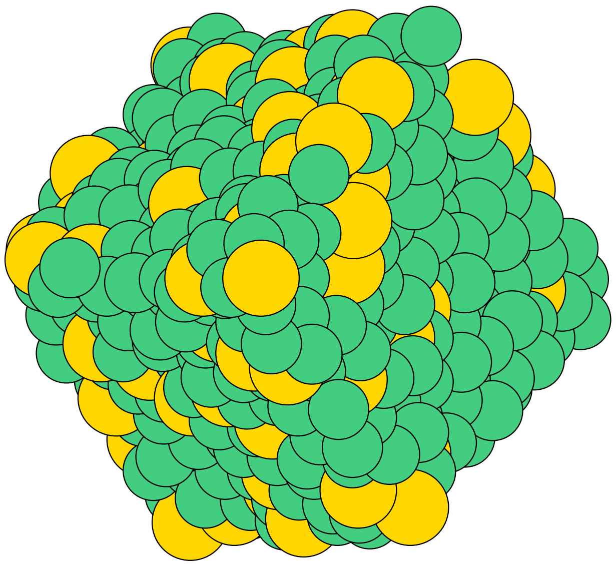
Relevant for SGR kind of approach

Test: couple an activated degree of freedom to a system undergoing plastic shear flow

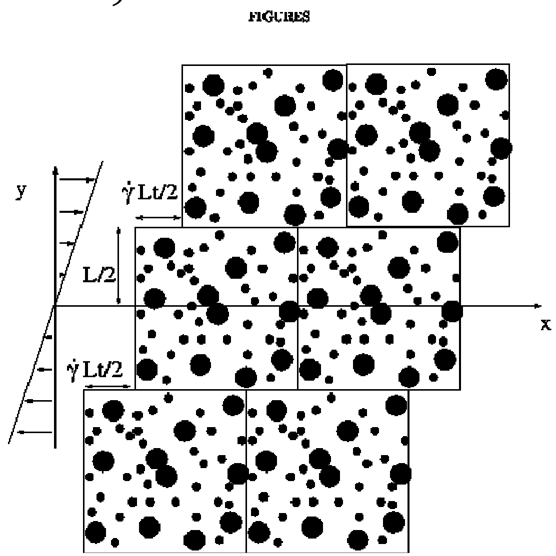
Model: Lennard-Jones mixture, originally model for metallic glasses.

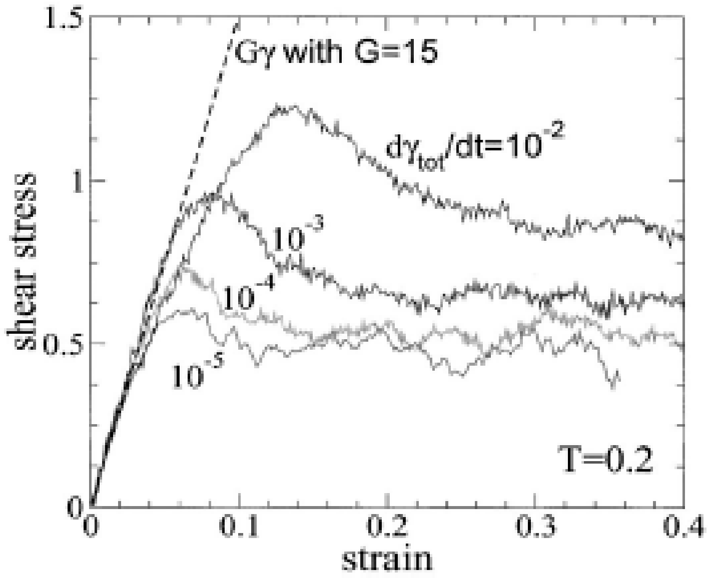
MD simulations at T=0.3 the system is a « computer glass » (aging in the absence of shear)

Periodic boundary conditions



Homogeneous Couette flow, thermostatted





Stress strain curves

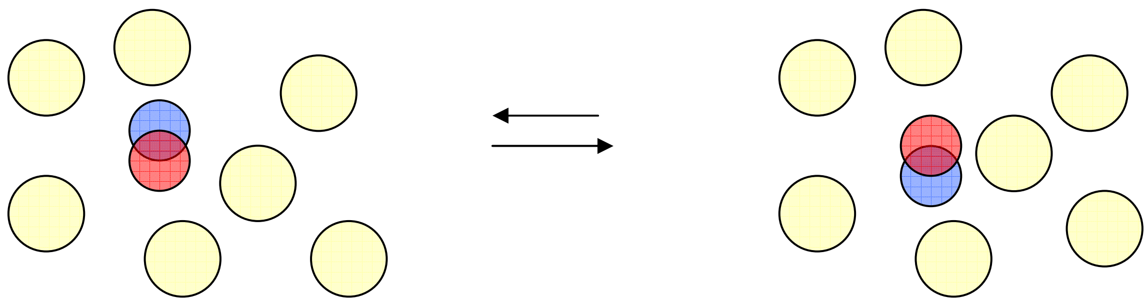
-Difficult to identify elementary events

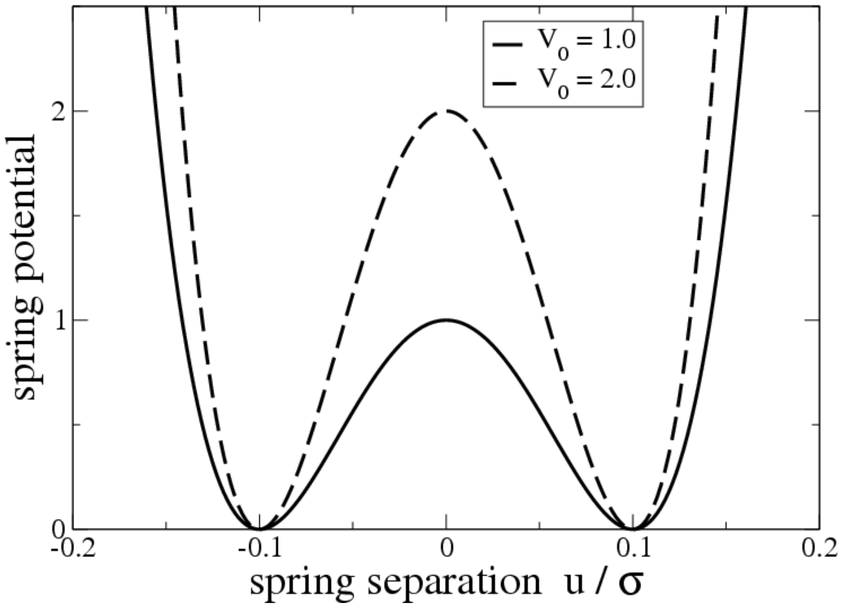
-Rate effects, similar to experiments

Activated process:

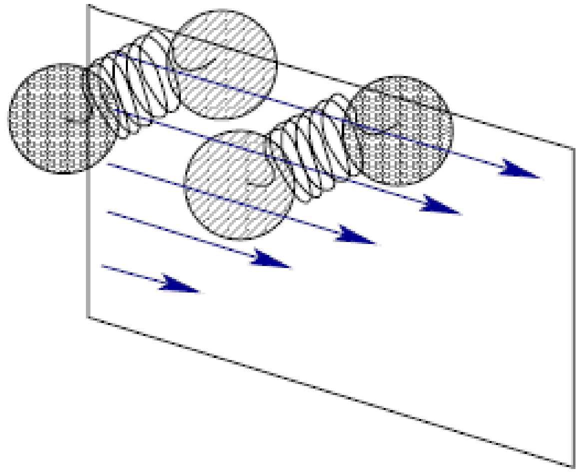
(P. Ilg, JLB Europhysics Letters, 2007)

Couple extra degree of freedom in a double well potential to the « bath » . Here, « dumbbell » particle has possibility to undergo « isomerization » reaction.

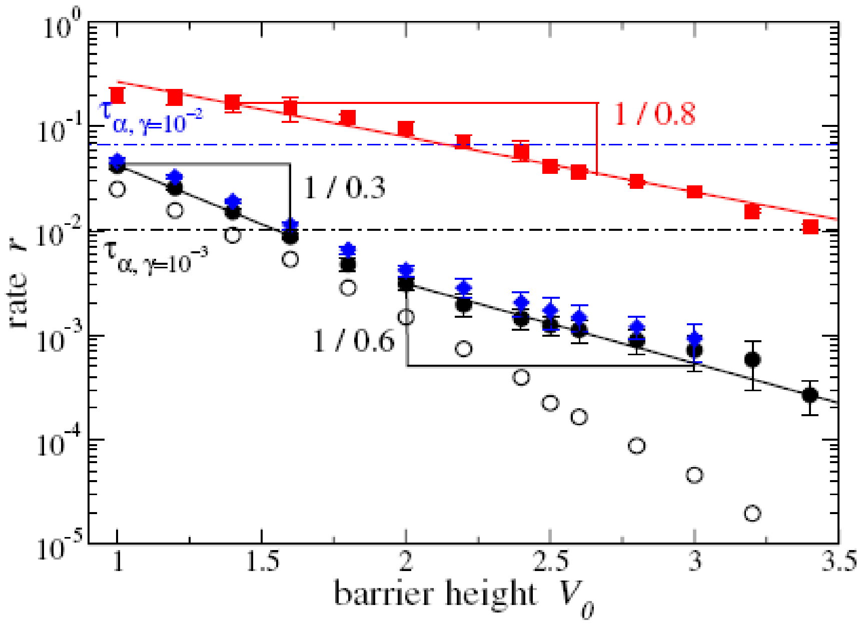




Potential seen by internal dumbbell coordinate



Compute « reaction rate » and probe Arrhenius like behaviour



$$\dot{\gamma} = 10^{-3}$$

$$T = 1. \quad k_{AB} \propto \exp(-V_0/1.01)$$

$$T = 0.3 \quad k_{AB} \propto \exp(-V_0/0.62)$$

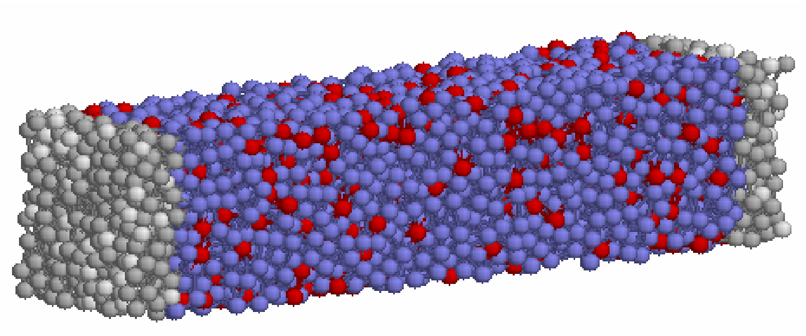
Summary

Slow « mechanical » noise from the flow can be described by an effective temperature higher than the actual (thermal bath) temperature.

Perspectives

- Consequences for rheology: Liu and Haxton PRL 2007 (effective T)
- Relation to fluctuation dissipation ratio ?
- Other activation effects : **shear driven nucleation** (A. Mokshin, JLB, PRE 2008)

Boundary driven system: shear banding, and yield stress



-Same glassy system as before

-Moving rough walls identical to the flowing material (no slip). Planar Couette flow with fixed distance between plates.

-Homogeneous flow is obtained *only above some critical shear rate*

-At small shear rate, **shear band formation**

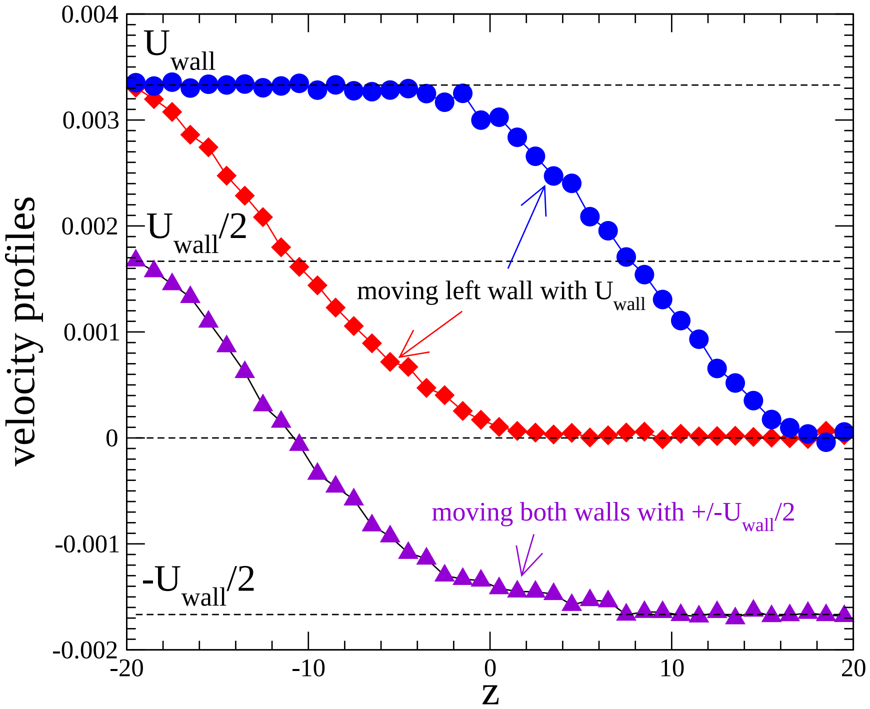
L. Berthier et al, PRL 90, 095702

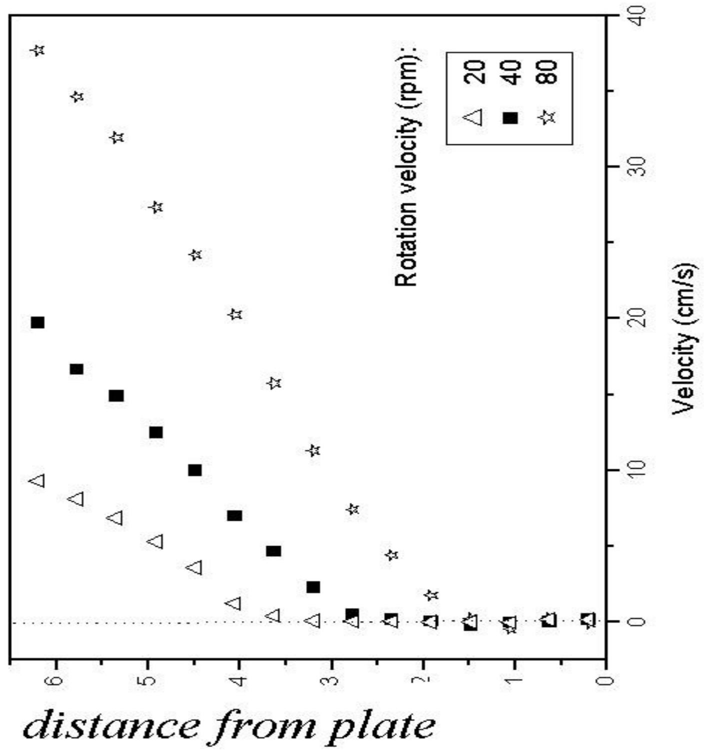
Couette flow: shear band velocity profile:

Simulation

MRI imaging of velocity profiles in bentonite (clay)

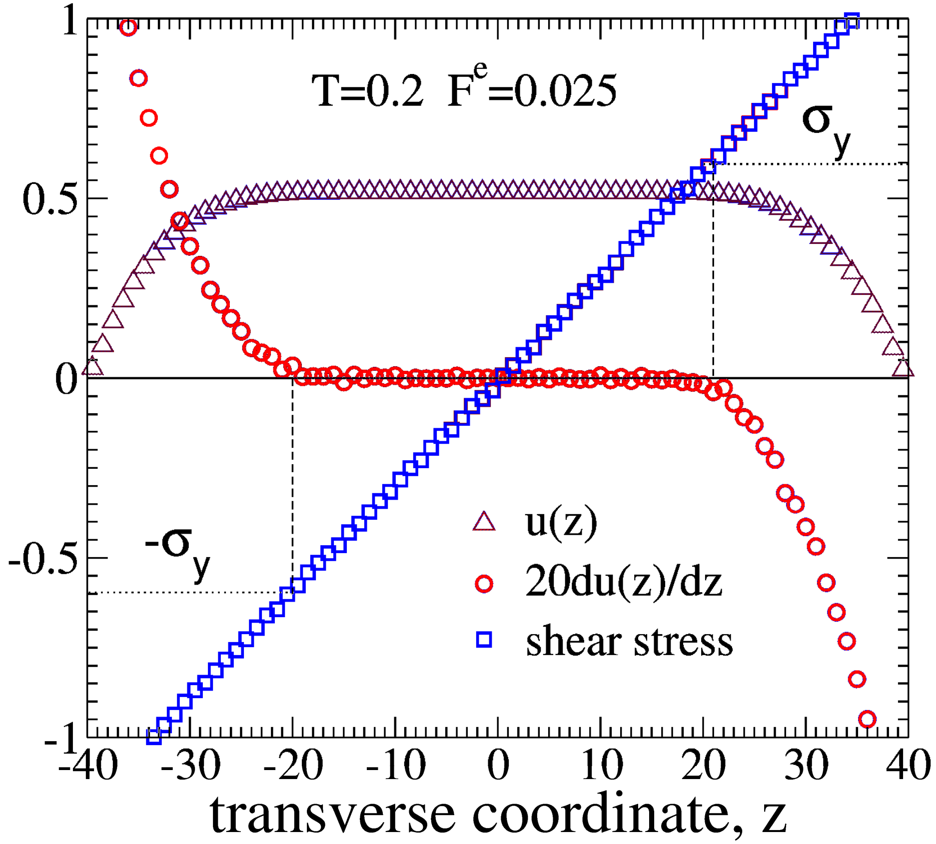
(Coussot et al, PRL 2001)





Pressure driven flow:

Poiseuille flow replaced by plug flow

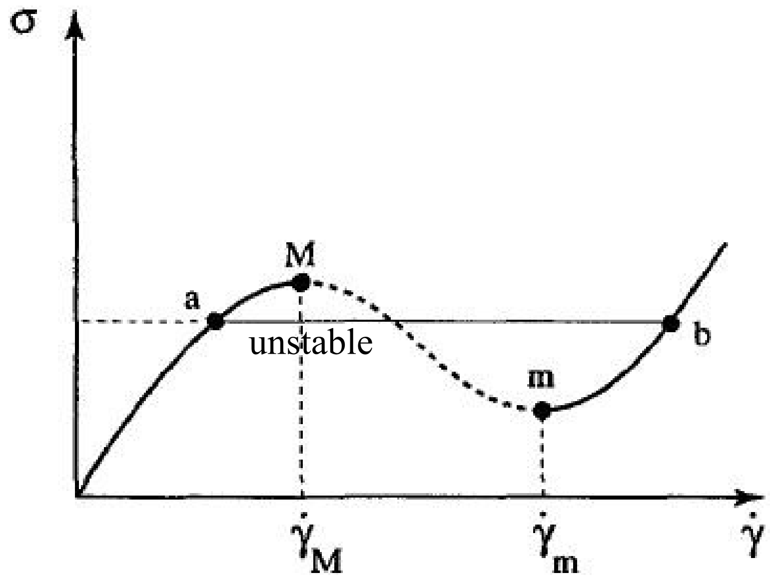


Shear bands are well known to form in systems with non monotonic flow curves (e.g. giant wormlike micelles) associated with coupling of flow with nematic order parameter

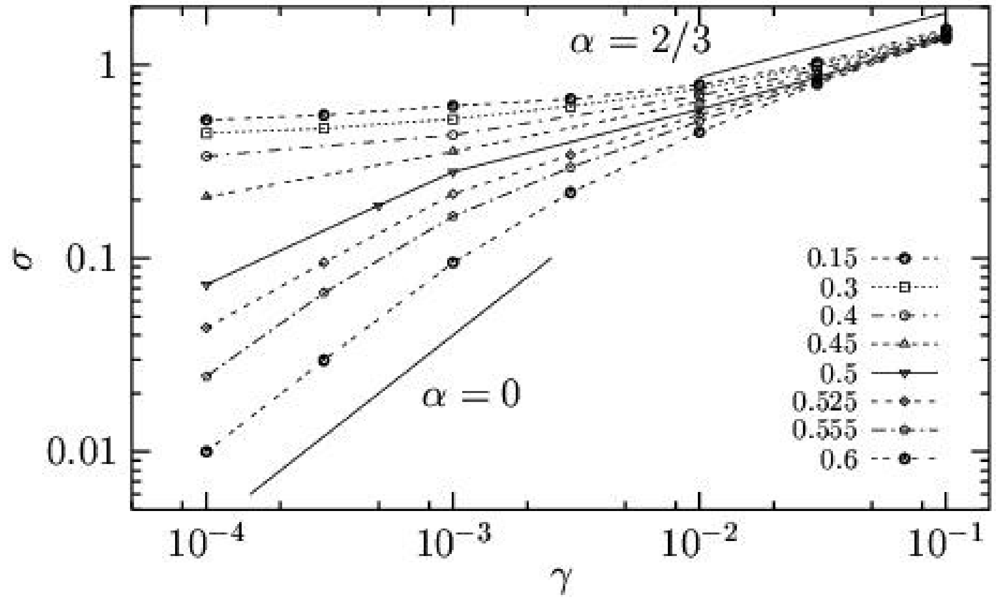
J. Phys. II France **7** (1997) 459–472 MARCH **1997**, PAGE 459

Inhomogeneous Flows of Complex Fluids: Mechanical Instability *Versus* Non-Equilibrium Phase Transition

Grégoire Porte (*), Jean-François Berret and James L. Harden



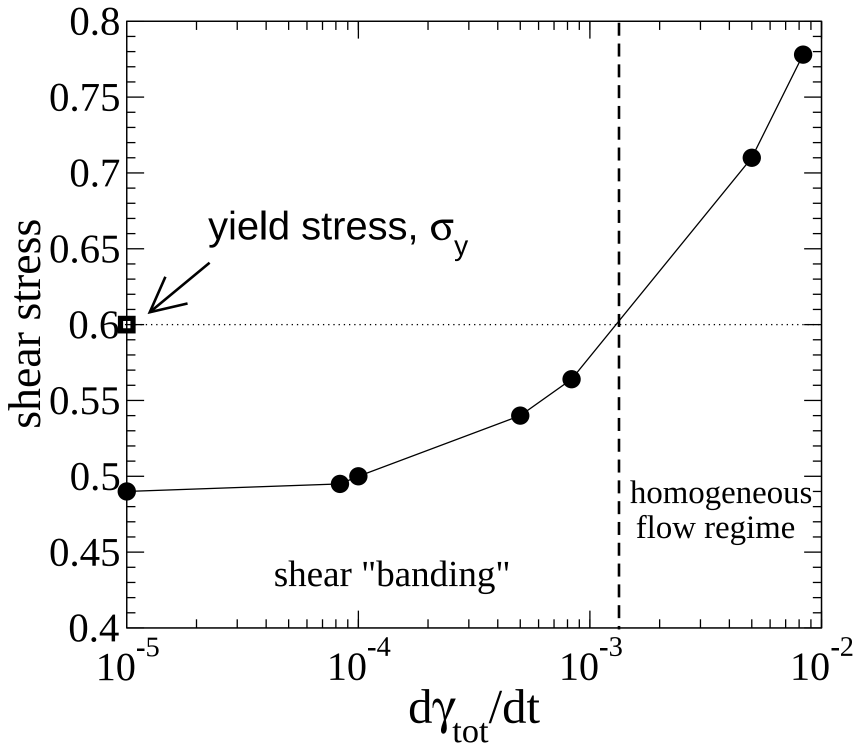
Here flow curve is monotonic !



Stress vs strain rate, different temperatures.

Flow curve with a finite yield stress

$$\sigma_Y > \lim_{\dot{\gamma}\to 0} \sigma_{homogeneous}(\dot{\gamma})$$



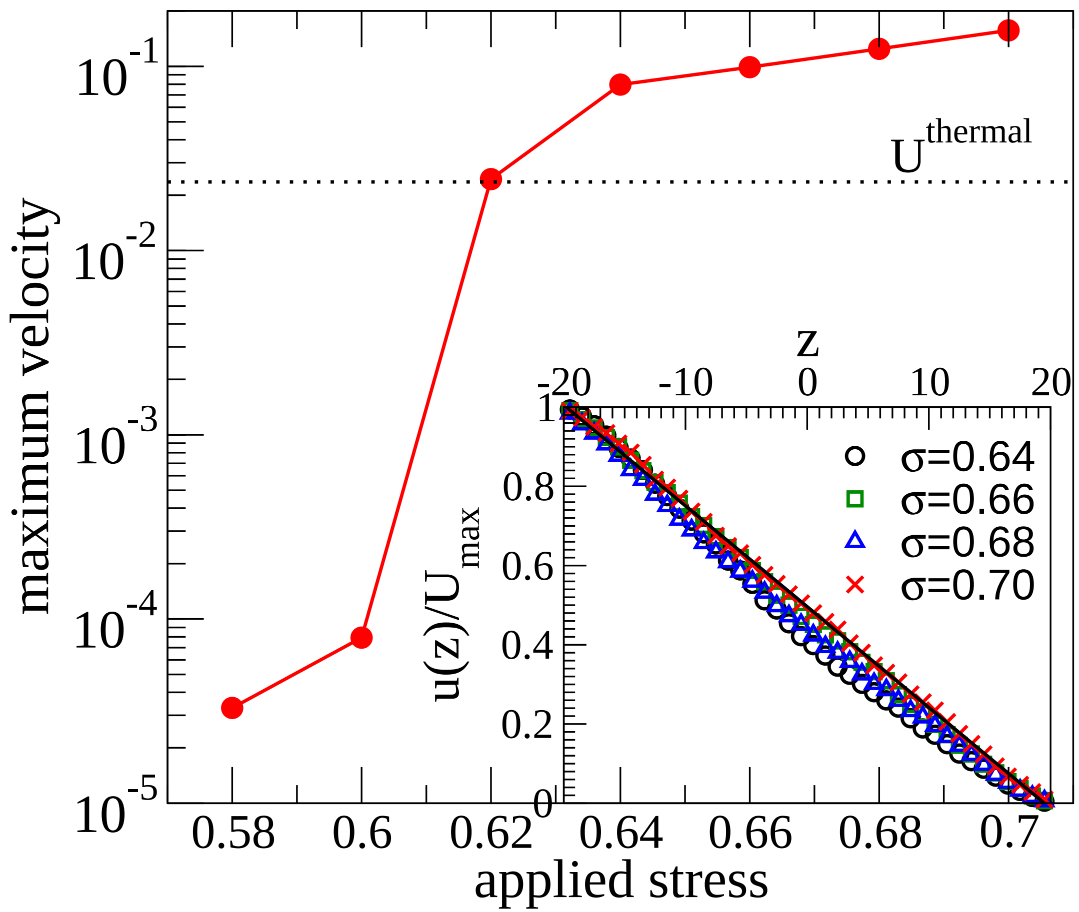
Full curve: homogeneous flow data.

Shear band formation and selection is an unsolved problem

Analogy with static/dynamic friction

No obvious order parameter

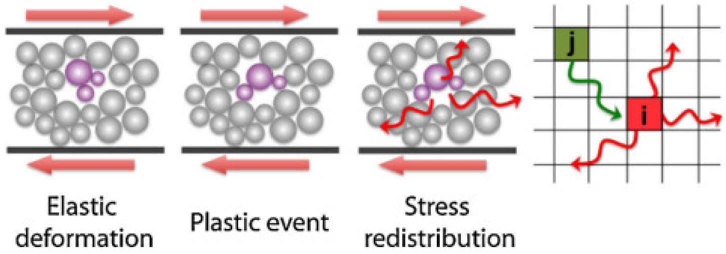
Definition of yield stress ? Apply an external stress (time scale τ_{exp}) and measure wall displacement $\Delta x = \Delta x_{el} + Vt$

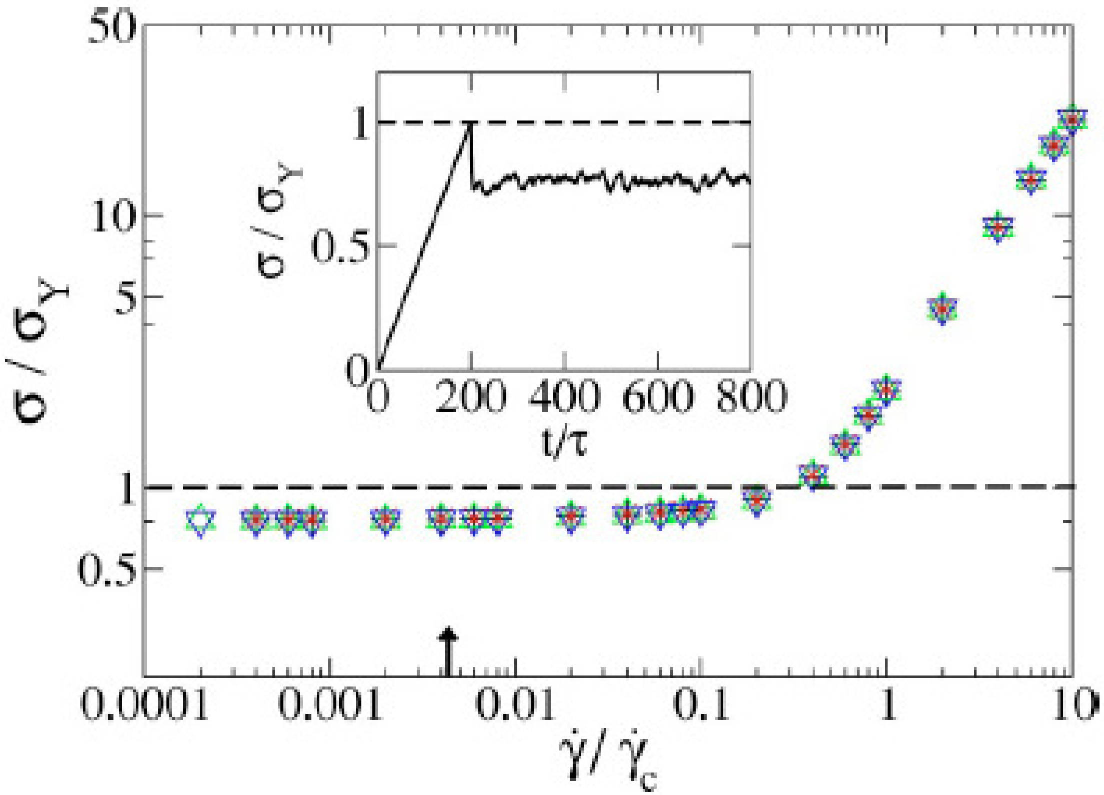


$\tau_{micro} \ll \tau_{exp} \ll \tau_{relax}$

F. Varnik et al, JCP 2004

Static/dynamic yield stress effect observed in Picard's model (but no permanent localisation)





$$\dot{\gamma}_c = \frac{\sigma_Y}{\mu \tau}$$

PHYSICAL REVIEW E **71**, 010501(R) (2005)

A promising route: coarse graining of elasto plastic models (Bocquet, Colin, PRL 2009)

$$\partial_t P_i(\sigma, t) = -G_o \dot{\gamma}_i \partial_\sigma P_i(\sigma, t) - \frac{\Theta(|\sigma| - \sigma_c)}{\tau} P_i(\sigma, t) + \Gamma_i(t)\delta(\sigma) + D_i \partial^2_{\sigma^2} P_i(\sigma, t).$$

$$\Gamma_i(t) = \int \frac{\Theta(|\sigma'| - \sigma_c)}{\tau} P_i(\sigma', t) d\sigma'.$$

$$D_i(t) = \frac{1}{2} \sum_{j \neq i} \Pi^2_{ij} \sigma_c^2 \Gamma_j(t).$$

Stress diffusion induced by plastic activity

$$D(\mathbf{r}, t) = m \Delta \Gamma(\mathbf{r}, t) + \alpha \Gamma(\mathbf{r}, t),$$

Coarse graining results in local stress strain relation coupled to nonlocal diffusion equation for fluidity *(resp. effective T, free volume)*. Basic ingredients to describe heterogeneous flow (see also Langer, Sollich Fielding and Cates).

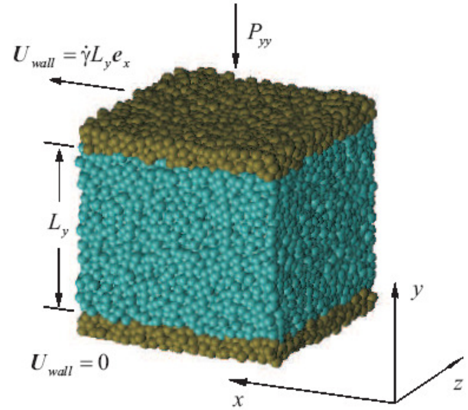
Still a lot of work: validity of coarse graining procedure, tensor aspects, 3d…

Perspectives

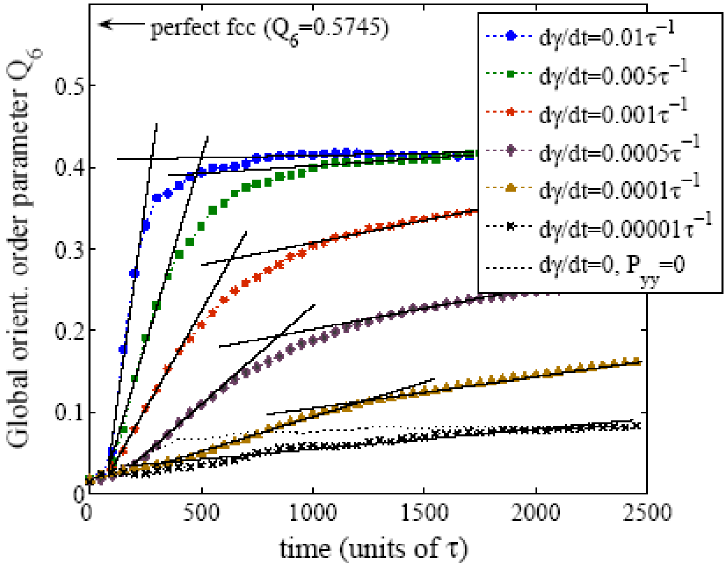
- Large scale simulation of elasto plastic models: understand collective behavior (correlation length), finite T, finite strain rate crossovers
- Conditions for strain localisation, continuum description with effective temperature diffusion, coarse graining to mean-field description
- Mappings: distribution of elastic moduli, distribution of local yield values, kinetic MC vs MD
- 3d

Shear induced crystallisation

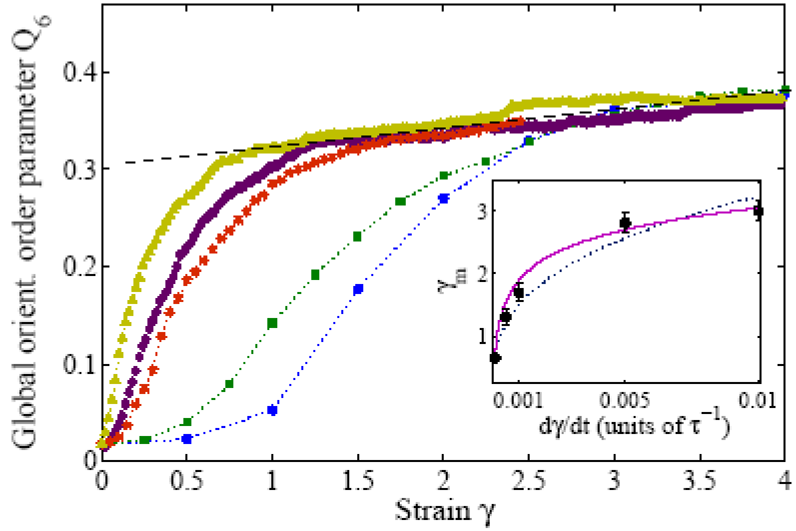
(A. Mokshin, JLB, PRE 2008)



Start from low T amorphous one component system



Order parameter vs time



Order parameter vs strain

=> **Stationary state: « nanocrystalline » material**