Athermal, Quasi-static Deformation of Amorphous Materials

Anaël Lemaître[1] and Craig Maloney[2]

[1]Institut Navier – France

[2]Department of Physics – UC Santa Barbara

Phys. Rev. Lett. 93, 016001 (2004)

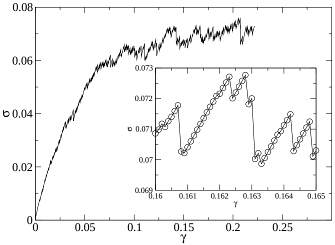
Phys. Rev. Lett. 93, 195501 (2004)

cond-mat/0410592

Acknowledgements: Jim Langer, Vasily Bulatov

Deformation of Small Systems

Numerical or Experimental observations (granular materials, foams, nanoindentation): Very intermittent response



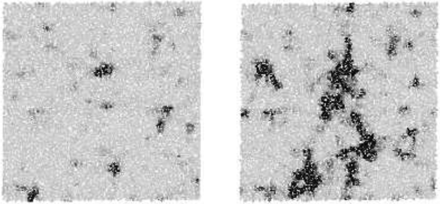
Intermittency smears out with:

- High temperature T
- High strain rate $\dot{\gamma}$
- Large system size N

Suggest that deformation is heterogeneous at a small (mesoscopic) scale

Spatial Organization of Deformation

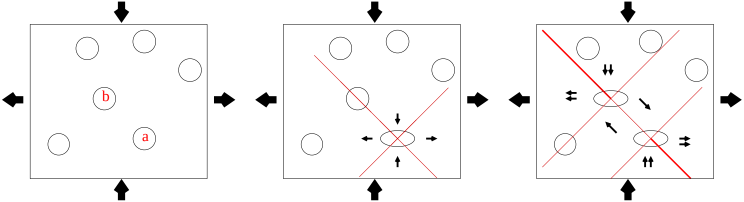
[Maeda & Takeuchi, (1978)]
Quasi-static Deformation (Numerics)
[Argon & Kuo (1979)]
Disordered bubble raft
[Falk & Langer (1998)]



- Shear occurs in localized spots = “Shear Transformation Zones”
- Elementary shear analogous to the nucleation of a dislocation loop (Argon (1979))

Avalanche Mechanism at Mesoscopic Scale

- Elementary shear associated with quadrupolar transformations
- Transfer of constraint between elementary shear transformations lead to localization [Bulatov & Argon (1994), Langer (2001), Baret *et al* (2002)]



Two Types of Theories

- Hydrodynamic Approaches:
  [Spaepen(1977)]
  [Argon (1979)]
  [Falk et Langer (1998)]
- Mesoscopic Models:
  [Bulatov et Argon (1994)]
  [Baret, Vandembroucq et Roux (2002)]
  [Picard *et al* (2004)]

Question: Does localization originates from a “hydrodynamic” instability or from mesoscopic transfer of constraints?
How can we test theories?

- No *a priori* identification of Shear Transformation Zones
- Few observations of elementary rearrangements (In dry foams [Kabla & Debreageas (2003)])

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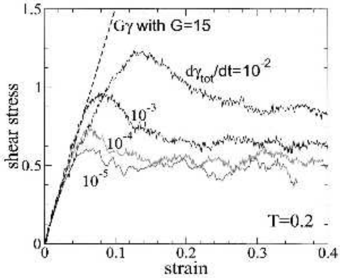
Recent Numerical works

- MD simulations
  - Yamamoto, Onuki (1997)
  - Falk, Langer (PRE 1998)
  - Rottler, Robbins (PRE 2002, PRE 2003)
  - Varnik, Bocquet, Barrat, Berthier (PRL 2003, JCP 2004)



- Athermal, Quasi-static simulations
  - Utz, Debenedetti, Stillinger (PRL 2000)
  - Malandro, Lacks (PRL 1998, JCP 2000)
  - Schuh, Lund (PRL 2003, Intermetallics 2004)

Athermal, Quasi-Static Limit

- Problem: intrinsic limitation of MD simulations: short timescales hence high shear rates
- Mimic experiments by taking the limits:
  - $T << T_g$: Limited role of Thermal Fluctuations
  - Small strain rate: $\dot{\gamma} << 1/\tau_{\text{aging}}$
- Protocol:
  - Minimize energy
  - Strain simulation cell
  - Start again

Shear-induced changes of PEL

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Relationships of shear-induced changes in the potential energy landscape to the mechanical properties of ductile glasses

Dennis L. Malandro and Daniel J. Lacks
Department of Chemical Engineering, Tulane University New Orleans, Louisiana 70118

(Received 20 August 1998; accepted 30 November 1998)

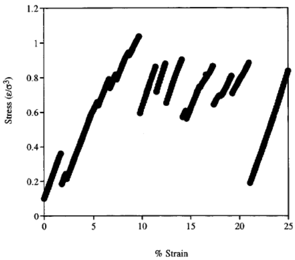
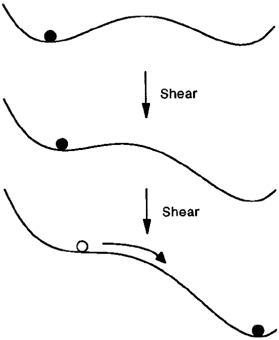


FIG. 1. Stress–strain diagram for a 500-atom system.



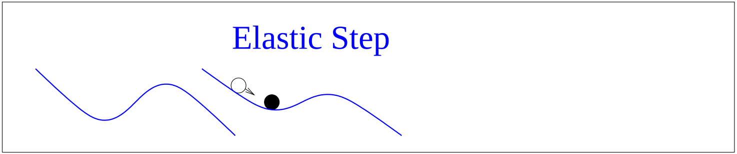
Indicate elementary transitions associated to localized rearrangements: $\delta\sigma \to 0$.

The PEL Picture

- Strain biases potential energy landscape

The PEL Picture

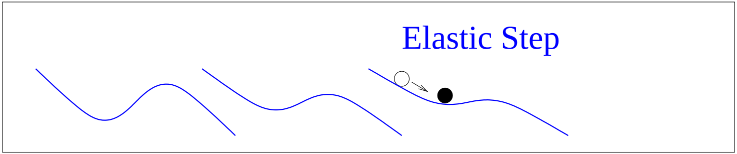
- Strain biases potential energy landscape



Elastic segment: System follows an energy minimum Reversible.

The PEL Picture

- Strain biases potential energy landscape



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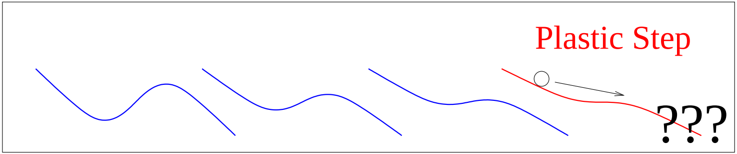
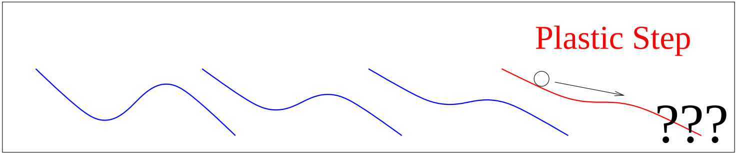


Elastic segment: System follows an energy minimum Reversible.

Plastic event: Local minimum annhiliates. Irreversible.

The PEL Picture

- Strain biases potential energy landscape



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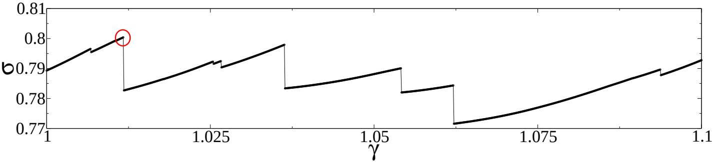
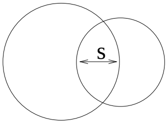
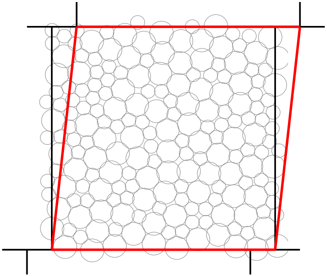


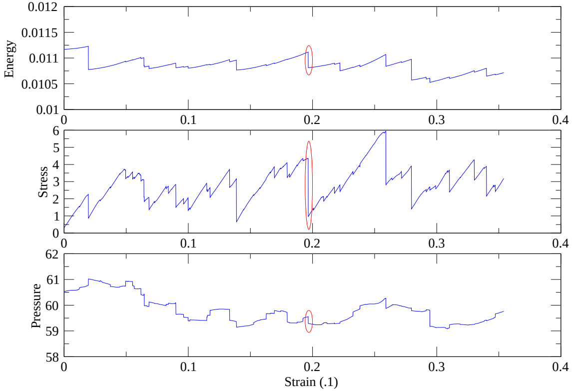
Atomistic Model and Algorithm

- Potentials:
  - Harmonic: $U = \frac{1}{2}ks^2$
  - Hertzian: $U = \frac{1}{2}ks^{5/2}$
  - Lennard-Jones: $U = k(r^{-12} - 2r^{-6})$
- Binary mixture.
- "Lees-Edwards" boundaries.
- Quasistatic Shearing: limit $T \to 0$, $\dot{\gamma} \to 0$
  - Apply uniform shear.
  - Minimize energy at fixed box.
  - Repeat.

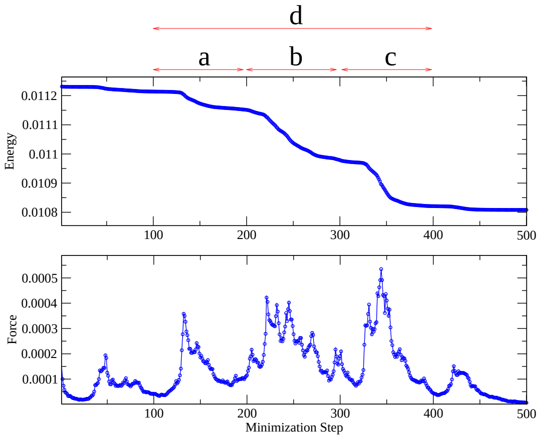




Stress-strain Curve



Small System – Small Events



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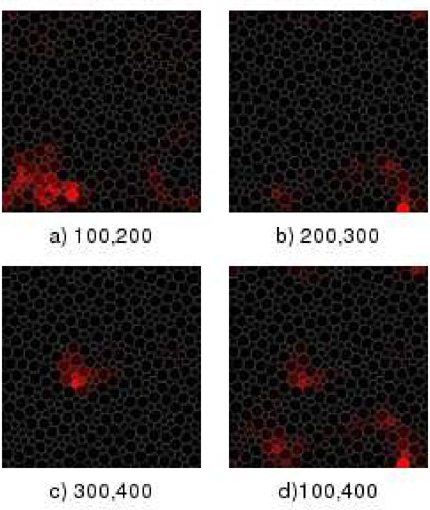
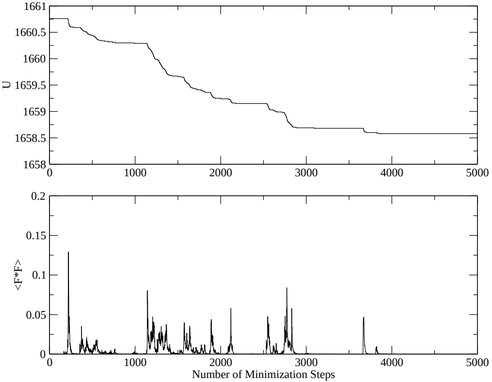
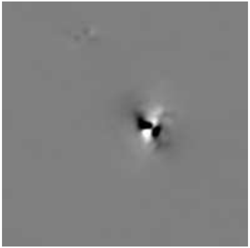
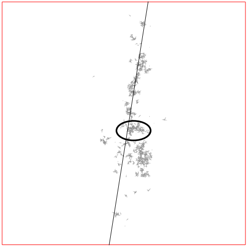


Observations on a Large System

Phys. Rev. Lett. 93, 016001 (2004)







An Issue about Localization

Europhys. Lett., **40** (1), pp. 61-66 (1997)

Nonlinear rheology of a highly supercooled liquid

R. YAMAMOTO and A. ONUKI
Department of Physics, Kyoto University, Kyoto 606-01, Japan

(received 25 May 1997; accepted in final form 29 August 1997)

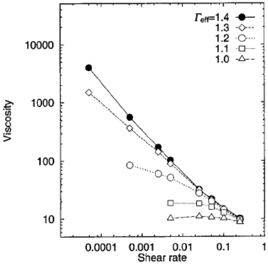


Fig. 1

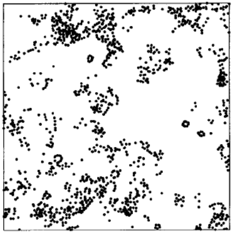
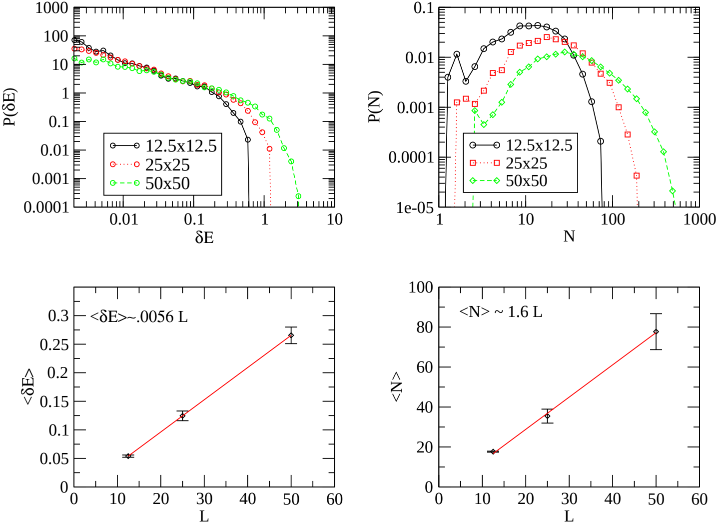


Fig. 2

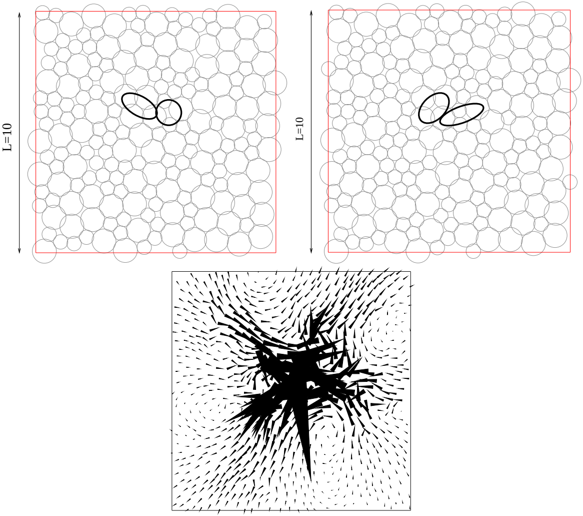
Fig. 1. – The viscosity $\eta(\dot{\gamma})$ *vs.* the shear rate $\dot{\gamma}$ at various $\Gamma_{\rm eff}$ in dimensionless units.

Fig. 2. – A snapshot of the broken bonds at $\Gamma_{\rm eff} = 1.4$ and $\dot{\gamma} = 0.5 \times 10^{-4}$. The time interval is $0.05\tau_{\rm b}$, so 5% of the initial bonds are broken here. The arrows indicate ξ. The horizontal axis is in the flow direction, while the vertical axis is in the velocity gradient direction.

Size of avalanches



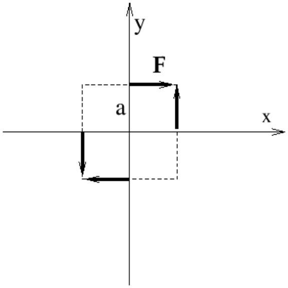
Zooming on the First Quadrupole



More about the Eschelby Calculation

Elastic consequences of a single plastic event :
a step towards the microscopic modeling of the flow of yield stress fluids.

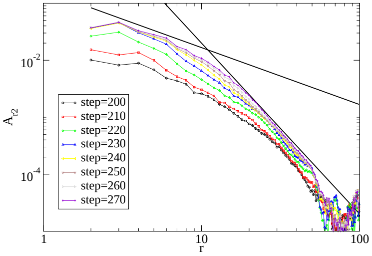
Guillemette Picard[1], Armand Ajdari[1*], François Lequeux[2], Lydéric Bocquet[3]
[1] *Laboratoire de Physico-Chimie Théorique, UMR CNRS 7083,*
[2] *Laboratoire de Physico-Chimie Macromoléculaire, UMR CNRS 7615,*
both at *ESPCI, 10 rue Vauquelin, F-75005 Paris, France*
[3] *Laboratoire PMCN, UMR CNRS 5586, Université Lyon I,*
43 Bd du 11 Novembre 1918, 69622 Villeurbanne Cedex, France



- Decay in $2D$:
  $\sigma_{xy} = \frac{2F\,a}{\pi\,r^2}\cos(4\theta)$
- With:
  - $F \sim a\mu\,\epsilon_0$
  - $\epsilon^{\mathrm{pl}} = a^2\,\epsilon_0$
  - Hence:
    $a\,F \sim a^2\,\mu\,\epsilon_0 \rightarrow$ Constant
    when $a \rightarrow 0$

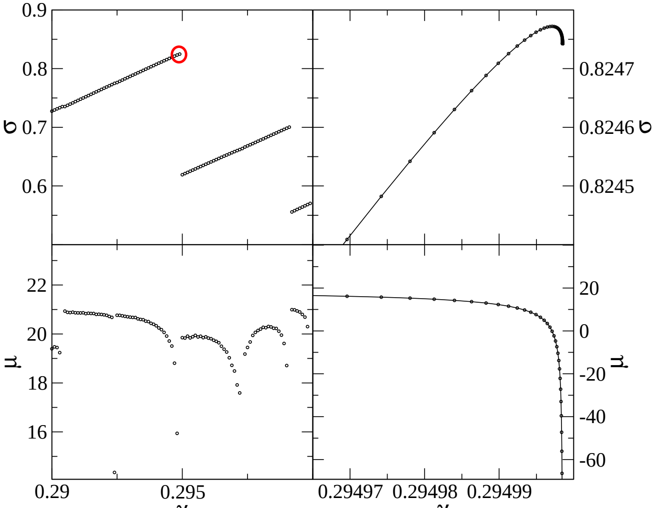
Fourier Analysis of the First Quadrupole

- Take radial component of displacement field
- Take its amplitude
- In $2D$: should decay as, $1/r^3$



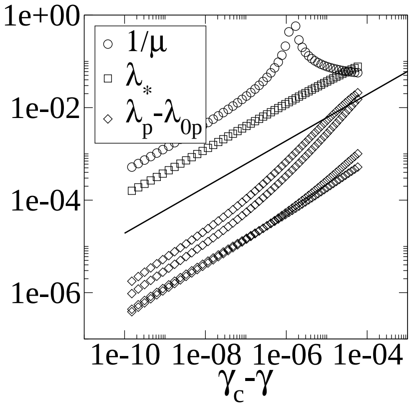
Catastrophes

- What happens when $\mathcal{H}$ becomes singular?
- $\frac{\mathrm{dr}}{d\gamma} \longrightarrow \infty$, $\frac{d\sigma}{d\gamma} \longrightarrow -\infty$.

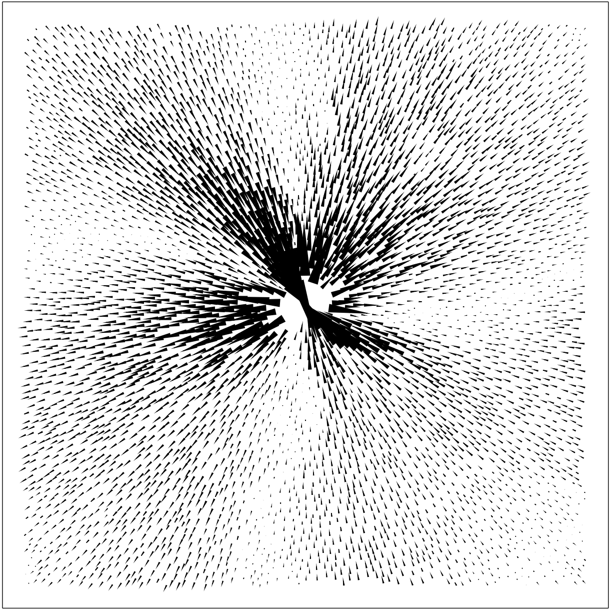


Scaling at the Onset of Failure

- Recall: $\frac{\mathrm{dr}}{d\gamma} = \mathcal{H}^{-1}.\Xi$
- At incipient failure: $\lambda^*(x) \sim ax$
  - $x(\gamma) \sim \sqrt{2(\gamma_c - \gamma)/a}$
  - $\lambda^*(\gamma) \sim \sqrt{2a(\gamma_c - \gamma)}$
  - $\widetilde{\mu} \sim -(\xi^*)^2/\sqrt{\gamma_c - \gamma}$



Critical Mode in Real Space



- $\frac{ds_{i\alpha}}{d\gamma}(\Delta\gamma \sim 10^{-9})$

Summary

- Elementary quadrupolar transformation can be observed at the onset of a cascade
- ...but they are difficult to separate at later stages
- A plastic event is a complex process: avalanche
  - Power-law distribution of avalanches sizes
  - Size of largest events determined by system size
  - Results from long-range elastic coupling
  - Speaking of criticality: are power laws a property of the quasi-static limit?
- Directions:
  - Need for 3D numerical studies
  - Finite strain-rates: departure from quasi-static limit
  - How timescales come into the picture?
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