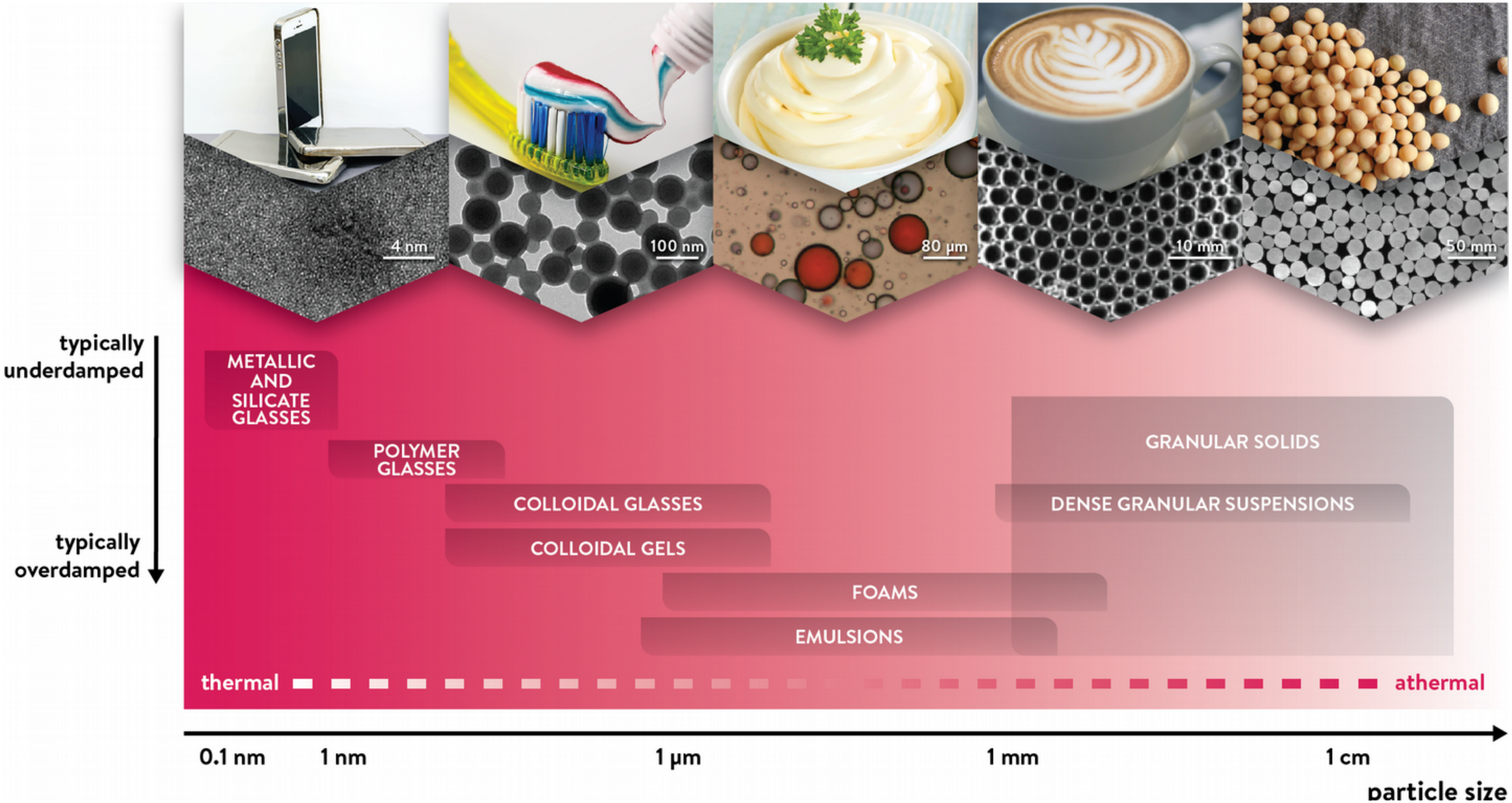
Deformation and flow of amorphous solids

(avalanche statistics and ductile-brittle transition)

Ezequiel Ferrero
Università degli Studi di Milano

Dipartimento di Biotecnologie Mediche e Medicina Traslazionale, UNIMI
November 16th 2017

Amorphous materials



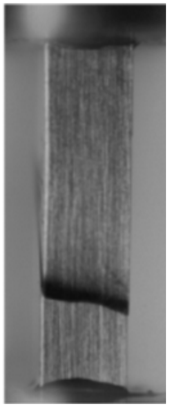
very diverse systems... but they share common features

Structurally ***disordered***

Solid-like (***elastic***) behavior below ***yield stress***

Flow under stress bigger than threshold

Yield stress systems

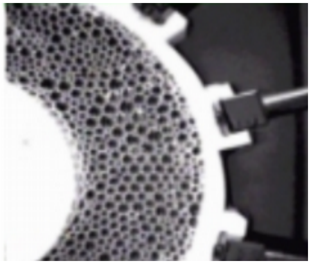


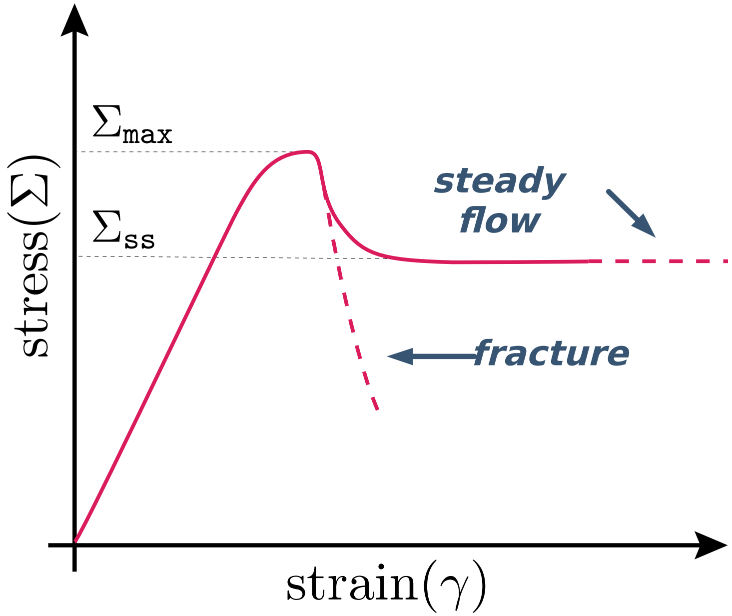
Bulk metallic glass
"hard" but somehow ductile

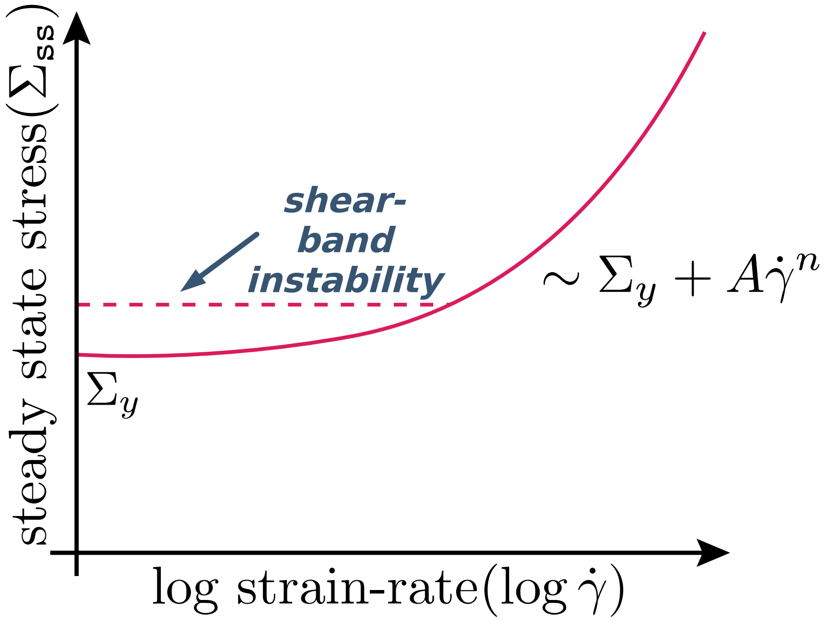
E~100 GPa

Soap foam
"soft"

E~100 Pa



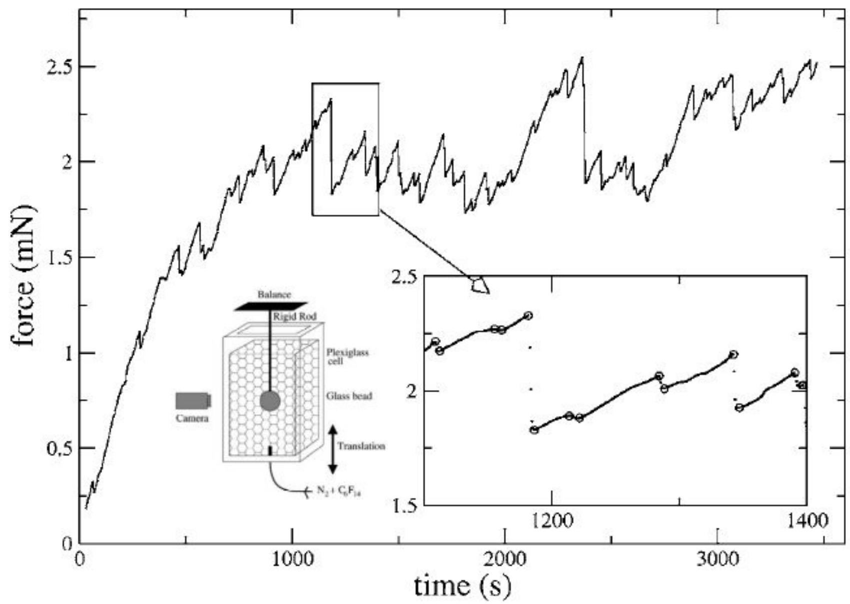




Phenomenology: 1. Local rearrangements

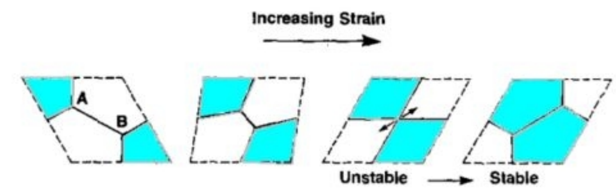
well identified, localized **"plastic events"**

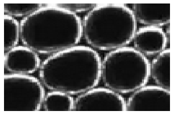
Foam moved at fix rate, exerting force on a bead



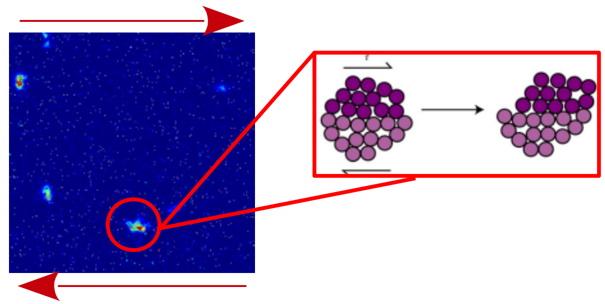
"jerky" aspect of the stress response

In foams: "T1 event" (4 bubbles)





In general: tens/hundreds of particles involved

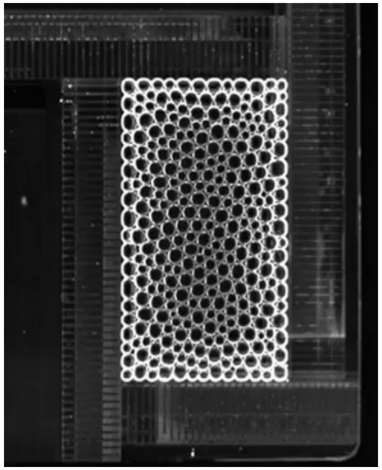


C. Derec et al. Phys. Rev. E **67** 61403 (2003)
I. Cantat and O. Pitois *Phys. Fluids* **18** 083302 (2006)

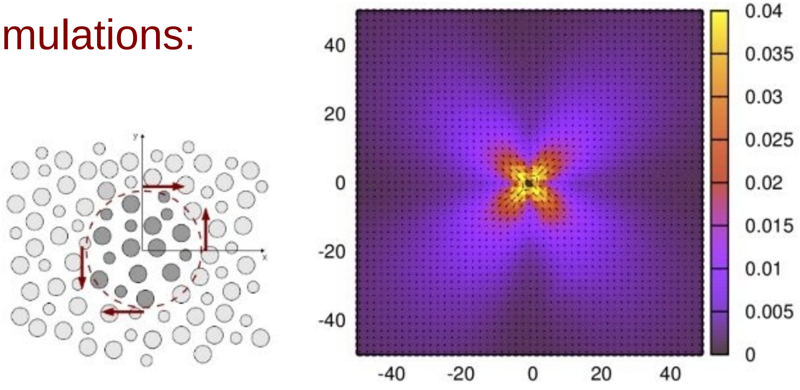
Princen and Kiss, *J Coll. Int. Sci.* **128** 176 (1989)
"T1 event in a densely packed foam" by M. van Hecke, youtube (2014)
A. Nicolas et. al EPJE **37** 50 (2014), A.S. Argon and H.Y. Kuo Mat. Sci. Eng. **39** 101 (1979)

Phenomenology: 2. Medium elastic response

A foam under shear strain



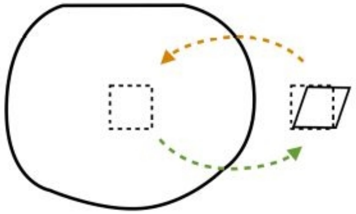
MD simulations:



imposed shear transformation and average displacement field

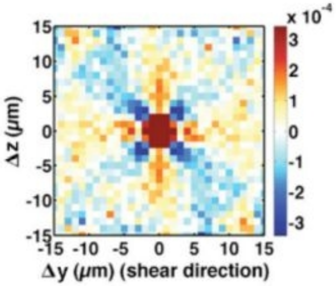
Continuum mechanics:

elastic response to a deformed inclusion

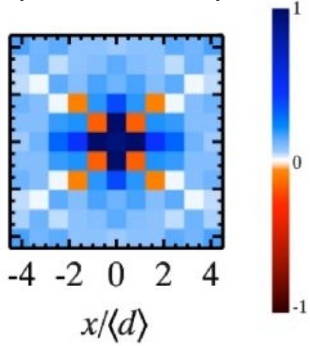


Experimental measurements:

correlations of local strain (sheared colloidal glass)



average stress change around an event (2D emulsion)



"Eshelby" propagator for the stress redistribution

$$G^{2D}(r,\theta) = \frac{1}{\pi r^2} cos(4\theta)$$

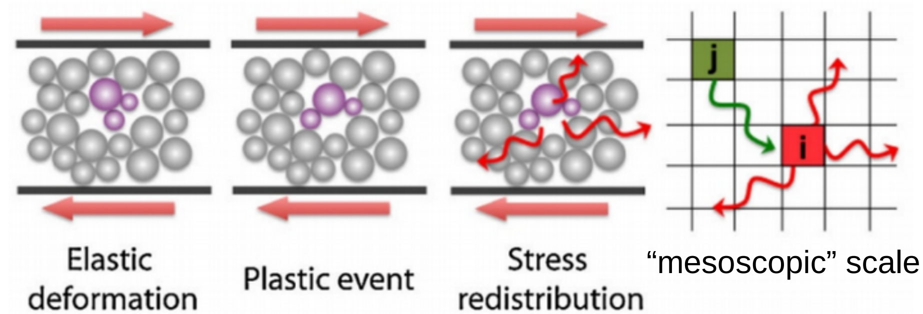
Quadrupolar in symmetry, ***dipolar*** in range

"Shearing a 2D foam" by M. van Hecke, youtube (2014)

Jensen et al, PRE **90**, 042305 (2014)   Desmond and Weeks, PRL **115**, 098302 (2015)

F. Puosi, J. Rottler, J.-L. Barrat PRE **89** 042302 (2014)
J.D. Eshelby Proc. Roy. Soc. A **241** 376 (1957)
Picard *et al*. EPJE **15** 371 (2004)

Coarse-grained Elasto-Plastic Models (EPM)



Simplifications:

- *Scalar*
- *Athermal*
- *Overdamped*

$$\partial_t \sigma_i(t) = \underbrace{\mu \dot{\gamma}^{\mathtt{ext}}}_{\text{external strain-rate}} - \underbrace{g_0 n_i(t) \frac{\sigma_i(t)}{\tau}}_{\text{local plastic yield}} + \underbrace{\sum_{j \neq i} G(i,j) n_j(t) \frac{\sigma_j(t)}{\tau}}_{\text{“mechanical noise” due to plastic activity elsewhere}}$$

Eshelby **propagator**

$$\boxed{G^{2d}_{(i,j)} = \cos(4\theta_{ij})/\pi r^2}$$

+ Dynamical **rules** for a local “**state**”

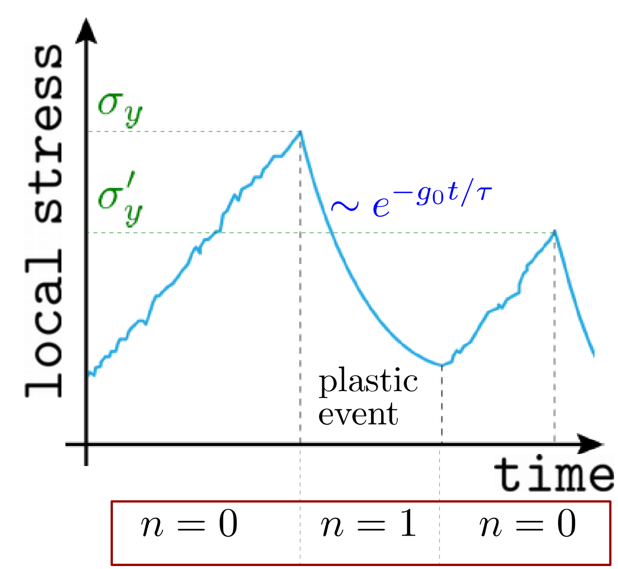


Fig. credit:
Bocquet *et al.* PRL **103**, 036001 (2009)

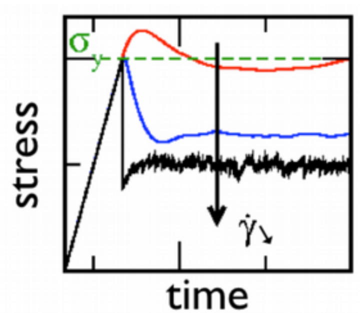
ADVERTISING

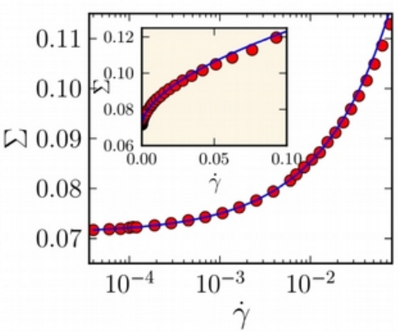
Deformation and flow of amorphous solids: a review of mesoscale elastoplastic models

Alexandre Nicolas, Ezequiel E. Ferrero, Kirsten Martens, Jean-Louis Barrat

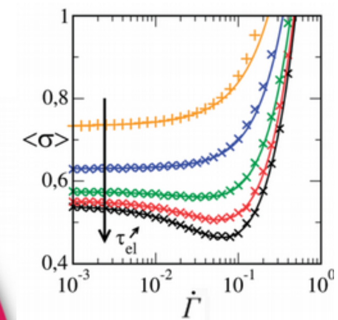
arXiv:1708.09194

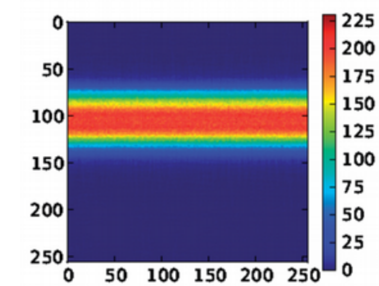
Stress-strain and flowcurves

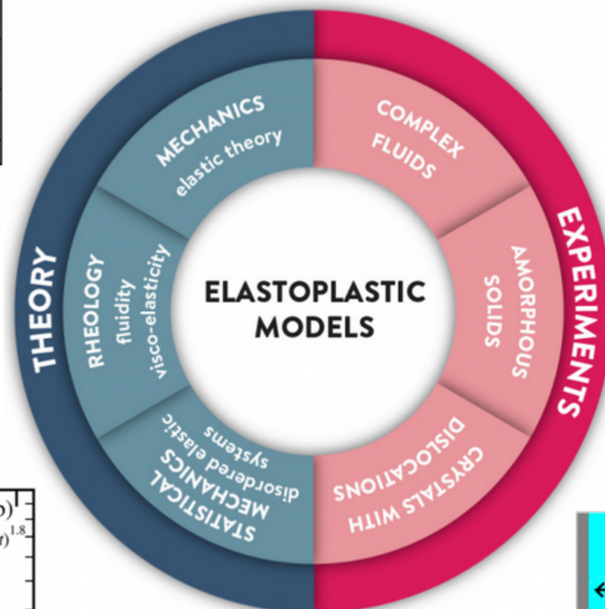




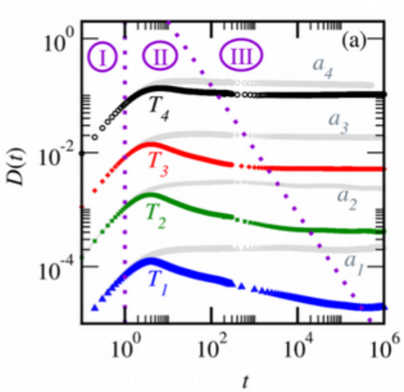
Shear localization

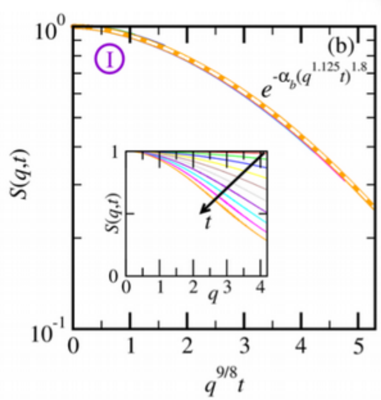




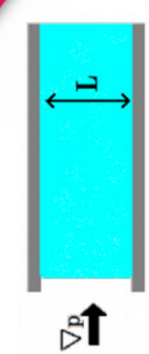


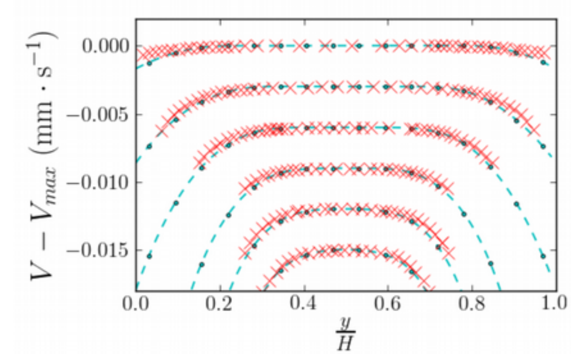
Relaxation in yield-stress systems





Flow and fluctuations in microchannels





Phenomenological, but also good “toy models” to do theoretical StatMech

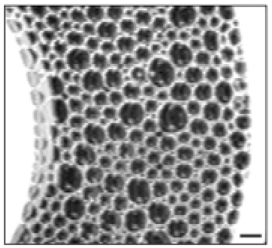
One example:

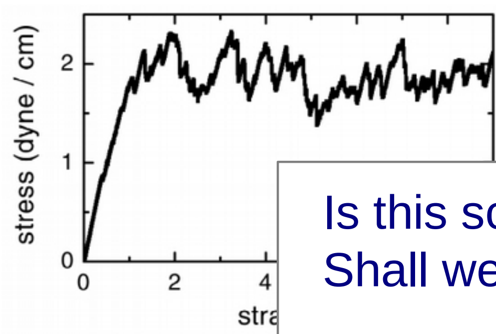
AVALANCHES

Avalanches: experiments

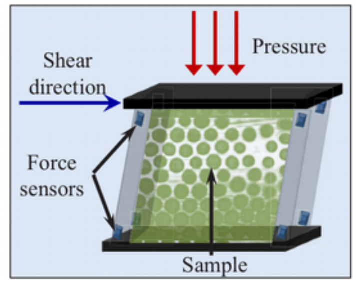
Plastic flow and stress drops

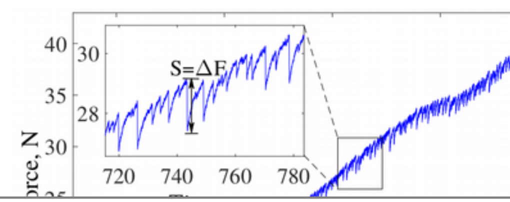
Foams



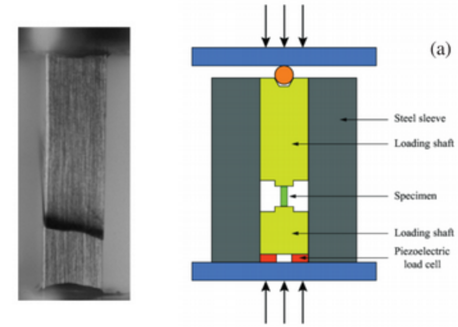


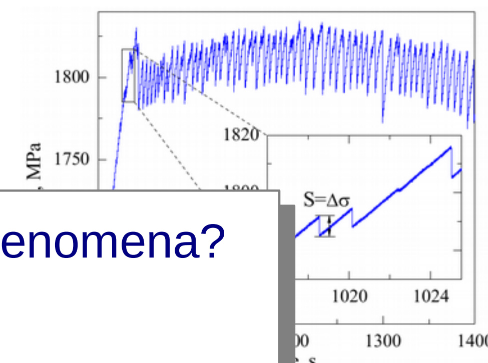
Granular systems



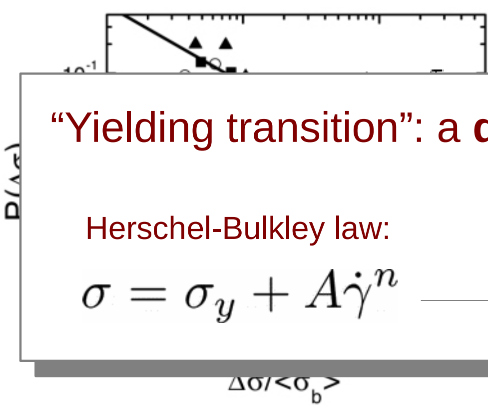


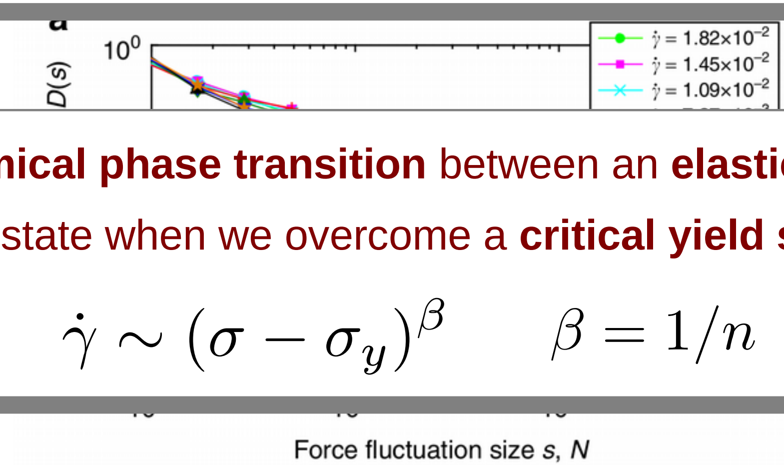
Bulk metallic glasses

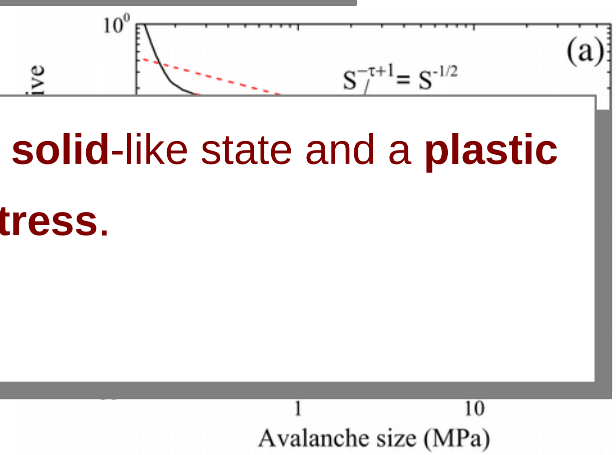




Is this scale freedom related to any kind of “critical” phenomena? Shall we expect universality?







“Yielding transition”: a **dynamical phase transition** between an **elastic solid**-like state and a **plastic flow** state when we overcome a **critical yield stress**.

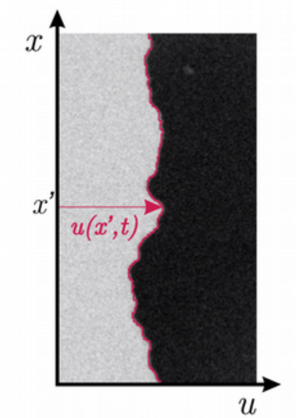
Herschel-Bulkley law:

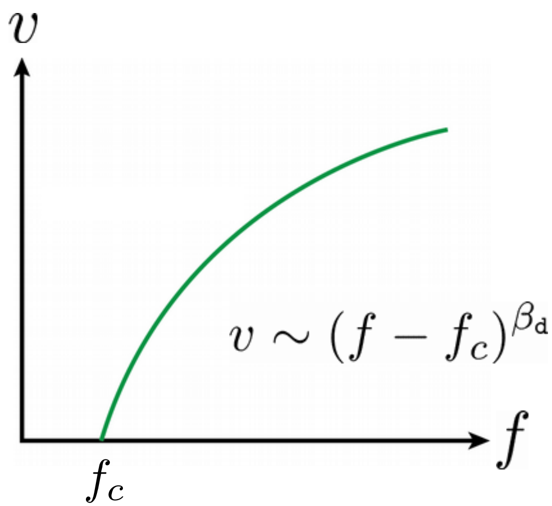
$$\sigma = \sigma_y + A\dot{\gamma}^n \longrightarrow \dot{\gamma} \sim (\sigma - \sigma_y)^\beta \qquad \beta = 1/n$$

J. Lauridsen et al. PRL **89** 098303 (2002) D. Denisov et al. NatComm **7**:10641 (2016), SciRep **7**:43376 (2017) J. Antonaglia et al. PRL **112** 155501 (2014)

Phase transition analogies

Depinning





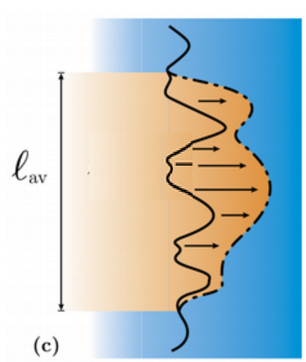
More than **30 years** of research

$$\eta \partial_t u(x,t) = c\partial_x^2 u(x,t) + F_p(u,x) + f$$

Interface is rough and self-affine at f_c
Divergent length and avalanches:

$$\ell \sim (f - f_c)^{-\nu} \ , \ \nu = \frac{1}{2-\zeta}$$

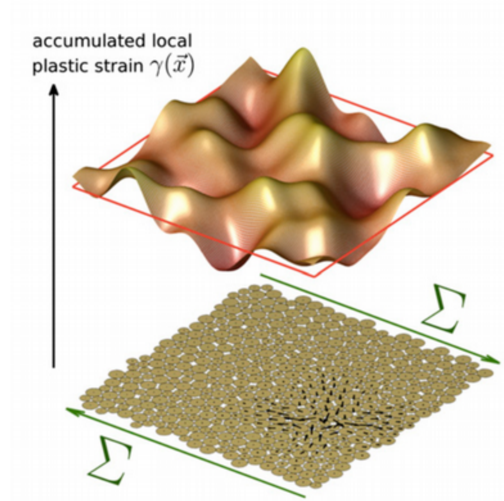
$$P(S) \sim S^{-\tau} \ , \ \tau = 2 - \frac{2}{d+\zeta}$$

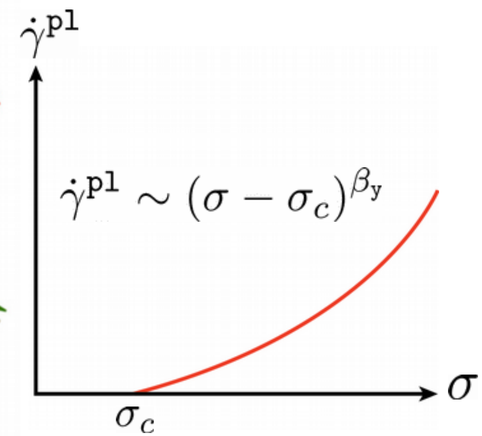


$$\tau_{\mathrm{MF}} = 3/2$$

D. Fisher Phys. Reports (1998)
EEF et al., Comp. Rend. Phys. (2013)

Yielding





Long-range depinning analogy proposals*

$$\eta \partial_t \gamma_i^{\mathrm{pl}} = \mu G_{ij} \gamma_j^{\mathrm{pl}} + F_p(\{\gamma_i^{\mathrm{pl}}, i\}) + \sigma$$

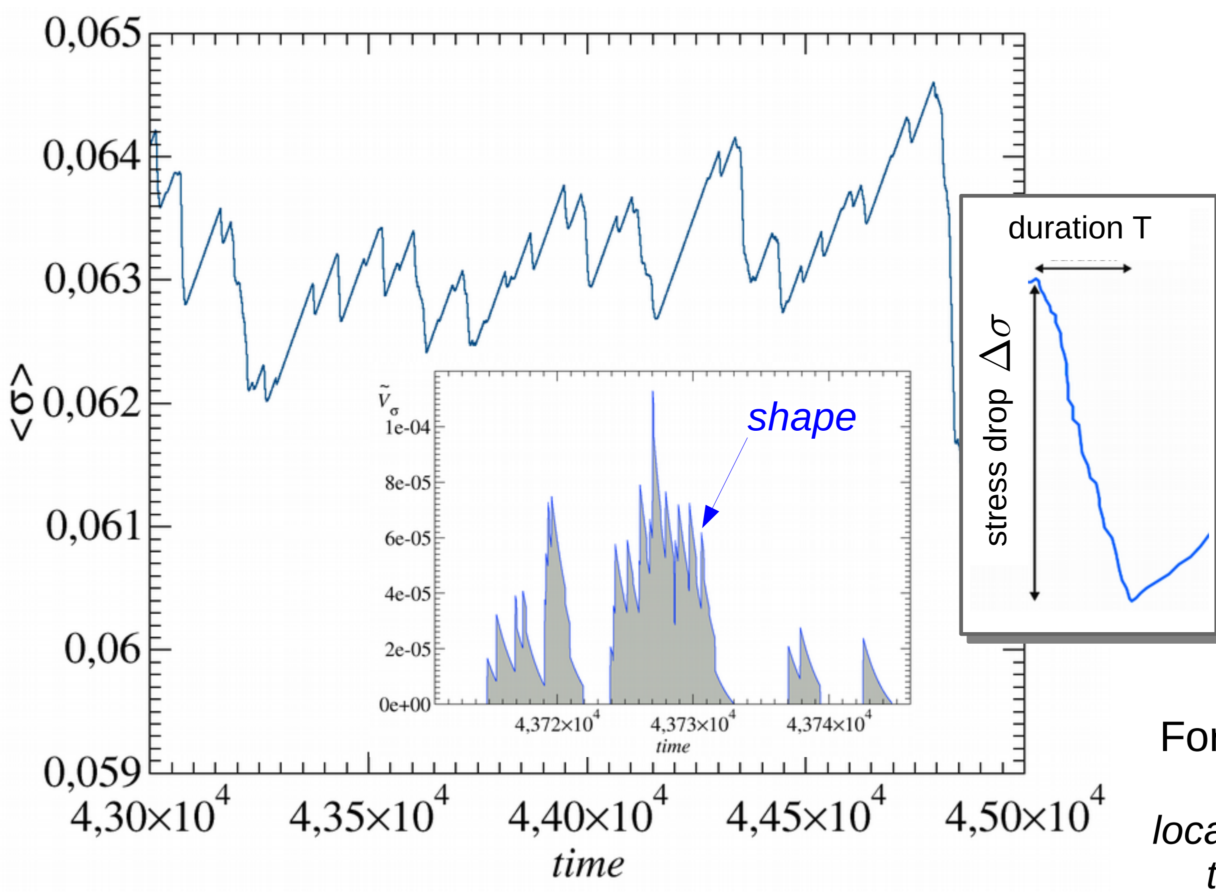
Divergent length scale and associated avalanche dynamics?

$$\xi \sim |\sigma - \sigma_c|^{-\nu} \ , \ \nu = ? \qquad S = ? \qquad \tau = ?$$

*e.g., J. Weiss et al. PNAS **111**, 6231 (2014)
Dahmen et al. PRL **102** 175501 (2009)

Avalanches: Simulations

We run our EPM for different imposed strain rates and system sizes...



Observables:

For **each event** (stress-drop *Δσ*) we compute:

duration $T = t_{\mathtt{end}} - t_{\mathtt{start}}$

size $S \equiv L^d \Delta\sigma$

shape $\tilde{V}_\sigma(t) = \left[-\frac{d\langle\sigma\rangle(t)}{dt} \right]_{t_{\mathtt{end}}}^{t_{\mathtt{start}}}$

For several **configurations** in time

local distances to threshold $\{x\}\ ,\ x_i \equiv \sigma_i^y - \sigma_i$

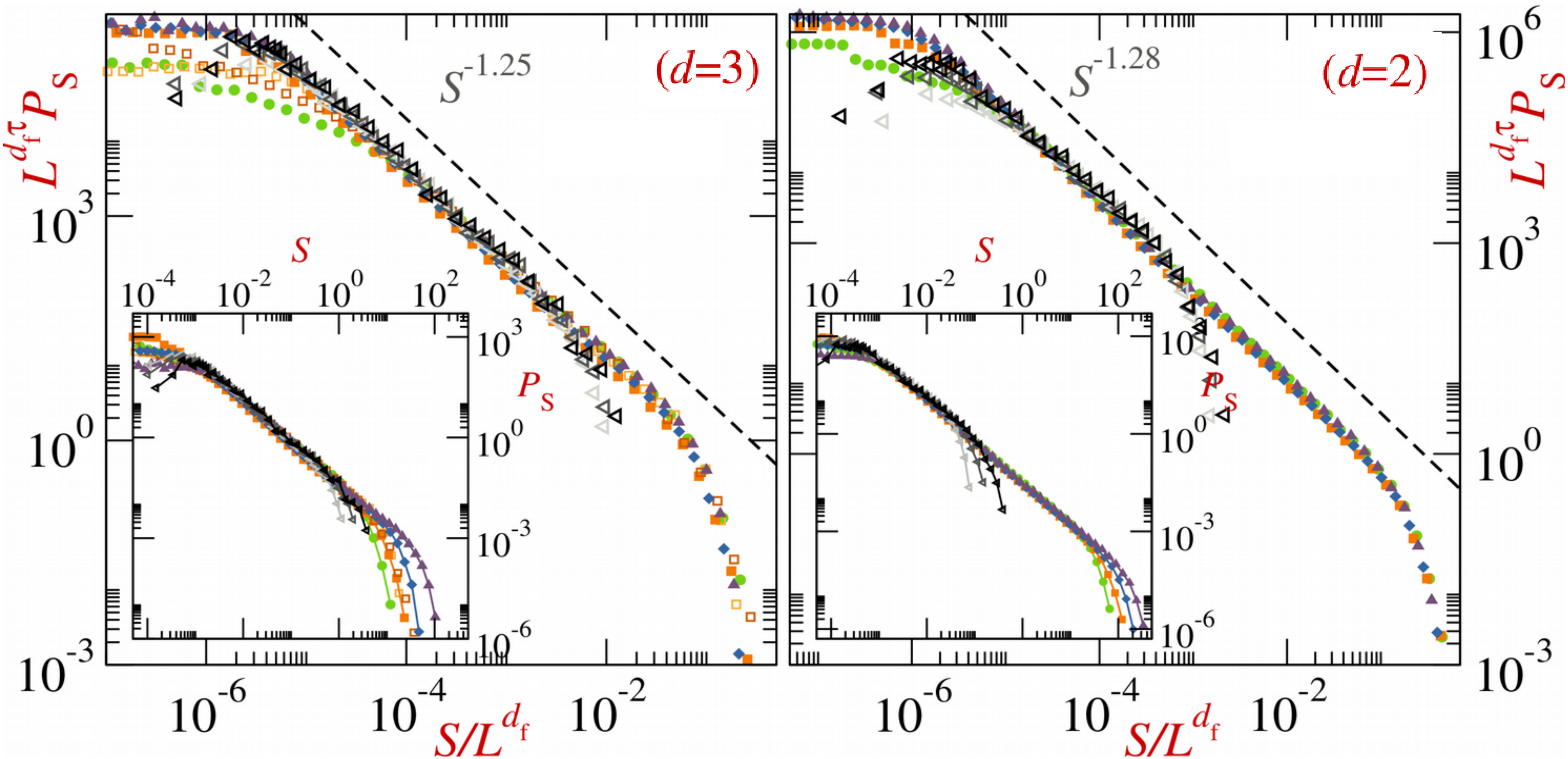
Massively parallel implementation on GPUs

C. Liu, EEF, F. Puosi, J-L Barrat, K Martens PRL 116 065501 (2016)

Results

Stress drop size distribution at very low shear rates

...for different system sizes, comparing with <u>quasistatic</u> **MD** simulations (grayscale triangles)



$\tau_{3D} \simeq 1.25 \neq \tau_{\mathtt{MF}}^{\mathrm{dep}}$

$d_f^{3D} \simeq 1.3$

$$P_S \propto S^{-\tau} f(S/S_c)\ ,\ \ S_c \simeq L^{d_f}$$

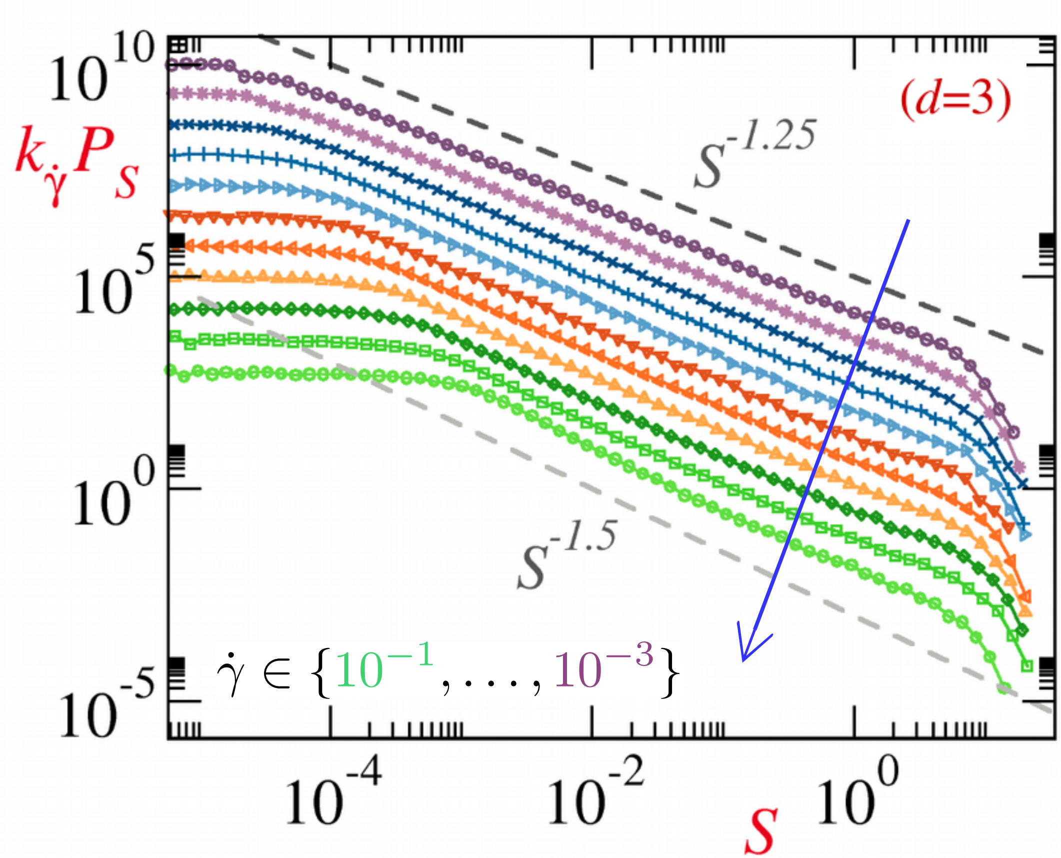
$\tau_{2D} \simeq 1.28$

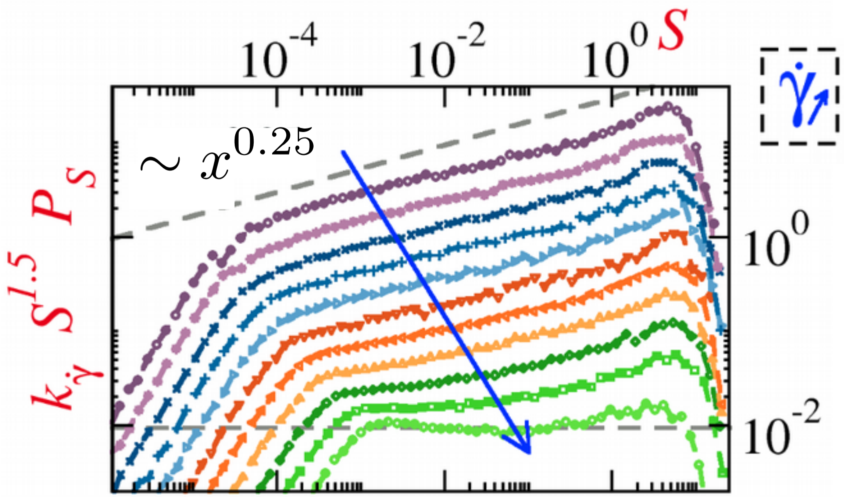
$d_f^{2D} \simeq 0.9$

scaling factor d_f: “fractal dimension”. *Slip-line* avalanche geometry

Results

Size distributions and crossover to mean-field behavior





(curves arbitrarily shifted by $k_{\dot\gamma}$)

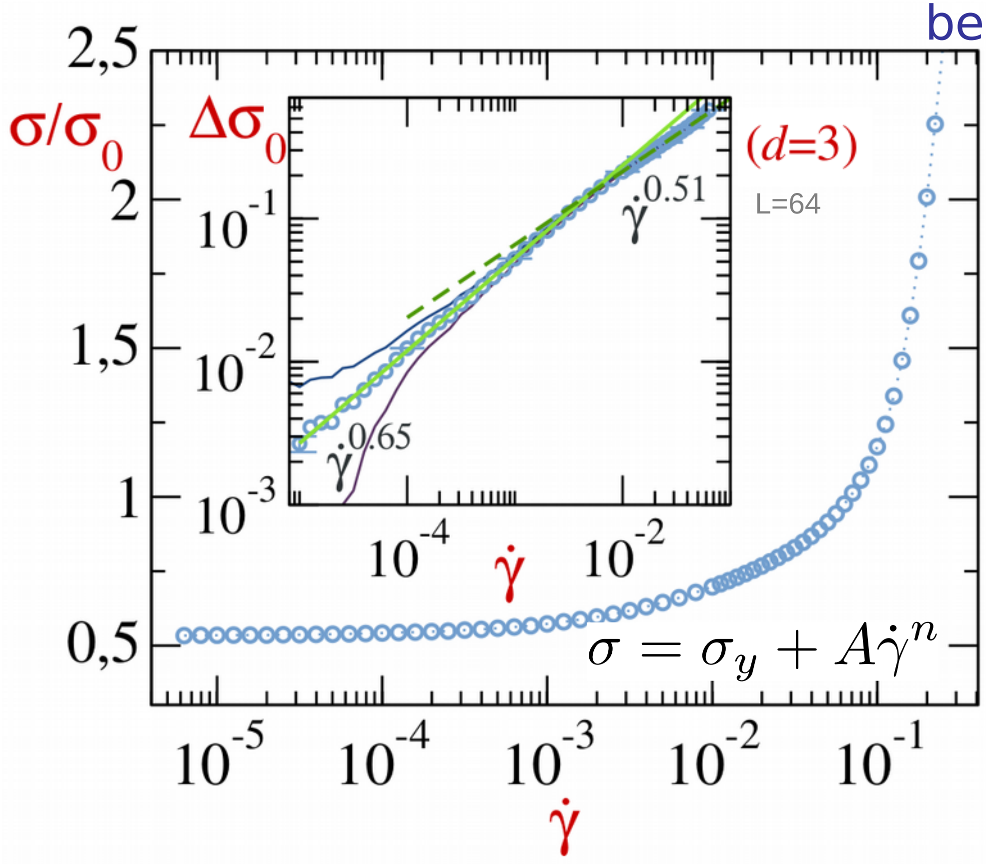
- Large strain-rates **"randomizes"** the stress signal, **by overlapping** uncorrelated plastic activity.
- **Crossover** to **depinning mean-field** exponent when we **go away** from the yielding point

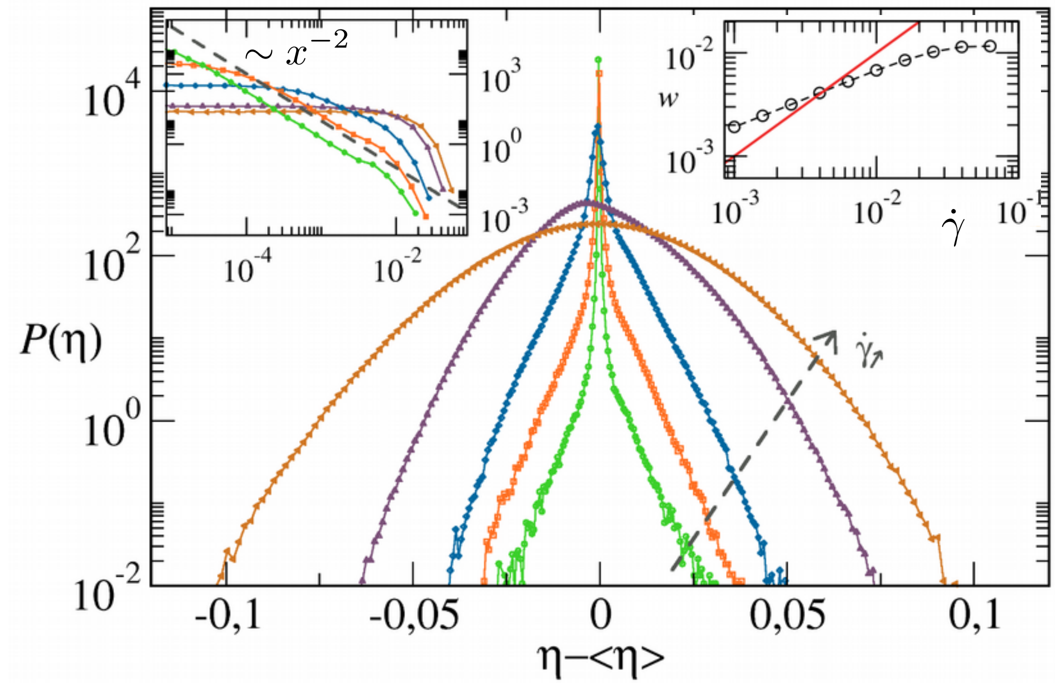
$$\tau : 1.25 \to 1.5$$

Be ξ^d the size of a "correlated event", with $\xi \sim |\langle\sigma\rangle - \sigma_c|^{-\nu} \sim \dot\gamma^{-\nu/\beta}$
Many events may "fit" in L^d. $\Delta\sigma$ results from this superposition.
$S \equiv \Delta\sigma L^d$ cutoff is controlled by L

Results

Flow-curve and crossover to mean-field “randomized” behavior





“Mechanical noise” → η_i

$$\partial_t \sigma_i = \mu\dot\gamma - g_0 n_i \frac{\sigma_i}{\tau} + \underbrace{\sum_{j\neq i} G_{ij} n_j \frac{\sigma_j}{\tau}}_{\eta_i}$$

$$\dot\gamma \sim (\sigma - \sigma_y)^\beta \qquad \beta = 1/n > 1$$

- β **crosses over toward the Hébraud-Lequeux mean-field** prediction when $\dot\gamma$ increases.

$$\beta \simeq 1.54 \to 2$$

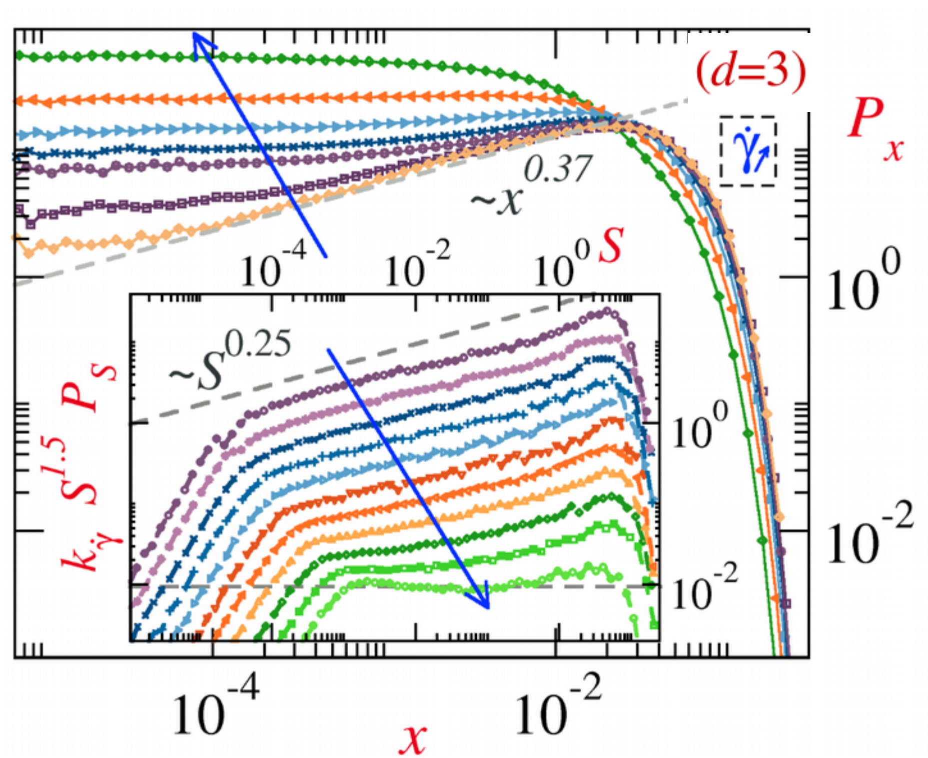
- At large rates, noise distribution turns Gaussian → **loss of non-trivial correlations**

- Variance grow slower than linear with $\dot\gamma$ → **drift dominates when** $\dot\gamma >\sim 0.004$

Results

Distribution of local distances to threshold (or "density of shear transformations")

$$x \equiv \sigma_y - \sigma$$



Expected: *"marginal stability"* pseudo-gap
(M. Wyart and co.)

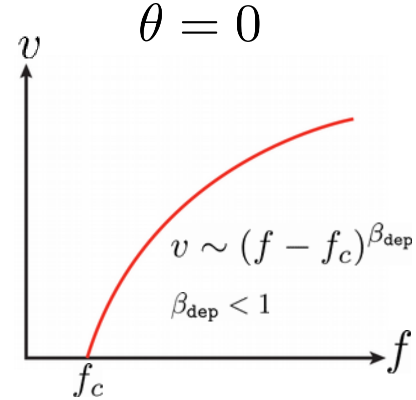
$$P_x \sim x^{\theta} \qquad \theta > 0$$

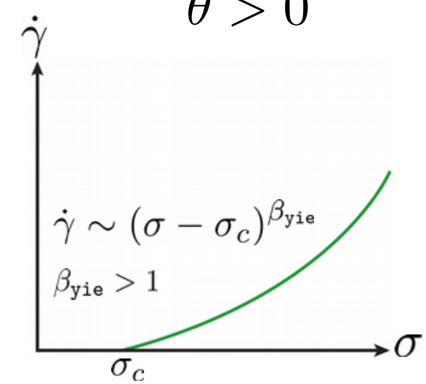
We observe:

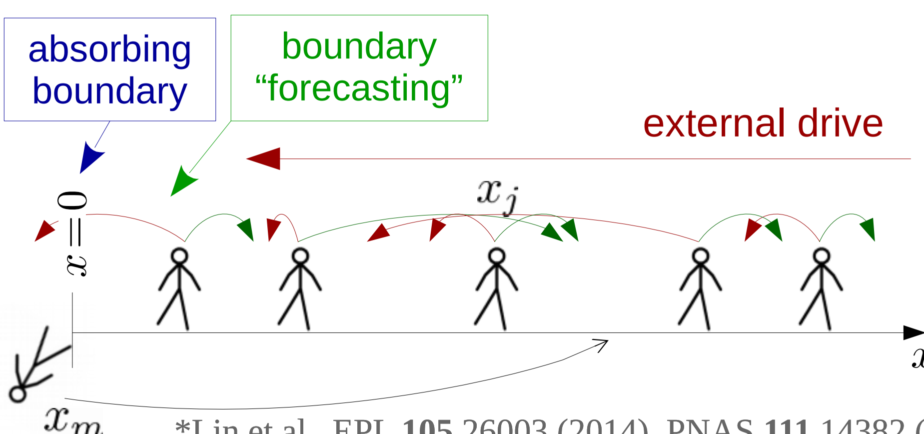
At $\dot\gamma \to 0$ $\quad \theta_{2D} \simeq 0.52 \quad \theta_{3D} \simeq 0.37$

When $\dot\gamma \gg 0$ $\quad \theta \to \theta^{\mathrm{dep}} = 0$

depinning	yielding
$\beta \leq 1$	$\beta > 1$
$d_f \geq d$	$d_f < d$
$\theta = 0$	$\theta > 0$







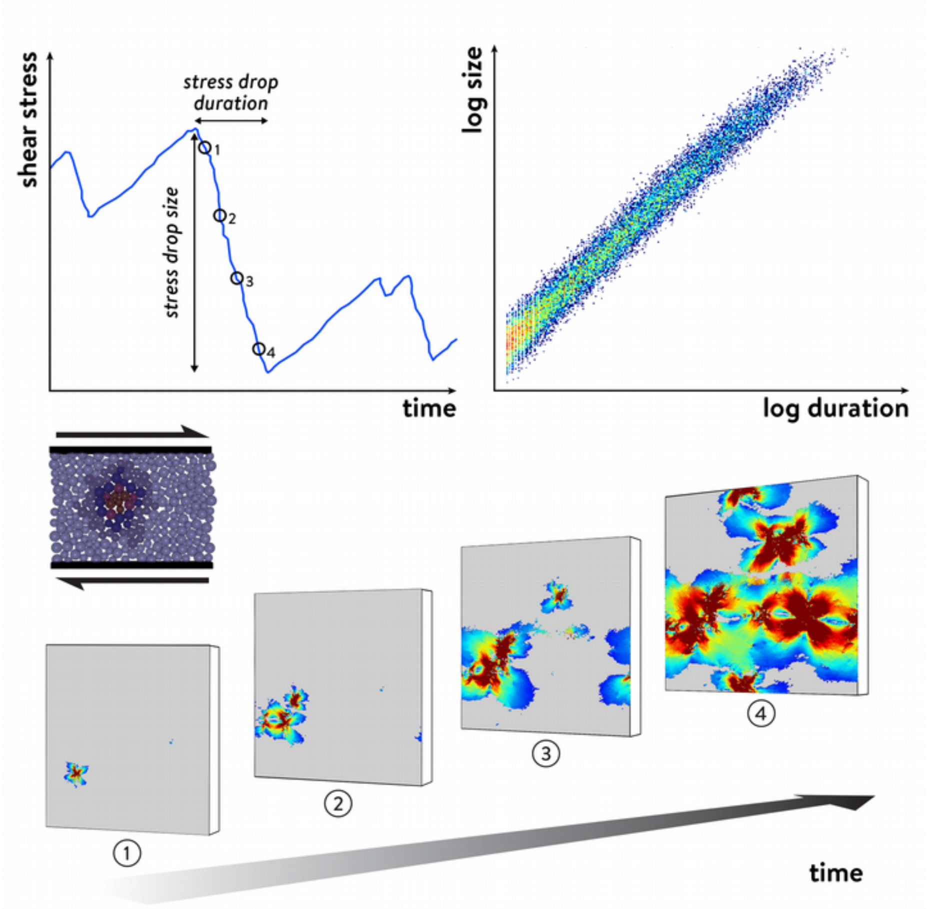
*Lin et al., EPL **105** 26003 (2014), PNAS **111** 14382 (2014)

Partial Summary

- Our results reinforce the idea of a **non-MF-depinning universality class** for the yielding transition below d=4.

- **Departing from** the **yielding** point, at **finite shear rates**, the rise of many independent regions with yielding activity randomizes the response and draw exponents **closer to MF expectations**.

- ***The density of STZs* crosses over** from yielding marginal stability ***P(x)~x***$^{\theta}$ to depinning-like ***P(x)~cst***. when increasing the external strain rate.



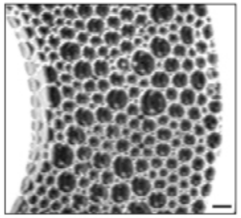
Driving Rate Dependence of Avalanche Statistics and Shapes at the Yielding Transition
Chen Liu, Ezequiel E. Ferrero, Francesco Puosi, Jean-Louis Barrat, Kirsten Martens
Phys. Rev. Lett. **116** 065501 (2016)

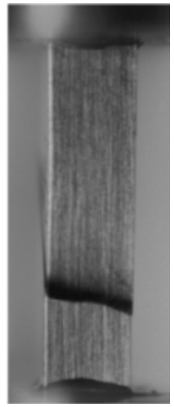
Inertia and universality of avalanche statistics: The case of slowly deformed amorphous solids
Kamran Karimi, Ezequiel E. Ferrero, Jean-Louis Barrat
Phys. Rev. E **95**, 013003 (2017)

Ductile vs brittle materials

Soap foam
“soft”

E~100 Pa



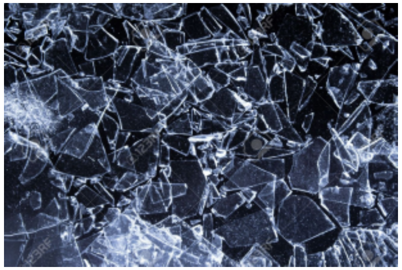


Bulk metallic glass
“hard” somehow ductile

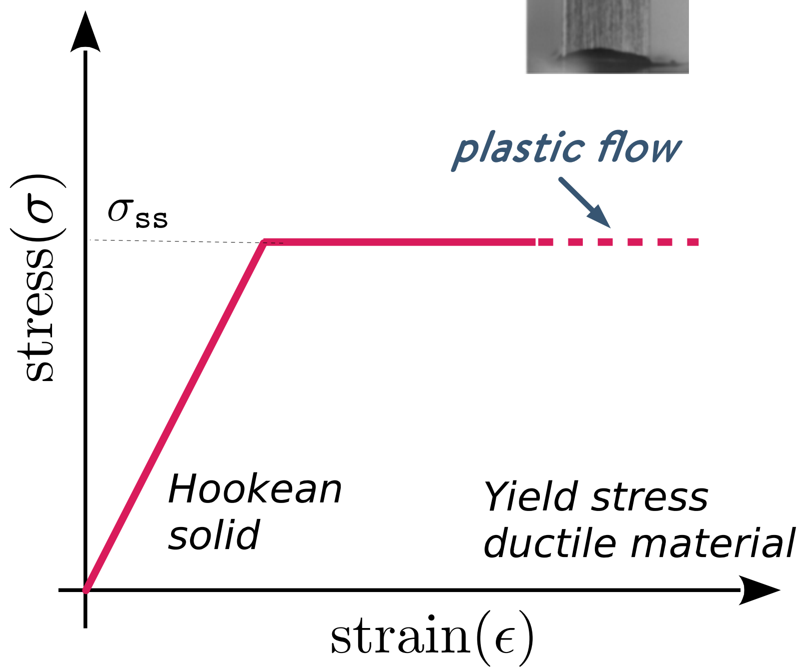
E~100 GPa

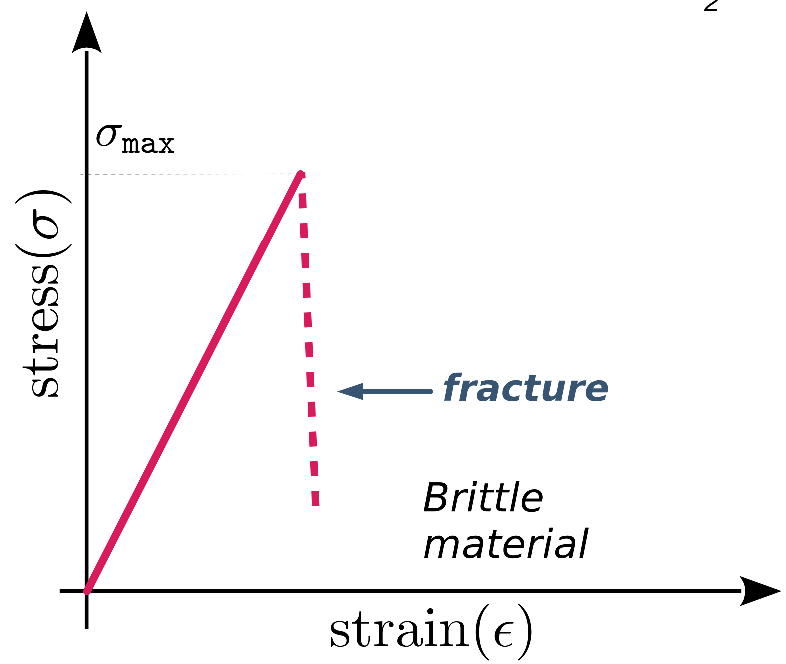
Silica glass
hard and brittle

E~70 GPa



a-SiO_2



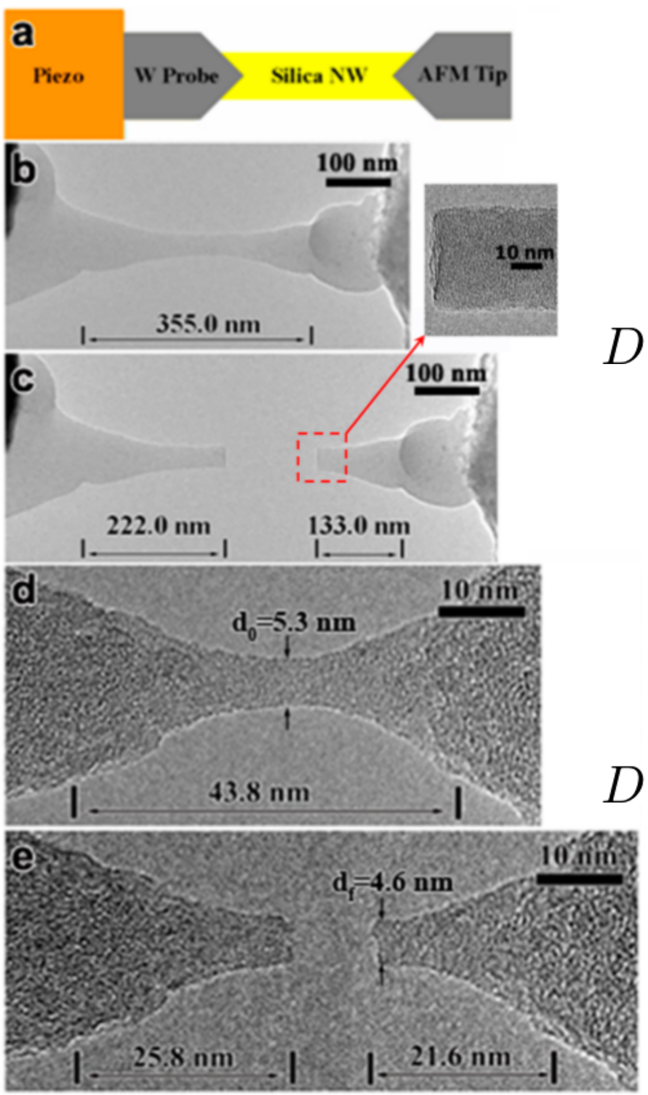


“Yielding transition” between a **solid state** and a **plastic flow** at a critical **yield strain**

Brittle fracture:
- *no “plastic plateau”*
- *no “yielding transition”*

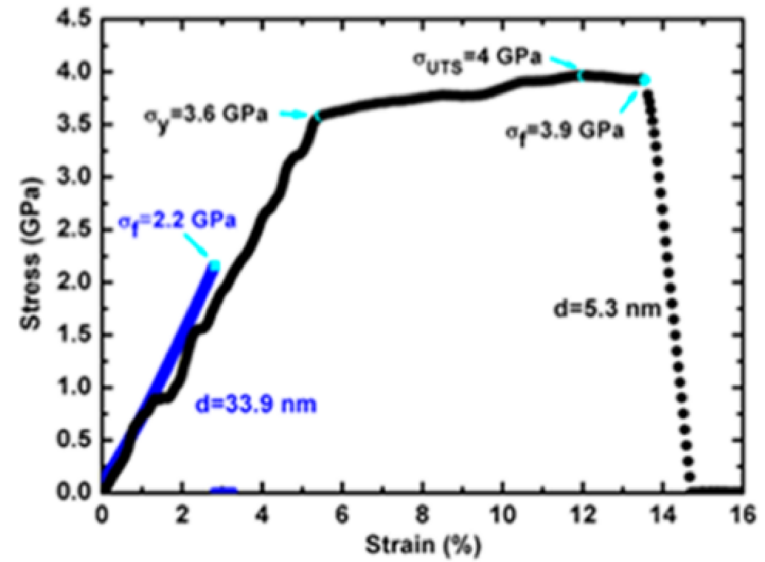
Plastic deformation of silica glass!
(at the nano-scale)

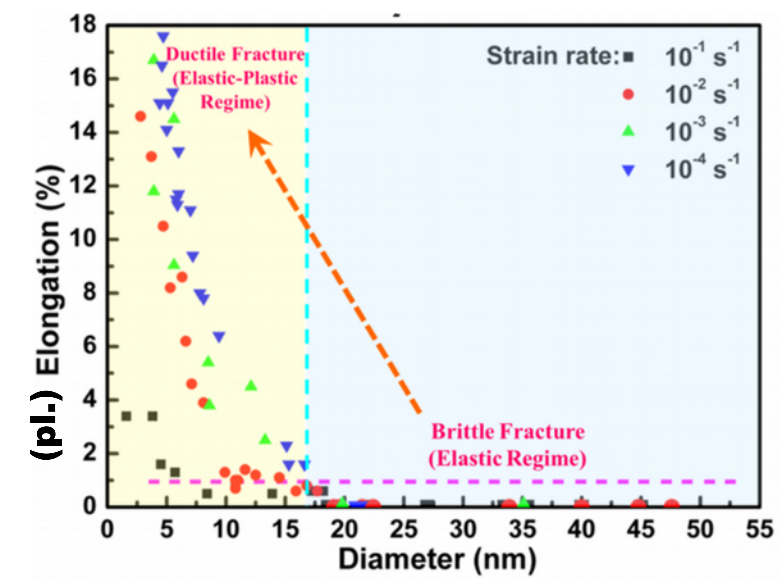
Tensile deformation of SiO_2 nanofibers



$$D = 33.9nm$$

$$D = 5.3nm$$





J. Luo et al. Nano Lett. **16**, 105 (2016)

Brittle-to-Ductile transition as diameter decreases

Molecular Dynamics simulations of a SiO_2 model

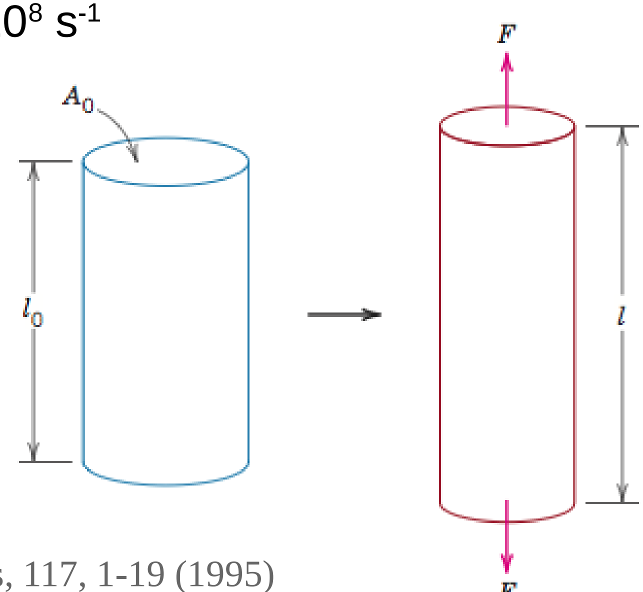
Size-driven brittle to ductile transition in the tensile deformation of silica glass

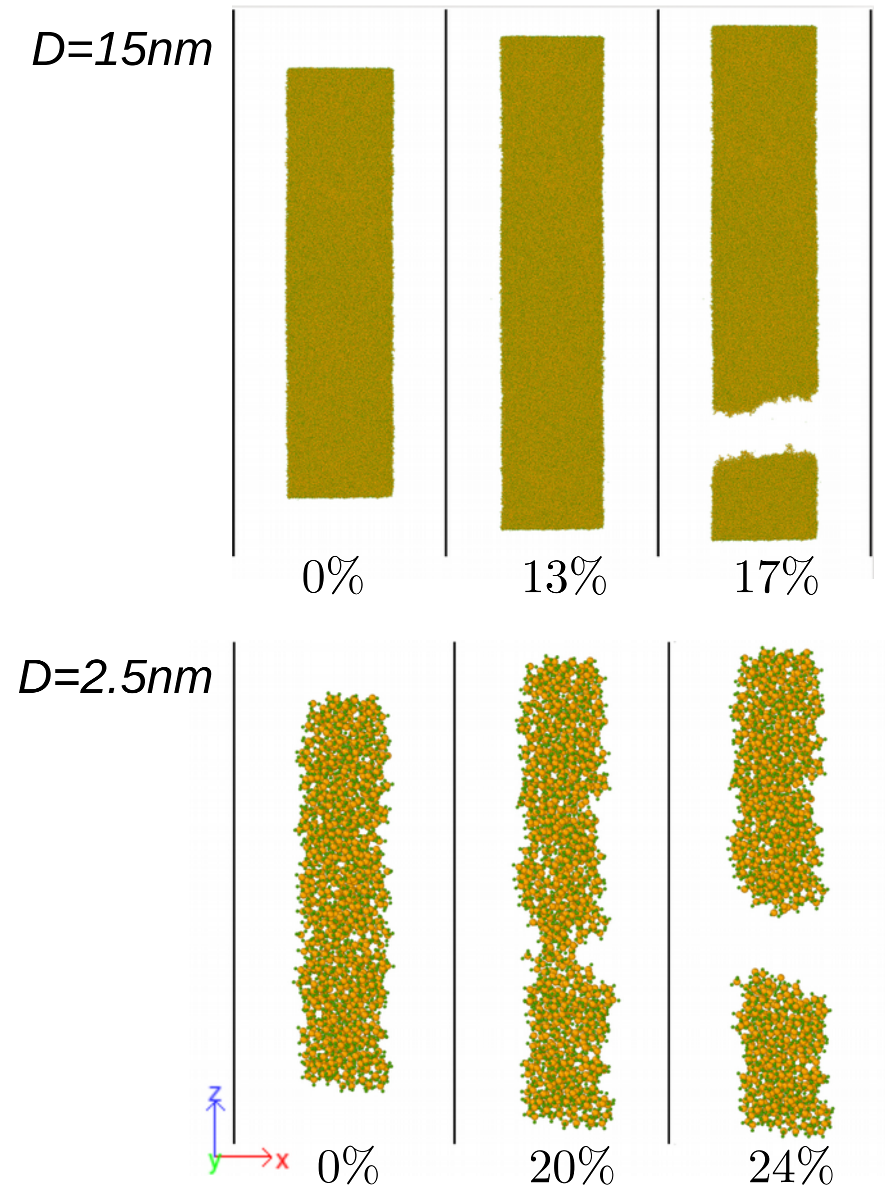
In preparation @CC&B, UNIMI

Tools:
- LAMMPS [1]
- Watanabe potential for *a*-silica [2]

Setup:
- Randomly distributed *Si* and *O* atoms (ratio 1:2) in a hard cylinder shell. Number matching correct density.
- Thermal annealing and subsequent equilibration.

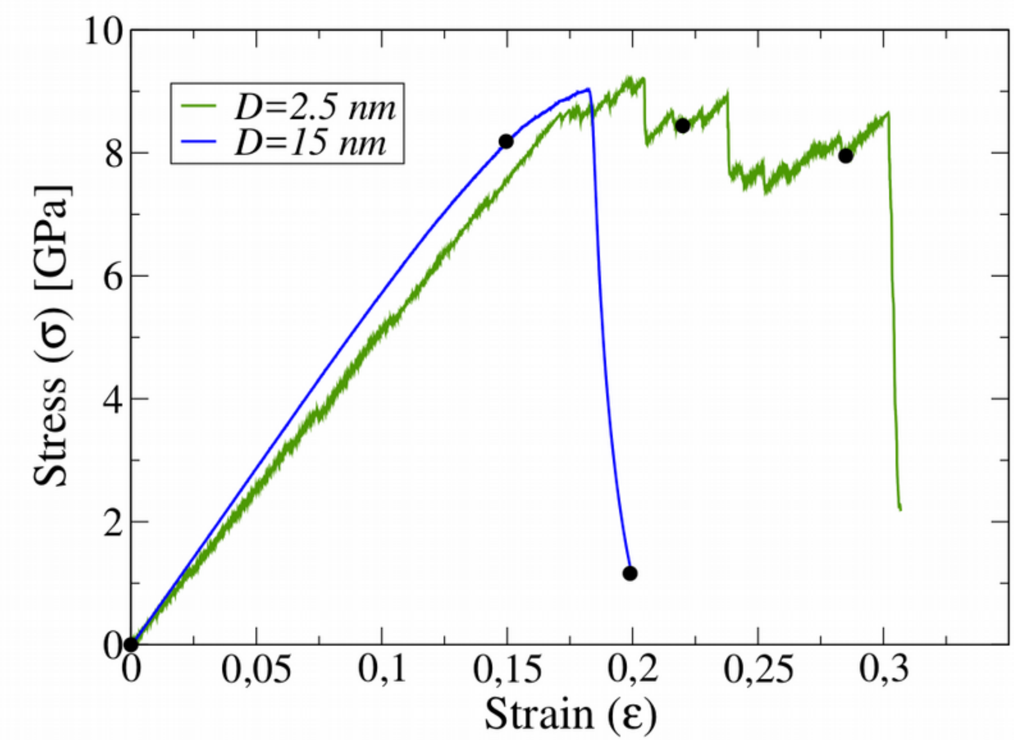
Deformation protocol:
- Uniaxial tensile deformation at cst. velocity
- Strain-rate ~ 2.5 10^8 s^{-1}
- T ~ 0 K

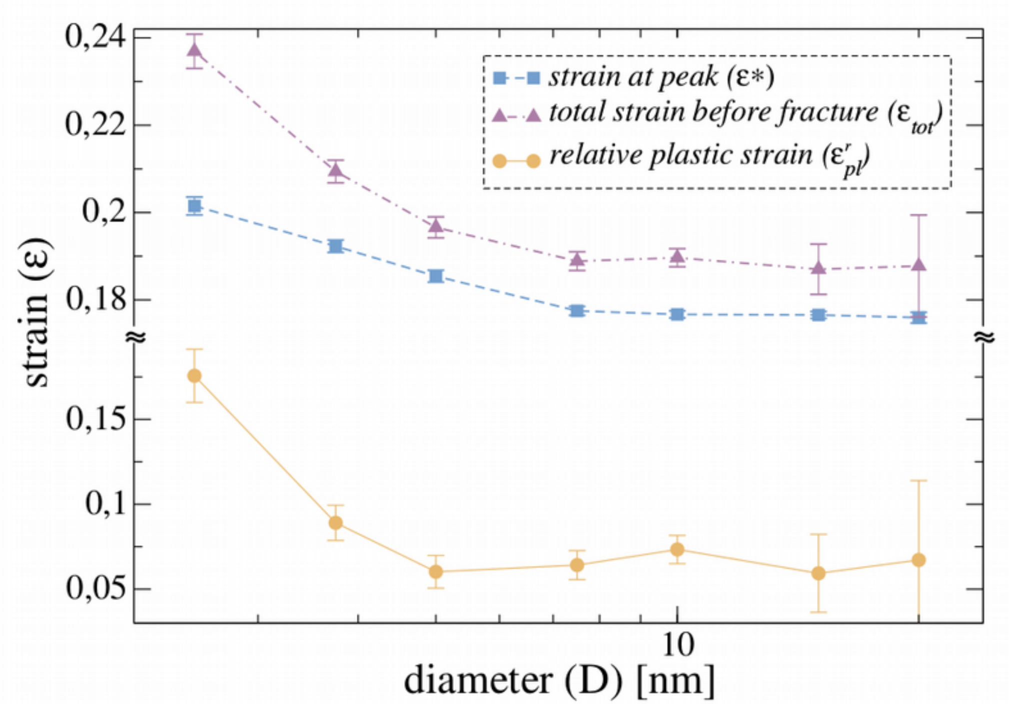




[1] S. Plimpton, J. Comp Phys, 117, 1-19 (1995)
[2] Watanabe et al. *Jap. Jour. of Appl. Phys. 38*, L366 (1999)

Brittle-to-ductile transition by size reduction





Total strain before fracture strongly enhanced for thin fibers

Typical paths to gain ductility:

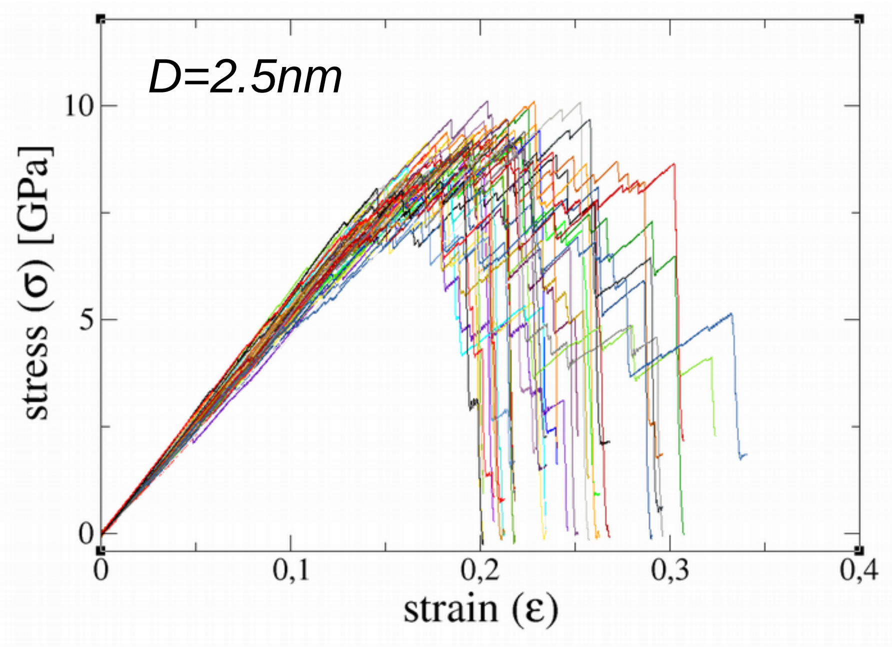
- Increase material heterogeneity
- Increase temperature
- Decrease strain rate

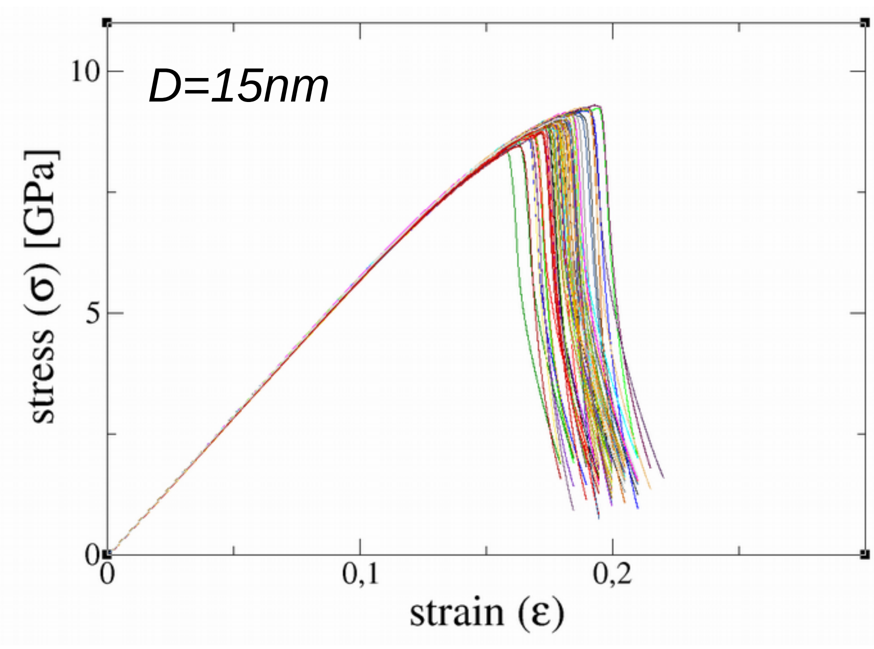
Novel approach:

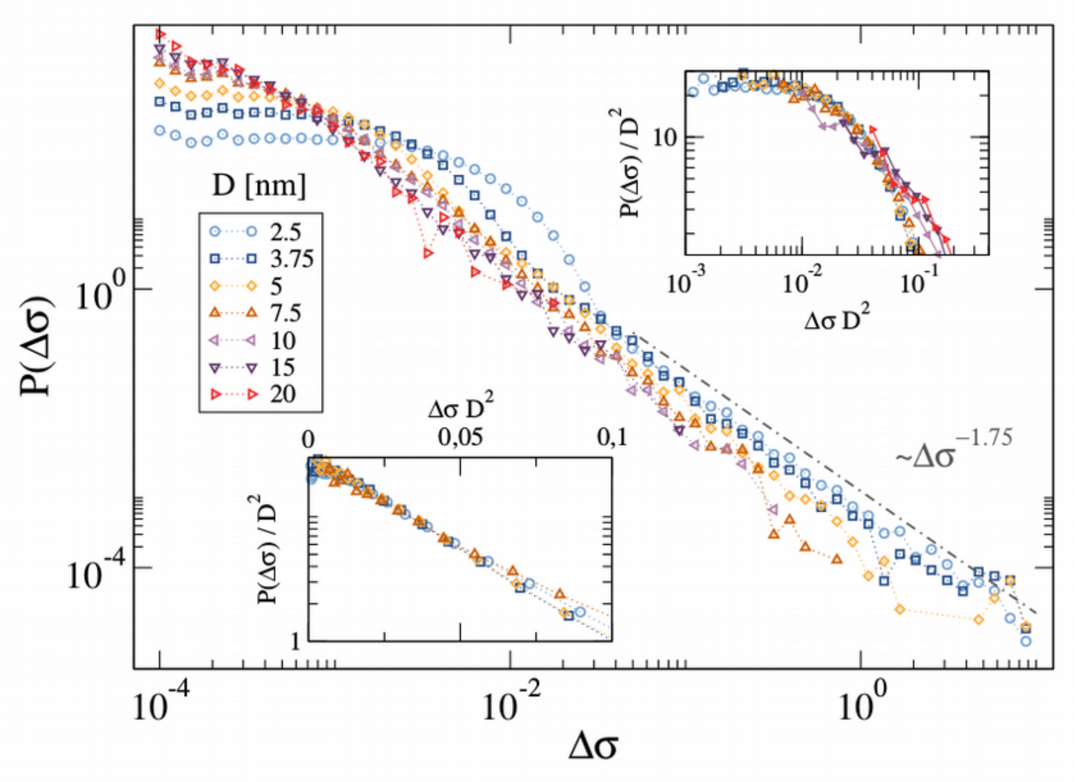
- Size reduction to the nano-scale
- Different physics involved

S. Bofanti, E.E. Ferrero, R. Guerra, A. Sellerio, S. Zapperi - in preparation

Stress drop distributions



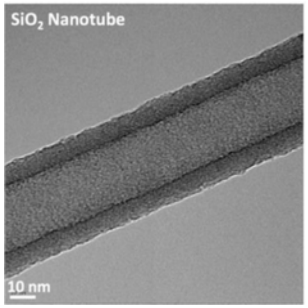




Avalanches in silica glass!

- Power-law range **longer for small samples**
- **Exponent** *a priori* **different** from bulk amorphous yielding
- Our **challenge**:
  - understand the exponents and scalings
- Changing **strain rate** seems to **affect** P(Δσ)

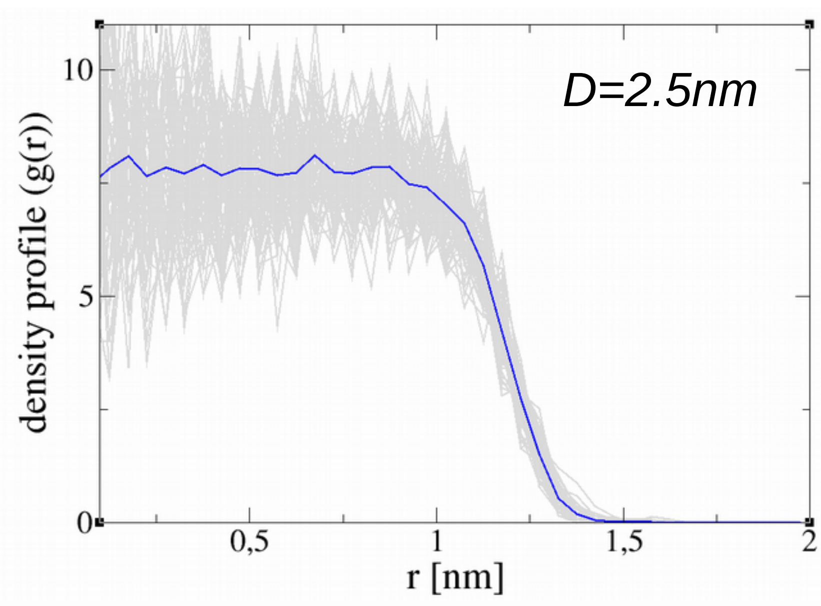
Surface vs bulk behavior

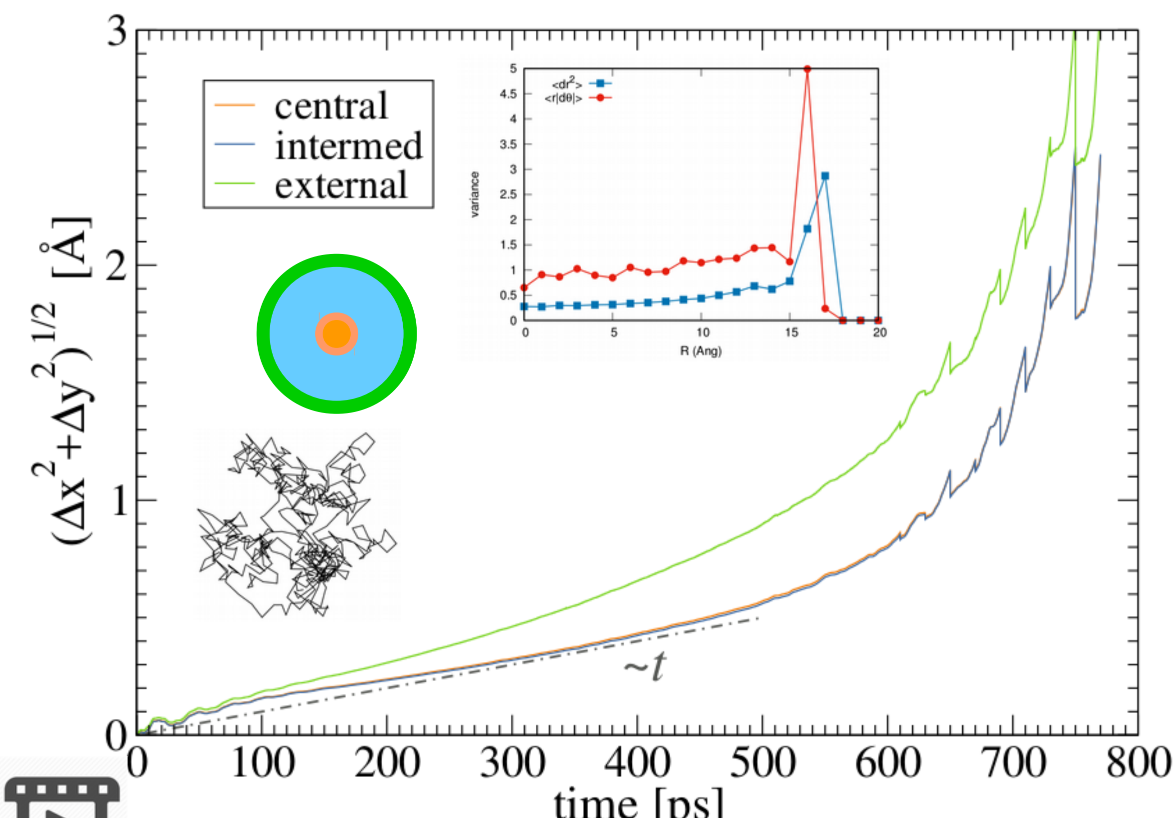


Reported at room temperature:
1 nm thick viscoelastic “fluid-like” surface layer

M. Wingert et al. Nano Lett., 16, 7545 (2016)

Displacements in different cross section “regions”

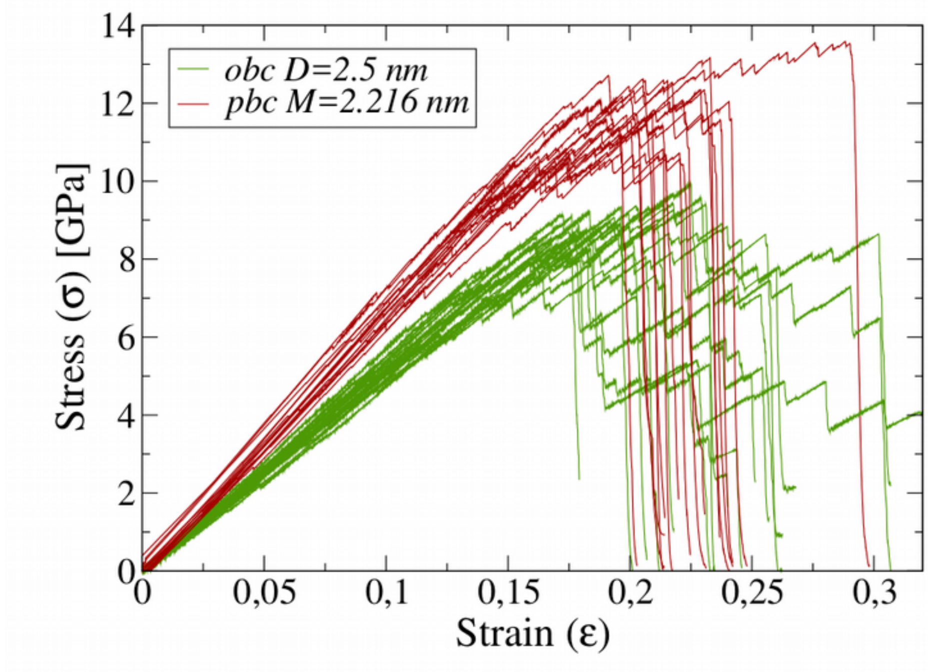




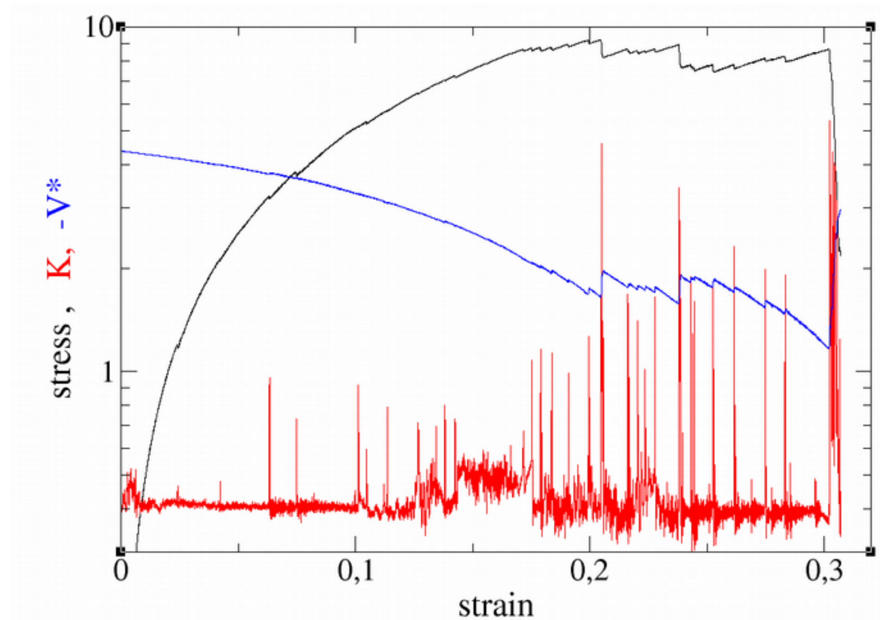
Observation:
- Surface layer ~0.5nm independent on sample diameter
--> *Small samples more affected by surface effect*

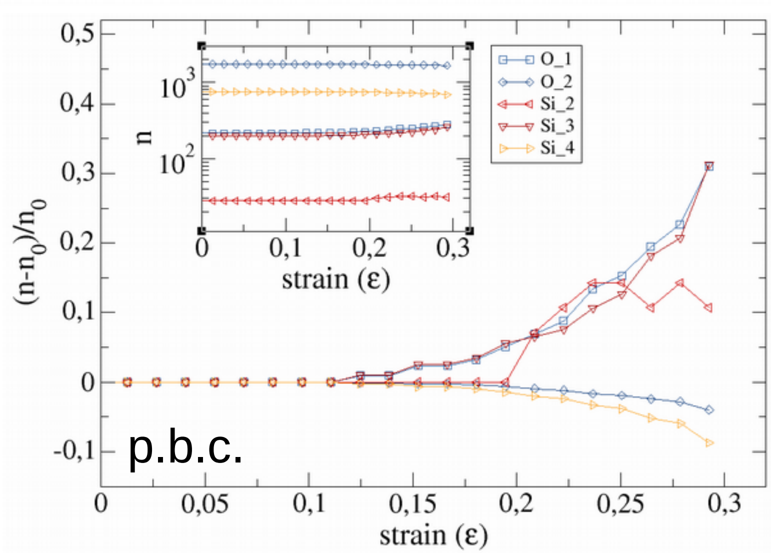
S. Bofanti, E.E. Ferrero, R. Guerra, A. Sellerio, S. Zapperi - in preparation

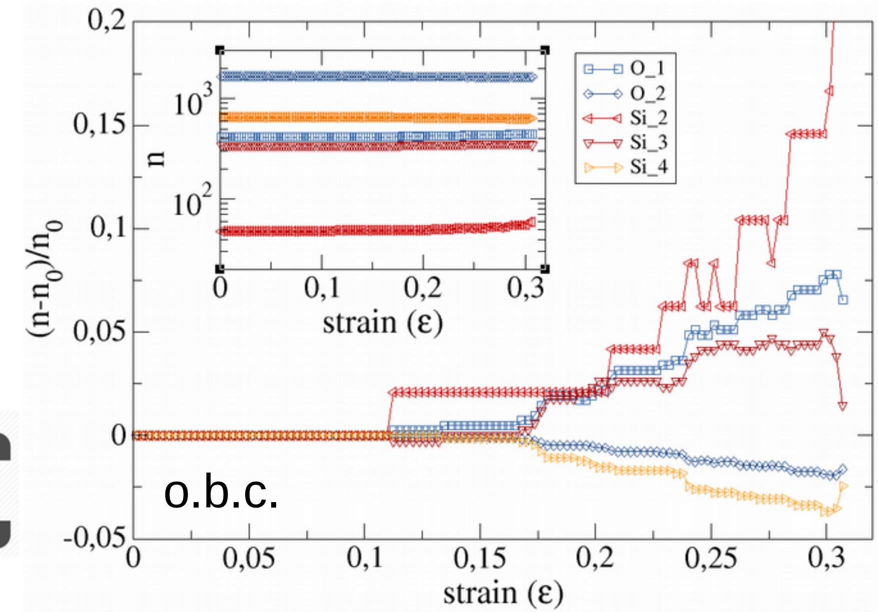
Plasticity even without surface effects!



Bond breaking and rewiring







Take home message

- Solid-like **amorphous materials may flow** under deformation

- A **theoretical framework built at the meso-scale**, describes the **yielding transition** and macroscopic phenomenology for bulk materials

- **At the nano-scale** even extremely brittle materials -like **silica glass**- can **flow plastically** before fracture, **showing avalanches** of plastic events.

- **Surface effects** are **relevant** for this ductility **but not** *sine qua non* condition. A theoretical description of this situation remains open.

Thanks !

www.ezequielferrero.com

"SIZEFFECTS"
No. ADG291002
European Research Council