Some results on Plasticity in **Amorphous Materials**

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I. Phenomenology

II. Mechanical Instability

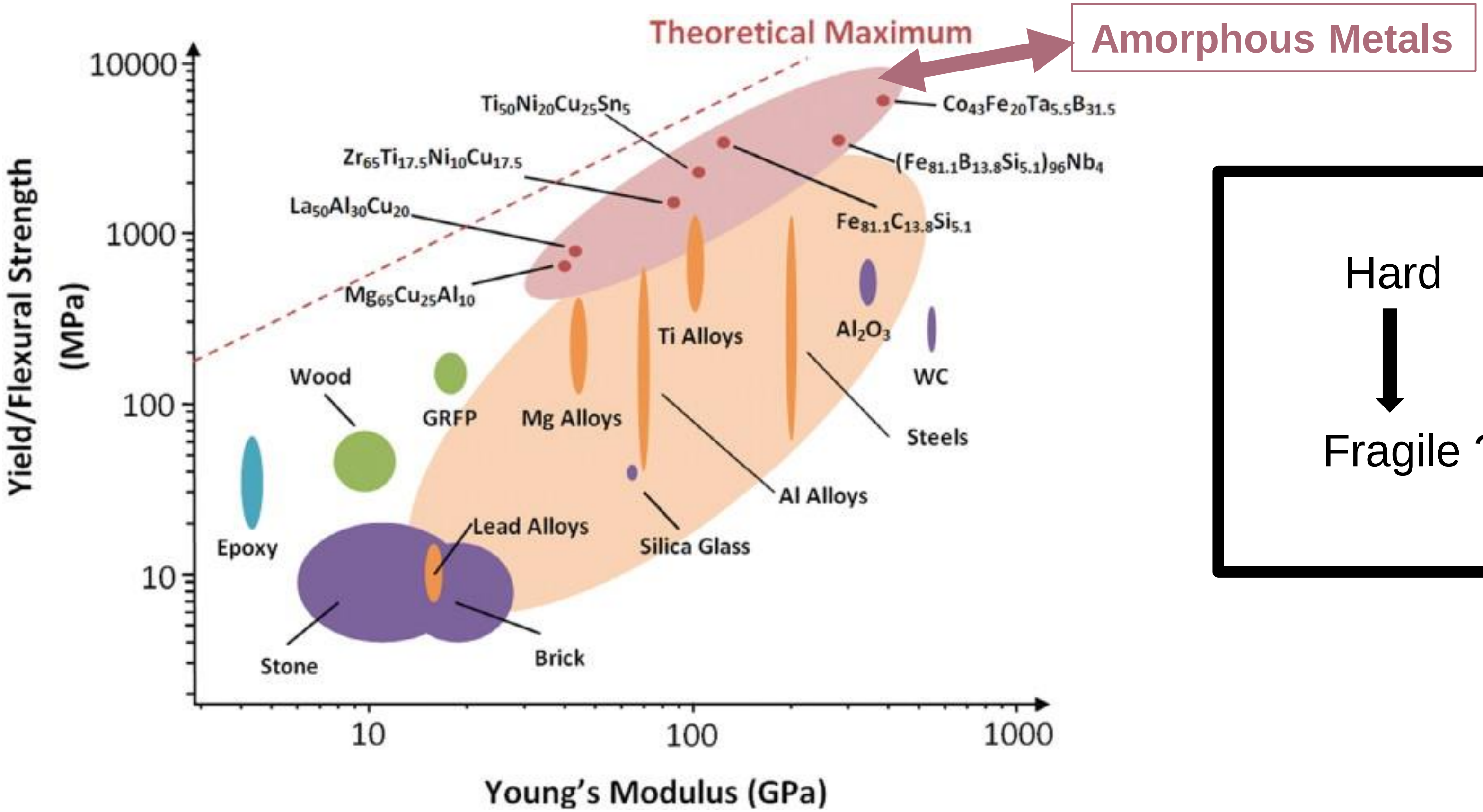
III. Plastic Flow

I. Phenomenology

II. Mechanical Instability

III. Plastic Flow

Amorphous materials are Very **hard** materials

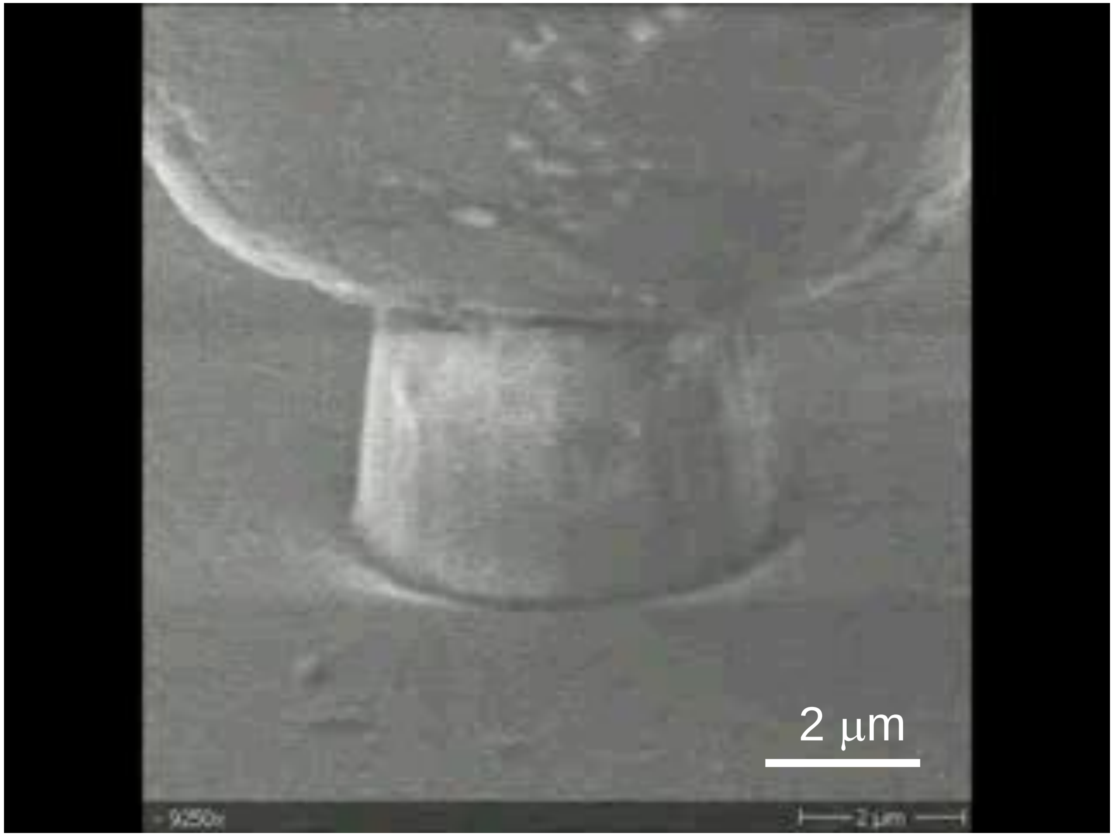


Hard

↓

Fragile ?

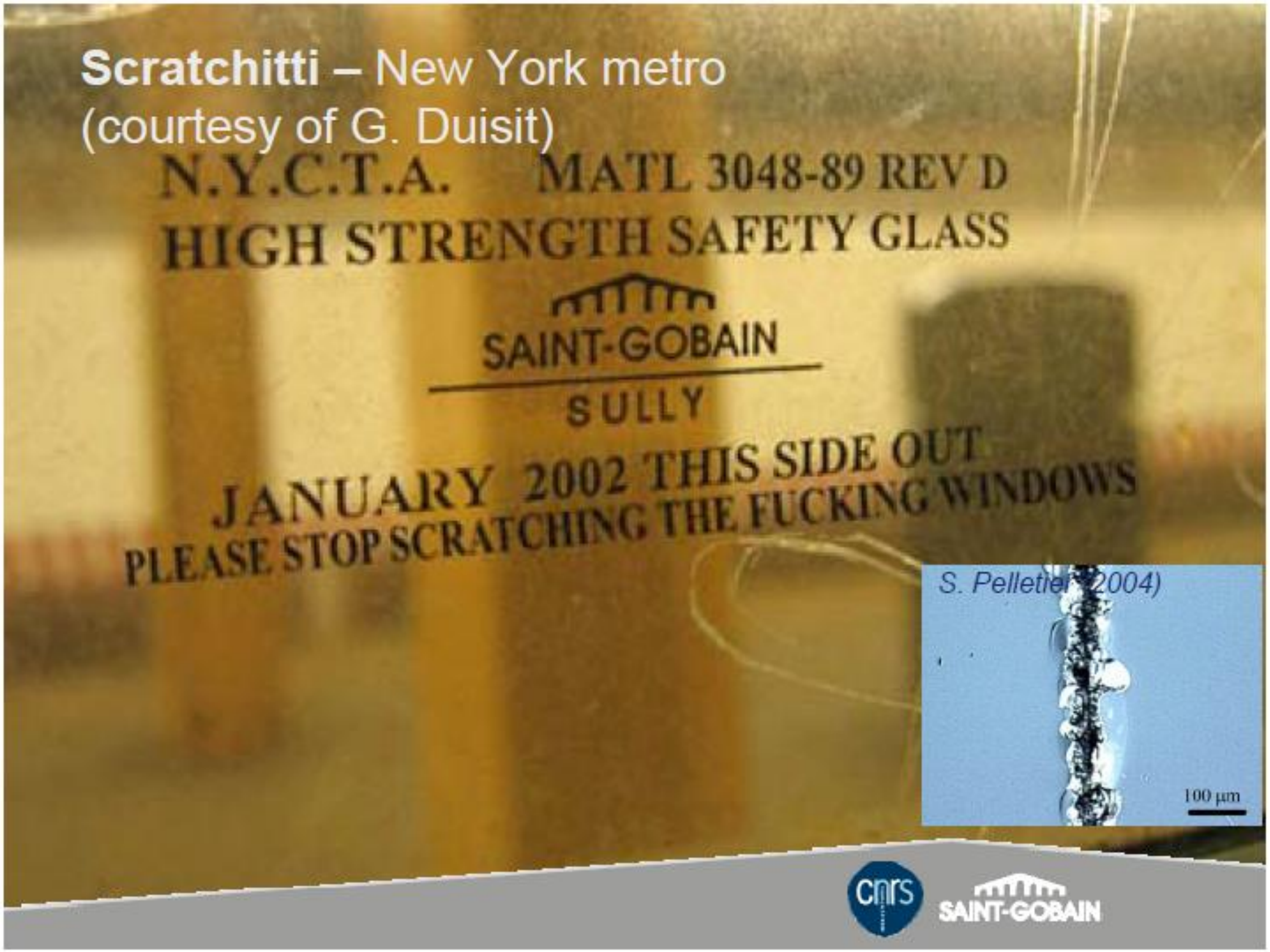
but they are **Ductile** at **small** scale



G. Kermouche, E. Barthel (2015)

Micropillar in pure silica glass

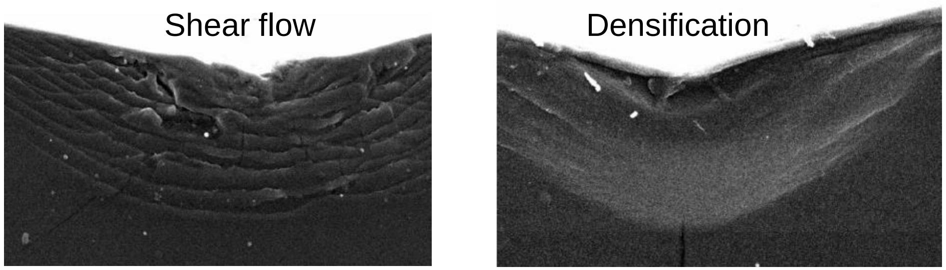
Scratchitti – New York metro (courtesy of G. Duisit)



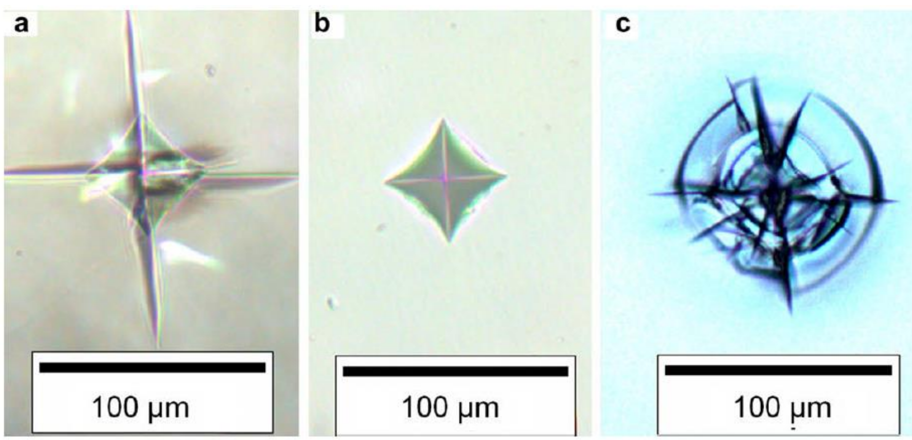
E. Barthel et al.

Their behaviour is **composition** and **loading** dependent

Composition

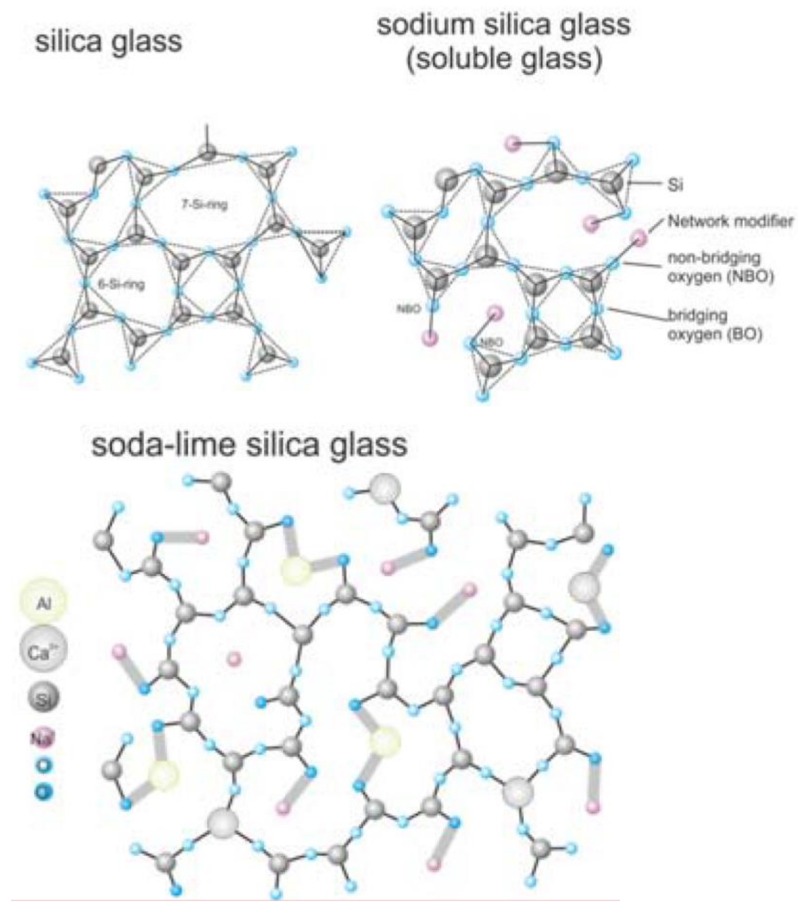


Soda-lime glass **Anomalous glass**



T.M. Gross et al. (2008, 2009)

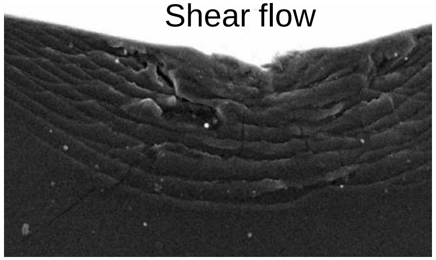
(a) 60% SiO_2 20% Al_2O_3 20% CaO; (b) 80% SiO_2 10% Al_2O_3 10% CaO; (c) 100% SiO_2



Their behaviour is **composition** and **loading** dependent

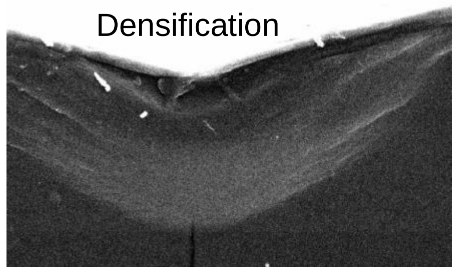
Composition

Shear flow

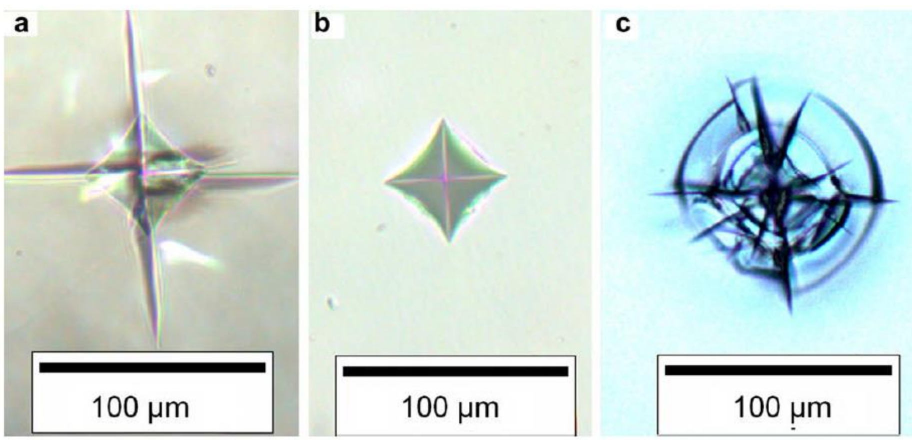


Soda-lime glass

Densification



Anomalous glass

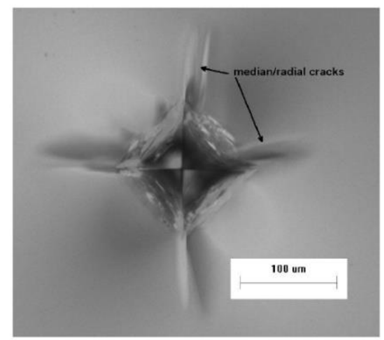


(a) 60% SiO_2 20% Al_2O_3 20% CaO; (b) 80% SiO_2 10% Al_2O_3 10% CaO; (c) 100% SiO_2

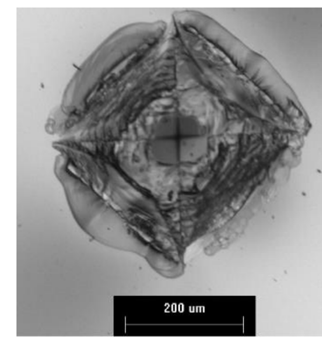
T.M. Gross et al. (2008, 2009)

Strain Rate

Quasi-static indentation (0.2 mm/mn, 69N)

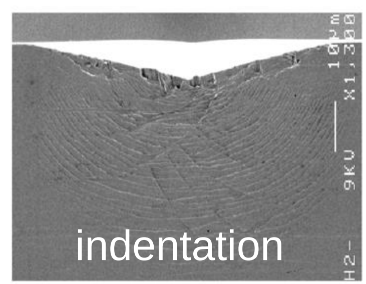


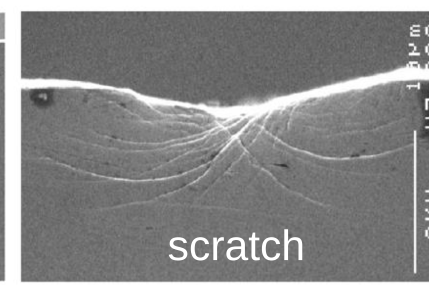
Impact velocity (410 mm/s, 562N)



T.M. Gross et al. (2013)

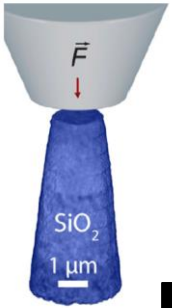
Applied Load





Bulk Metallic Glass

V. Keryvin et al. (2008)

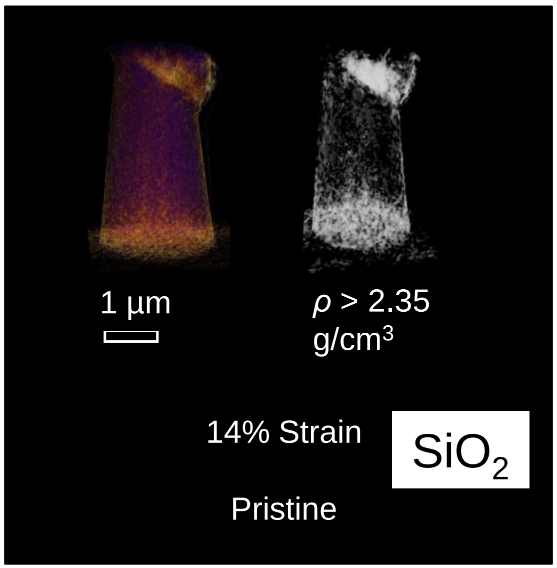


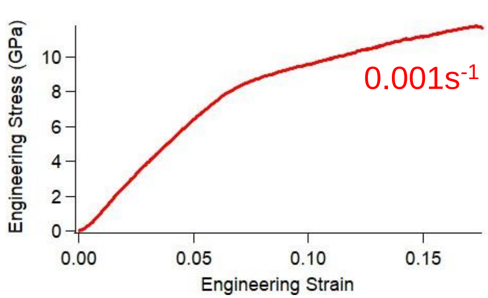
Their behaviour is **temperature** and **loading** dependent

0.001 s^{-1}

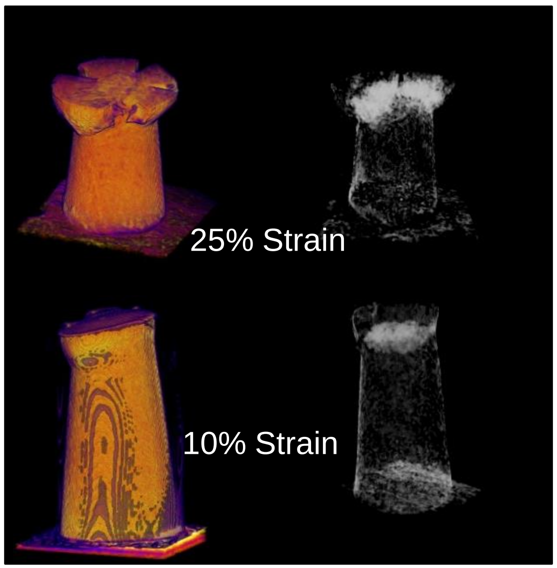
1 s^{-1}

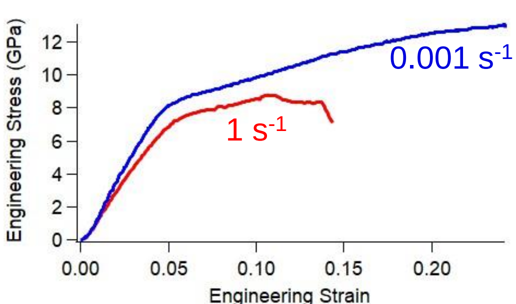
T=25°C



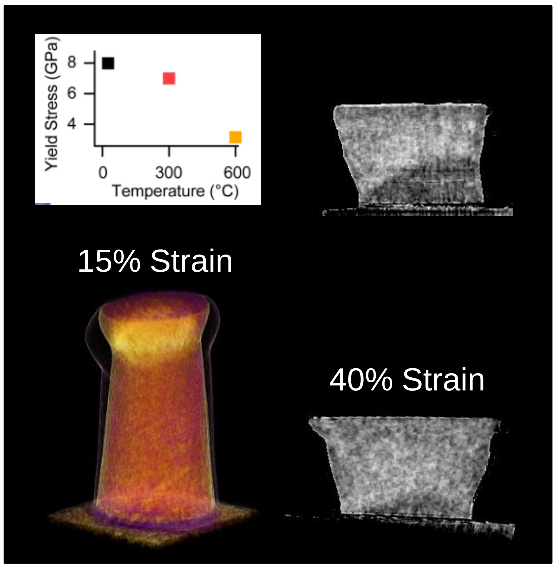


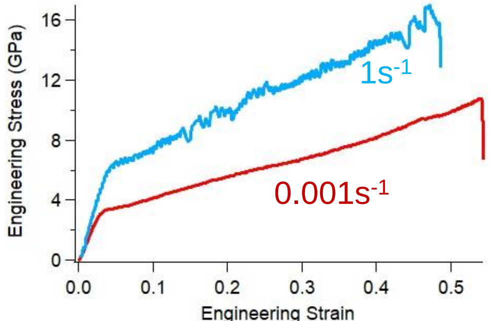
T=300°C





T=600°C

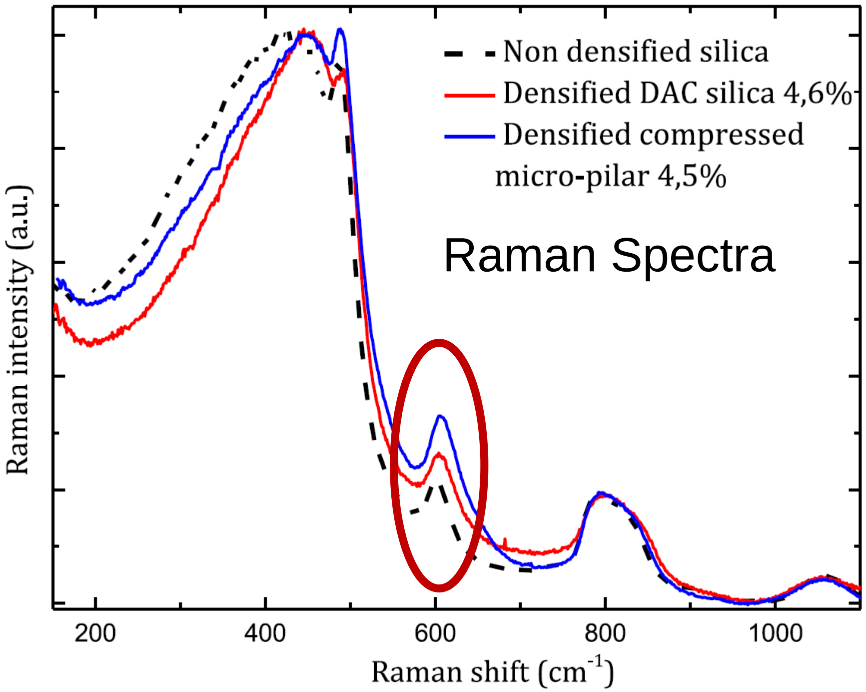


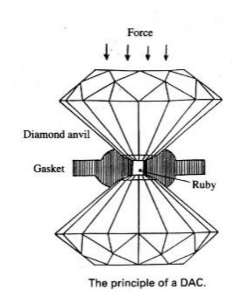


R.N. Widmer et al. (2022)

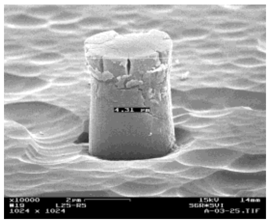
Their behaviour depends on the **loading history**

Comparison between different **densification processes** in SiO_2

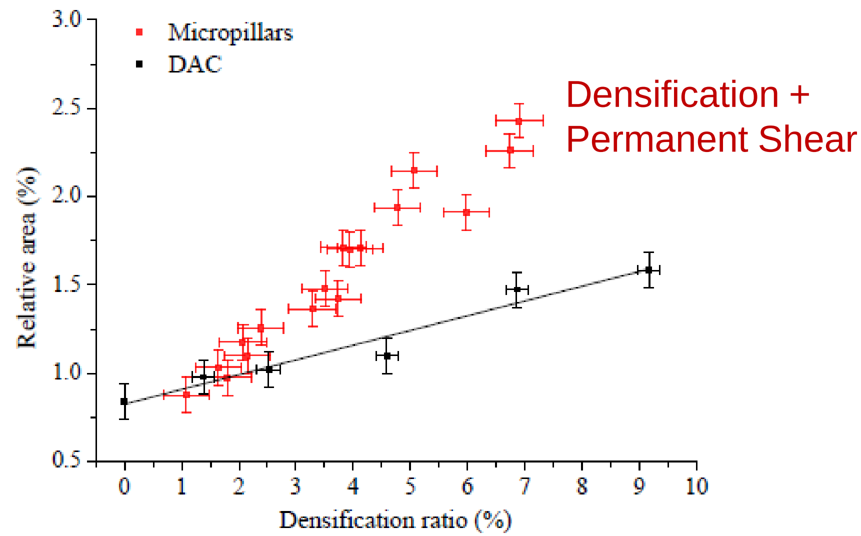




DAC Exp.



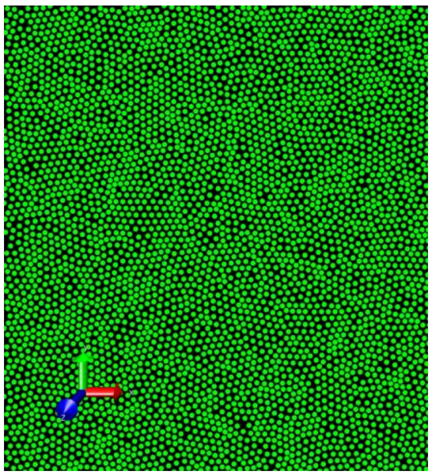
Micropillar Exp.



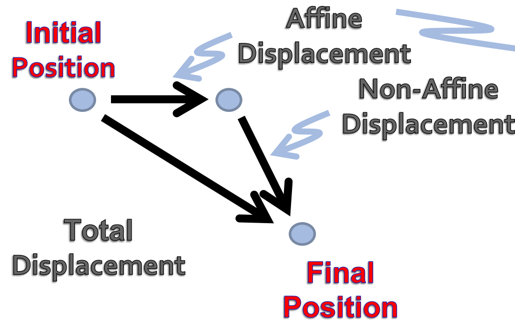
C. Martinet et al. (2020)

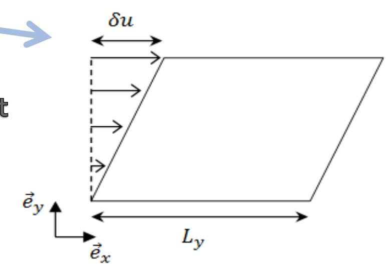
What happens **inside** a **disordered material** ?

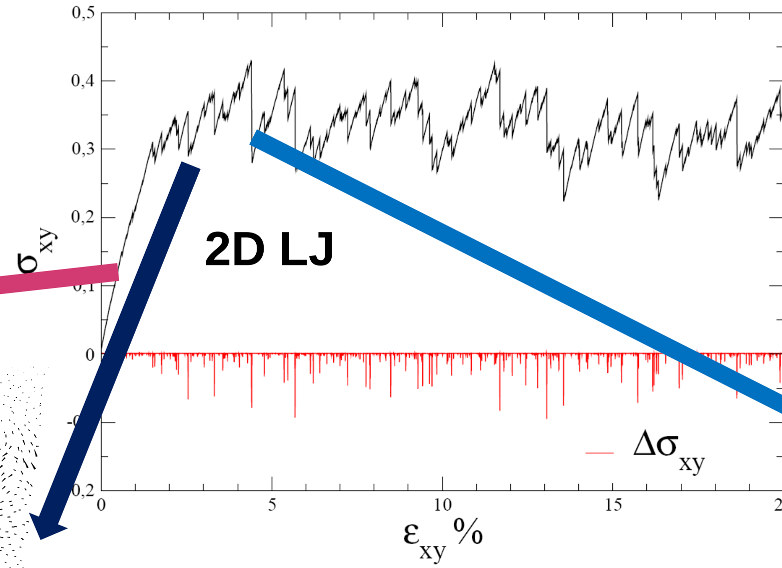
Non-affine displacement:



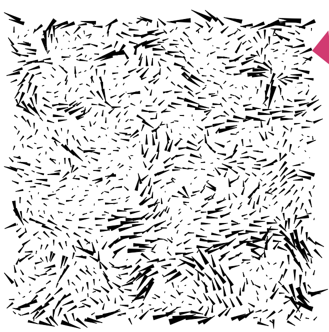
2D
LJ Glass



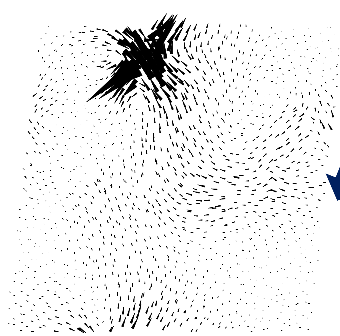




Athermal Quasi-static shear deformation



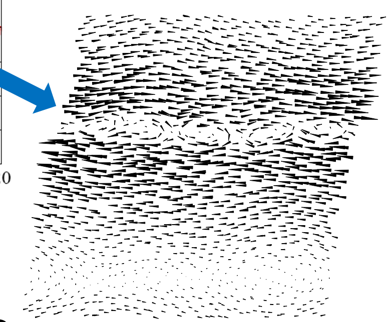
Non-affine **reversible** displacements (x10³)



Local shear **ir**reversible (x40) quadrupolar event

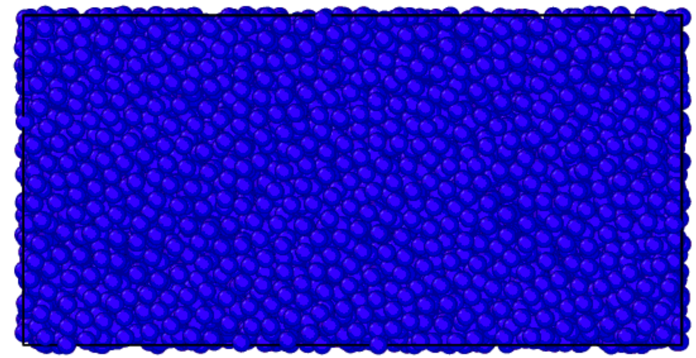
The strong **localisation** of the deformation prevent **stress losses**

A.Tanguy et al. (2002, 2006)



Elementary Shear band (x0.4)

C1 LOADING

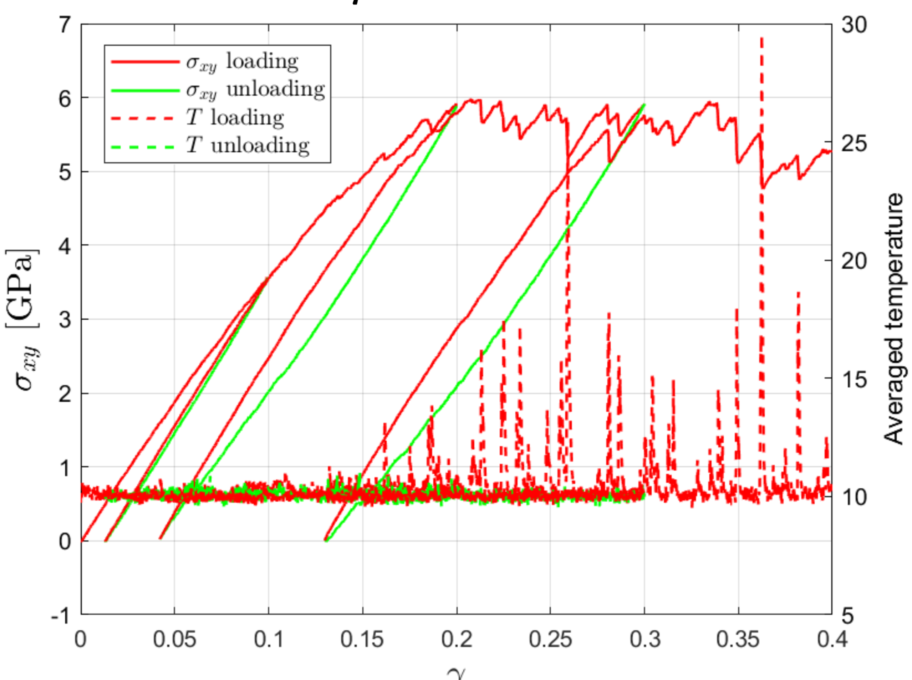


3D
CuZr Glass
$T = 10$ K

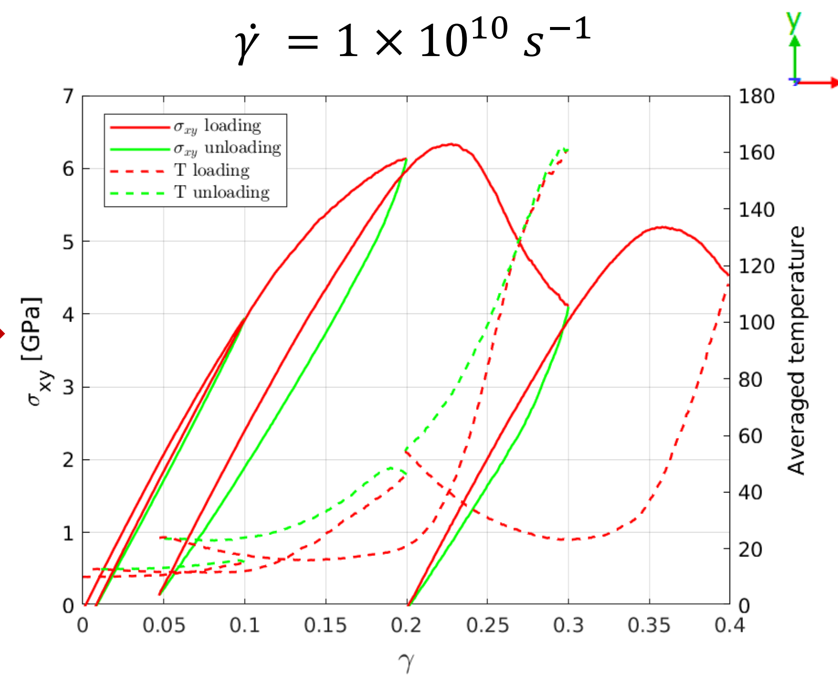
Local or collective **thermal** increases are a signature of a **collective instability**

Elementary vs. **permanent** shear bands

$\dot{\gamma} = 1 \times 10^{8}\ s^{-1}$



$\dot{\gamma} = 1 \times 10^{10}\ s^{-1}$



M. Sepulveda et al. (2022)

At equilibrium, an **amorphous** solid is prepared in a **metastable** state.
A **mechanical equilibrium** corresponds to a local minimum of the **potential energy**.
At fixed **temperature**, it is kept in a local minimum of the **thermodynamic potential**.
The external driving deforms the energy landscape, up to the loss of equilibrium

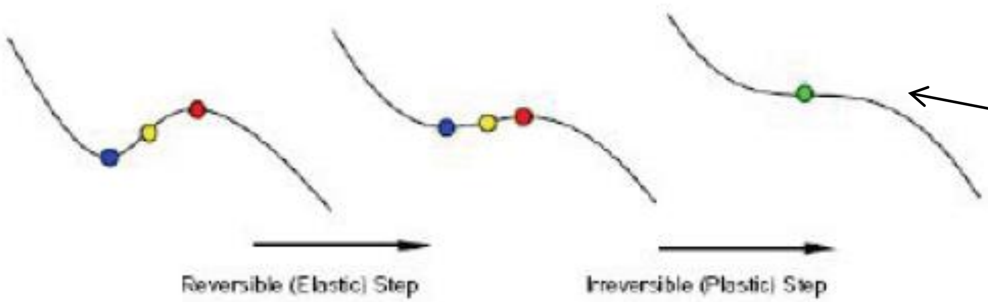
Hill's Criterion for Crystals Stability (1962) in Continuous Media

Helmholtz Free Energy $$F(Y) \equiv F(X) + \Omega(X)\left\{ \tau_{ij}(X)\,\eta_{ij} + \frac{1}{2} C_{ijkl}(X)\,\eta_{ij}\eta_{kl} + \cdots \right\}$$

Stability Criterion $$\min_{\{\underline{w},\underline{k}\}} \left(C_{ijkl} w_i w_k k_j k_l \right) \geq 0$$

$\eta_{ij} \propto w_i k_j$

Burgers Vector (w_i), Slip Plane (k_j)



Spinodal Limit

R.E. Miller and D. Rodney(2008)

Atomistic description in an Amorphous material:

$$m_i \frac{\partial^2 u_\alpha}{\partial t^2}(\underline{r_i}, t) = -\sum_{j,\beta} M_{ij}^{\alpha\beta} . u_\beta(\underline{r_j}, t) \quad \text{at T=0K}$$

with $M_{ij}^{\alpha\beta} = -\frac{\partial^2 E_{total}}{\partial r_{i\alpha}\partial r_{j\beta}}$ including external forces

$$\underline{V}(\underline{r_i})e^{i\omega t} = \sqrt{m_i}\,\underline{u}(\underline{r_i}, t)\,,\; D_{ij}^{\alpha\beta} = \frac{M_{ij}^{\alpha\beta}}{\sqrt{m_i m_j}}$$

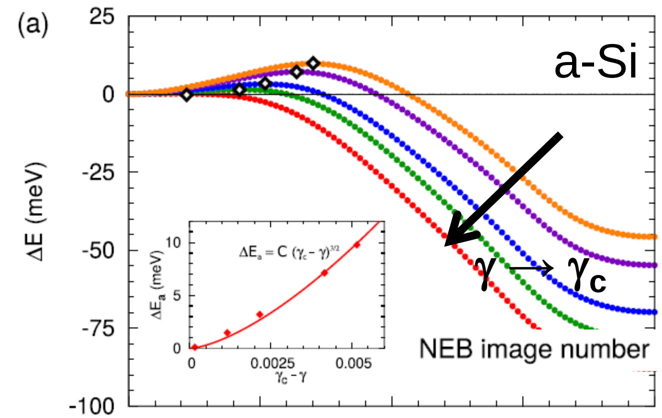
Dynamical Matrix

$$\boxed{\omega^2 \underline{V} = \overline{\overline{D}}.\underline{V}}$$

$\omega \rightarrow 0$ **Instability**

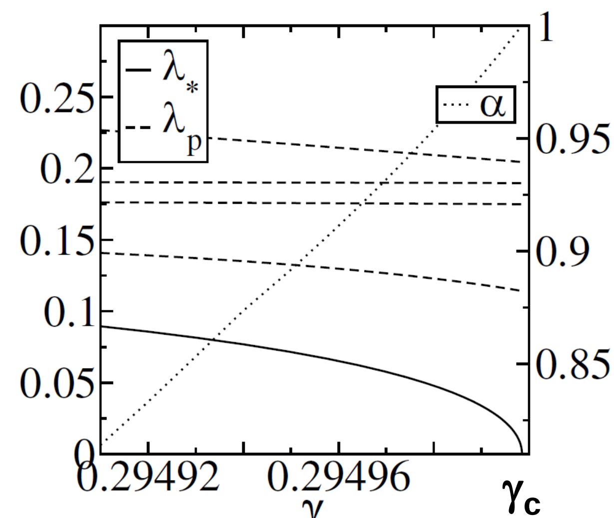
Energy Barriers

T. Albaret et al (2018)



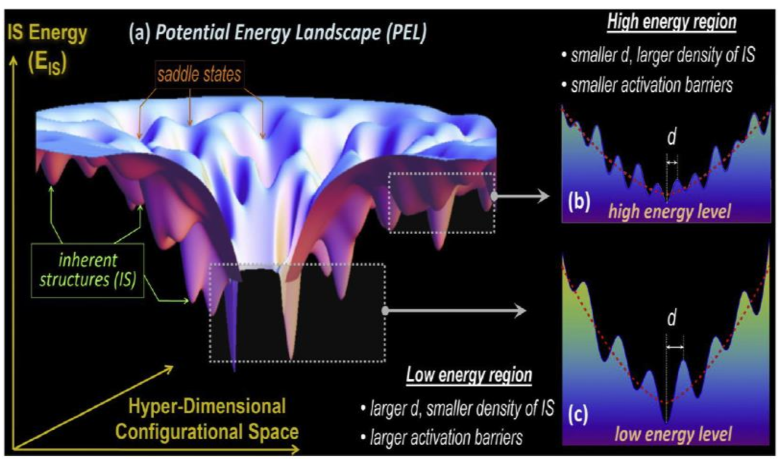
Eigenvalues of the Dyn. Mat.

C. Maloney et et al (2004)



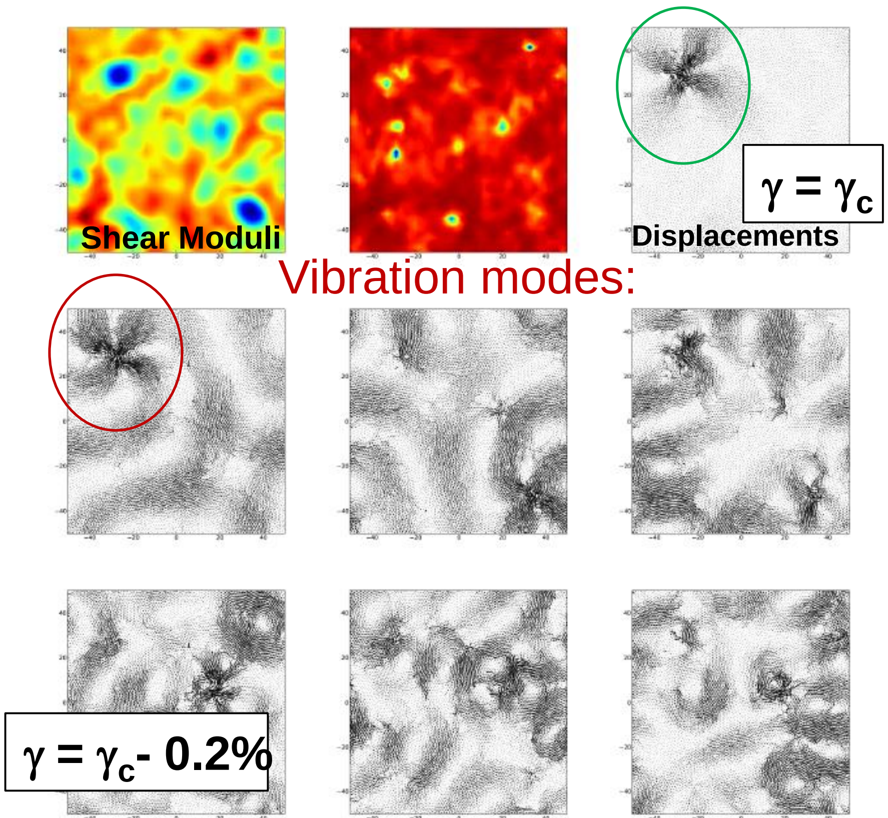
Potential Energy Landscape

C. Liu et al. (2018)
D. Rodney et et al (2011)



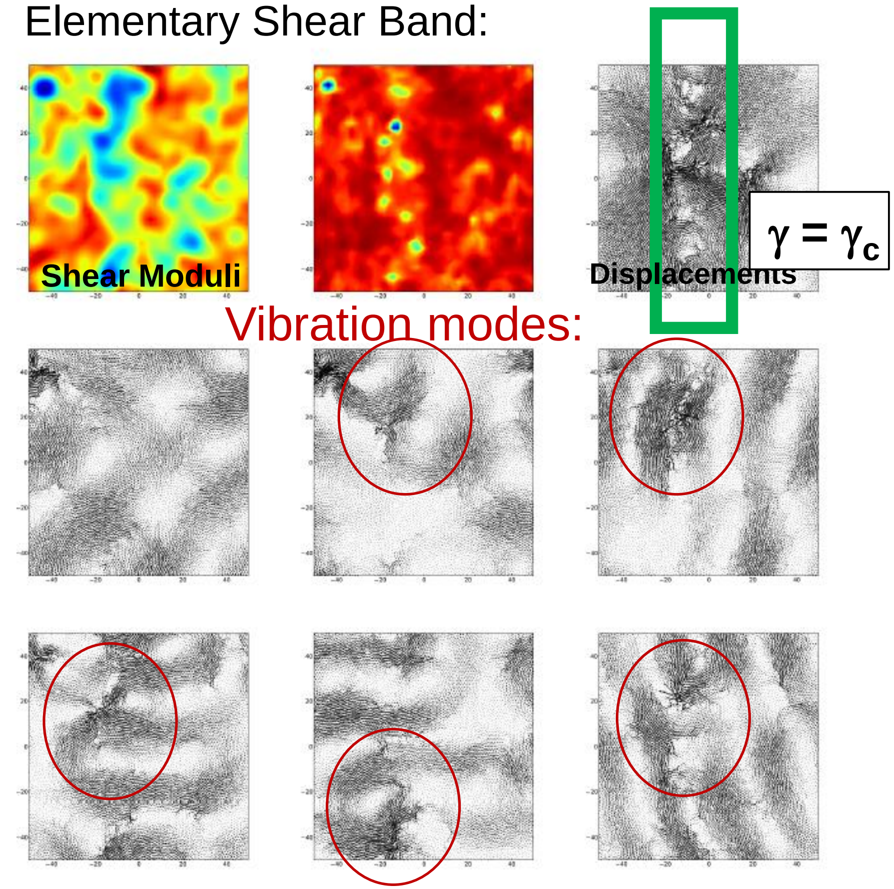
Prediction of plasticity through ***soft* vibration modes** and **local elastic moduli** in a 2D Lennard-Jones glass:

Quadrupolar Local Rearrangement (STZ):



A *single* localized mode

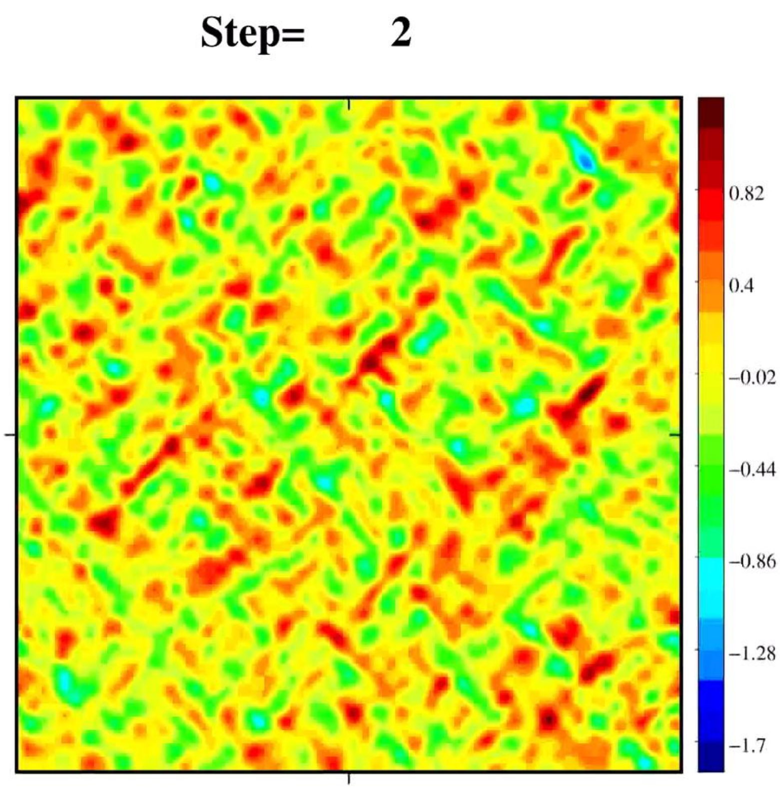
Elementary Shear Band:

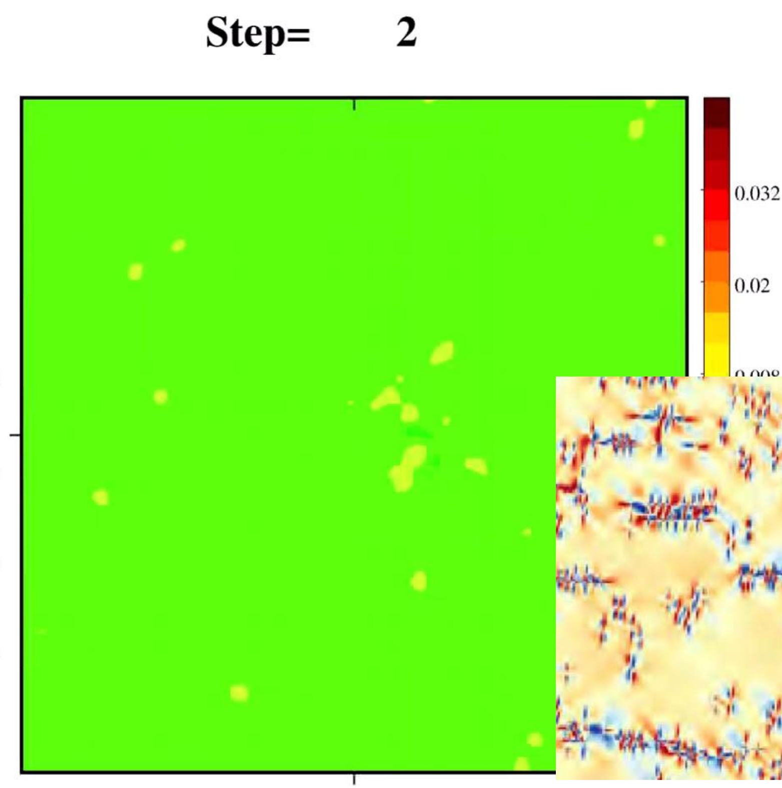


Superposition of localized modes, on percolating soft zones

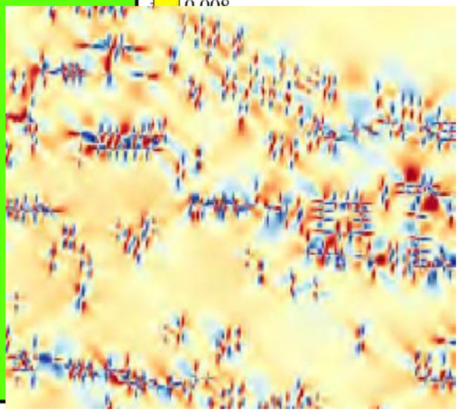
A. Tanguy et al. (2010)

Signature of Plasticity in **the local shear stress components** in a 2D LJ Glass





T=0K



Pristine micro-crystal
L. Truskinovsky et al. (2021)

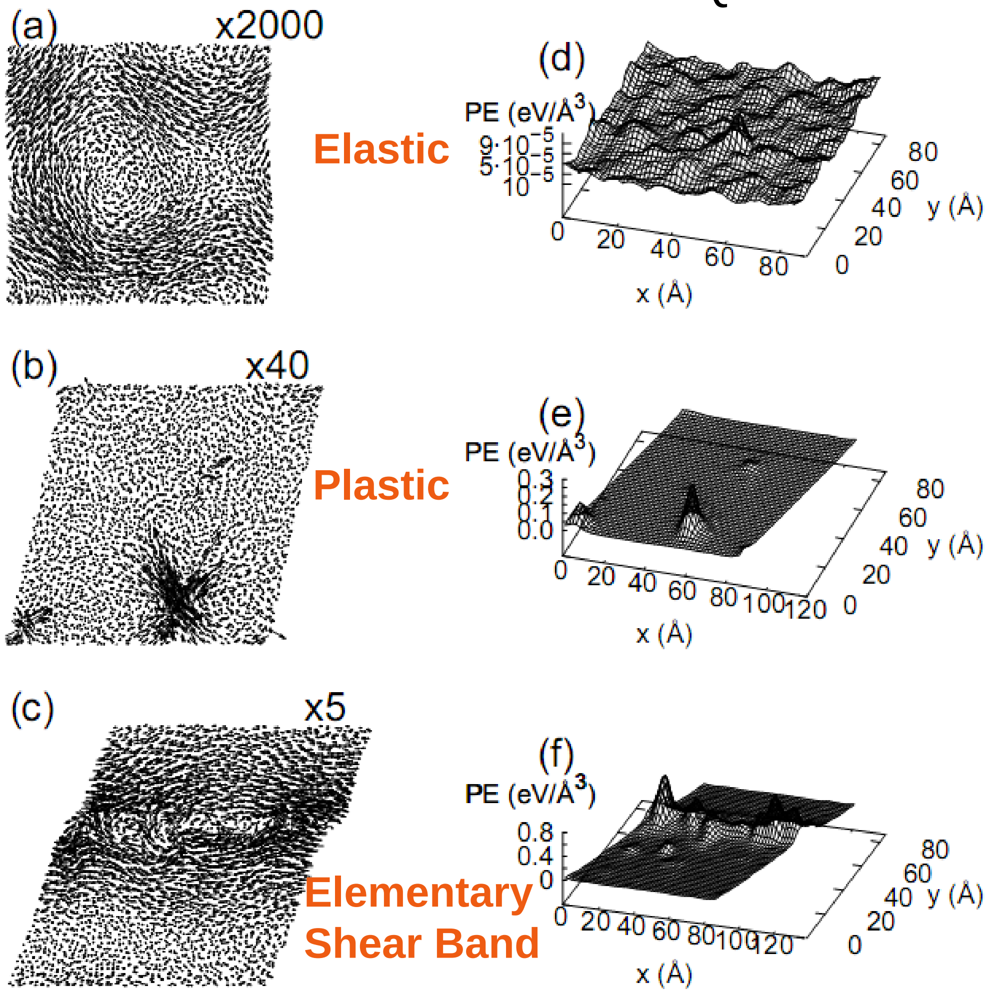
Total Local **Shear Stress**
Incremental + Quenched Stress

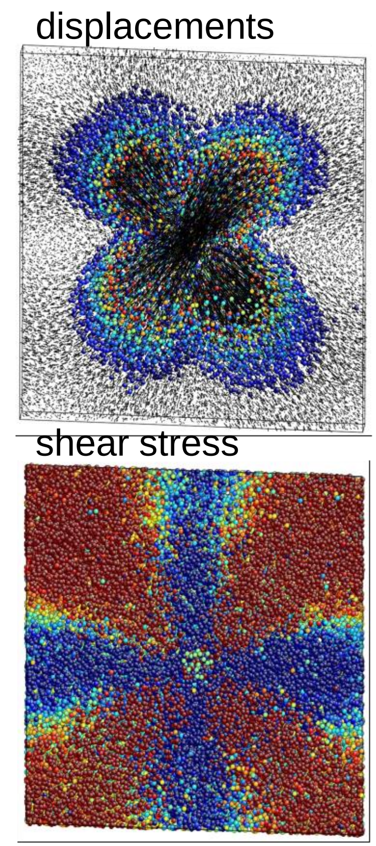
Incremental Local **Shear Stress**

M. Tsamados et al. (2008)

Elementary Rearrangements in **Plastic** Deformation

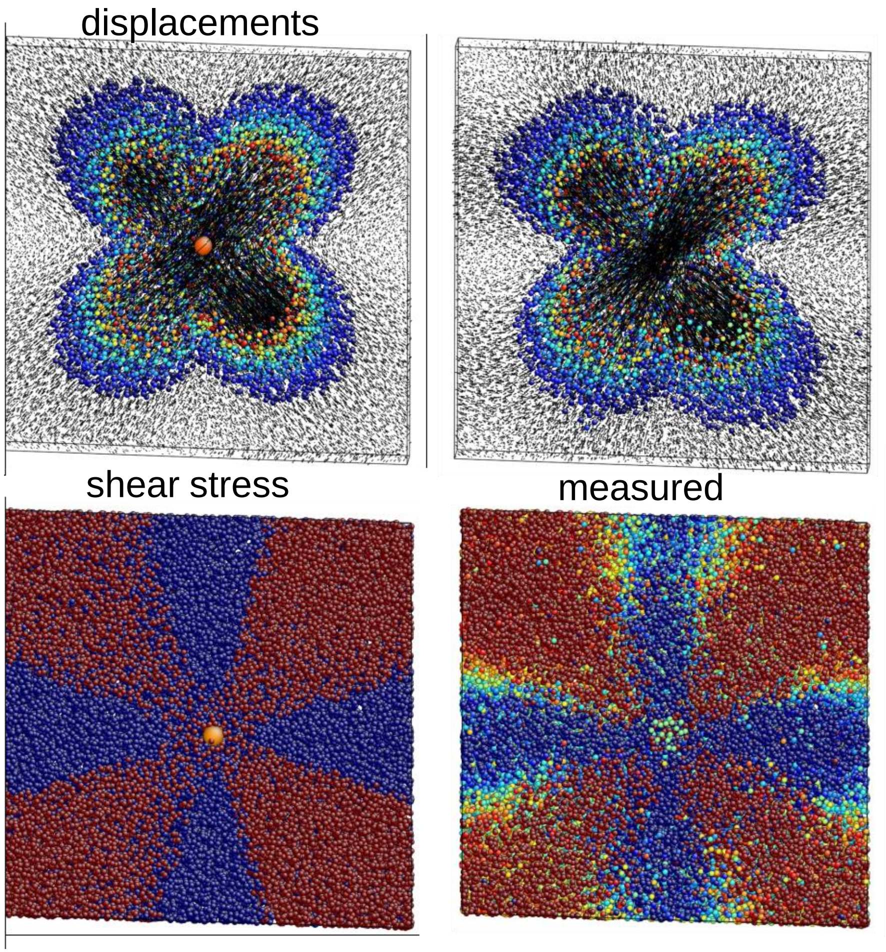
Athermal Quasi-Static deformation of a-Si



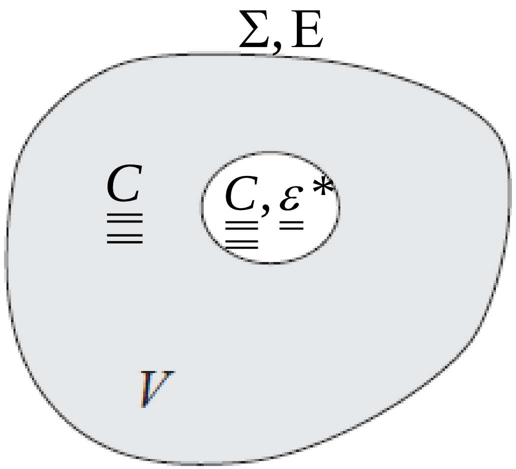


T. Albaret et al. (2016)

Local Irreversible **Plastic** deformation



T. Albaret et al. (2016)



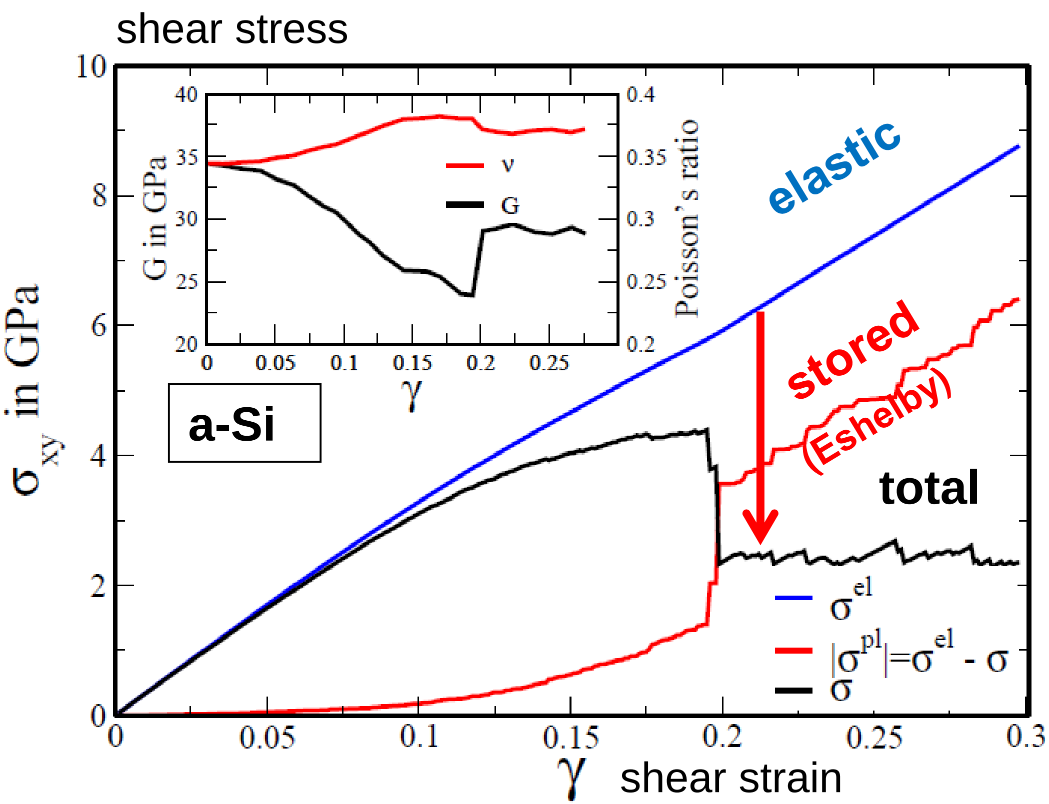
Eshelby-like Inclusion

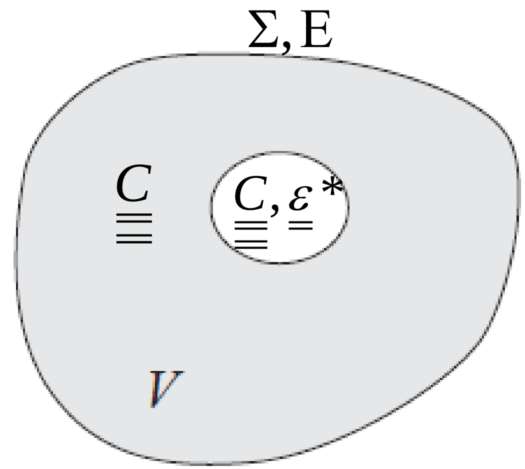
$$div\,\underline{\underline{\sigma}}^{I} = 0 \Leftrightarrow div\left(\underline{\underline{\underline{\underline{C}}}} : \underline{\underline{\varepsilon}}\right) + f\left(\underline{\underline{\varepsilon}}^{*}\right) = 0$$

$$f\left(\underline{\underline{\varepsilon}}^{*}\right) = \underline{\underline{\underline{\underline{C}}}} : \underline{\underline{\varepsilon}}^{*} . \underline{n}\,\delta\left(S^{I}\right) \Rightarrow \underline{\underline{\varepsilon}} = \underline{\underline{\underline{\underline{S}}}} : \underline{\underline{\varepsilon}}^{*}$$

T. Albaret et al. (2016)

Local Irreversible **Plastic** deformation



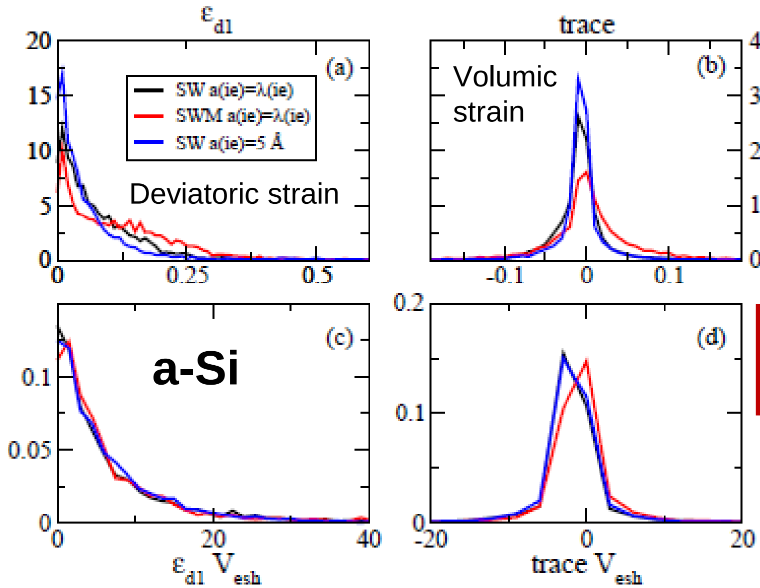


Eshelby-like Inclusion

$$\delta\sigma_{xy} = 2G(\gamma)\delta\varepsilon_{xy} - 2G(\gamma)\delta\varepsilon_{xy}^{*}$$

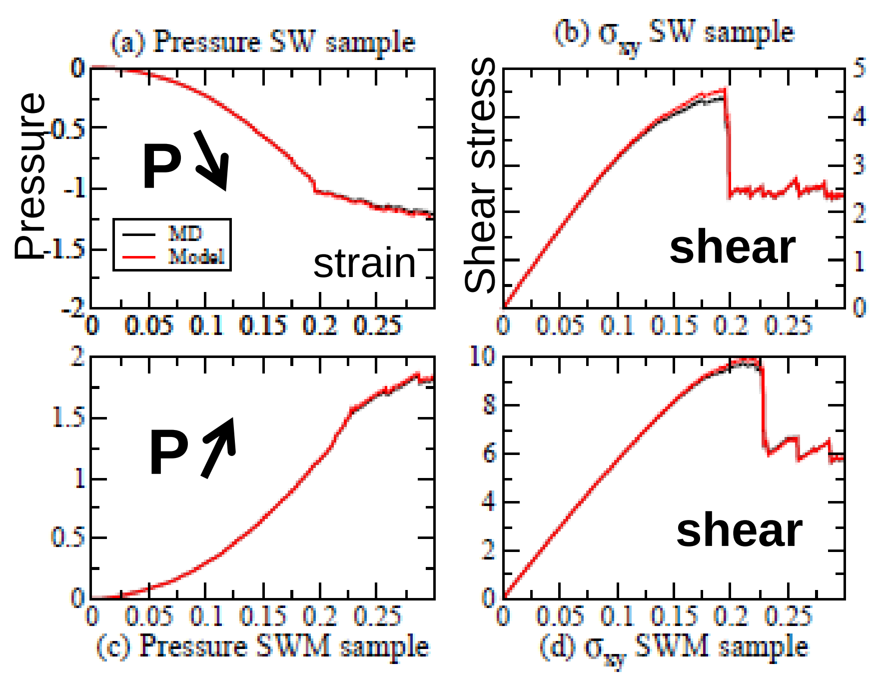
T. Albaret et al. (2016)

Fitting **Eshelby** tensor vs. **Constitutive** Laws: the example of **a-Si**



$$\delta_i \epsilon_{xy} = \delta_i \epsilon^{el}_{xy} + \delta_i \epsilon^{pl}_{xy}$$

$$\delta_i \sigma_{xy} = 2G(\gamma_i)\delta_i \epsilon_{xy} - 2G(\gamma_i)\delta_i \epsilon^{*}_{xy} = \delta_i \sigma^{el}_{xy} - \delta_i \sigma^{pl}_{xy}$$



Bonds Bending Rigidity

→ Constitutive Law

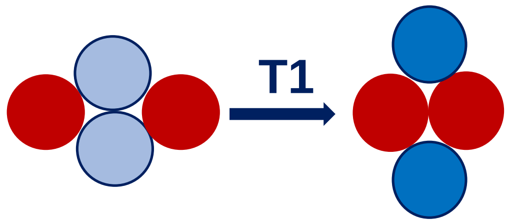
Elementary bricks for Mesoscopic Modeling

T. Albaret et al. (2016)

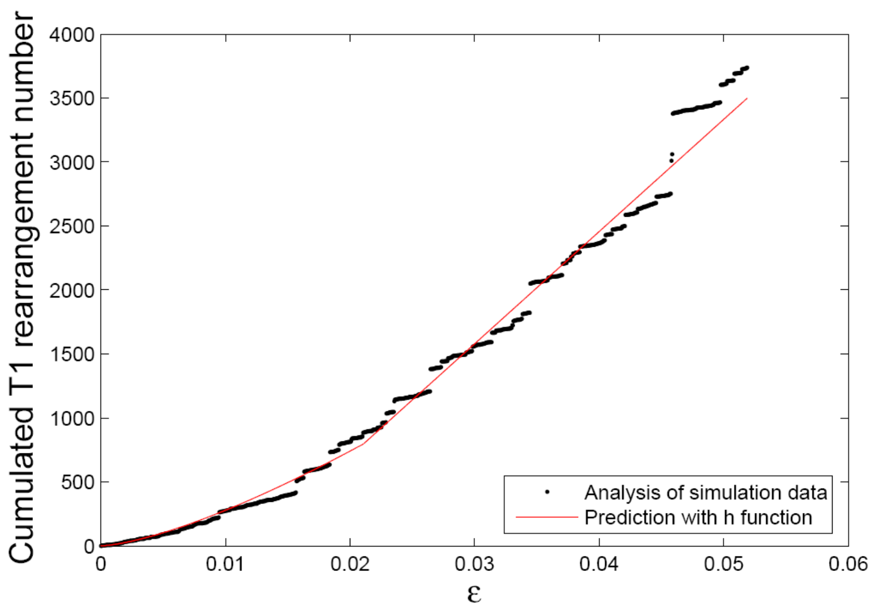
Example of a **2D Lennard-Jones** glass

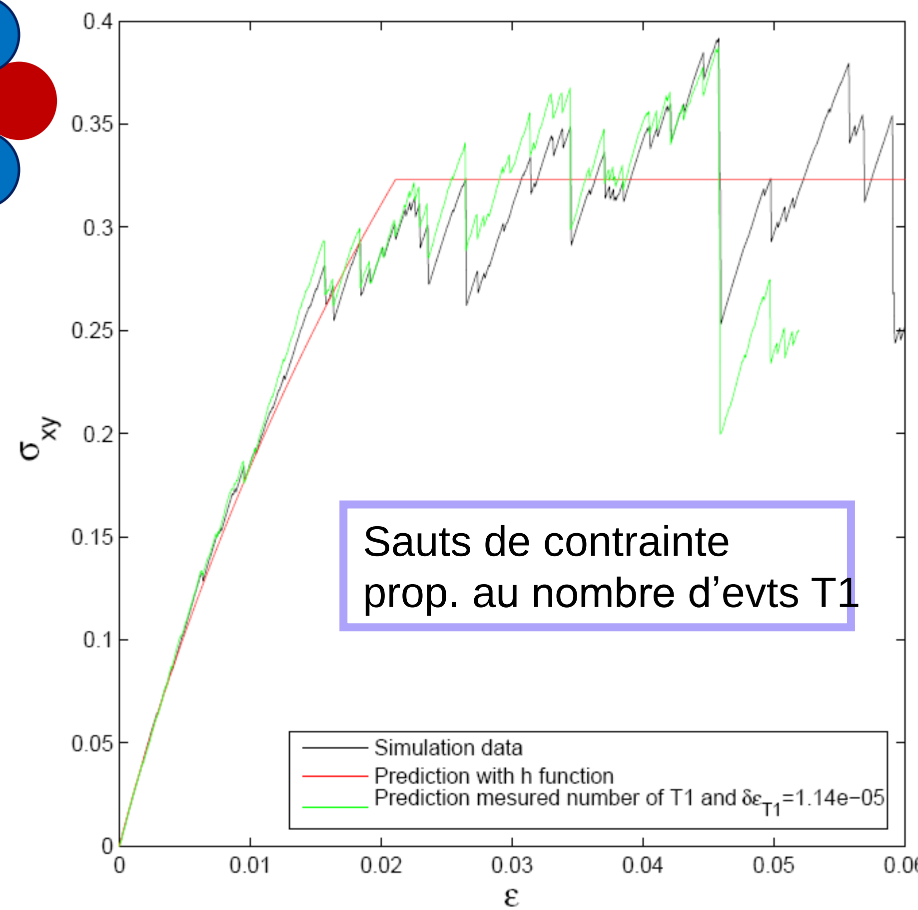
$$\dot{\varepsilon} = \underbrace{\dot{U}}_{\text{él.}} + \underbrace{\dot{\varepsilon}_p}_{\text{pl.}}$$

$$\varepsilon_p = N^{T1}\delta\varepsilon^{T1}$$



$$\sigma = \mu(\varepsilon - N^{T1}\delta\varepsilon^{T1})$$





Sauts de contrainte
prop. au nombre d'evts T1

P. Marmottant et al. (2007)

T1 rearrangement in a 2D **silica glass**

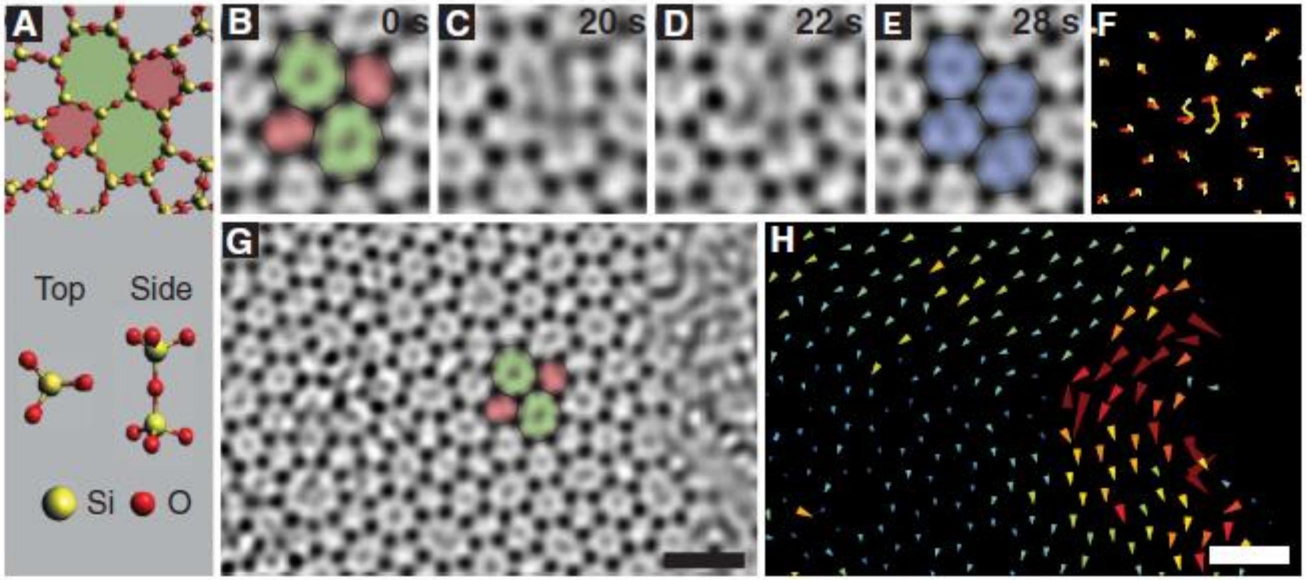
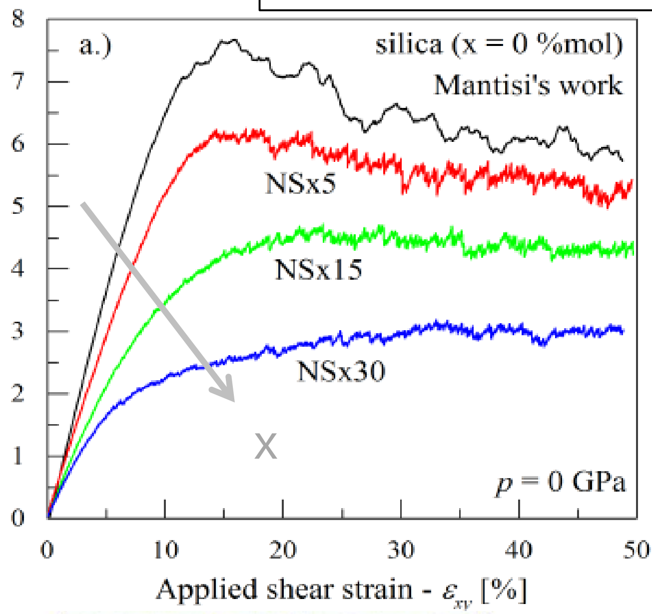
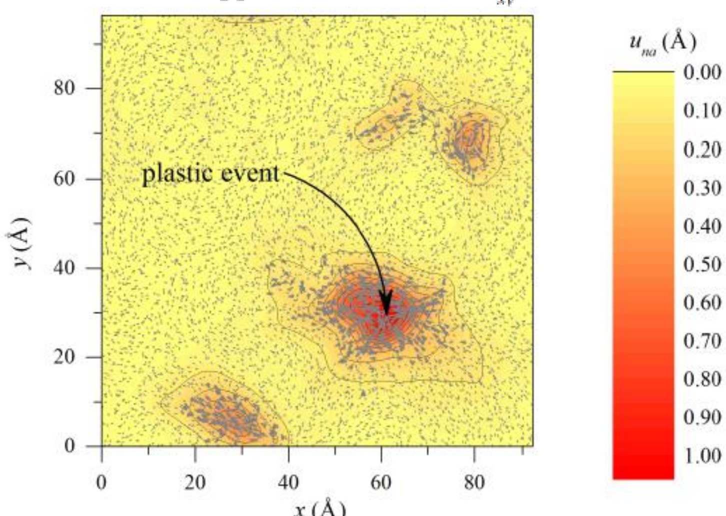


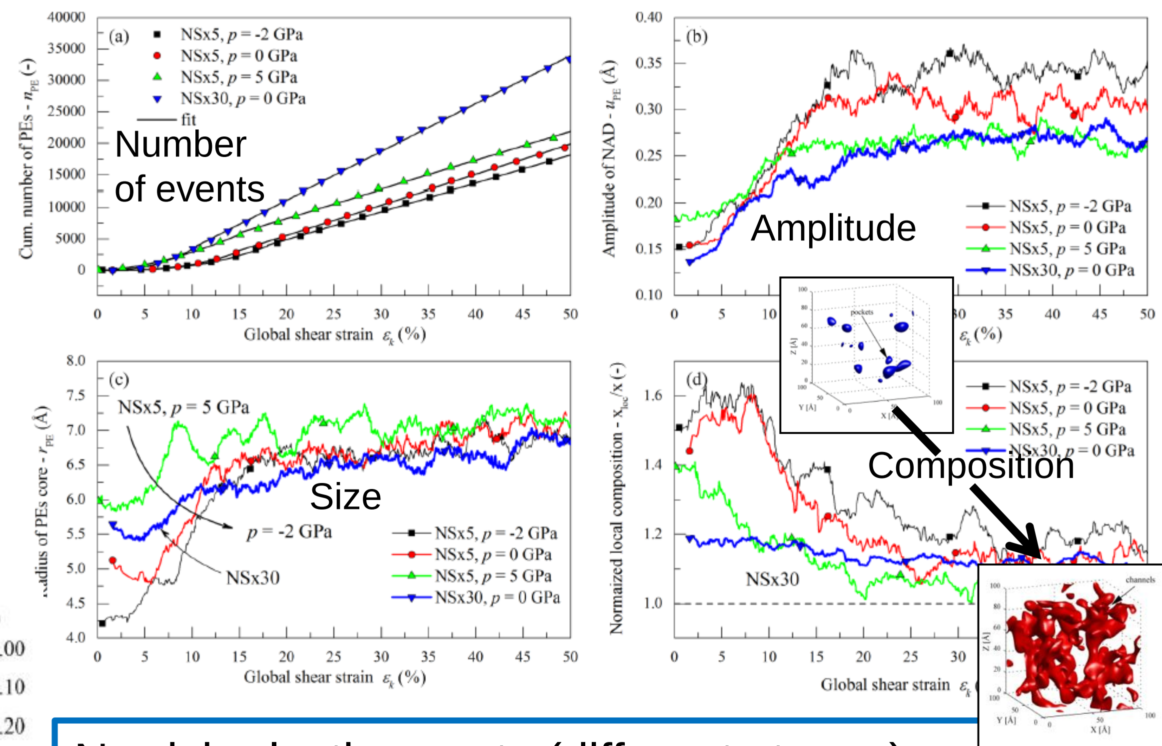
Fig. 1. Elastic and plastic deformation in ring exchange. (**A**) Cartoon models of the 2D silica structure. (**B** to **E**) TEM images showing a ring rearrangement that transforms a 5-7-5-7 cluster into a 6-6-6-6 cluster. The dark spots are Si-O-Si columns that correspond with the top and side views in (A). Images have been smoothed and Fourier-filtered to remove the graphene lattice background [see figs. S2 and S3 and (*17*)]. (**F**) A trajectory map of the atomic sites. Color (red to yellow) indicates time of motion. (**G**) Larger view of the region from (A), and (**H**) corresponding first-to-last frame displacement map. The arrows have been enlarged ×2 to increase visibility; color indicates size of displacement, from 0 (dark blue) to ≥1.3 Å (red). The region between the bond rearrangement and the edge of the sheet exhibits strong local rotation. Scale bars: 1 nm. See also movies S1 and S2.

Huang et al. Science (october 2013)

Sensitivity to **Composition** and **Pressure** in (1-**x**) SiO_2 + **x** Na_2O







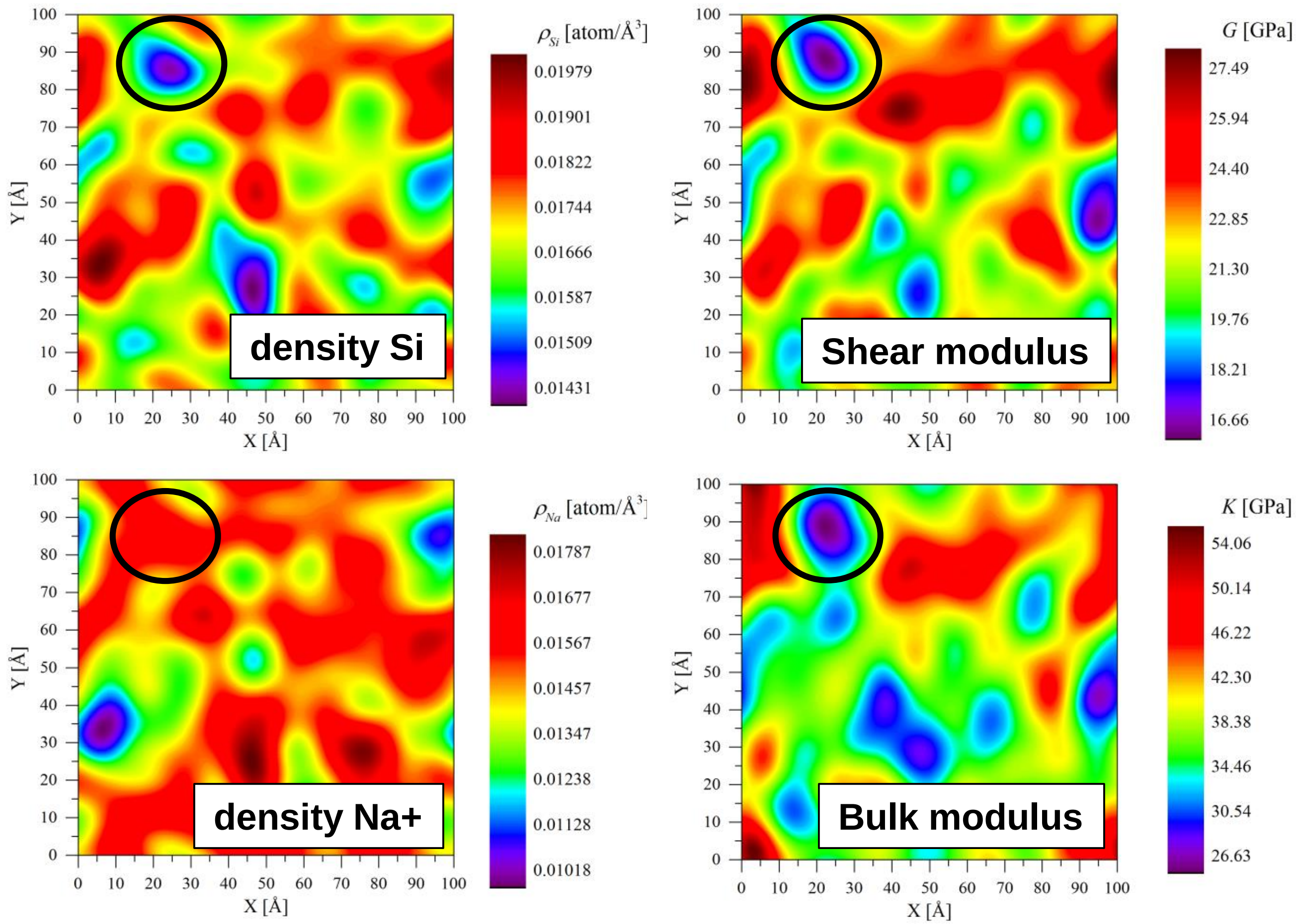
Na-rich plastic events (different stages)

Composition controls the number of events

Their size and amplitude are **pressure** dependent

G. Molnar et al. (2017)

Elastic Moduli in a **sodo-silicate** glass $(1\text{-}x)SiO_2 + xNa_2O$:

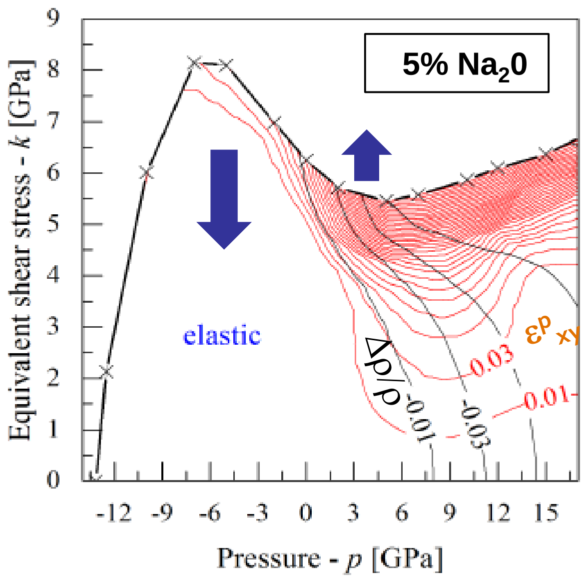


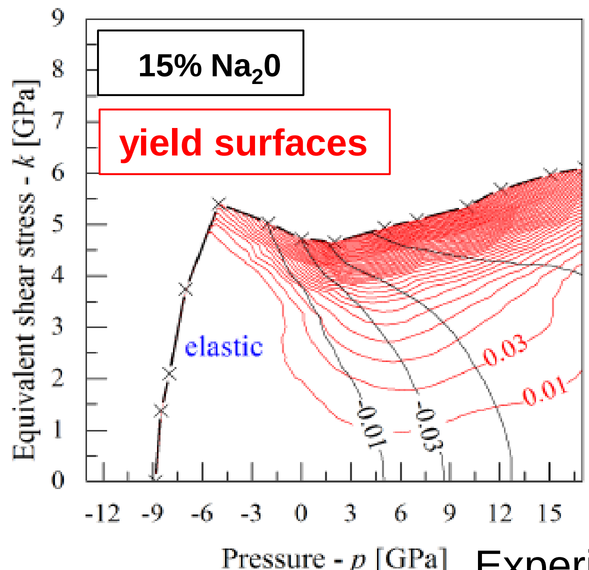
High loca Na+ density↔ Low Elastic Modulus

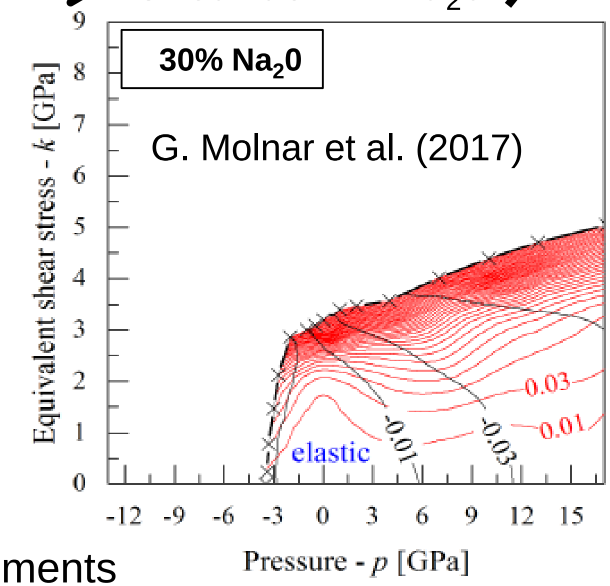
G. Molnar et al. (2016)

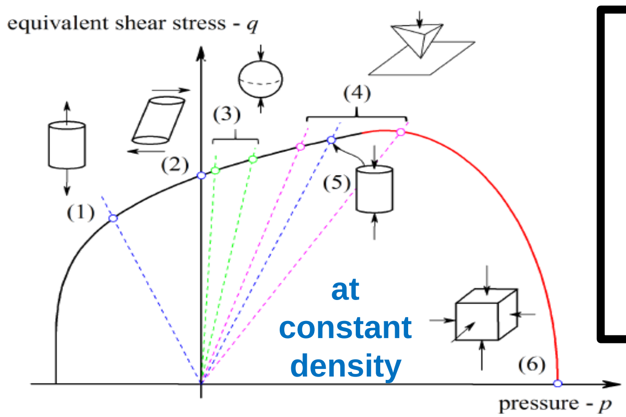
Sensitivity to **Composition** and **Pressure** in (1-x) SiO_2 + **x Na_2O**

Densification → Shear as % Na_20 ↗



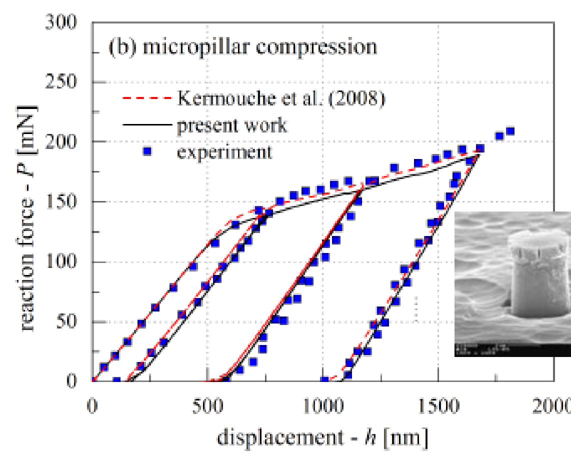


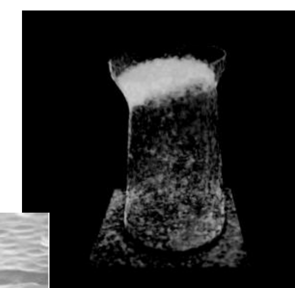




Adapt the **parameters** of the **yield surfaces** to experimental results

Experiments





G. Kermouche. (2022)

I. Phenomenology

II. Mechanical Instability

III. Plastic Flow

nature COMMUNICATIONS

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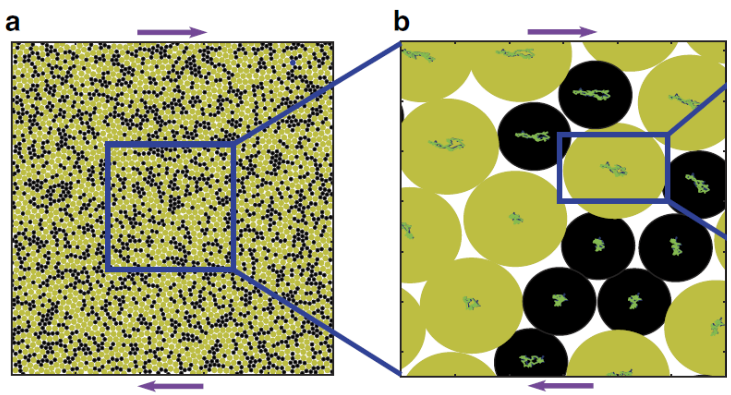
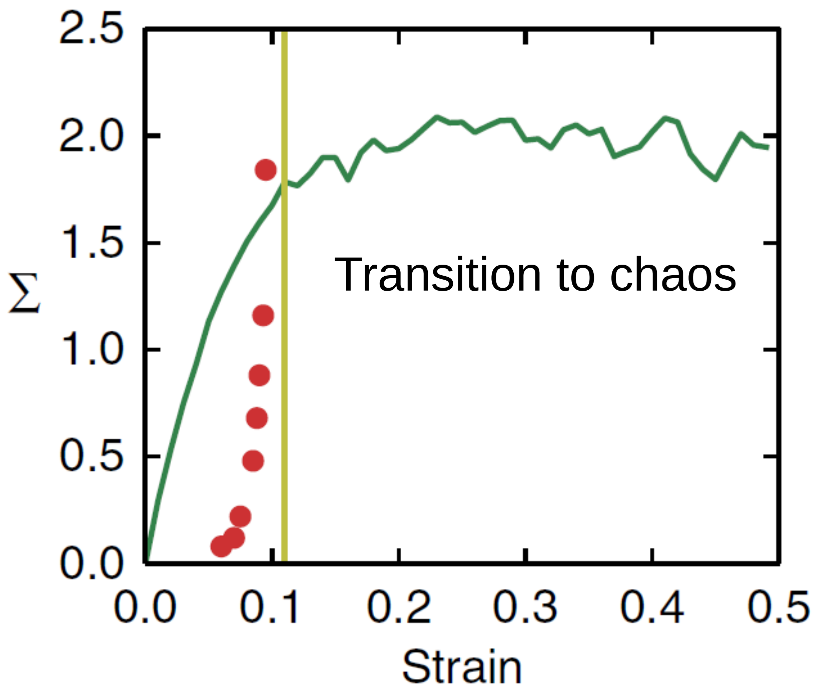
OPEN

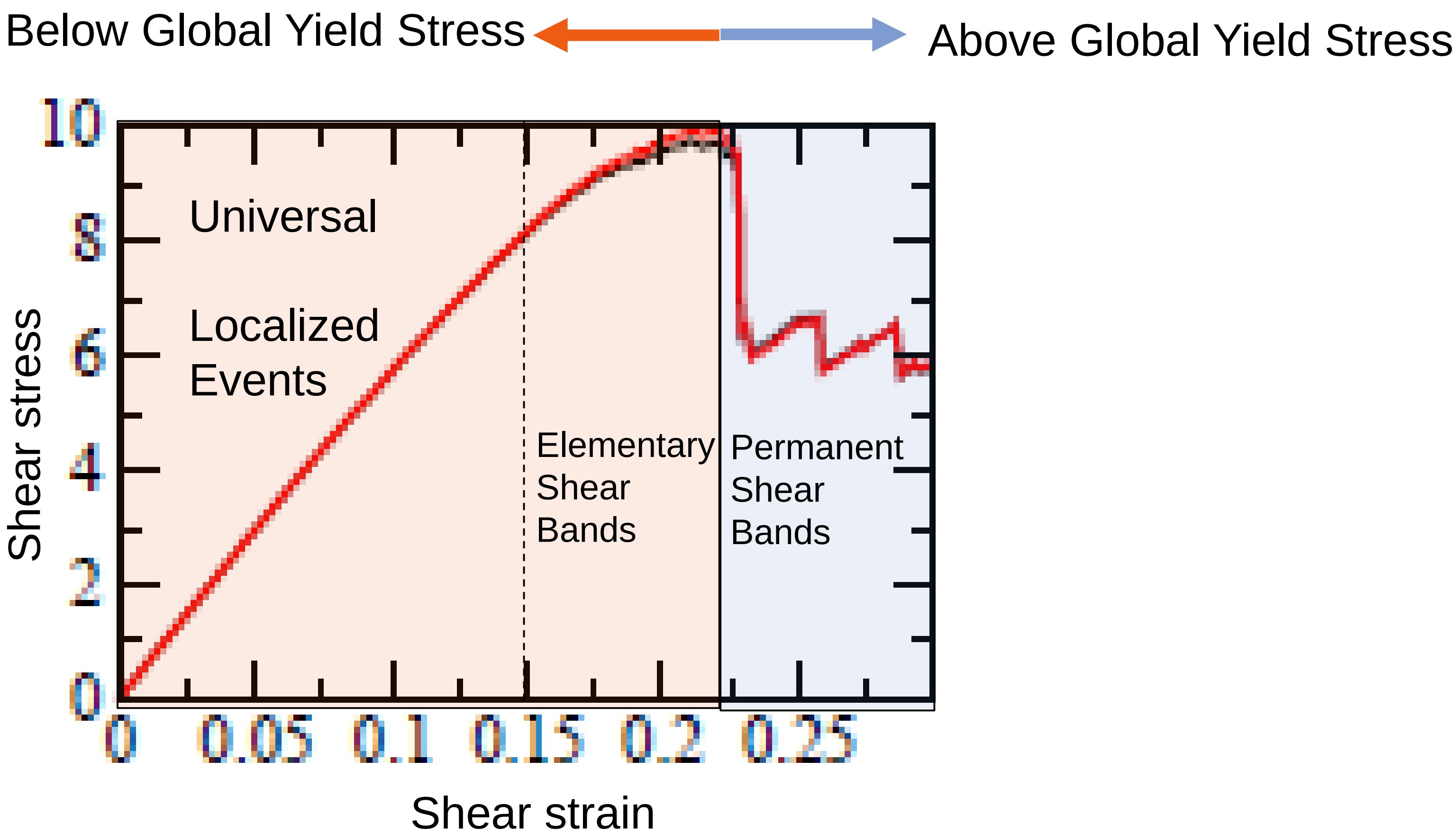
Reversibility and criticality in amorphous solids

Ido Regev[1,2,3], John Weber[4], Charles Reichhardt[2,3], Karin A. Dahmen[4] & Turab Lookman[2,3]



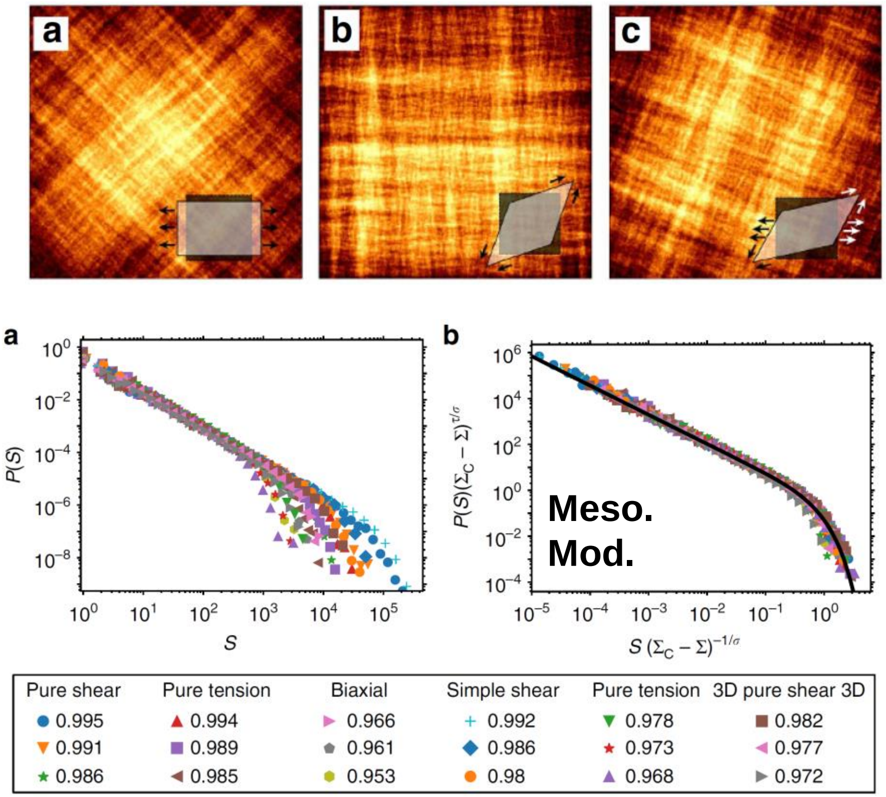


General Behaviour for **Plastic Flow** in **Amorphous** materials



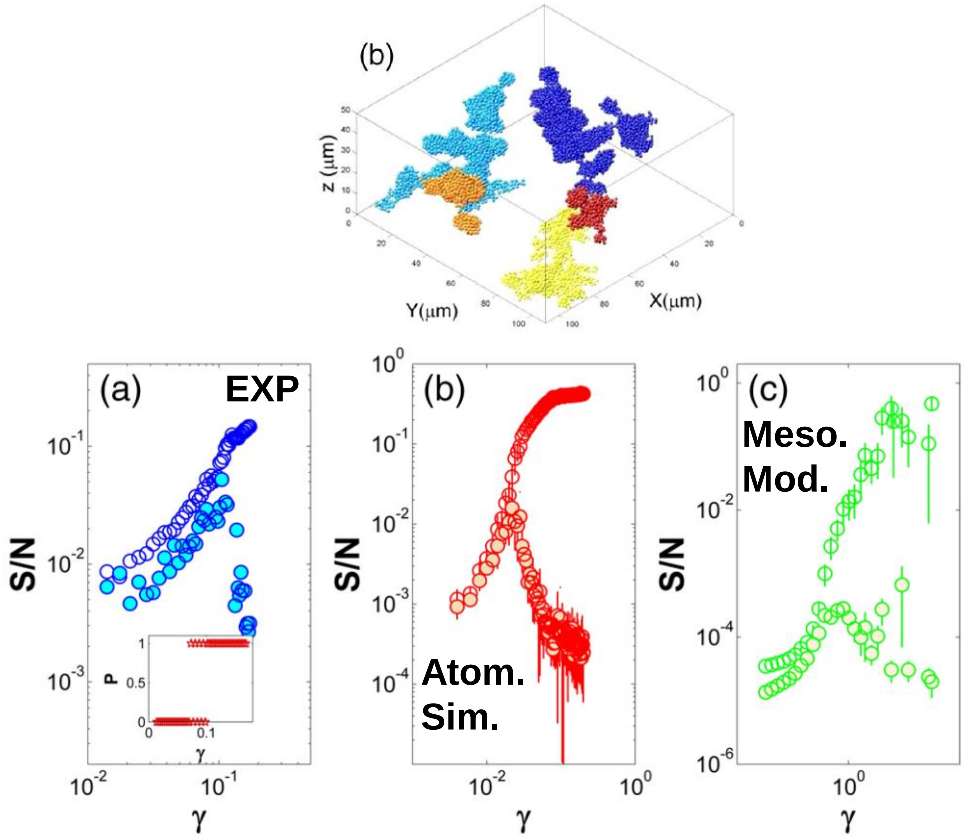
Critical Behaviour **below Yielding**

Avalanche Size distribution



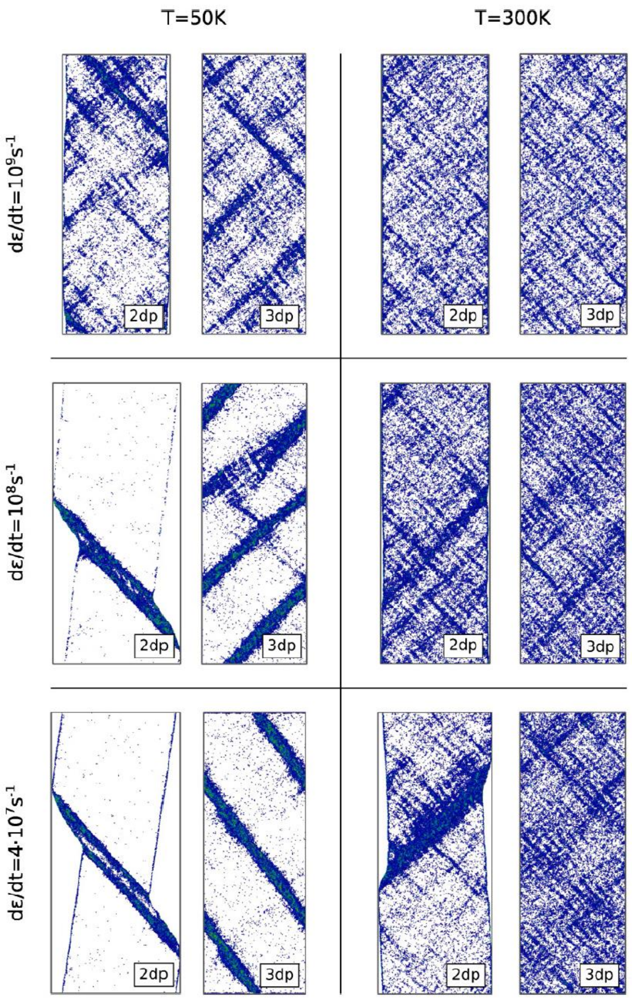
Z. Budrikis et al. (2017)

Percolation of Active Clusters



P. Schall et al. (2017)

The Occurrence of **Permanent Shear-Banding** in Non-Universal



$Cu_{64}Zr_{36}$ K. Albe et al. (2013)

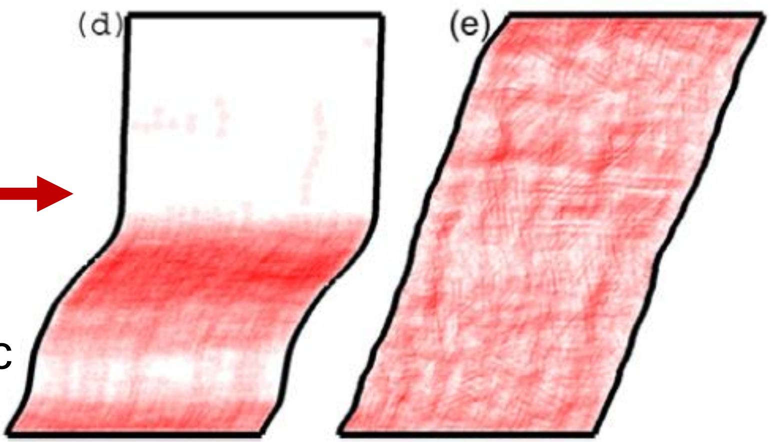
Role of Temperature

Strain Rate, Free Boundaries

Non-universal Process

Importance of Self-Softening

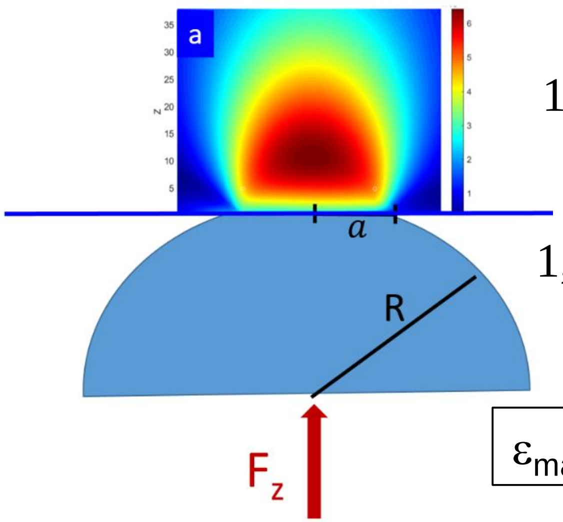
« Free Volume » creation at Plastic Rearrangement



E. Homer et al. (2013)

Sensitivity to Local Disorder

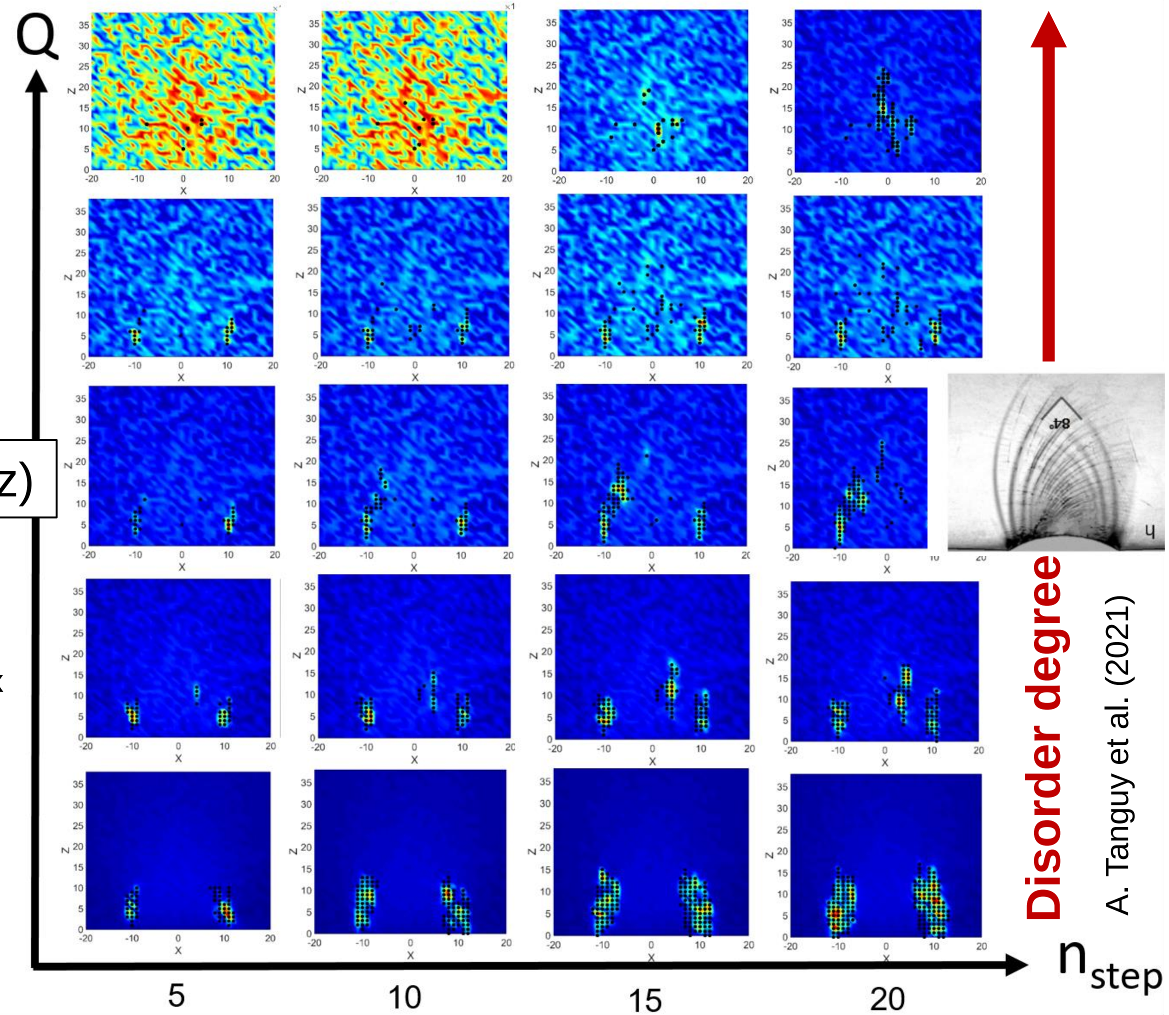
Example of **shear banding** in a **contact** problem



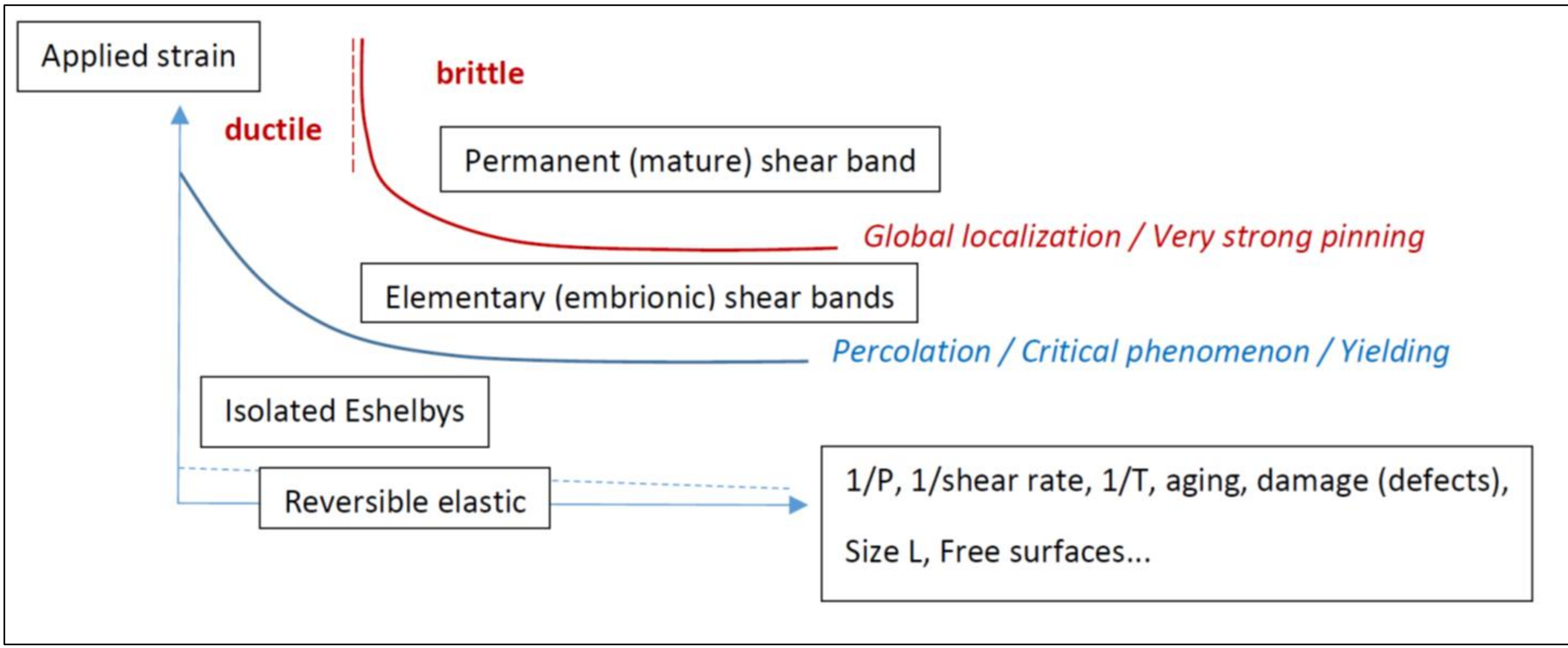
$\varepsilon(i) > \varepsilon^d_{thresh}(i)$: plastic event
then : $\varepsilon(i) = \varepsilon(i) + d\varepsilon$
with stress redistribution

Random threshold:
$\varepsilon^d_{thresh}(i) = \varepsilon^0_{thresh} + Q.ran(i)$

with initial surface defects



Summary



A. Tanguy (2021)

Conclusion

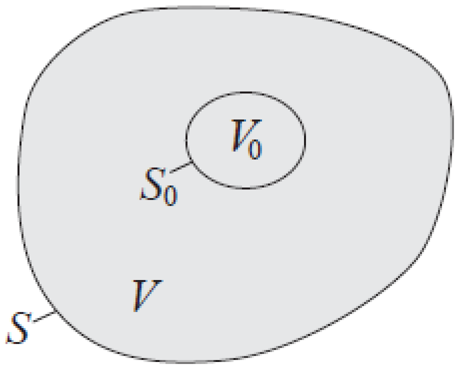
Universal features:
Plasticity as a Mechanical Instability (atomistic buckling)
Elementary events (Eshelby inclusions and Elementary – embrionic - shear bands)
Critical behaviour before yielding

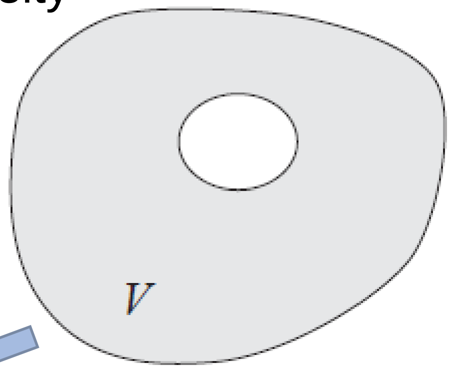
Non-universal features have engineering importance:
Structural signature of plastic rearrangements
Number and spatial distribution of plastic events as a function of temperature,
as a function of composition, and as a function of strain rate
Importance of Self-softening or strong heterogeneities for permanent shear-banding
Sensitivity of the permanent – mature – shear-banding to the boundary conditions

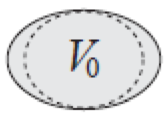
Comparison to crystals:
Difficulty to identify a permanent structural signature of plasticity
Coupling between shear and densification
No order to disorder transition

Eshelby Inclusion (1957)

Linear Elastic Heterogeneity
with ellipse shape
in a Linear Elastic matrix

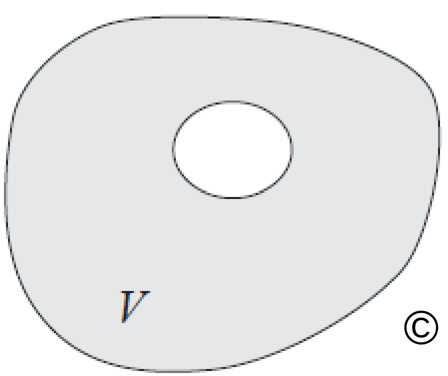


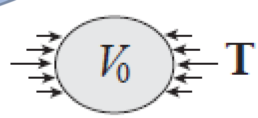




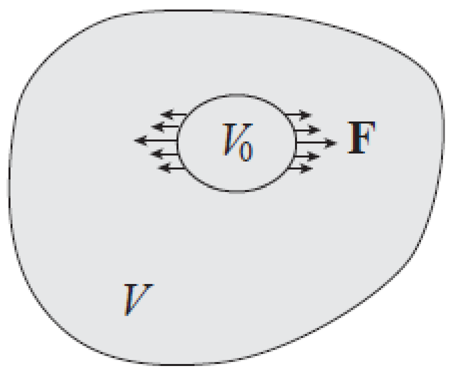
matrix	inclusion
$e_{ij}=0$	$e_{ij}=e^*_{ij}$
$\sigma_{ij}=0$	$\sigma_{ij}=0$
$u_i=0$	$u_i=e^*_{ij}x_j$

ε* is the « eigenstrain »
or stress-free strain
Inside the inclusion





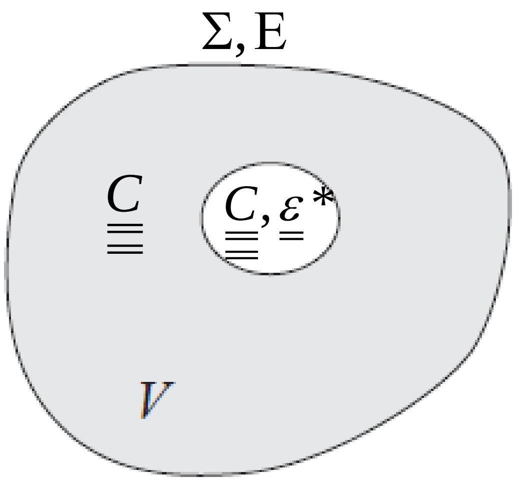
matrix	inclusion
$e_{ij}=0$	$e_{ij}=e^{\mathrm{el}}_{ij}+e^*_{ij}=0$
$\sigma_{ij}=0$	$\sigma_{ij}=C_{ijkl}e^{\mathrm{el}}_{ij}=-C_{ijkl}e^*_{ij}=-\sigma^*_{ij}$
$u_i=0$	$u_i=0$



matrix	inclusion
$e_{ij}=e^{\mathrm{c}}_{ij}$	$e_{ij}=e^{\mathrm{c}}_{ij}$
$\sigma_{ij}=\sigma^{\mathrm{c}}_{ij}$	$\sigma_{ij}=\sigma^{\mathrm{c}}_{ij}-\sigma^*_{ij}=C_{ijkl}(e^{\mathrm{c}}_{kl}-e^*_{kl})$
$u_i=u^{\mathrm{c}}_i$	$u_i=u^{\mathrm{c}}_i$

Similar Cases:

1) Uniform Load at infinity:

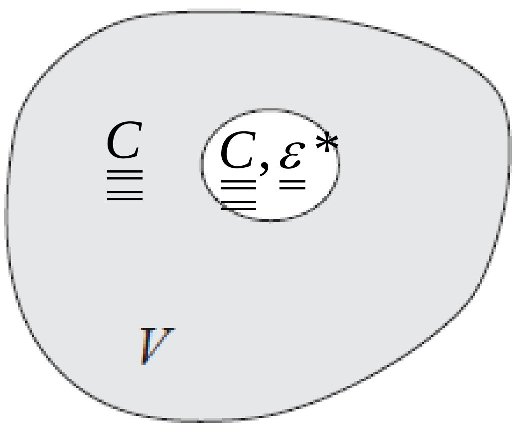


$$\underline{\underline{\sigma}}^I = \boxed{\underline{\underline{\Sigma}}} + \underline{\underline{\underline{\underline{C}}}} : \left(\underline{\underline{\underline{\underline{S}}}} - I \right) : \underline{\underline{\varepsilon}}^*$$

$$\underline{\underline{\varepsilon}} = \boxed{\underline{\underline{E}}} + \underline{\underline{\underline{\underline{S}}}} : \underline{\underline{\varepsilon}}^*$$

$$\underline{\underline{\sigma}}^M = \underline{\underline{\Sigma}} + \underline{\underline{\underline{\underline{C}}}} : \underline{\underline{\underline{\underline{S}}}} : \underline{\underline{\varepsilon}}^*$$

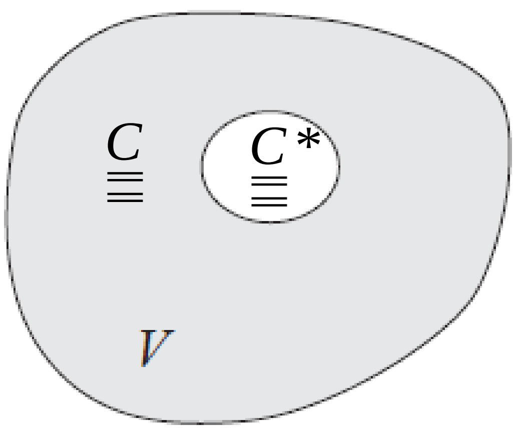
2) Empty Inclusion:



$$\underline{\underline{\Sigma}} + \underline{\underline{\underline{\underline{C}}}} : \left(\underline{\underline{\underline{\underline{S}}}} - I \right) : \underline{\underline{\varepsilon}}^* = \boxed{0}$$

$$\underline{\underline{\sigma}}^M = \underline{\underline{\Sigma}} + \underline{\underline{\underline{\underline{C}}}} : \underline{\underline{\underline{\underline{S}}}} : \underline{\underline{\varepsilon}}^*$$

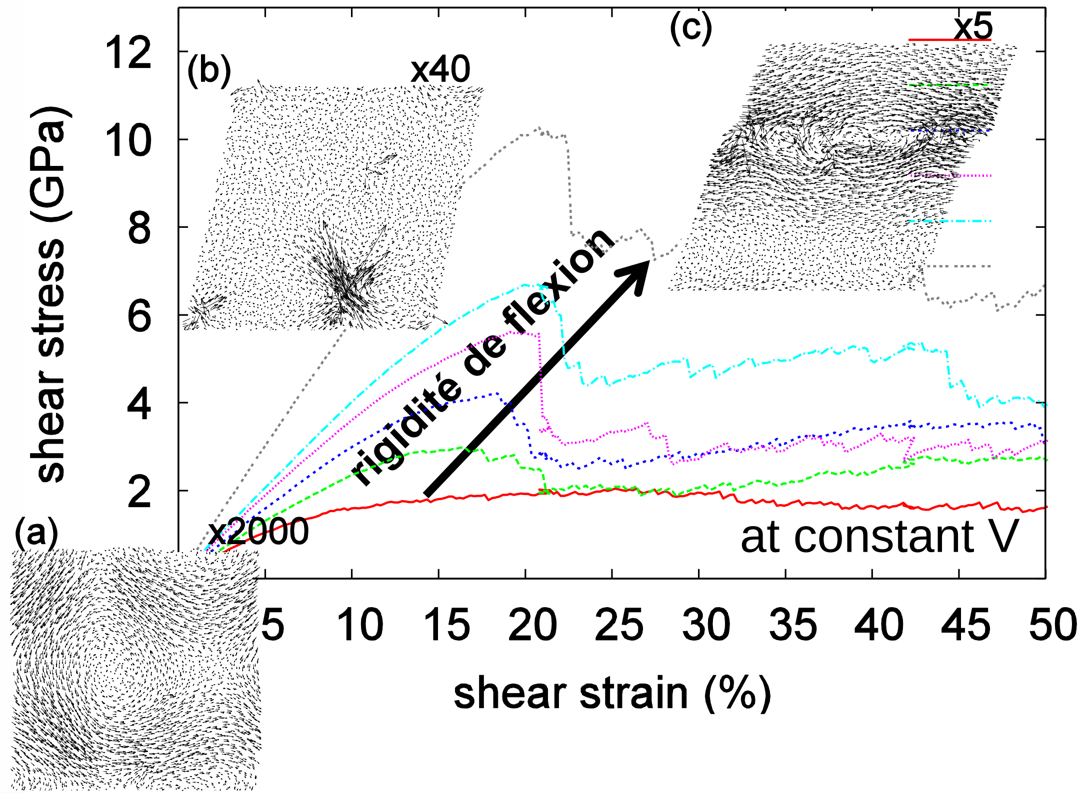
3) Elastic Inhomogeneity:

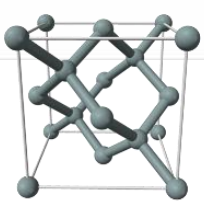


$$\underline{\underline{\sigma}}^I = \underline{\underline{\Sigma}} + \underline{\underline{\underline{\underline{C}}}} : \left(\underline{\underline{\underline{\underline{S}}}} - I \right) : \underline{\underline{\varepsilon}}^* = \boxed{\underline{\underline{\underline{\underline{C}}}}^*} : \underline{\underline{\varepsilon}}^I$$

$$\underline{\underline{\varepsilon}}^I = \underline{\underline{E}} + \underline{\underline{\underline{\underline{S}}}} : \underline{\underline{\varepsilon}}^*$$

The Example of Amorphous Silicon





$$E_{SW} = \Sigma_{(i,j)} f(r_{ij}) + \Sigma_{i,j,k} \Lambda.. \left(\cos\theta_{jik} + \frac{1}{3} \right)^2 .e^{\gamma.(r_{ij}-a)^{-1}+\gamma.(r_{ik}-a)^{-1}}$$