Coarse-graining amorphous plasticity: shear-banding and rejuvenation

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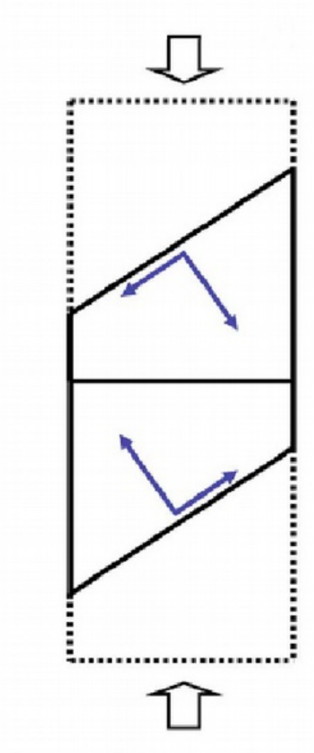
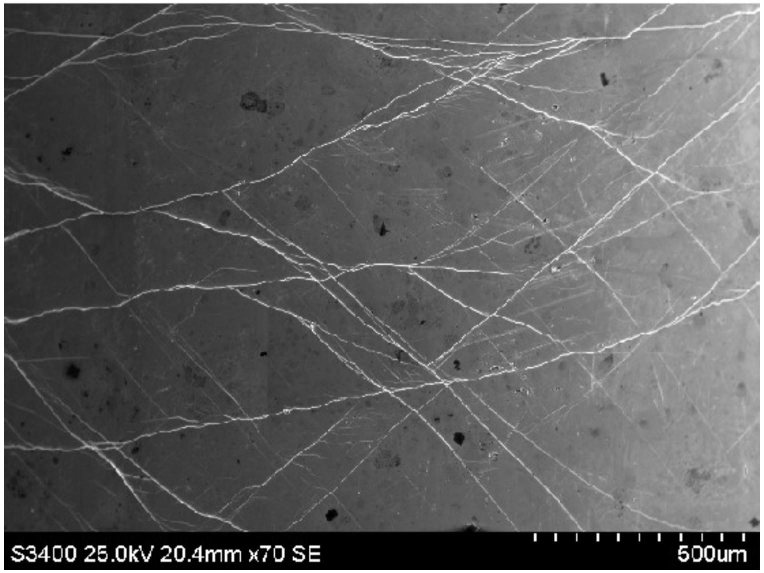
Yielding vs Depinning in Disordered Systems
Paris, October 22-24, 2018

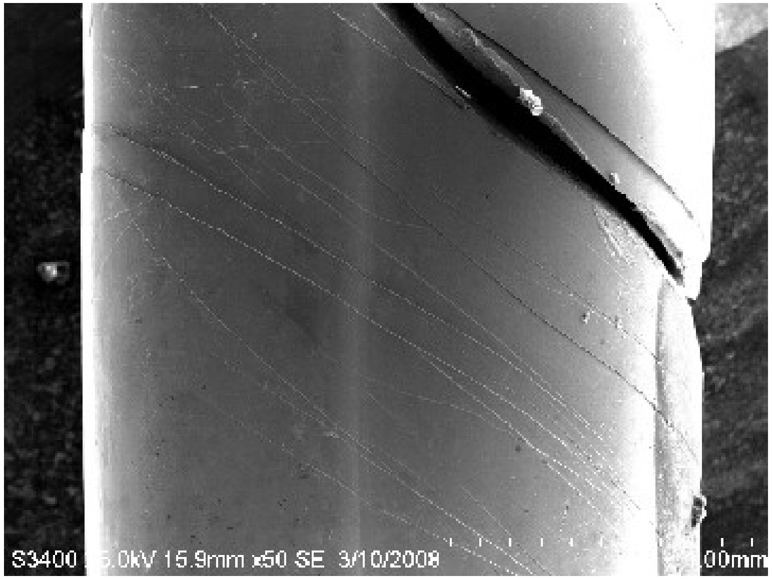
SIMONS FOUNDATION

Compression of metallic glass

- High yield strength but brittle
- Localization and shear-banding behavior
- Dependence on thermal and mechanical history

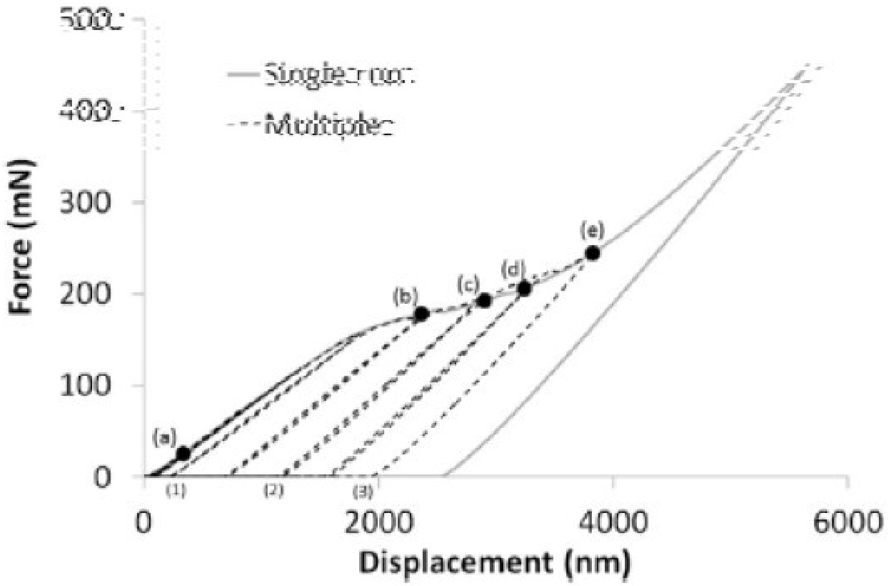


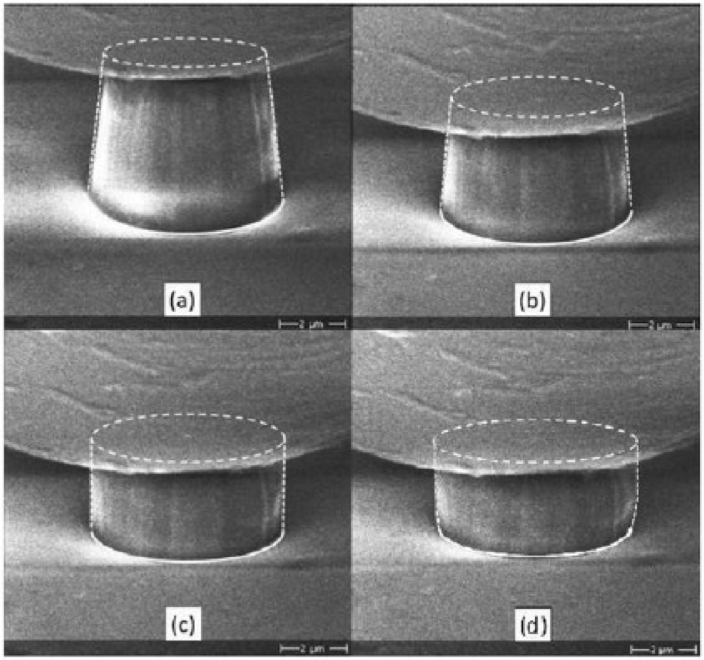


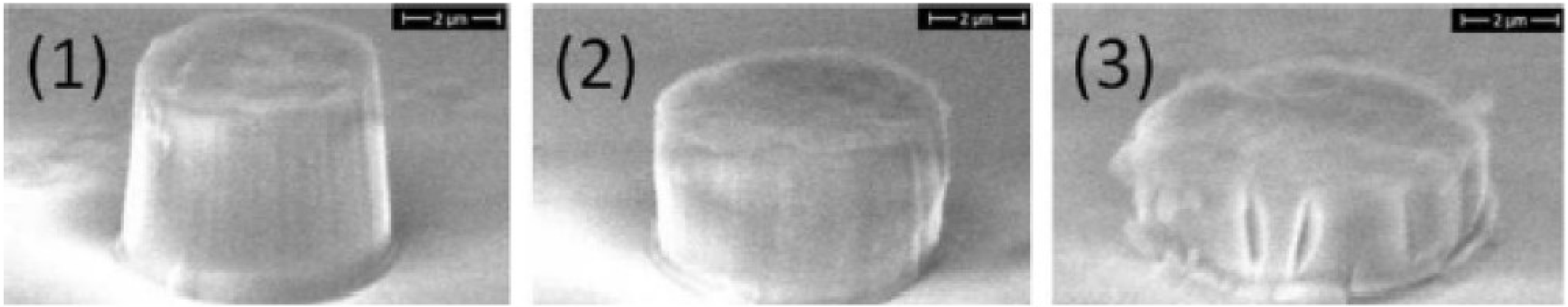


J. Zhang et al, Scripta Mater. **61**, 1145 (2009)

Compression of silica glass

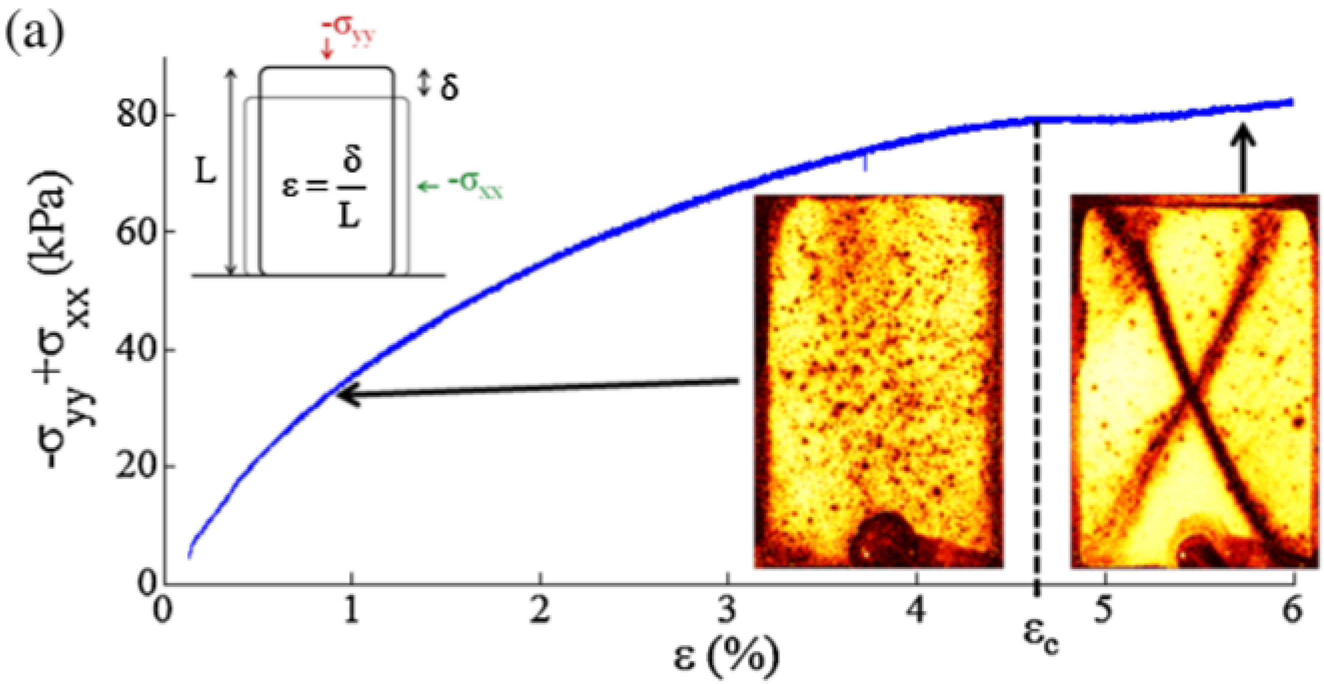


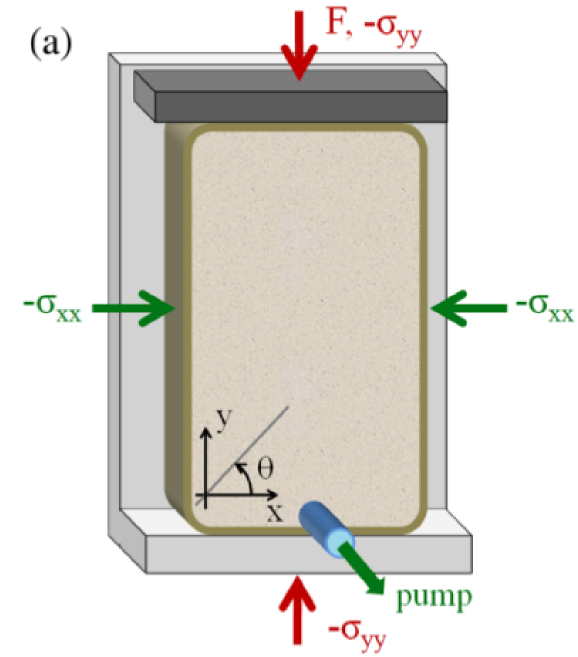




G. Kermouche et al. Acta Mater. 114, 146 (2016)

Compression of granular matter



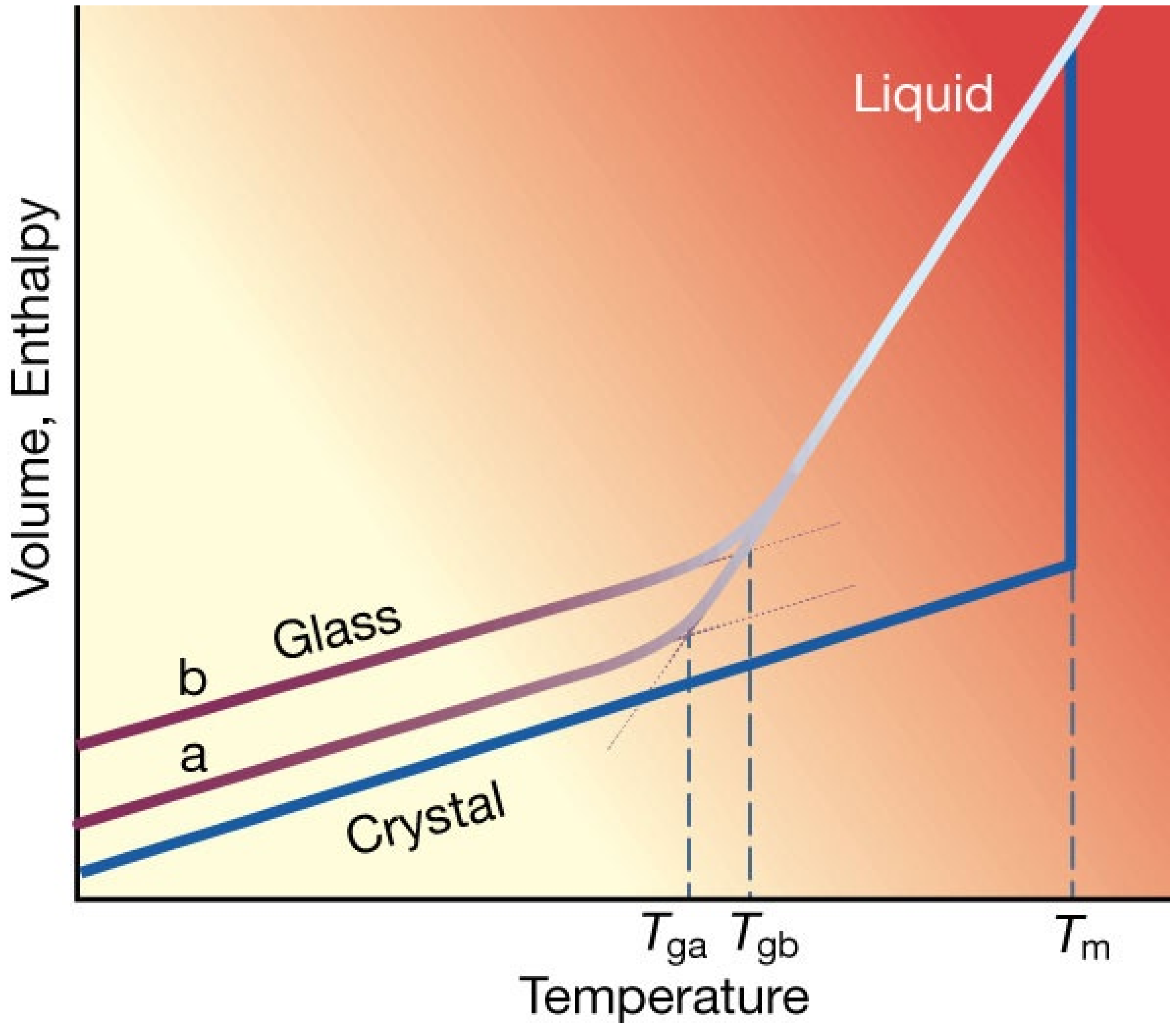


PRL **112,** 246001 (2014) PHYSICAL REVIEW LETTERS week ending 20 JUNE 2014

Emergence of Cooperativity in Plasticity of Soft Glassy Materials

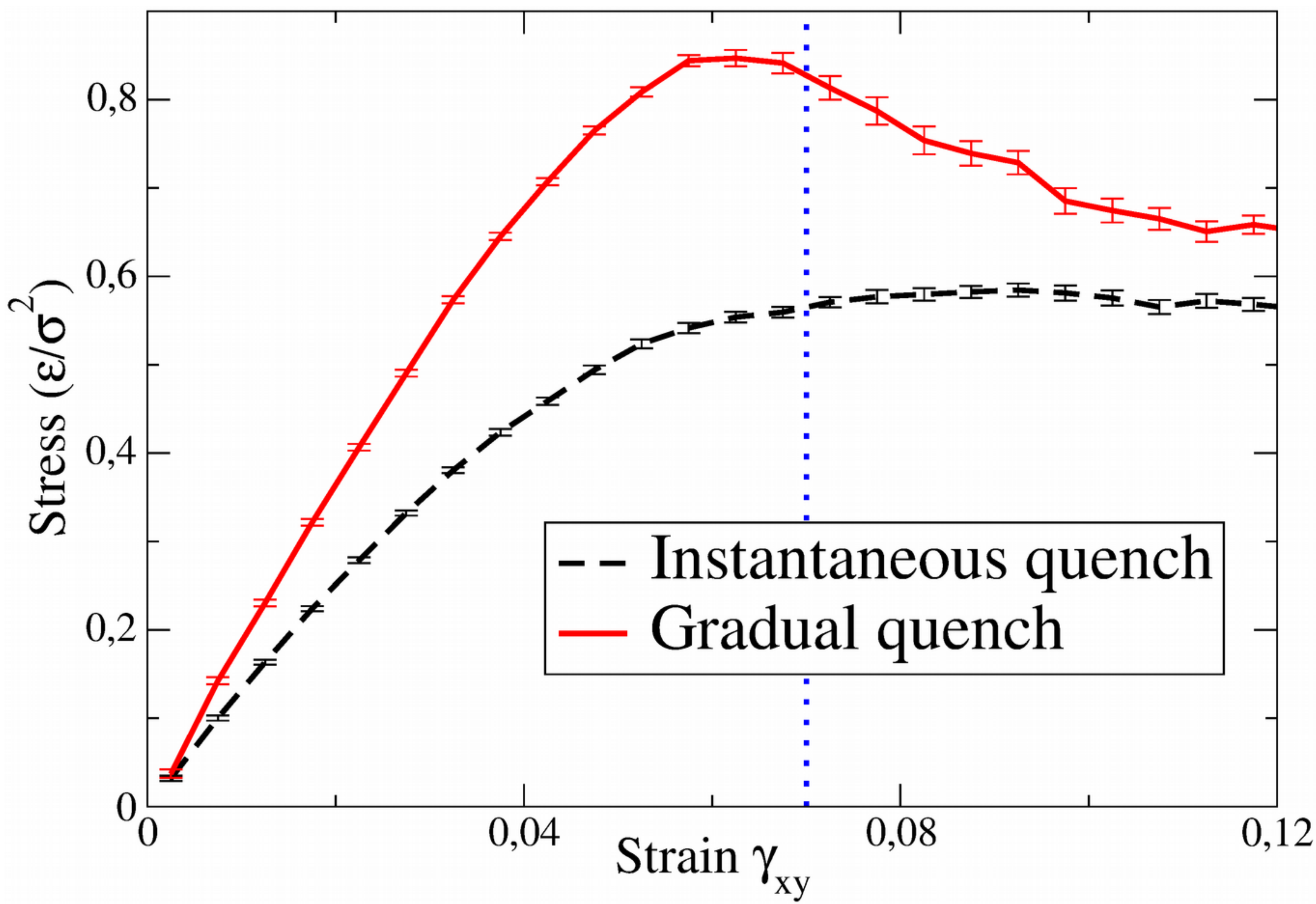
Antoine Le Bouil, Axelle Amon, Sean McNamara, and Jérôme Crassous
Université de Rennes 1, Institut de Physique de Rennes (UMR UR1-CNRS 6251),

Glass making: quench from liquid

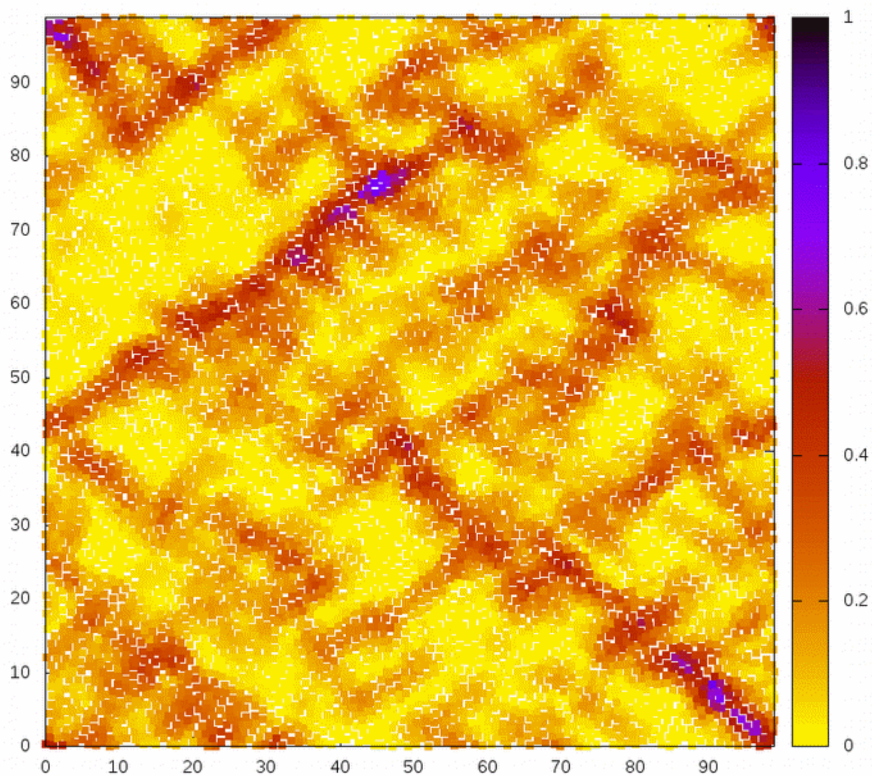


P. G. Debenedetti and F. H. Stillinger Nature **410**, 259 (2001)

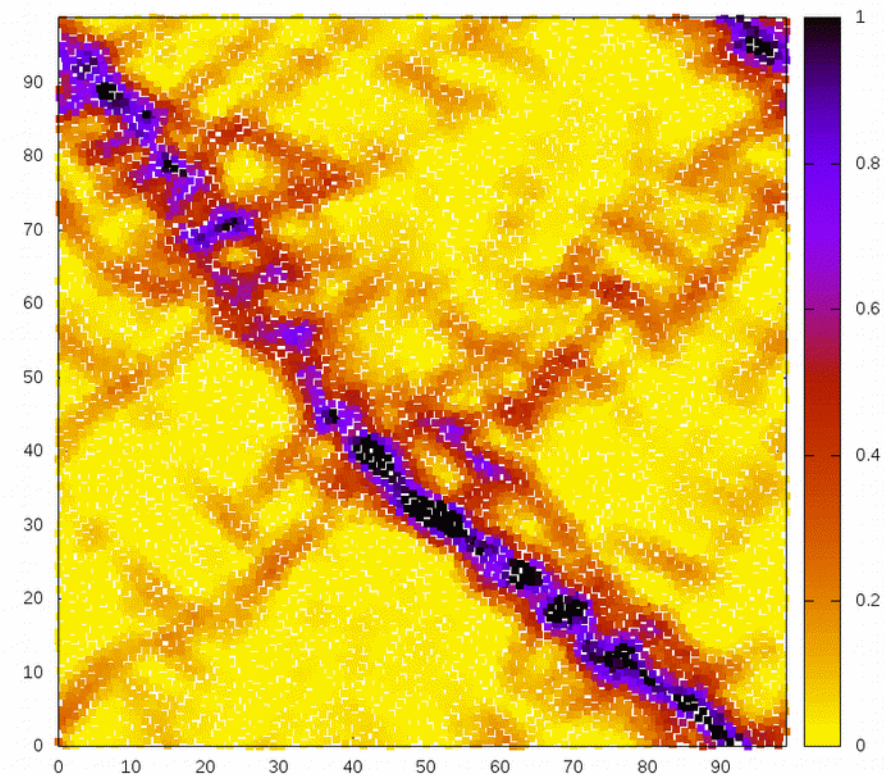
Plastic behavior depends on thermal history



Shear banding depends on thermal history

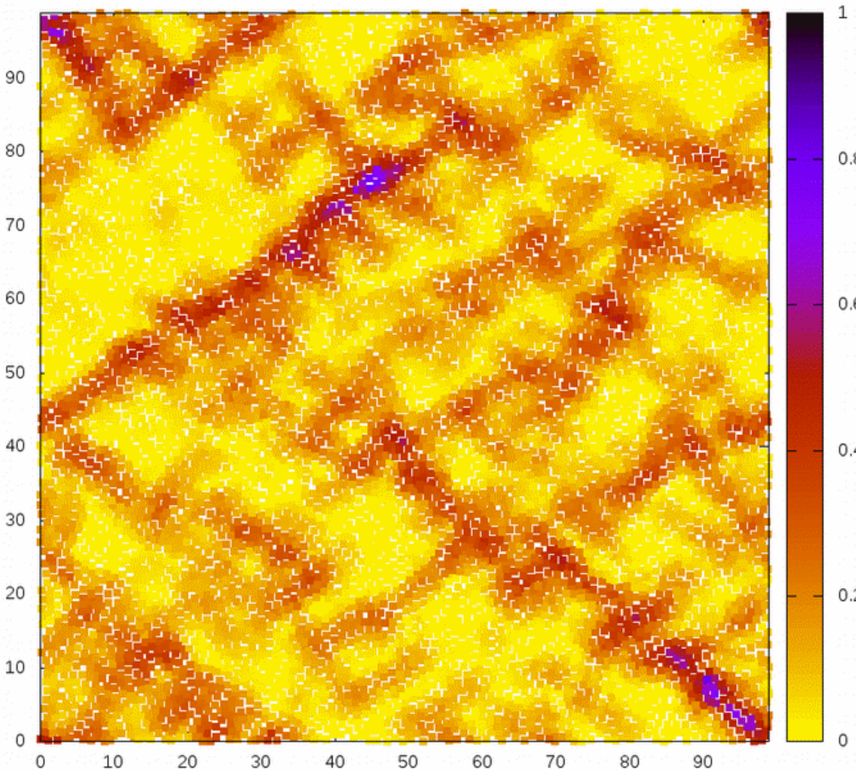


Fast quench

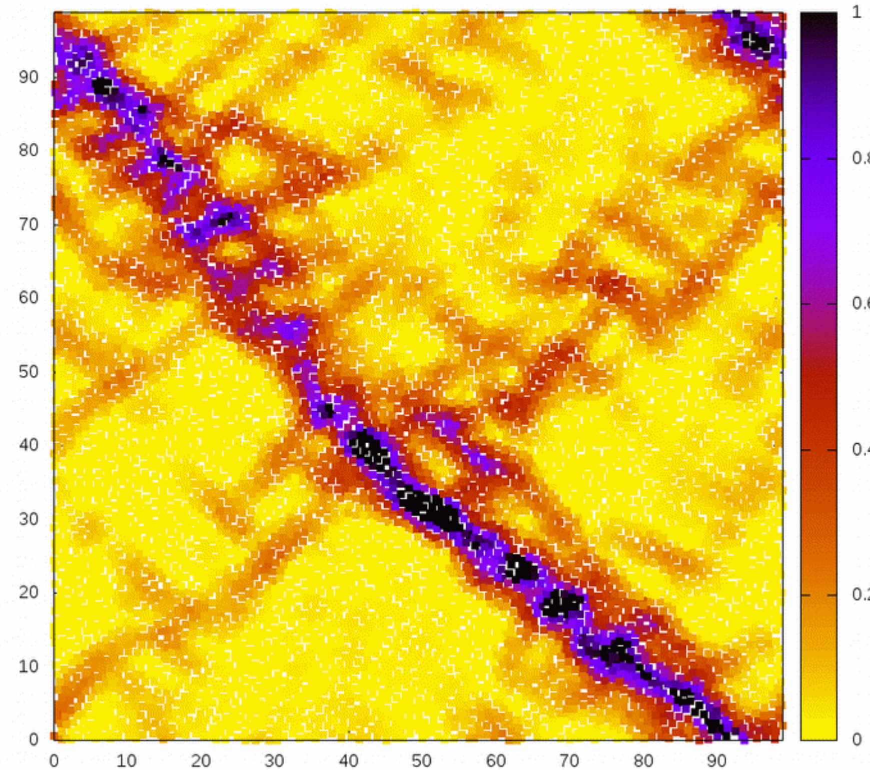


Slow quench

Shear banding depends on thermal history



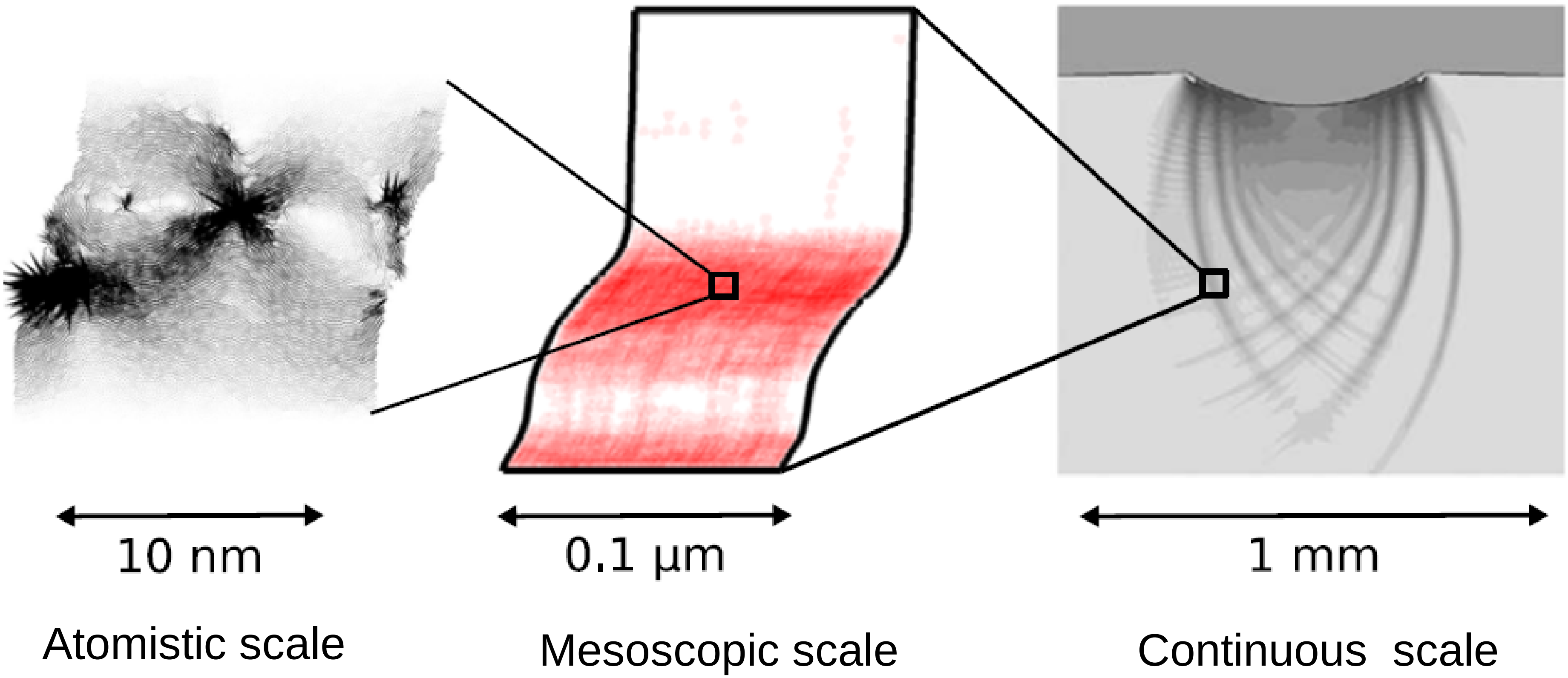
Fast quench



Slow quench

But structure of glass almost identical to that of the liquid i.e. no clear dependence on glass preparation !

Multi-scale modeling methods



D. Rodney, A. Tanguy and D. Vandembroucq, Modelling Simul. Mater. Sci. Eng. ***19*** *083001 (2011).*

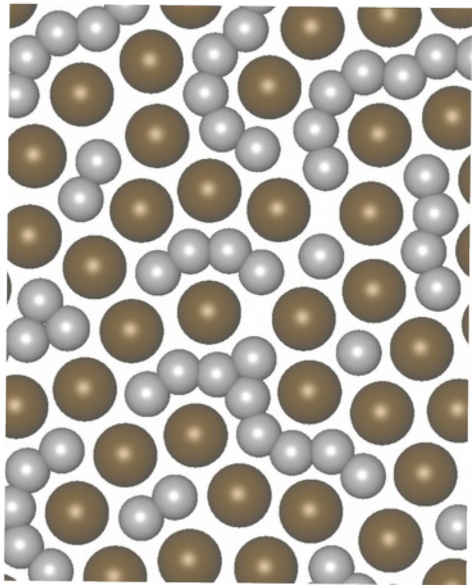
Atomistic simulation of a 2D model glass

System:

- Two-dimensional binary glass
- 10^4 atoms, ρ=1,024, PBC
- Lennard-Jones potentials *(+smoothing function)*

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \; r < r_c$$

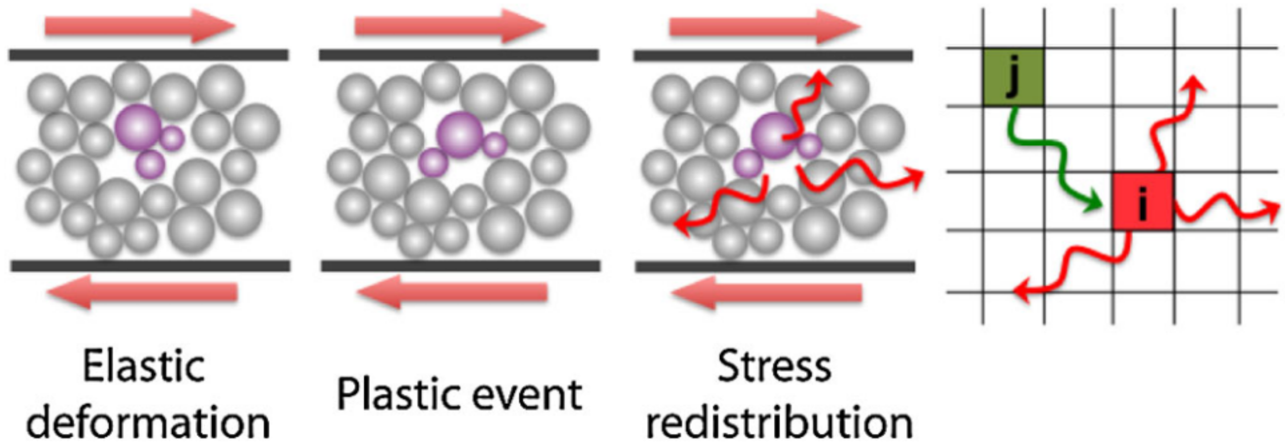
Falk, M. L. et al. *Phys. Rev. E* **57,** 7192 (1998).
Shi, Y. et al., *Phys. Rev. Lett.* **98,** 185505 (2007).



Simulation methods:

- Synthesis of the glass: NVT quench from liquid
- Loading: Athermal Quasi-Static shear

Lattice models of amorphous plasticity

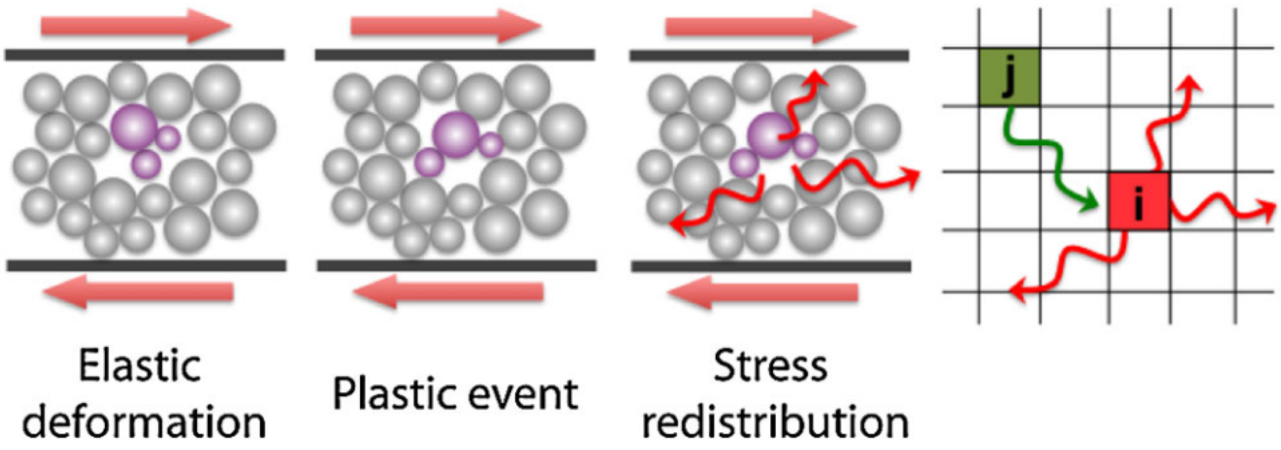


Bocquet et al PRL 2009

- Aim: build at mesoscopic scale a minimal model that reproduces the salient features of amorphous plasticity
- Two main ingredients:
  - Local threshold dynamics – plastic events
  - Eshelby quadrupolar elastic interaction
- Various implementations: Boston, Erlangen, Grenoble, Helsinki, Lausanne, Milano, Paris...

A. Nicolas et al, Rev. Mod. Phys (2018)

Mesoscopic models of amorphous plasticity



Bocquet et al PRL 2009

2D, scalar. Inclusions on lattice sites.

Local slips of inclusions (**threshold**-related): $\boxed{\sigma_{ij} > \sigma_{ij}^{th}}$ **disorder**

Plastic strain associated to each inclusion: $\epsilon_{ij}^{p} \rightarrow \epsilon_{ij}^{p} + \delta\epsilon^{p}$

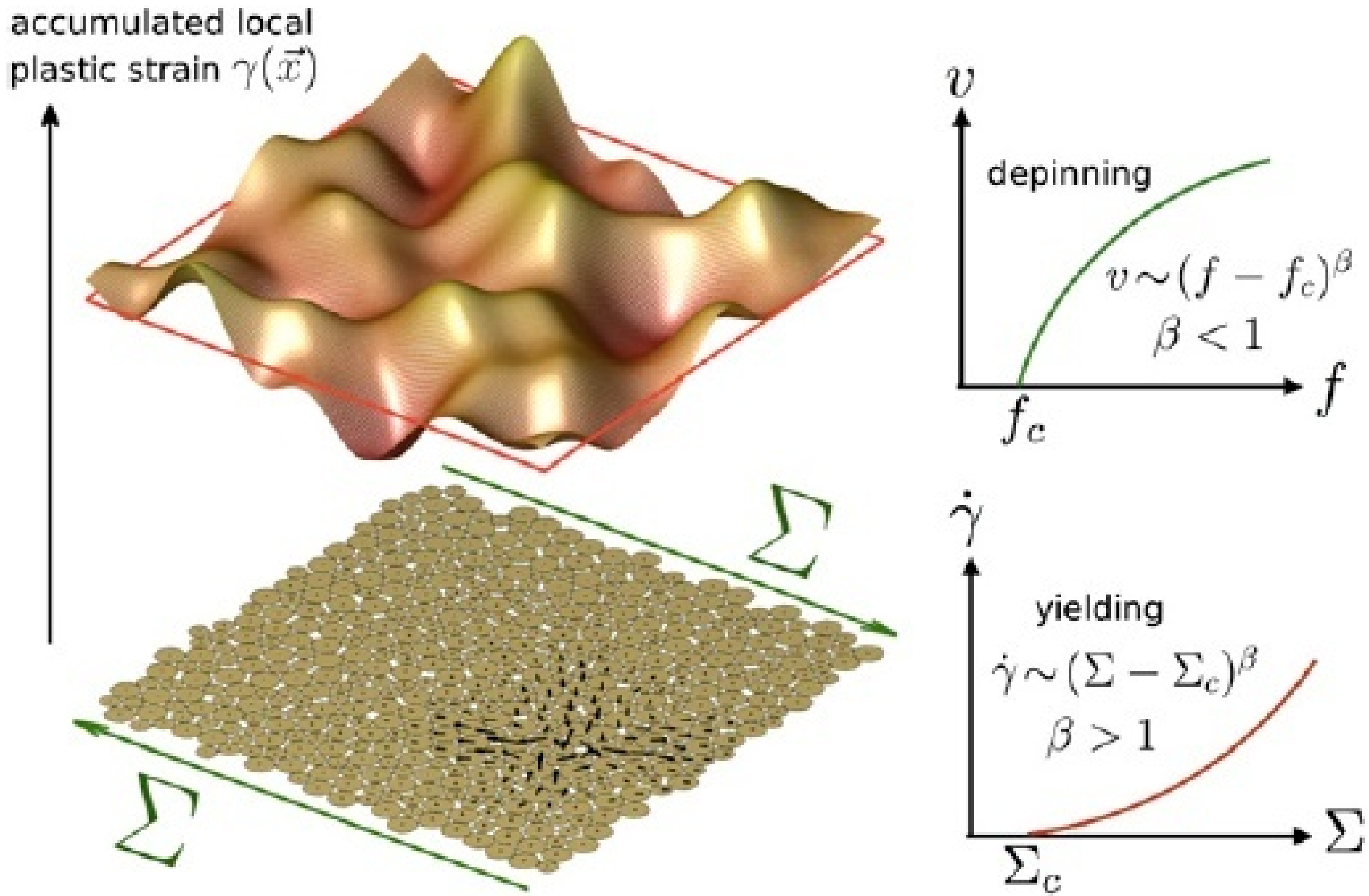
$$\sigma_{ij} \rightarrow \sigma_{ij} + G * \delta\epsilon^{p}$$

Elastic interaction between inclusions: via the **elastic kernel**

$$\boxed{G(\vec{r}) \propto \frac{\cos 4\theta}{r^2}}$$

elasticity

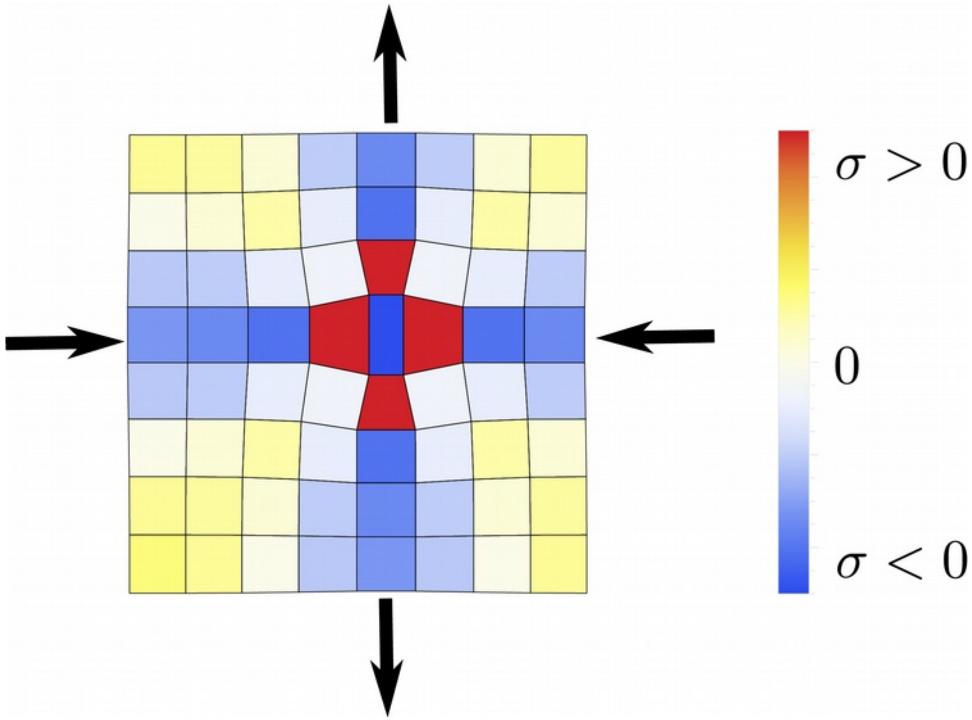
Yielding vs Depinning



Plastic strain field as an elastic manifold
moving in a *random medium*

Lin et al, PNAS (2014)

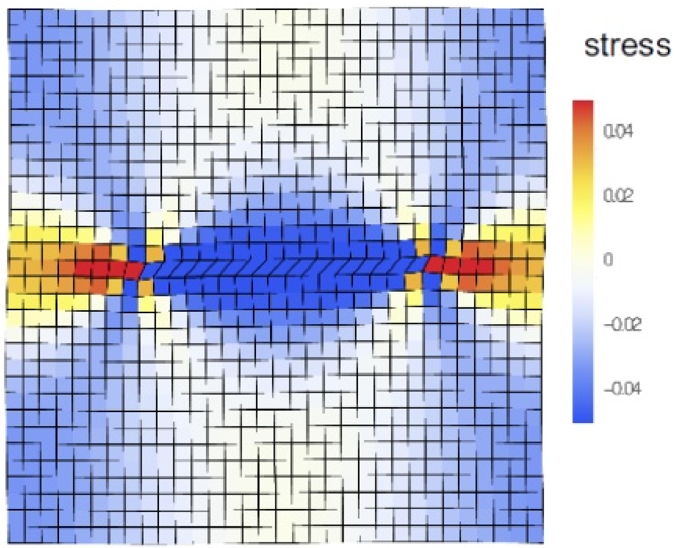
Yielding vs Depinning



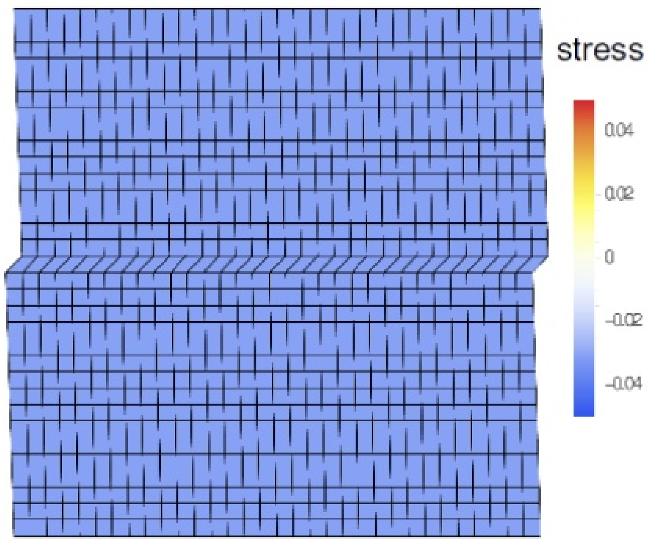
$$G(\vec{r}) \propto \frac{\cos 4\theta}{r^2}$$

Eshelby inclusion :
anisotropic stress interaction

Yielding vs Depinning



partial shear band

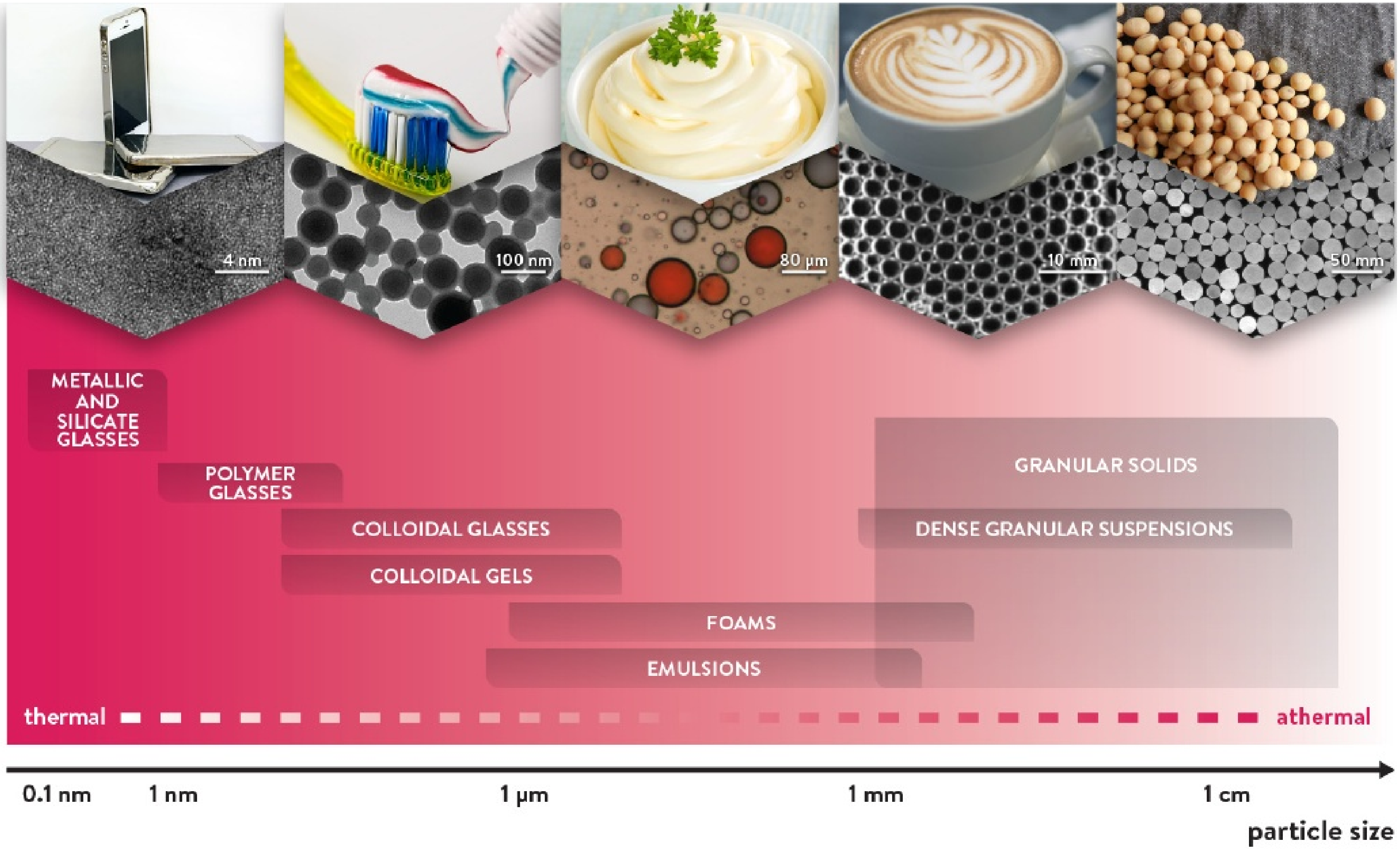


full shear band

- **Depinning**: Any fluctuation of the line/manifold induces a restoring force
- **Plasticity**: Any unit shear-band in a maximum shear stress direction induces <u>no elastic stress</u>

B. Tyukodi et al **93** 063005 PRE 2016

How disordered are disordered materials ?



A. Nicolas et al, Rev. Mod. Phys (2018)

How disordered are disordered materials ?

A tentative classification

- **Heterogeneous materials :**
  - Mechanical properties = invariant along the ε_{pl} / z direction
  - Quenched disorder : $\sigma_Y[x,y,\varepsilon_{pl}(x,y)] = \sigma_Y(x,y,0)$
  - Composites ? Polycrystals ? Earthquakes ?

  => Localization on extremal/minimal path (Chen, Bak & Obukhov PRA 91)

- **Disordered materials :**
  - Mechanical properties = weakly dependent on the ε_{pl} / z direction
  - Stationary disorder : $P(\sigma_Y[\varepsilon_{pl}]) = P(\sigma_Y[\varepsilon_{pl}=0])$
  - ???

  => Avalanches (most lattice models of yielding)

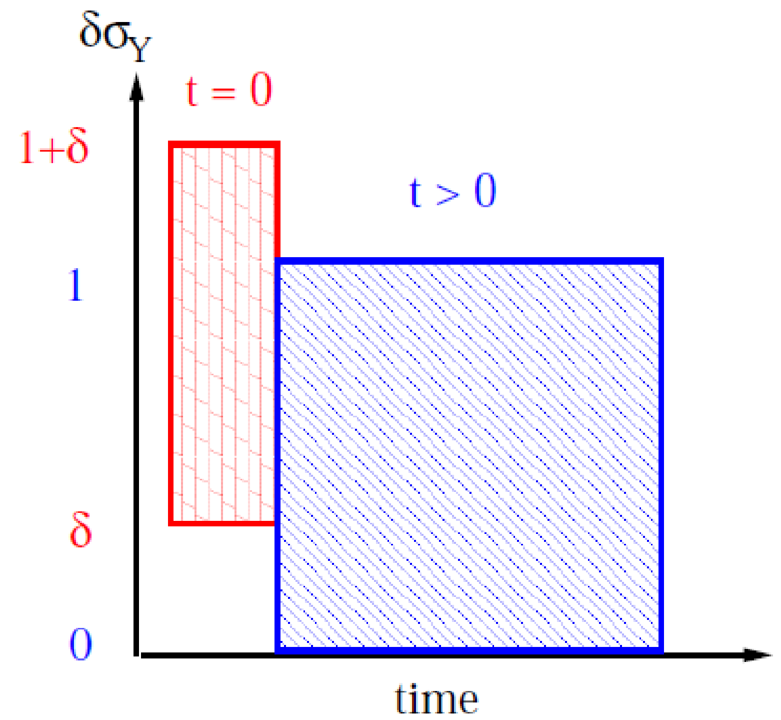
- **Glassy materials :**
  - Mechanical properties = strongly dependent on the ε_{pl} / z direction
  - Thermal/Mechanical aging and rejuvenation
  - Non-stationary disorder : $P(\sigma_Y[\varepsilon_{pl}]) \neq P(\sigma_Y[\varepsilon_{pl}=0])$
  - BMG & oxide glasses, pastes, complex fluids...

  => Homogeneous deformation (mech. Aging/hardening) or Shear-Banding (rejuvenation/softening) (Dahmen, Uhl, Ben-Zion PRL 09)

Shear-banding and Rejuvenation in a lattice model of plastic yielding

Mimicking aging with changing initial conditions

- Introduction of an age-like parameter δ
- Initial state characterized by a biased distribution of barriers $\delta\sigma_Y^i \in rand[\delta, 1+\delta]$
- Under shear $\delta\sigma_Y^i$ still renewed in $rand[0,1]$;



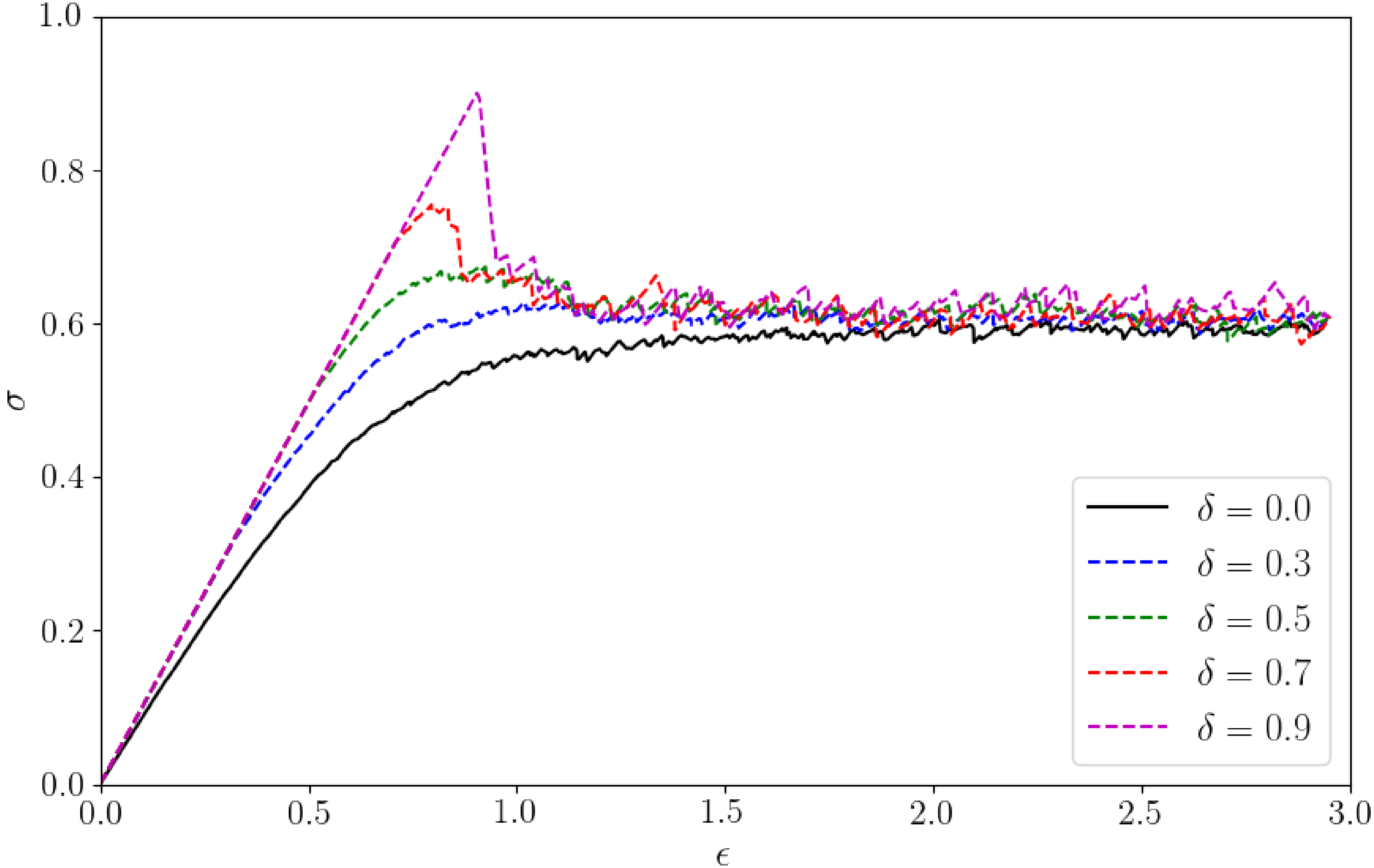
Random barriers

Aged structure = higher energy barriers ?

Don't change anything but the initial condition

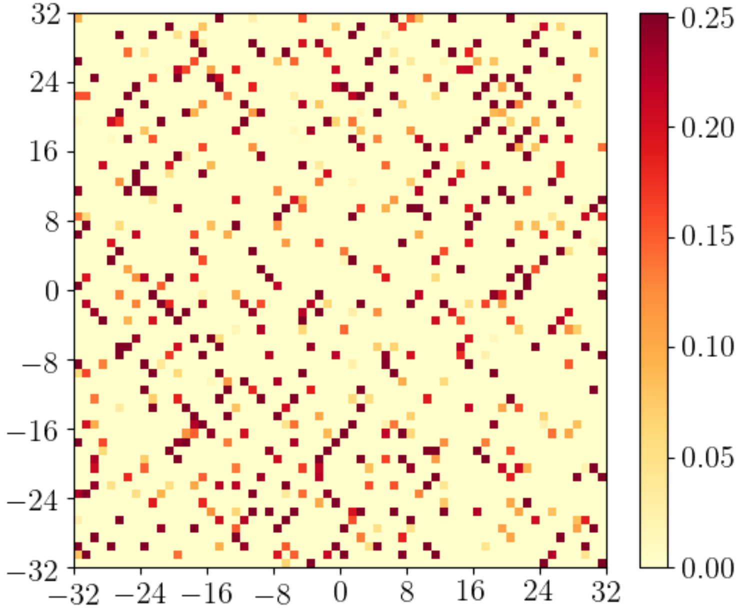
D. Vandembroucq & S. Roux, Phys Rev. B (2011)

Age-dependent stress-strain curves

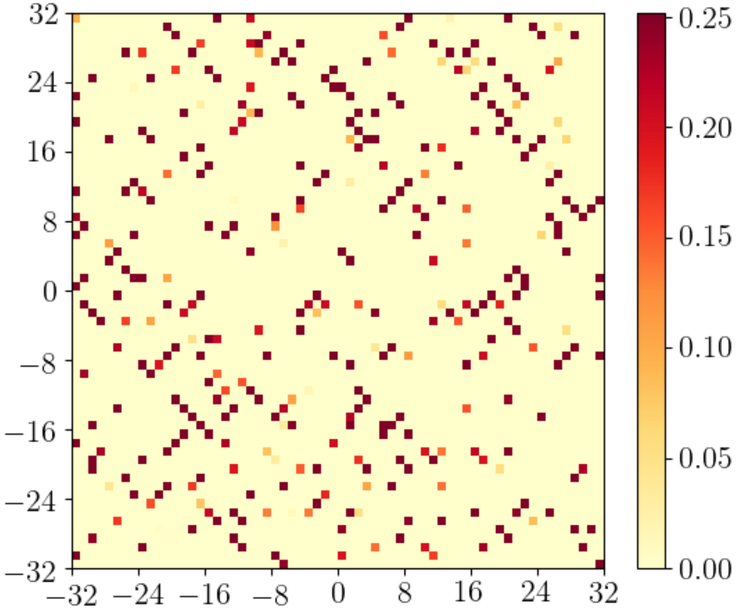


Plastic strain ε_{pl}

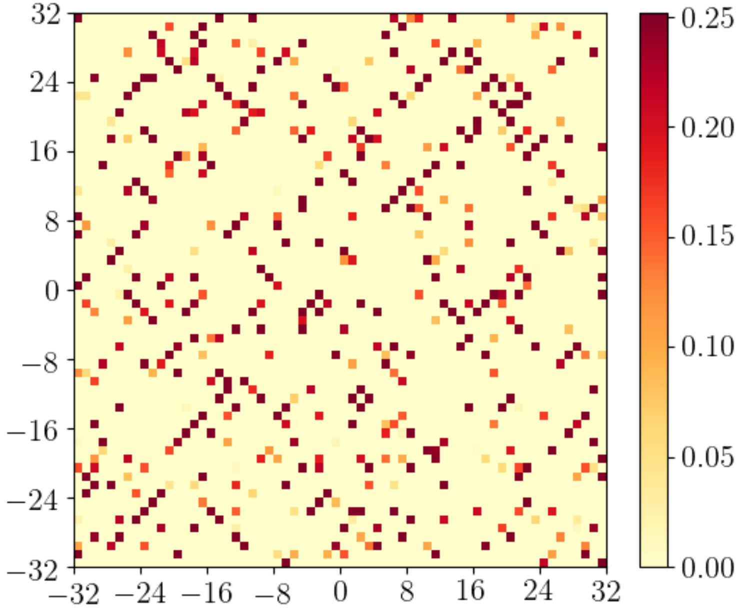
δ = 0.3



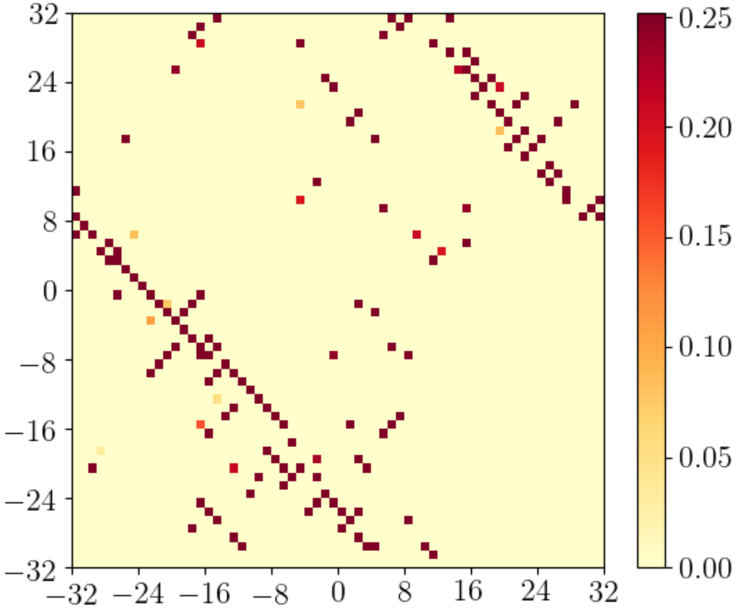
δ = 0.7



δ = 0.5

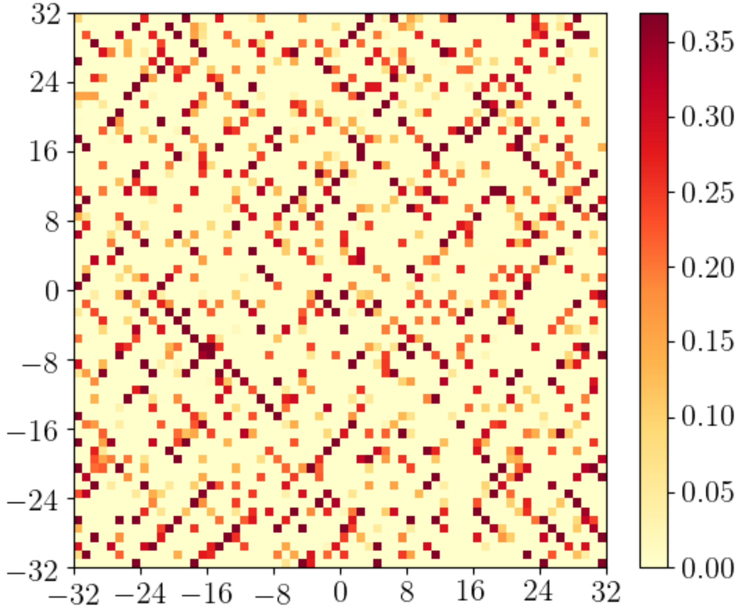


δ = 0.9

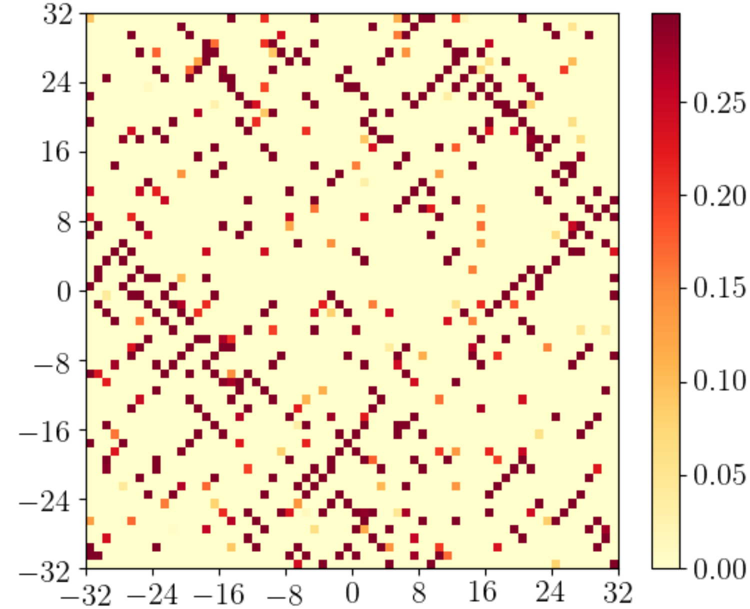


Plastic strain ε_{pl}

δ = 0.3



δ = 0.7



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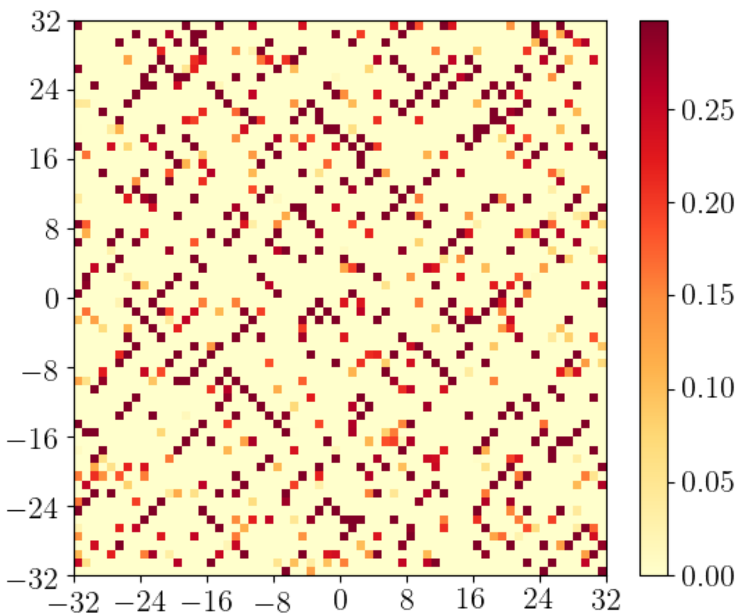

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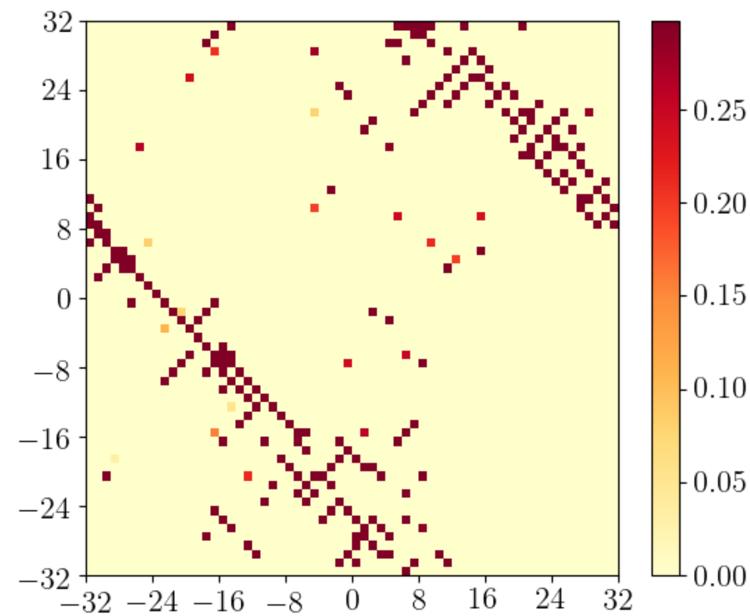
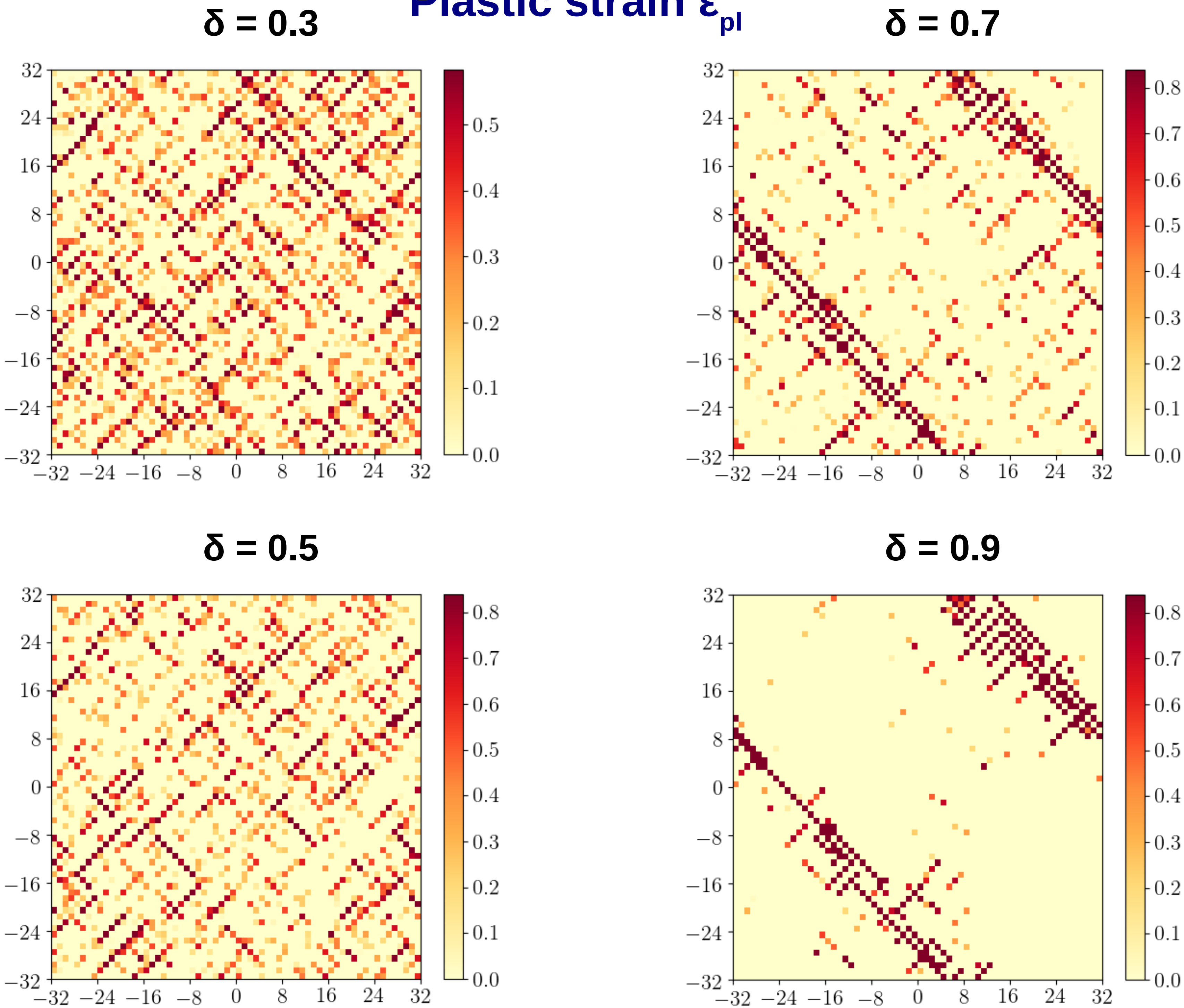
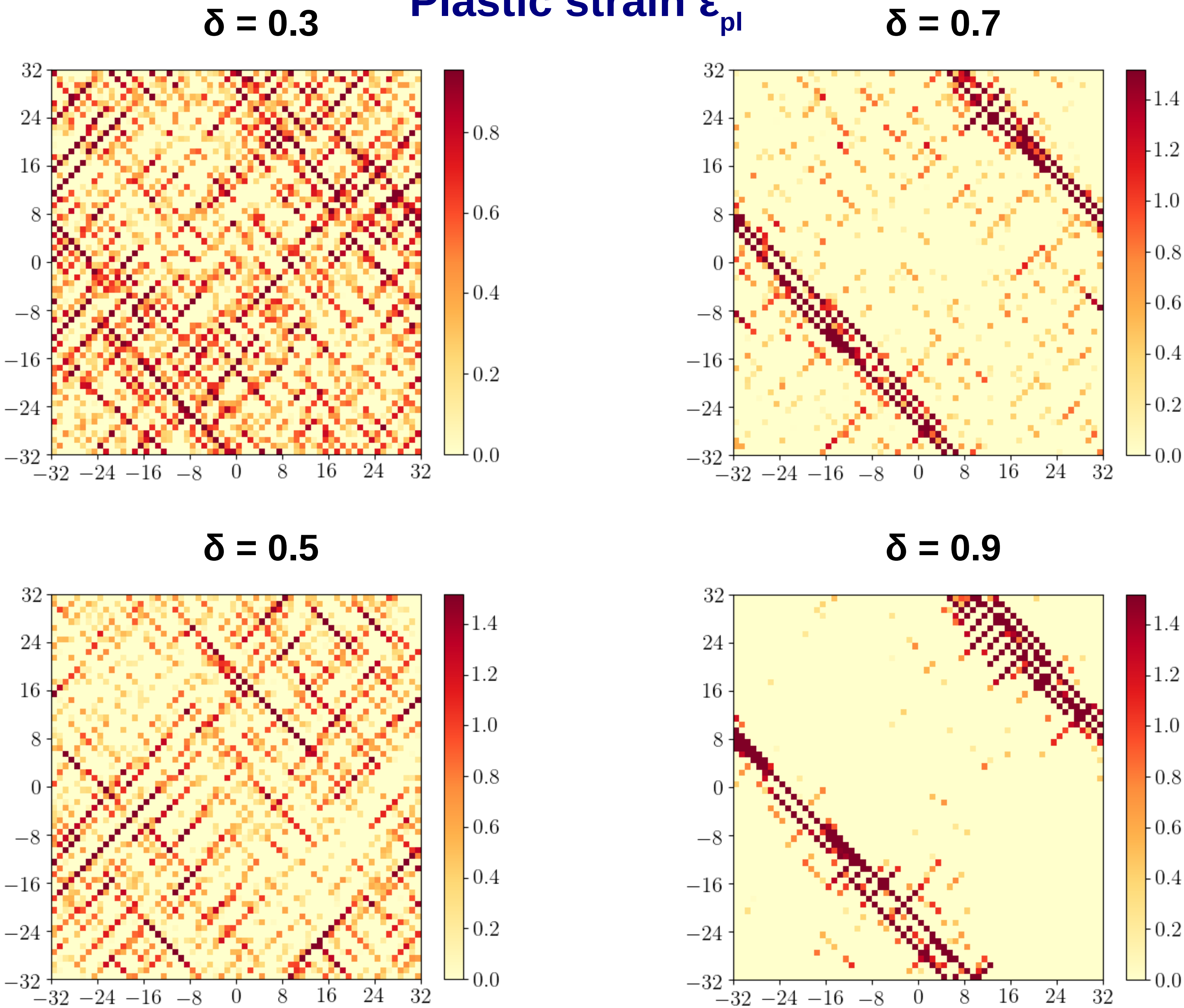


Plastic strain ε_{pl}



Plastic strain ε_{pl}



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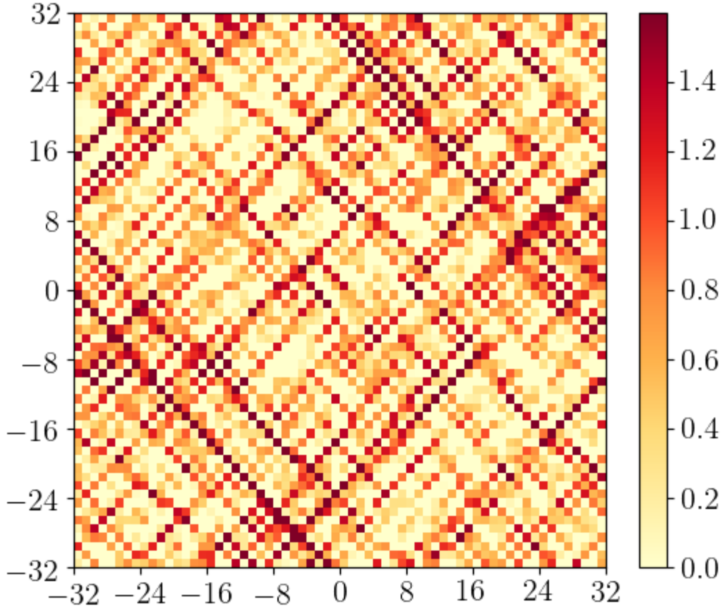

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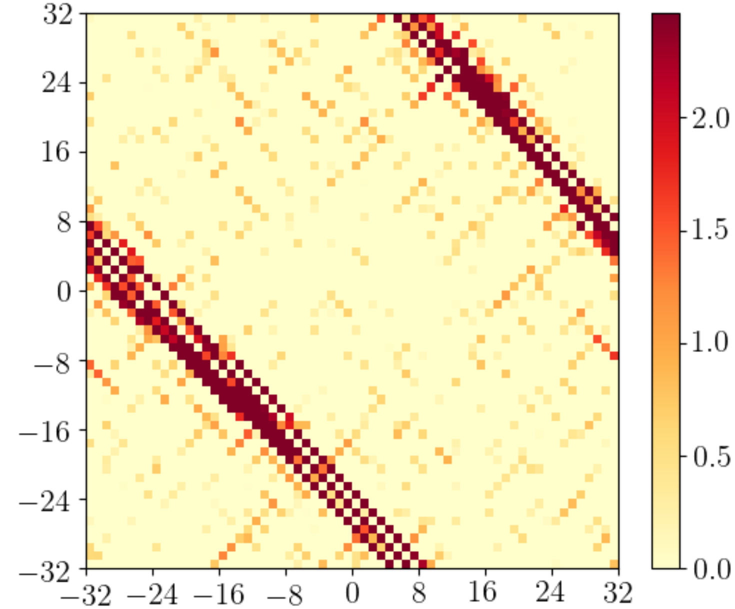

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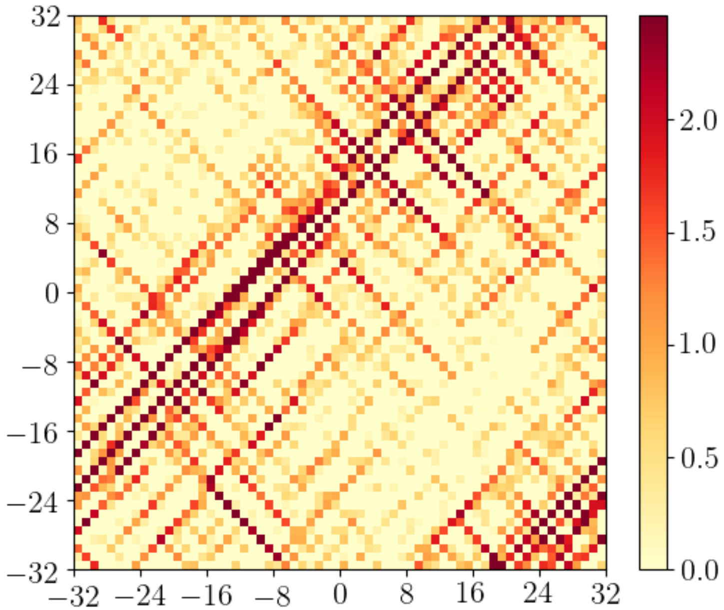
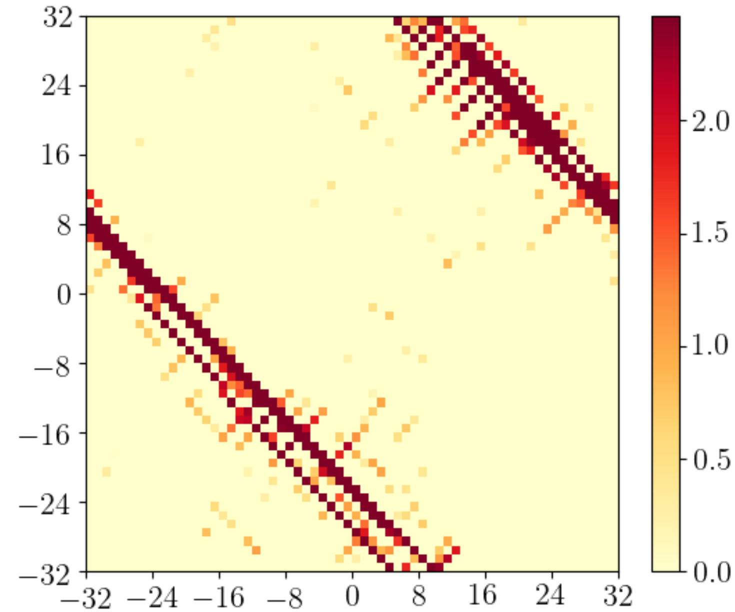
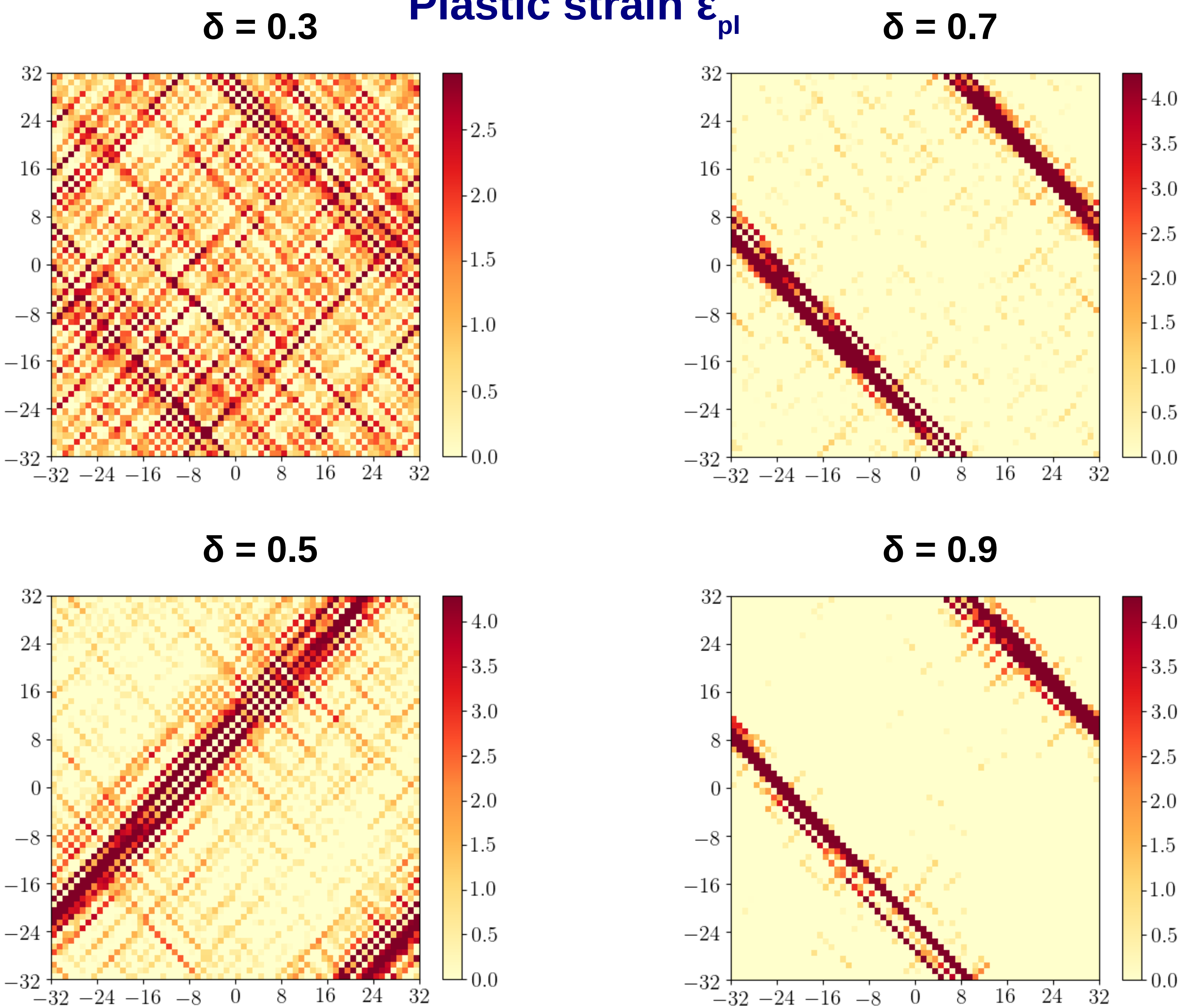


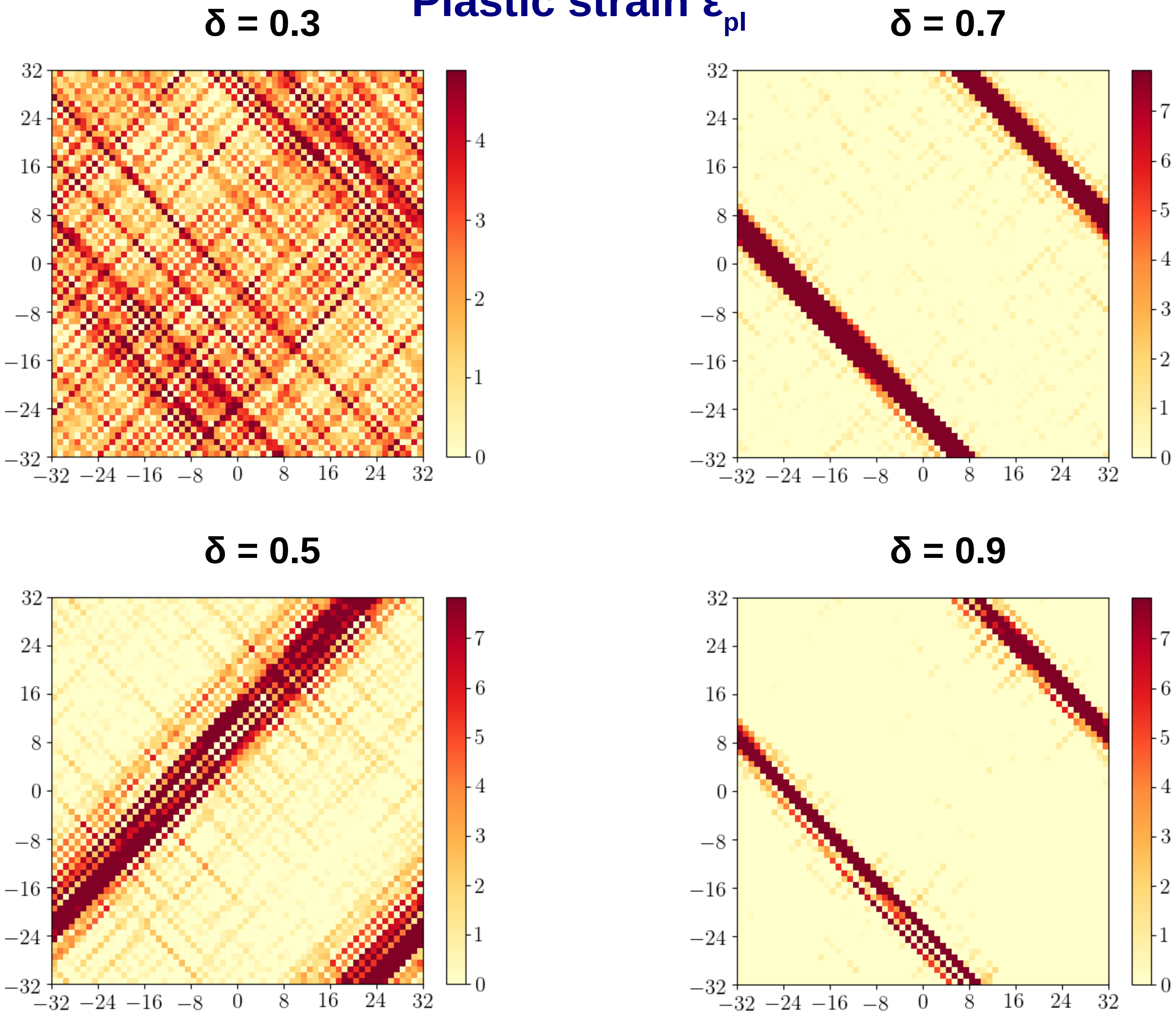
δ = 0.9



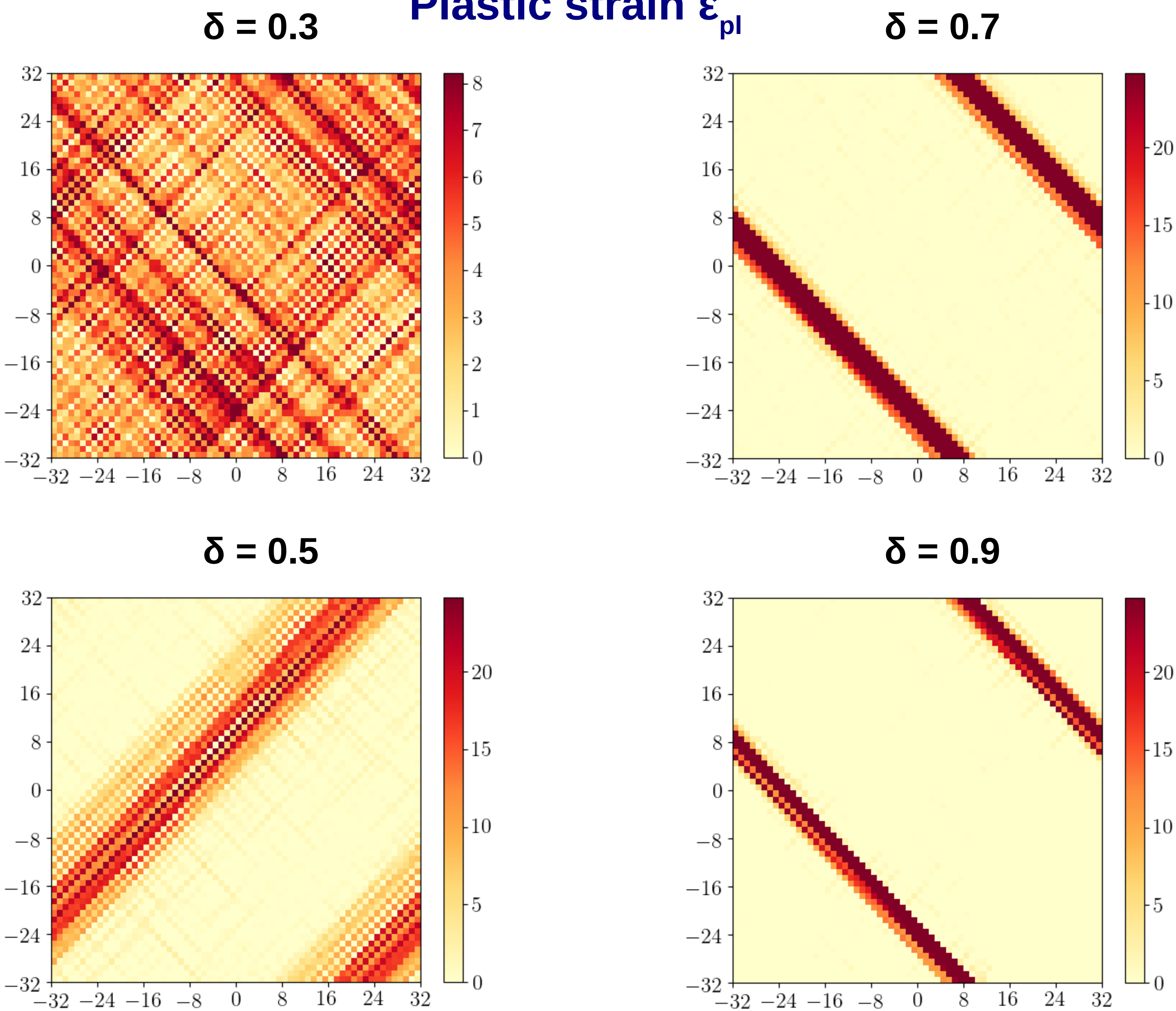
Plastic strain ε_{pl}



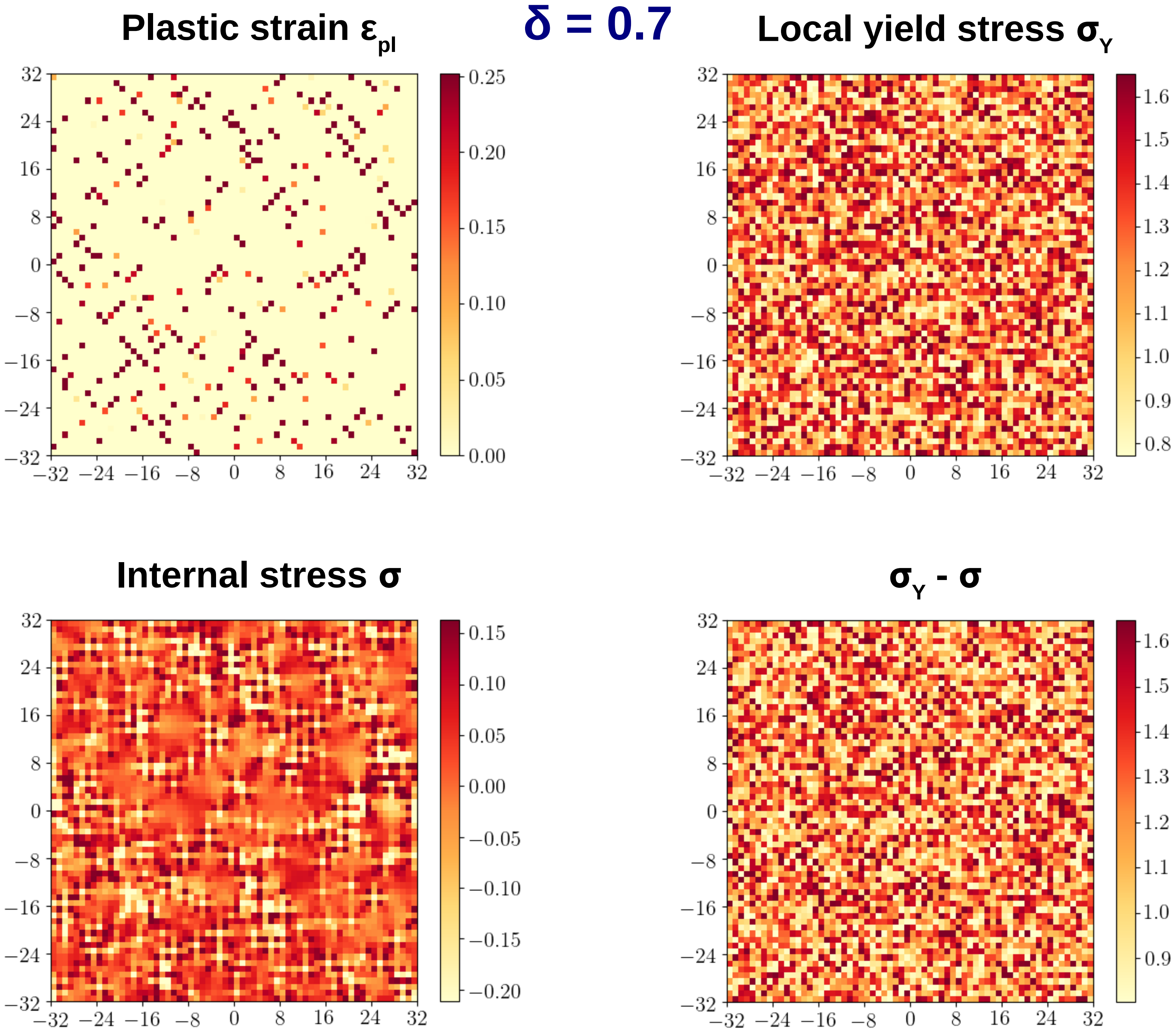
Plastic strain ε_{pl}



Plastic strain ε_{pl}

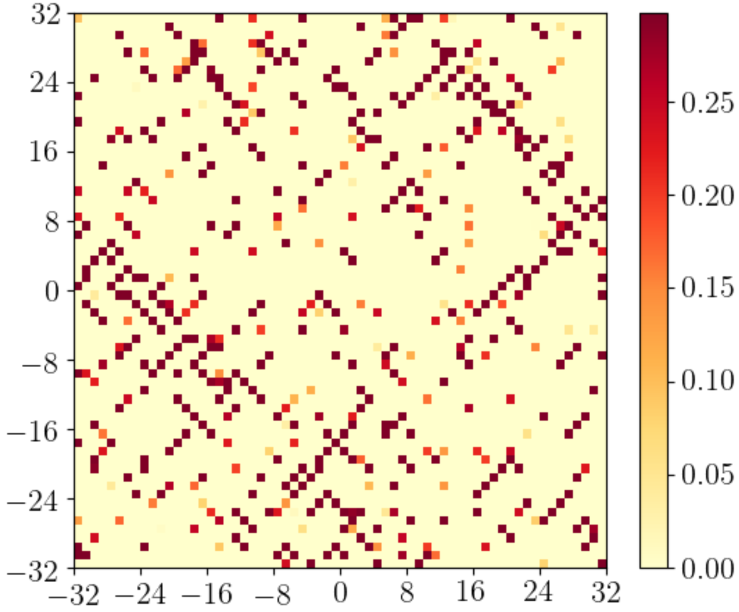


- The higher δ, i.e. the older/the more slowly quenched the glass,
  - The higher the stress peak,
  - The thinner the shear-band
  - The slower the broadening of the band
- Connection with other observables ?
  - Plastic thresholds : σ_Y
  - Internal stress : σ
  - Local plastic criterion : $\sigma_Y - \sigma$

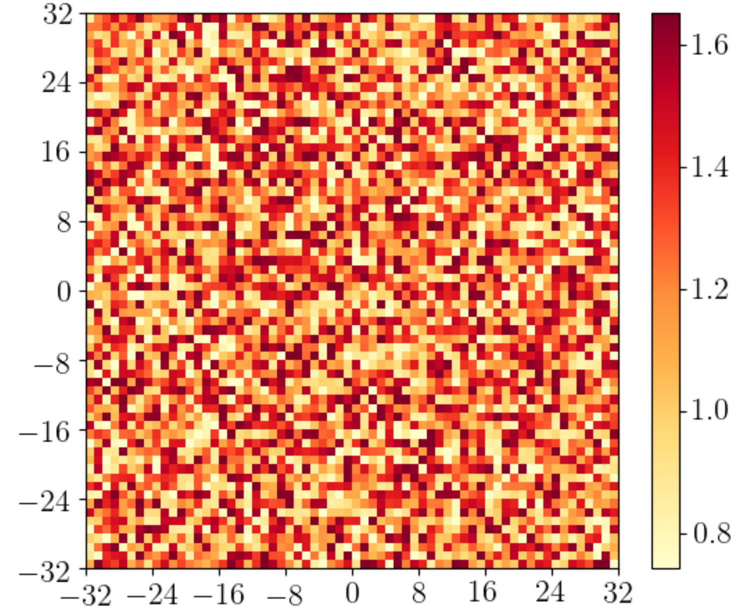

$\delta = 0.7$
Plastic strain ε_{pl}
Local yield stress σ_Y
Internal stress σ
σ_Y - σ

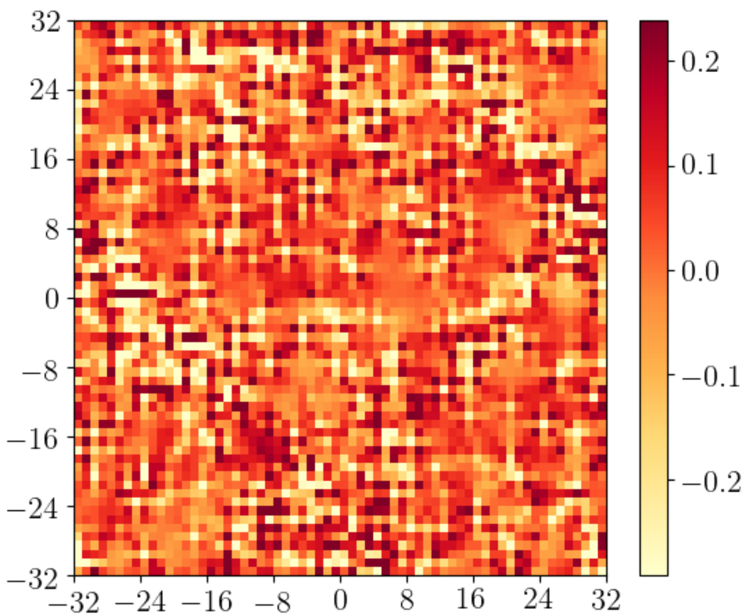
$\delta = 0.7$

Plastic strain ε_{pl}

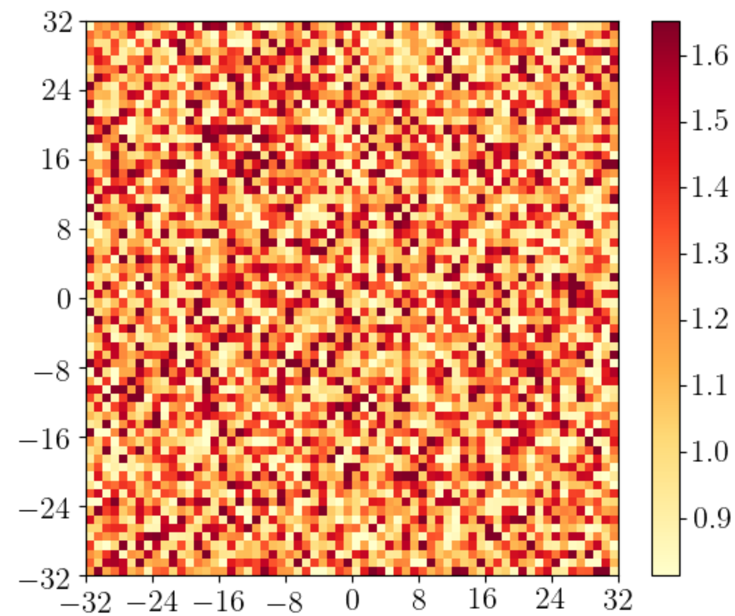


Local yield stress σ_Y



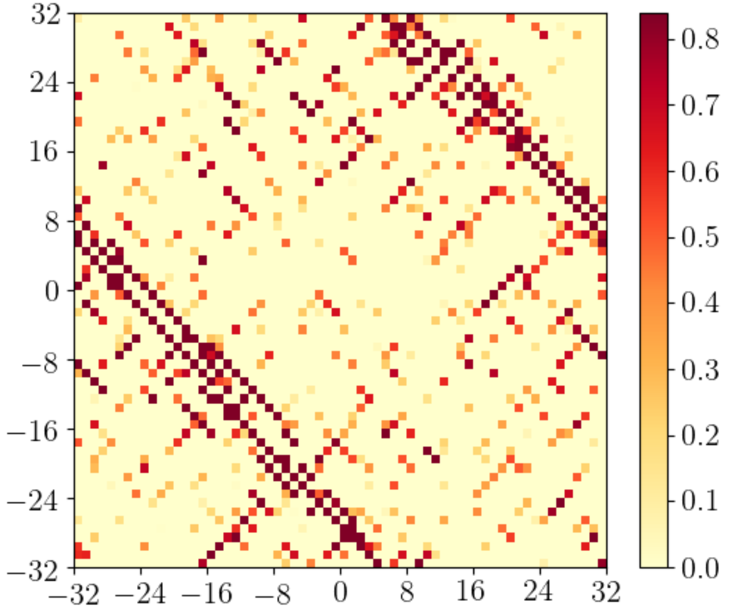


σ_Y - σ

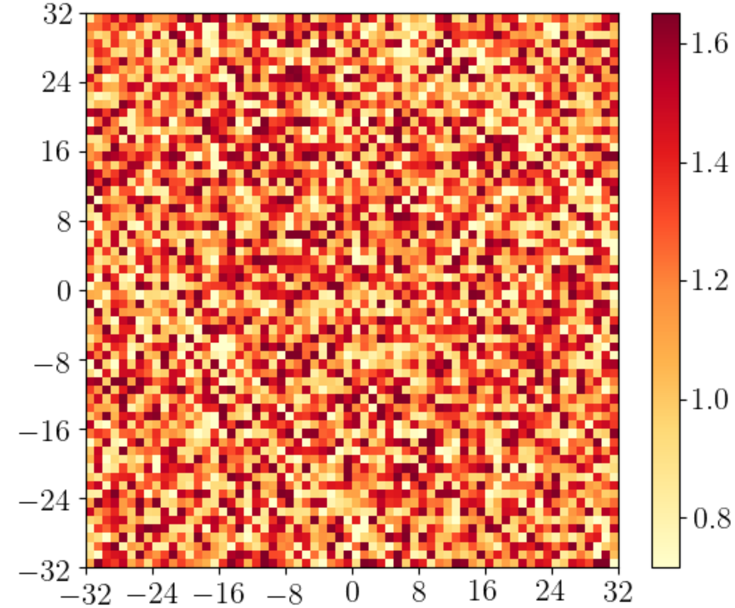


$\delta = 0.7$

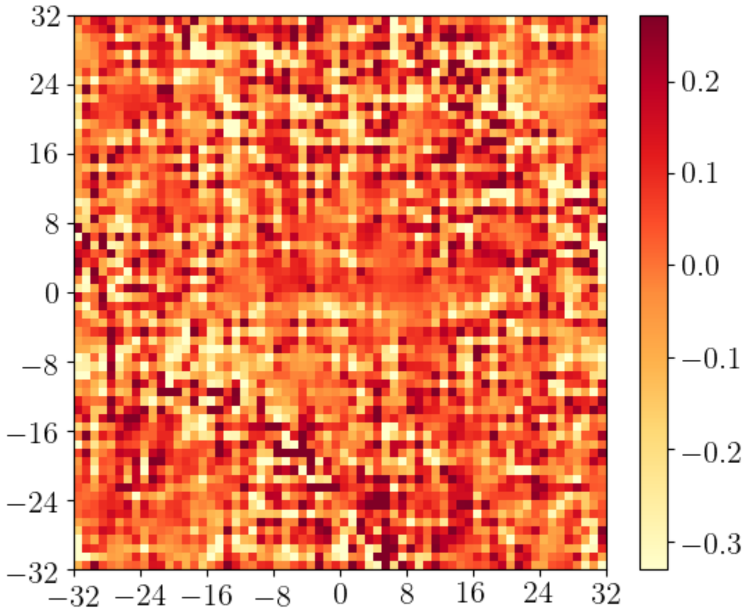
Plastic strain ε_{pl}



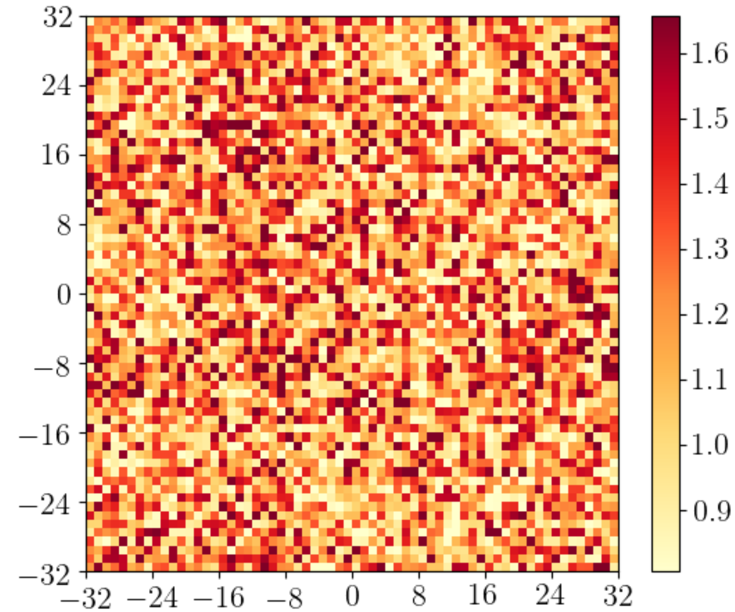
Local yield stress σ_Y



Internal stress σ

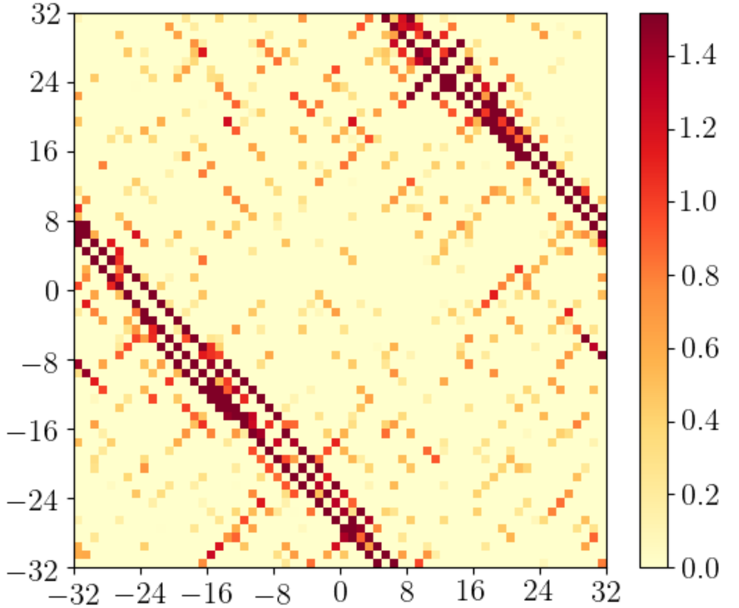


σ_Y - σ

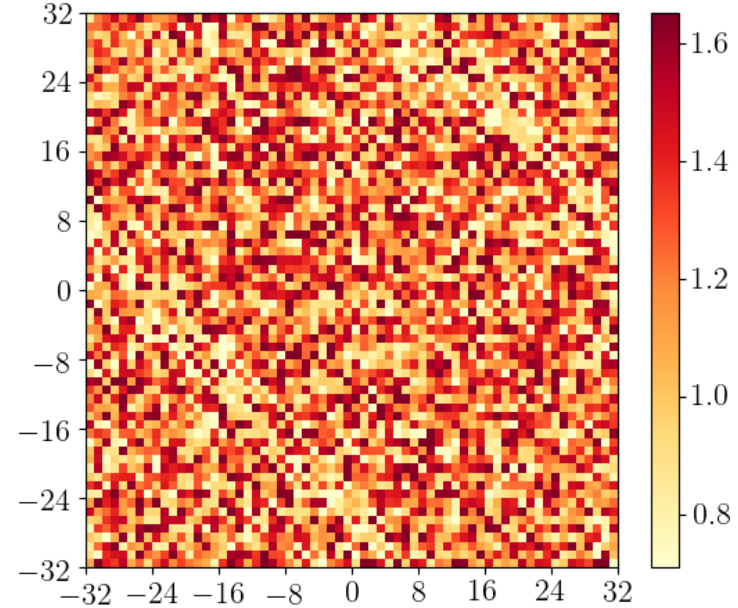


$\delta = 0.7$

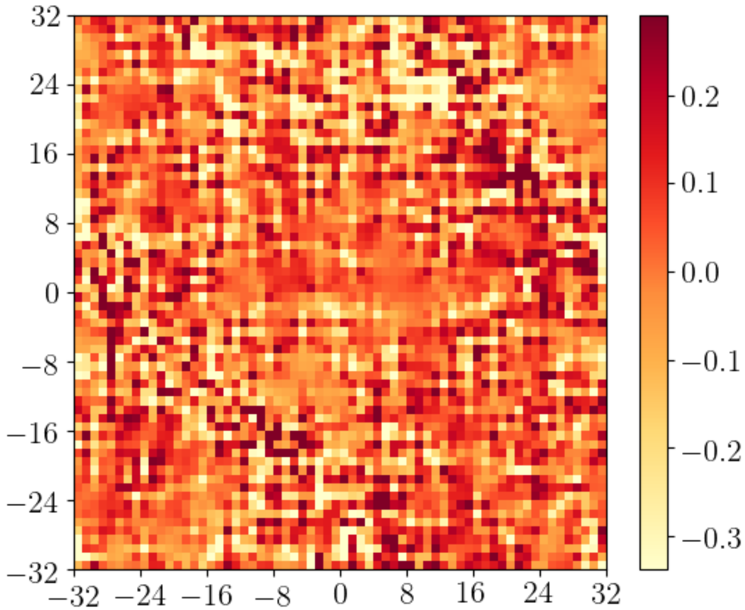
Plastic strain ε_{pl}



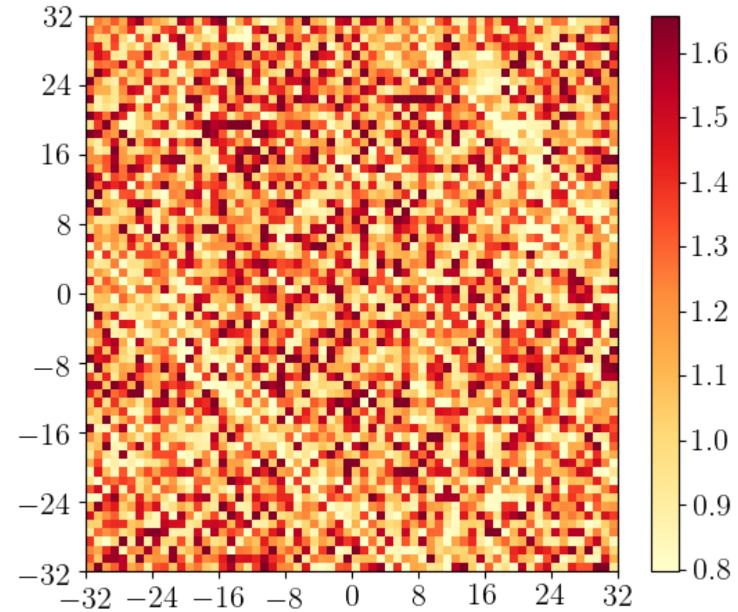
Local yield stress σ_Y



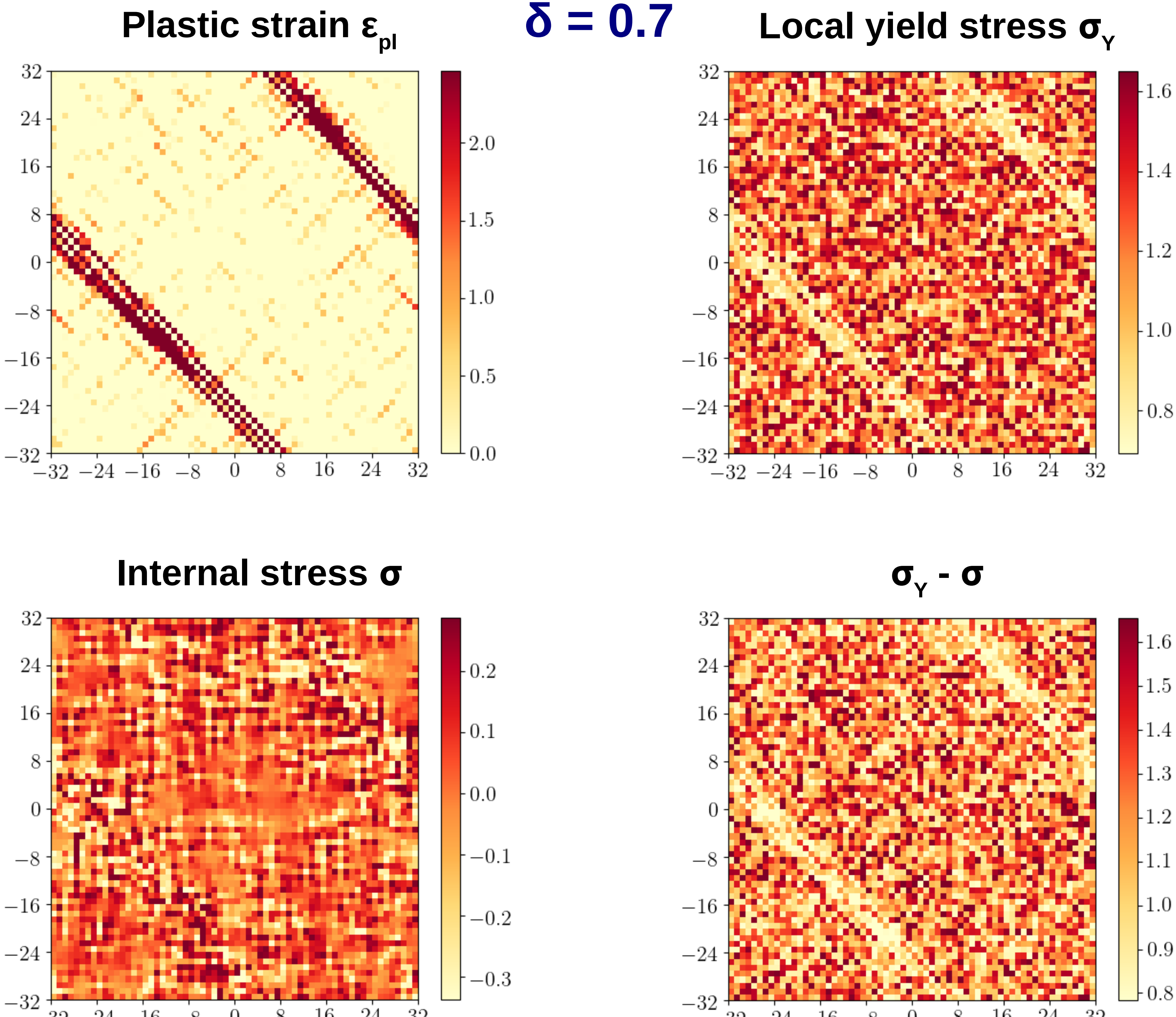
Internal stress σ



$\sigma_Y - \sigma$



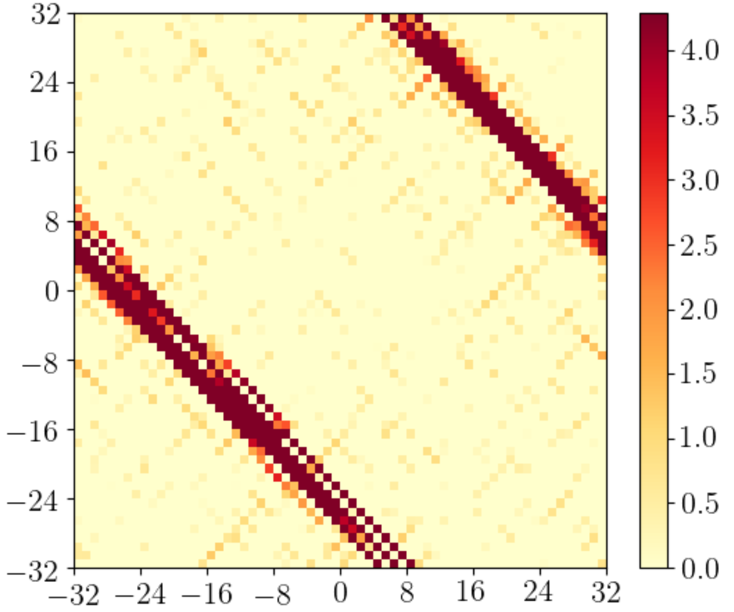
$\delta = 0.7$



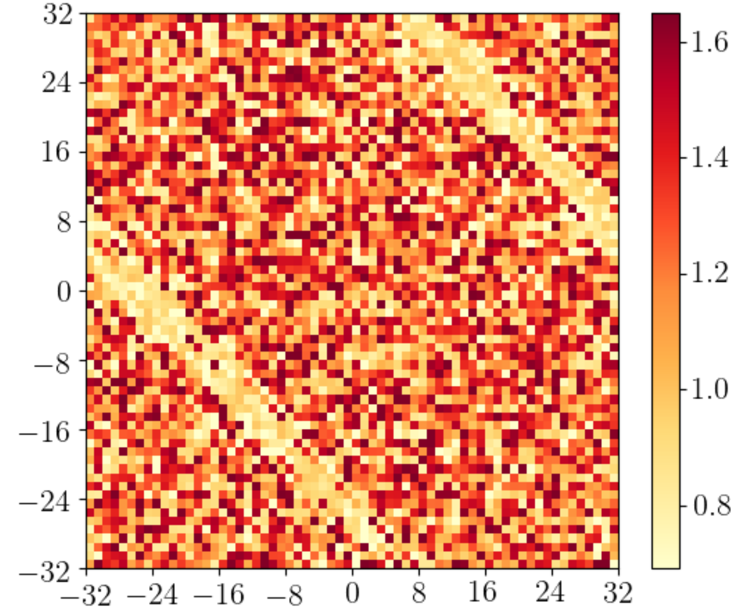
Plastic strain ε_{pl}
Local yield stress σ_Y
Internal stress σ
σ_Y - σ

$\delta = 0.7$

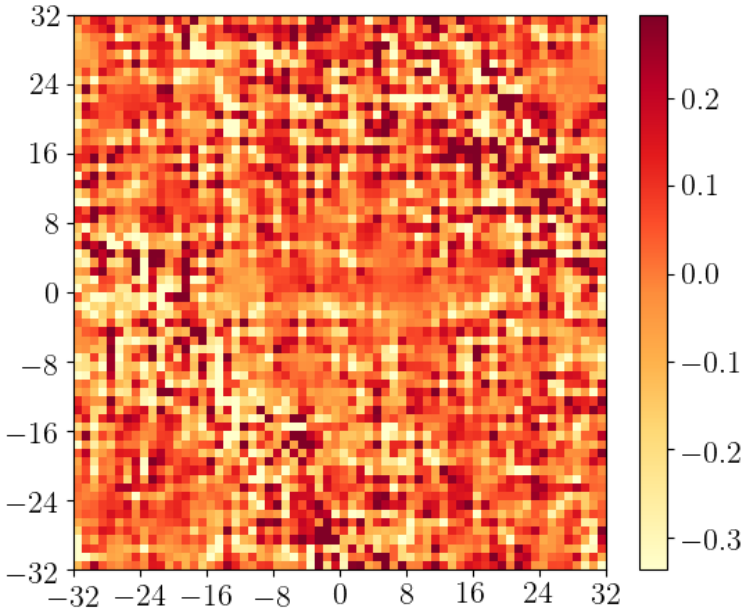
Plastic strain ε_{pl}



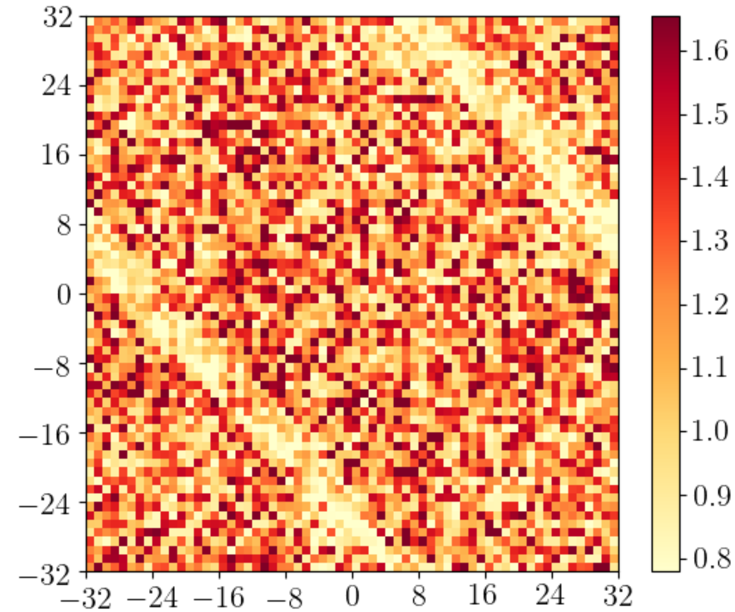
Local yield stress σ_Y



Internal stress σ

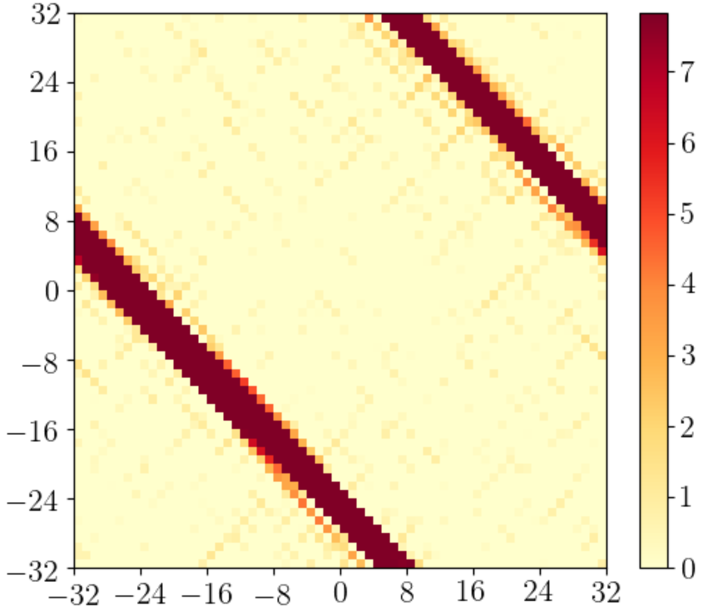


σ_Y - σ

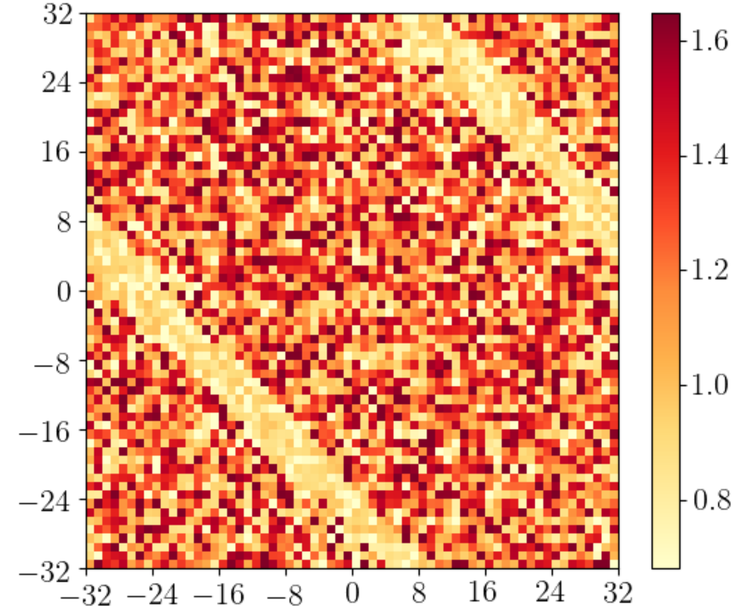


$\delta = 0.7$

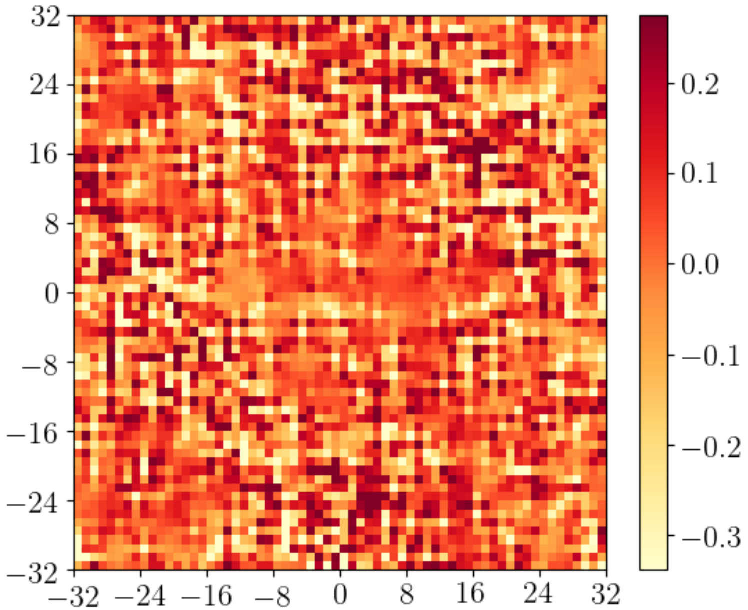
Plastic strain ε_{pl}



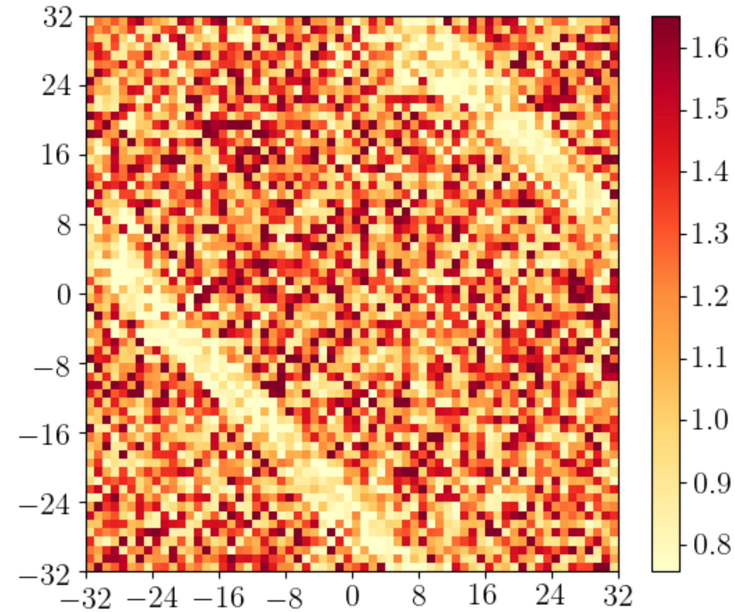
Local yield stress σ_Y



Internal stress σ



σ_Y - σ



$\delta = 0.7$

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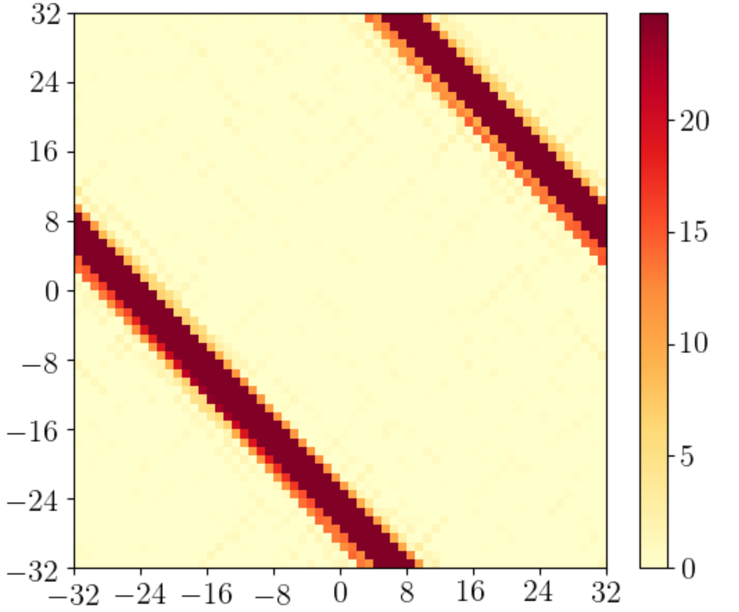
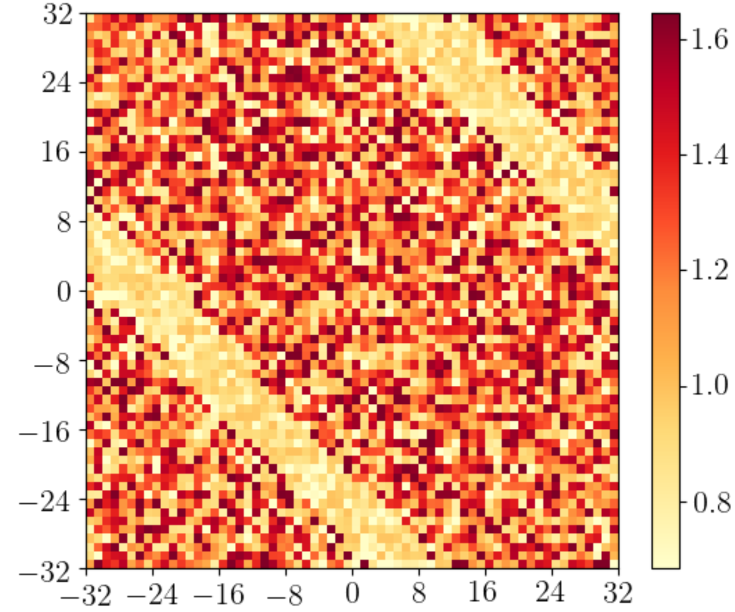
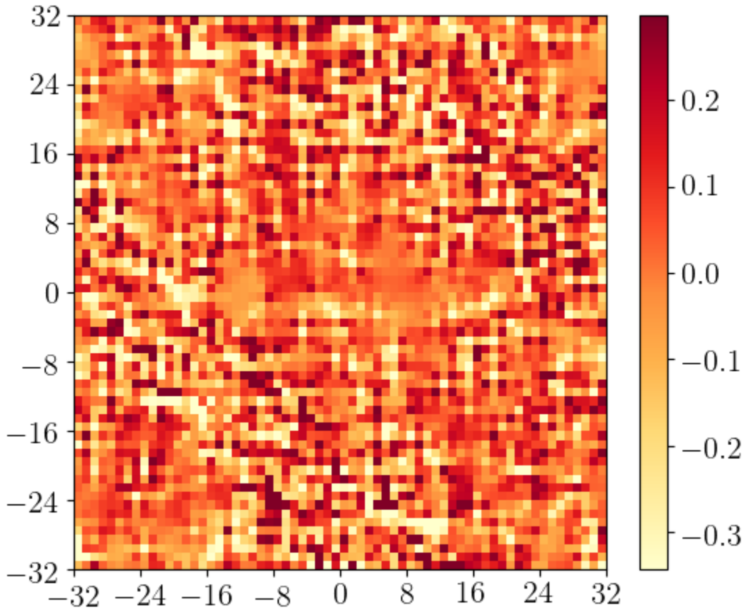


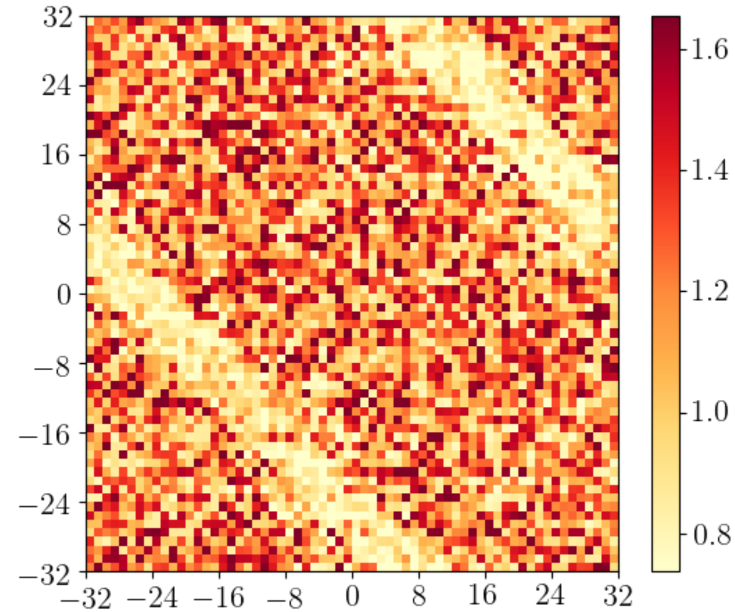
Local yield stress σ_Y

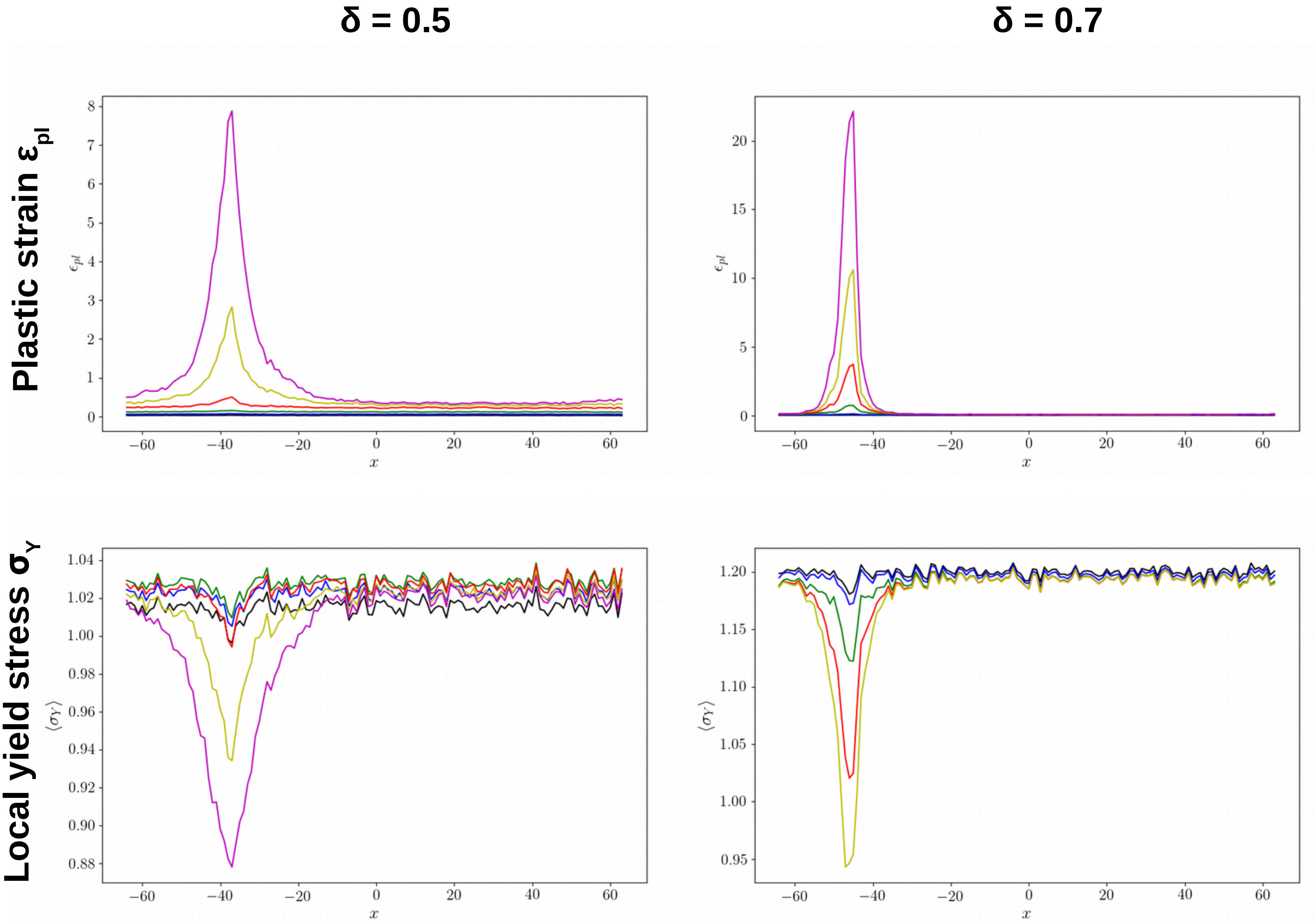


Stress σ

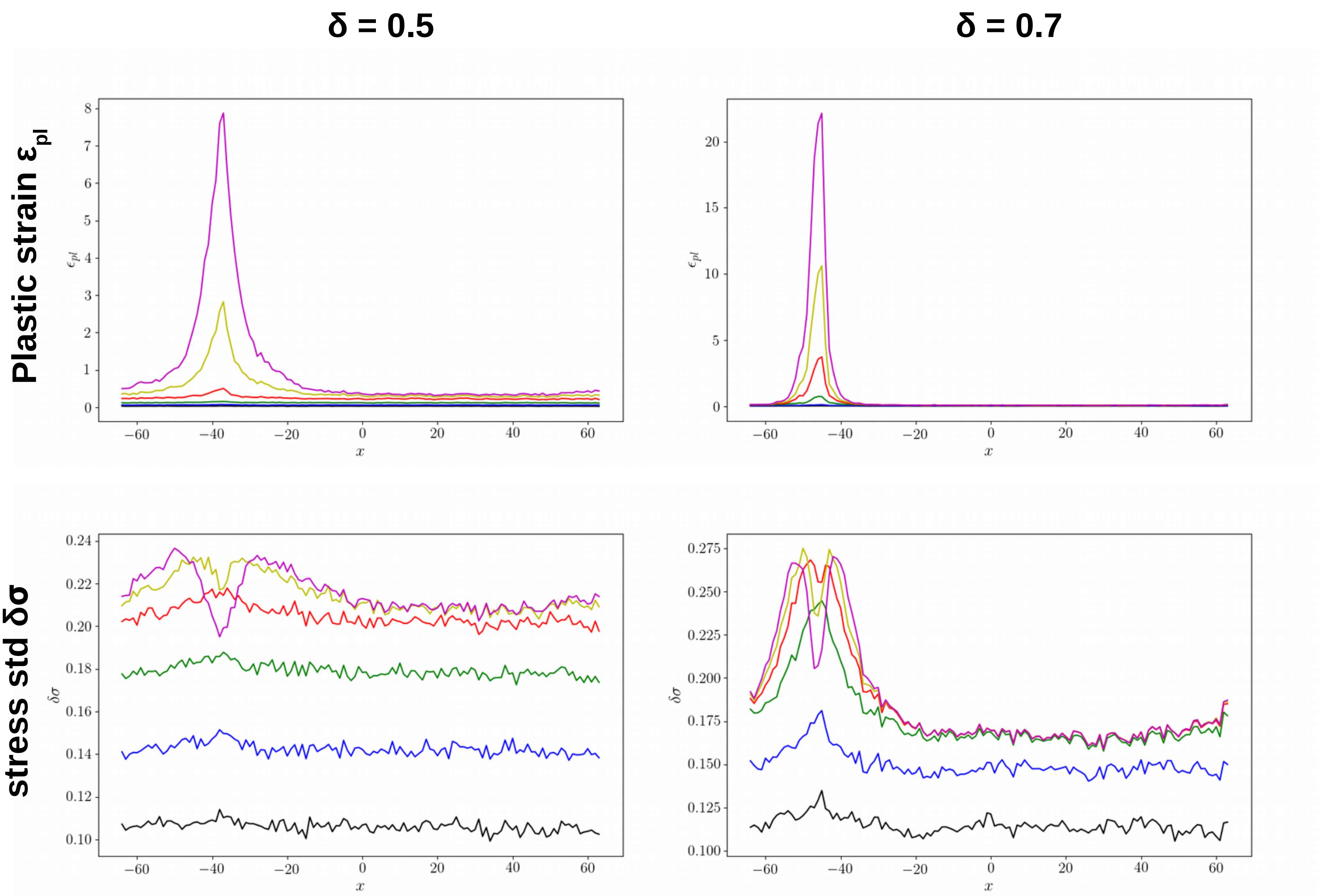


σ_Y - σ



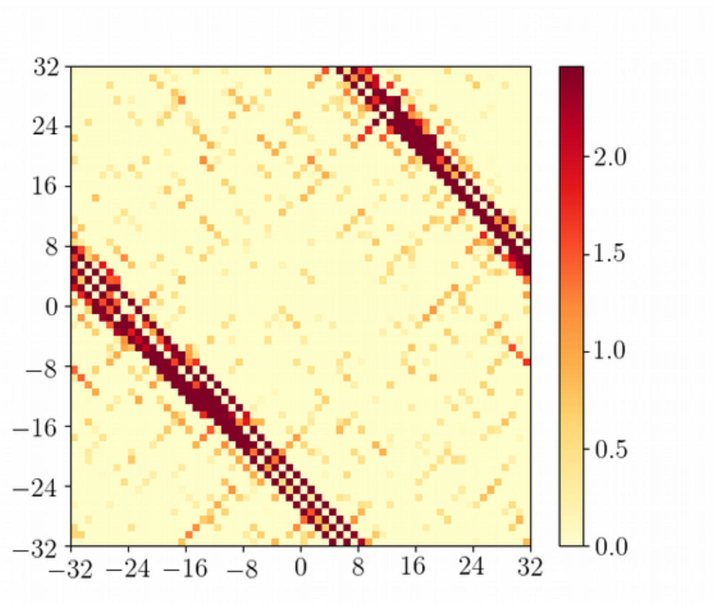


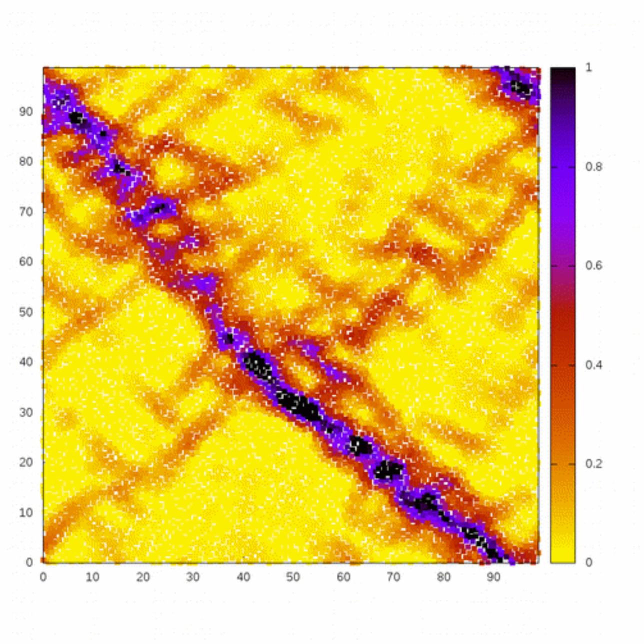
δ = 0.5
δ = 0.7
Plastic strain ε_{pl}
Local yield stress σ_Y
ϵ_{pl}
$\langle\sigma_Y\rangle$
x


δ = 0.5
δ = 0.7
Plastic strain ε_{pl}
stress std δσ
ϵ_{pl}
$\delta\sigma$
x

Avalanche behavior and/or Shear-banding can be obtained in lattice models via the simple distinction between :

- Initial distribution of plastic thresholds (aging, quench)
- Renewal distribution of plastic thresholds (stationary glass)



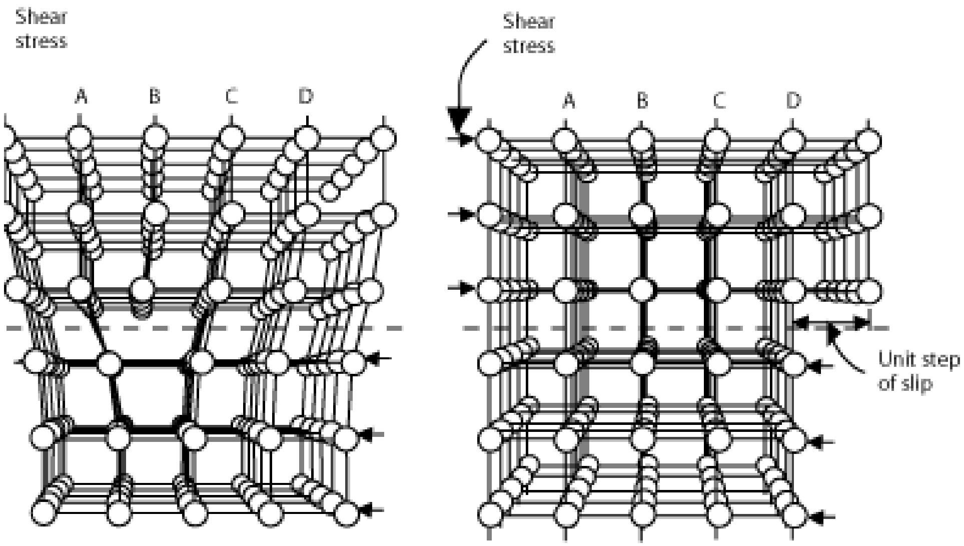


Link with atomistic simulations ?

A local probe of plasticity in model amorphous materials

Microscopic mechanisms of plasticity

Crystals



Dislocation

Amorphous Solids

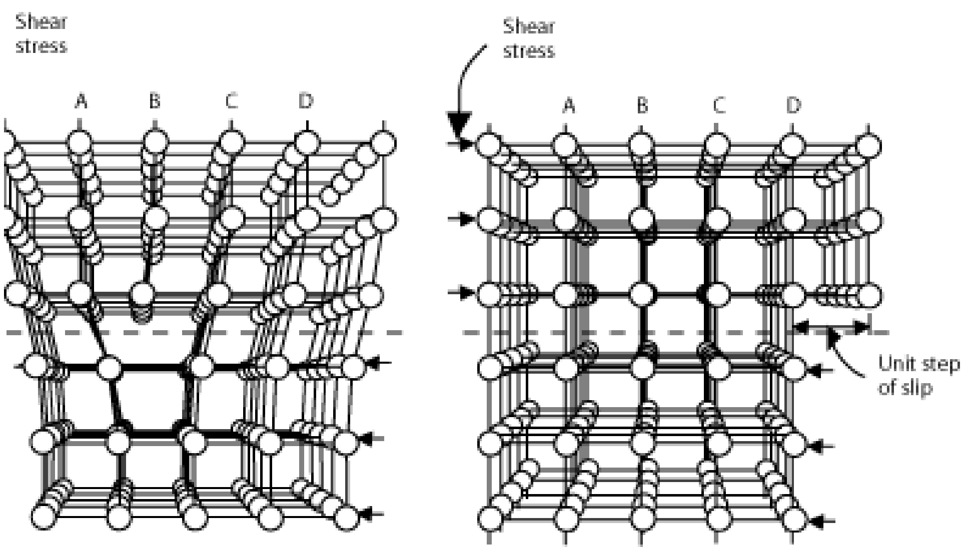
Localized rearrangement

V. Volterra, Ann. Ec. Norm. Sup., **24**, 401 (1907)

A. Tanguy, F. Leonforte and J.-L. Barrat, Eur. Phys. J. E, **20**, 355 (2006)

“Flow defects” at atomic scale

Crystals



Dislocation

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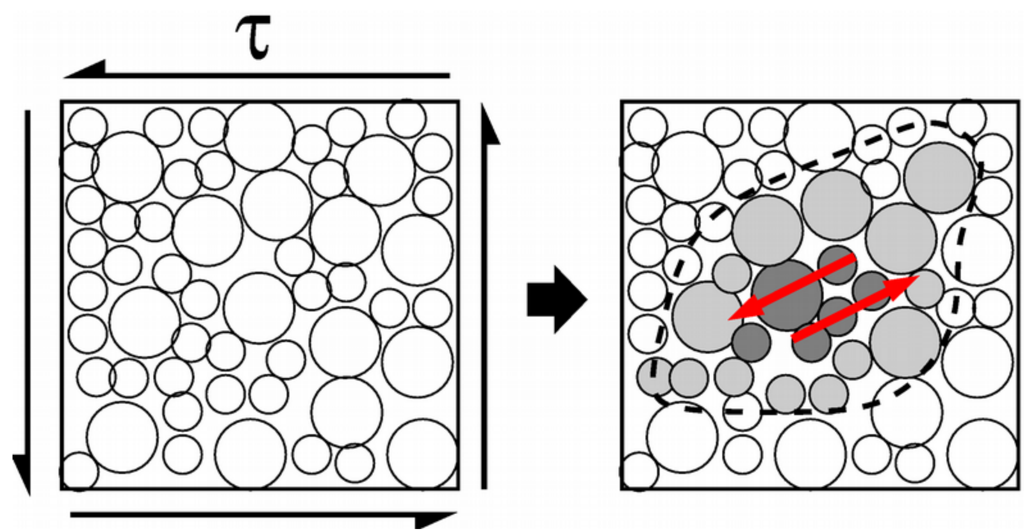
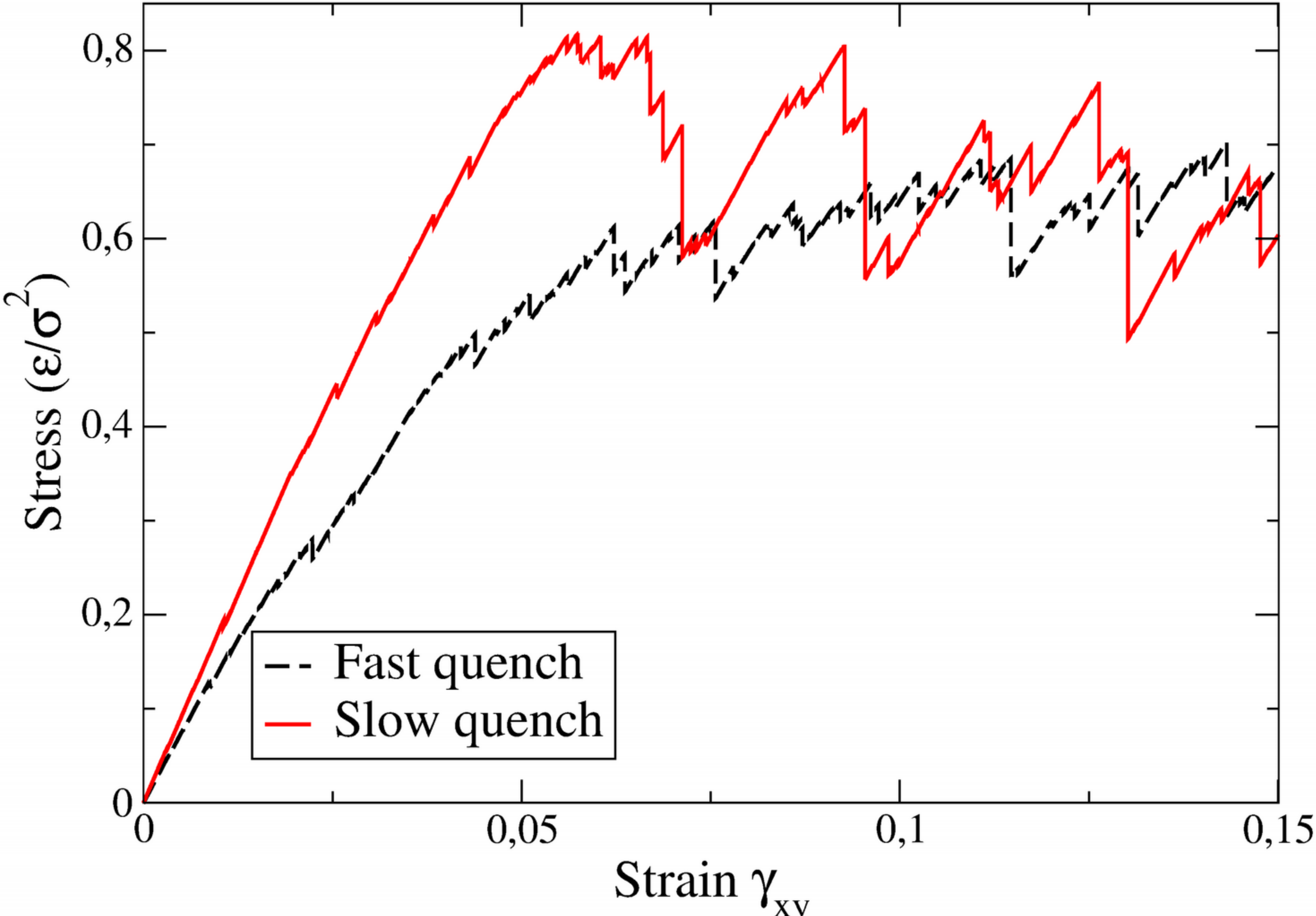


Shear Transformation Zone (STZ)

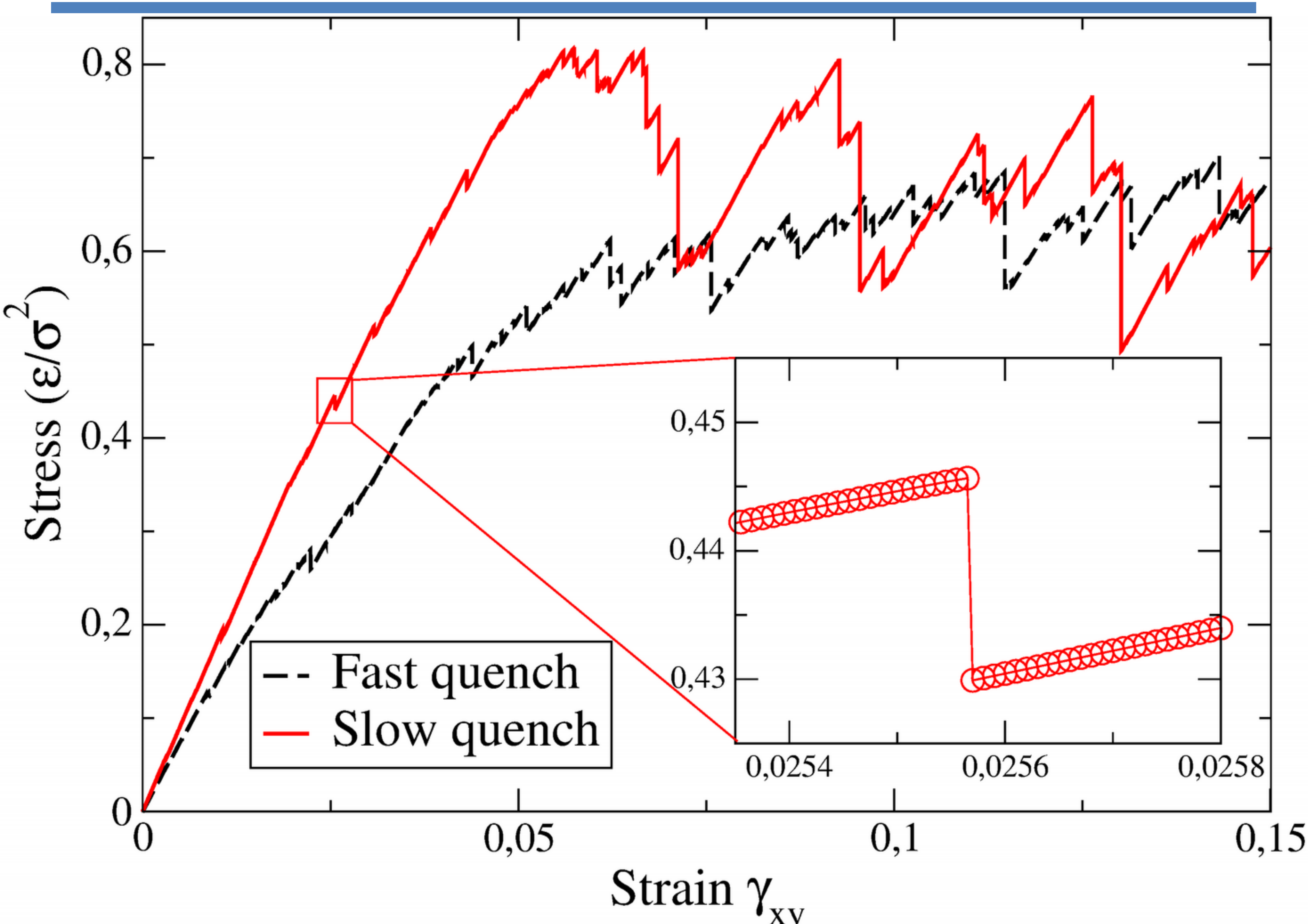
V. Volterra, Ann. Ec. Norm. Sup., **24**, 401 (1907)

M. L. Falk and J. S. Langer, Phys. Rev. E, **57**, 7192 (1998)

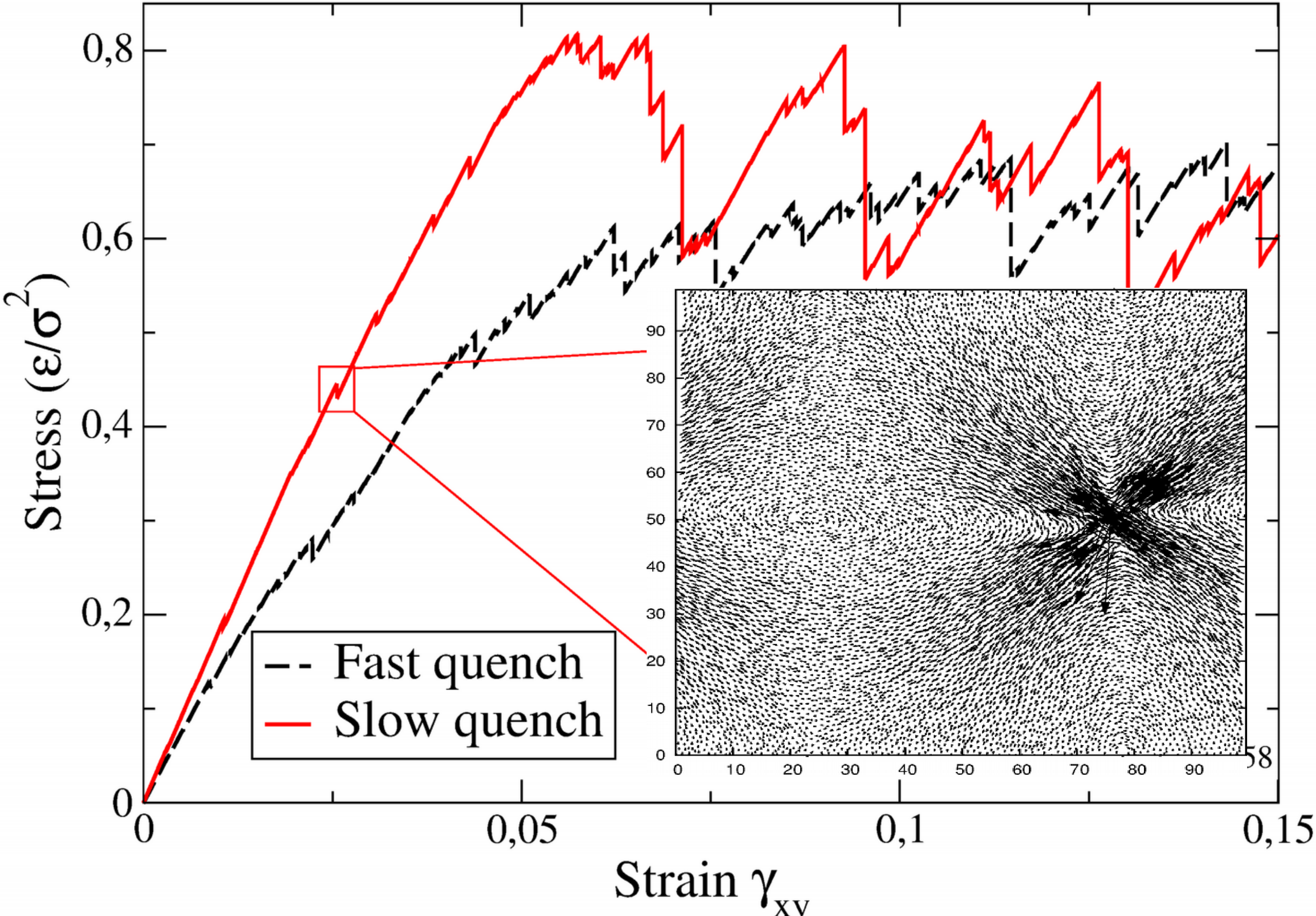
Plastic events under simple shear



Plastic events under simple shear

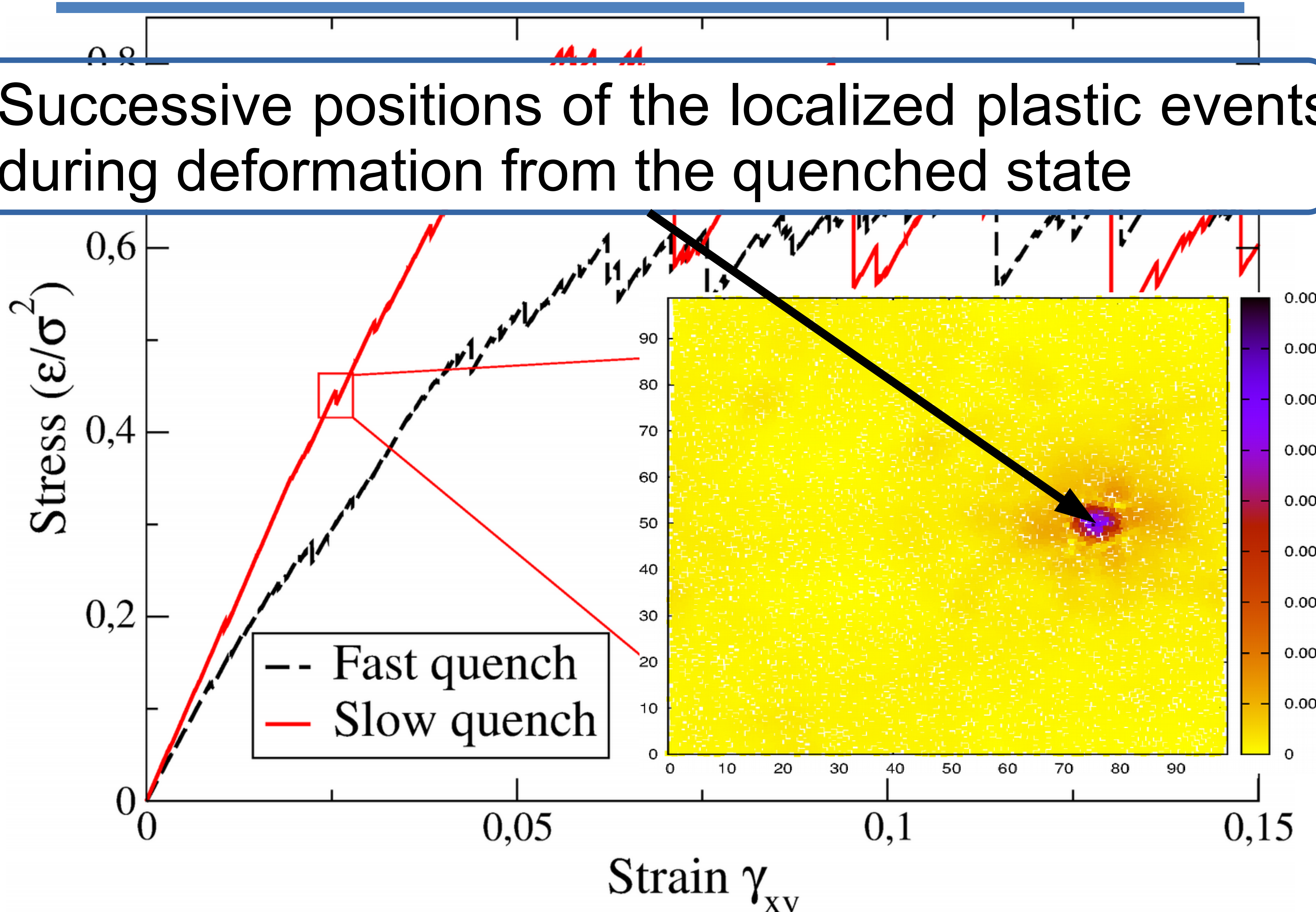


Plastic events under simple shear



Plastic events under simple shear

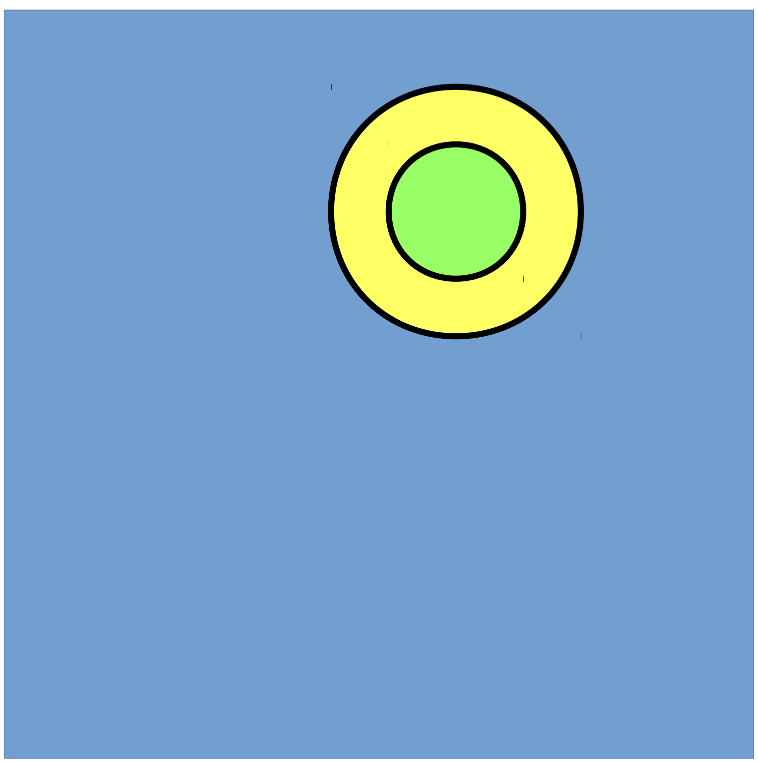
- Successive positions of the localized plastic events during deformation from the quenched state



A direct method to probe the local yield stresses

Idea:
- Probe the local plastic rearrangement with a local loading
- Extension of the P. Sollich's “Virtual strain method”

P. Sollich, MultiScale Modelling of Amorphous Materials workshop, Dublin, Ireland (2011).



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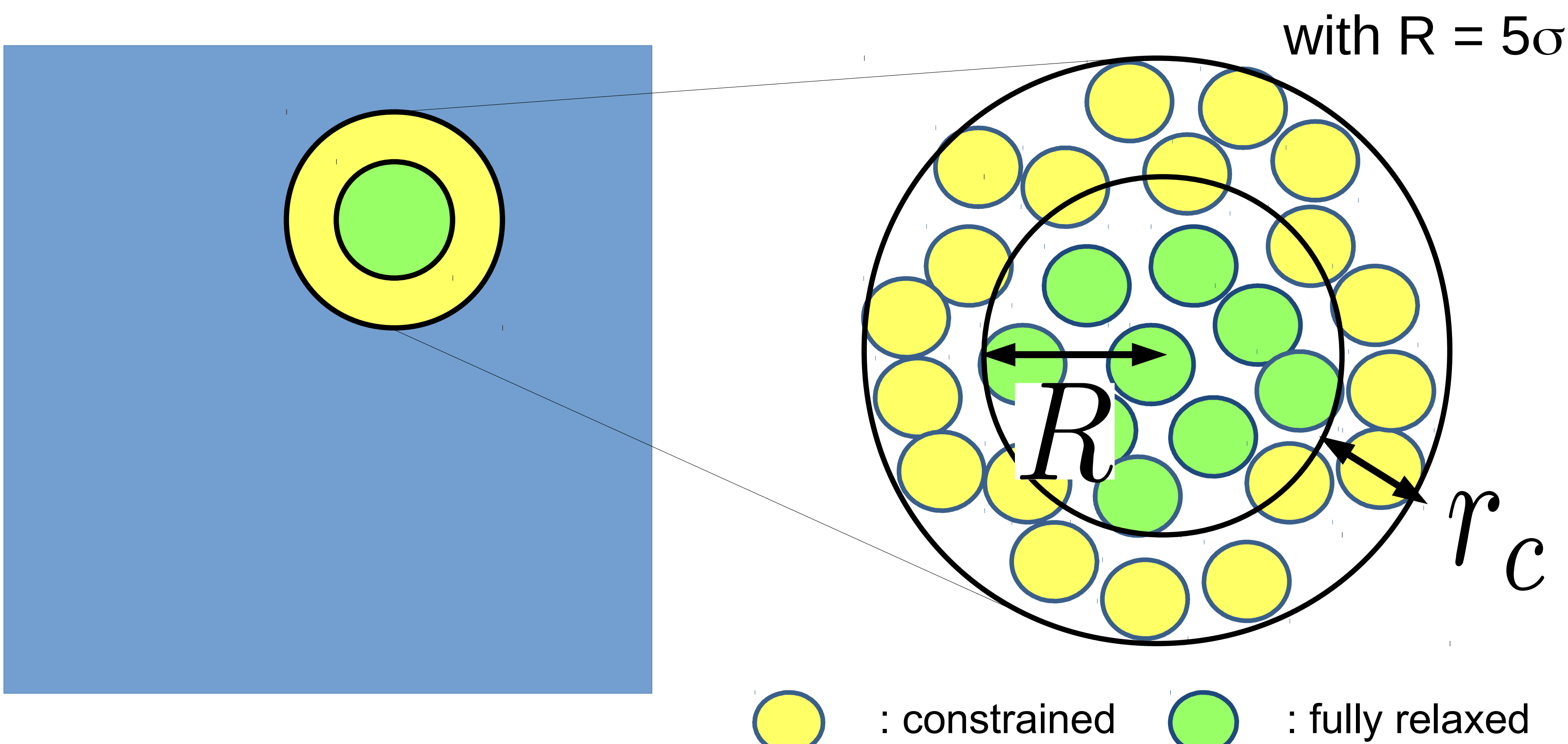

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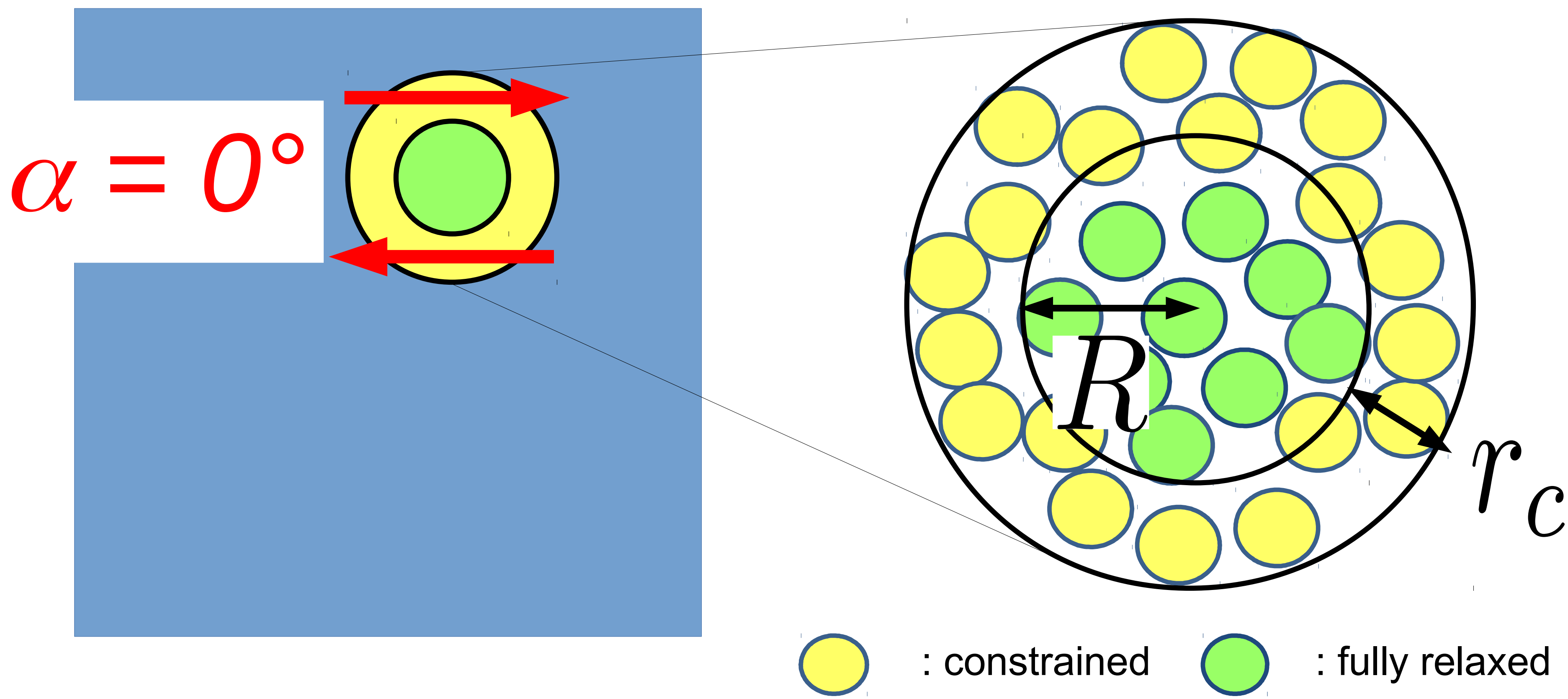
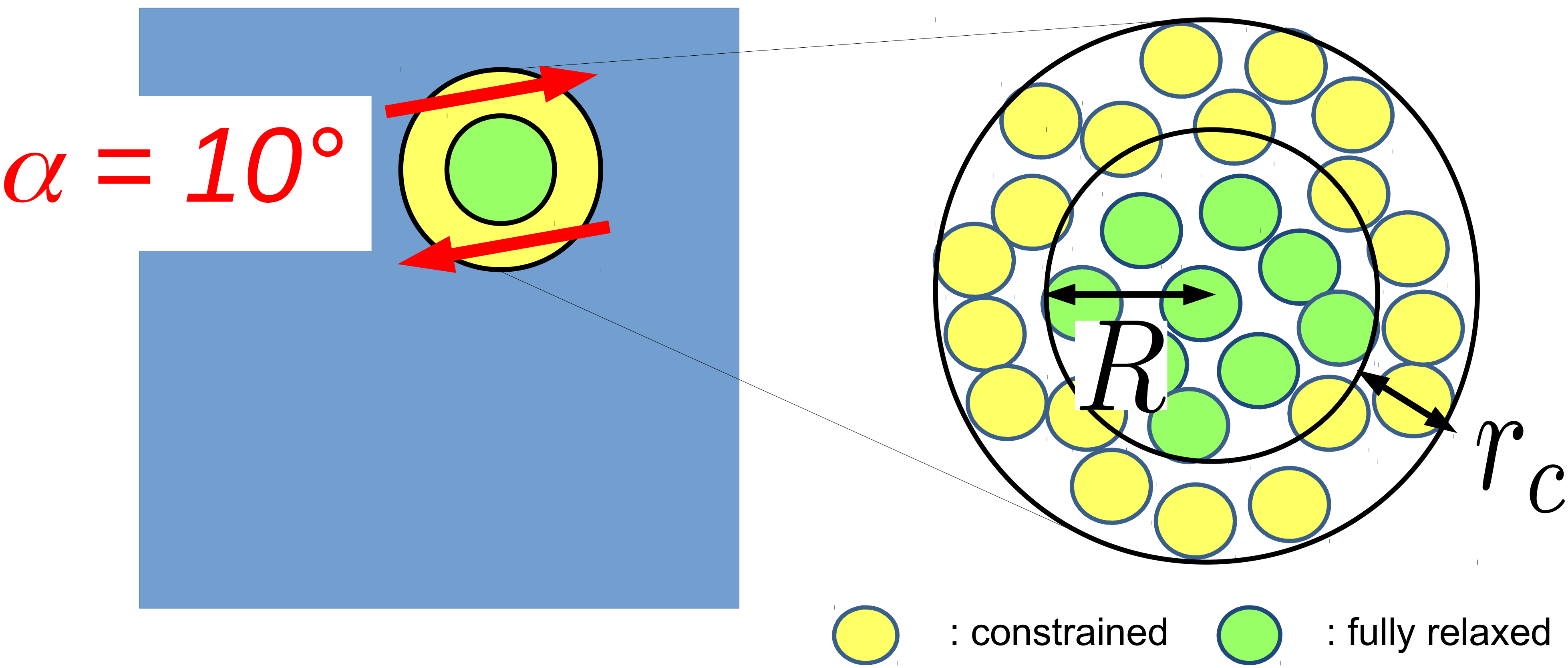


A direct method to probe the local yield stresses

- This operation is performed systematically for orientations from α = 0° to 170° every $\Delta\alpha$ = 10° and for each atom in the system



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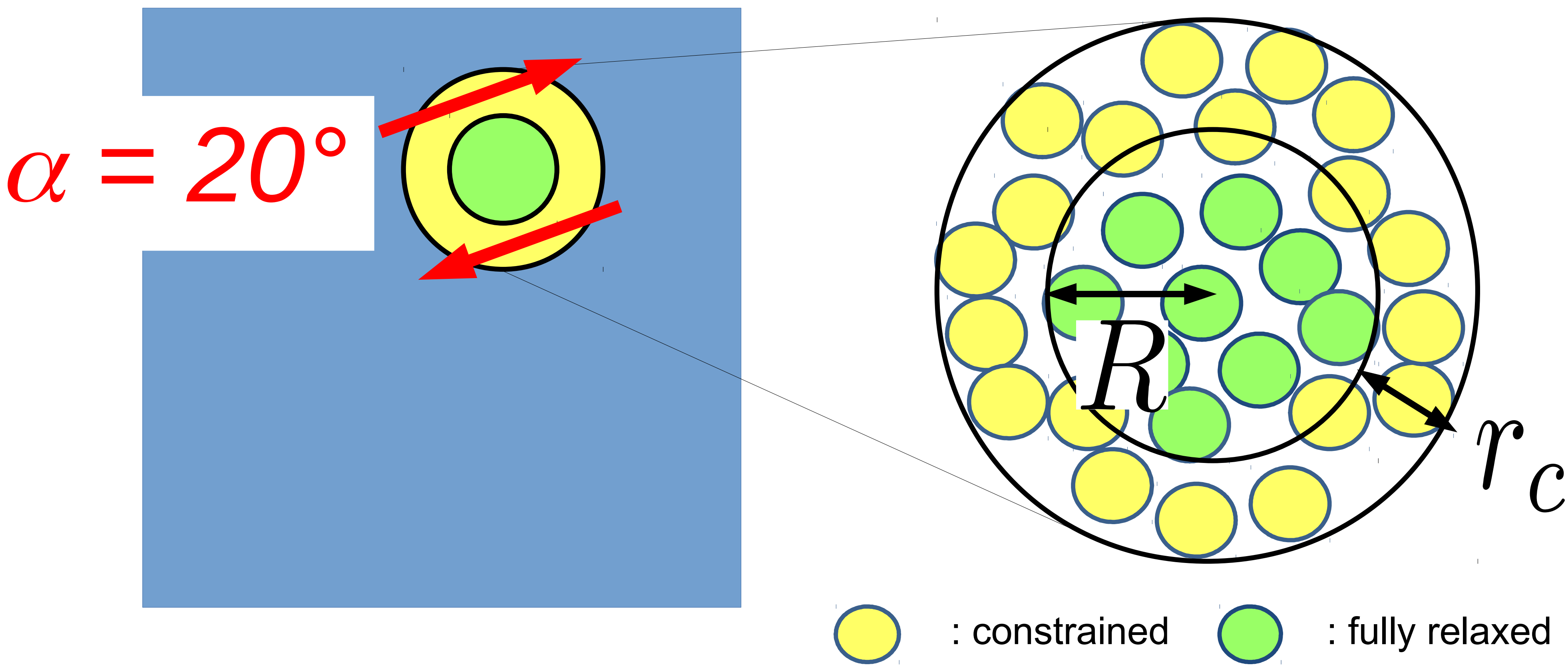

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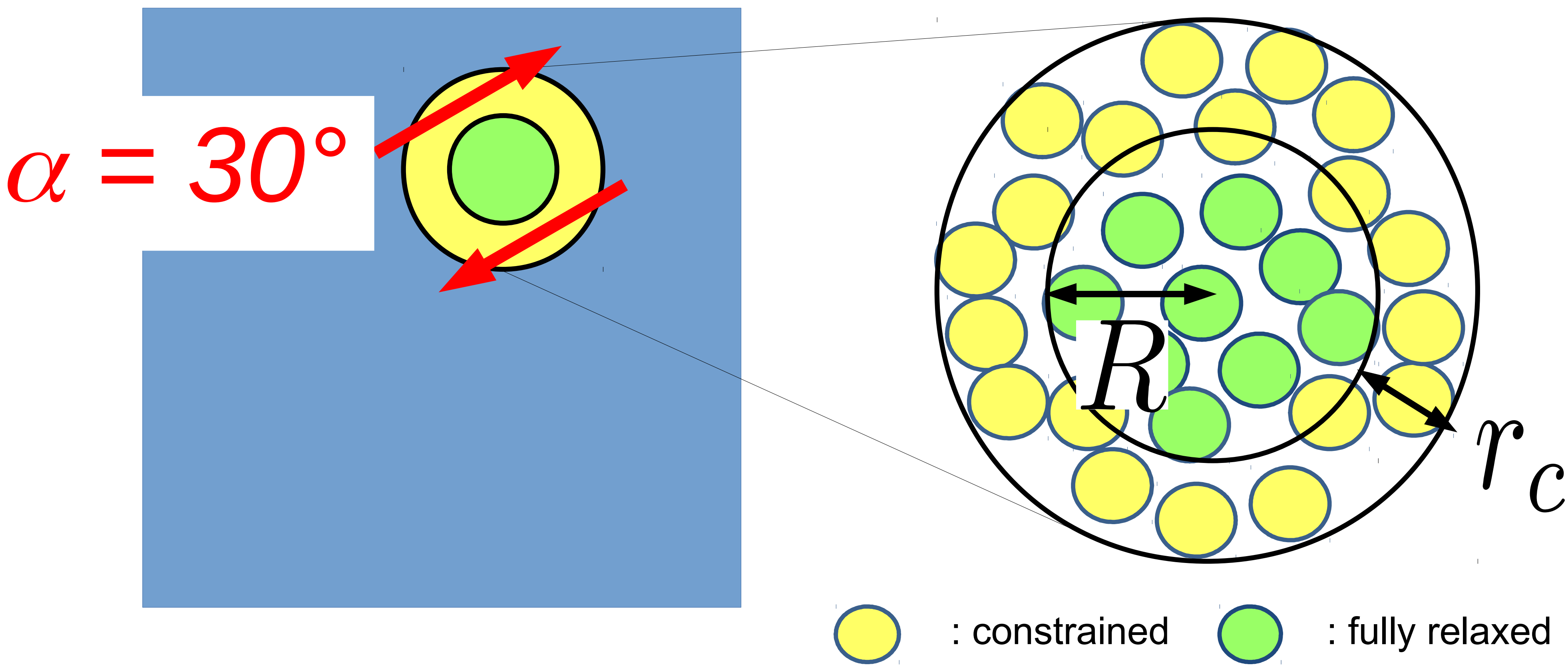

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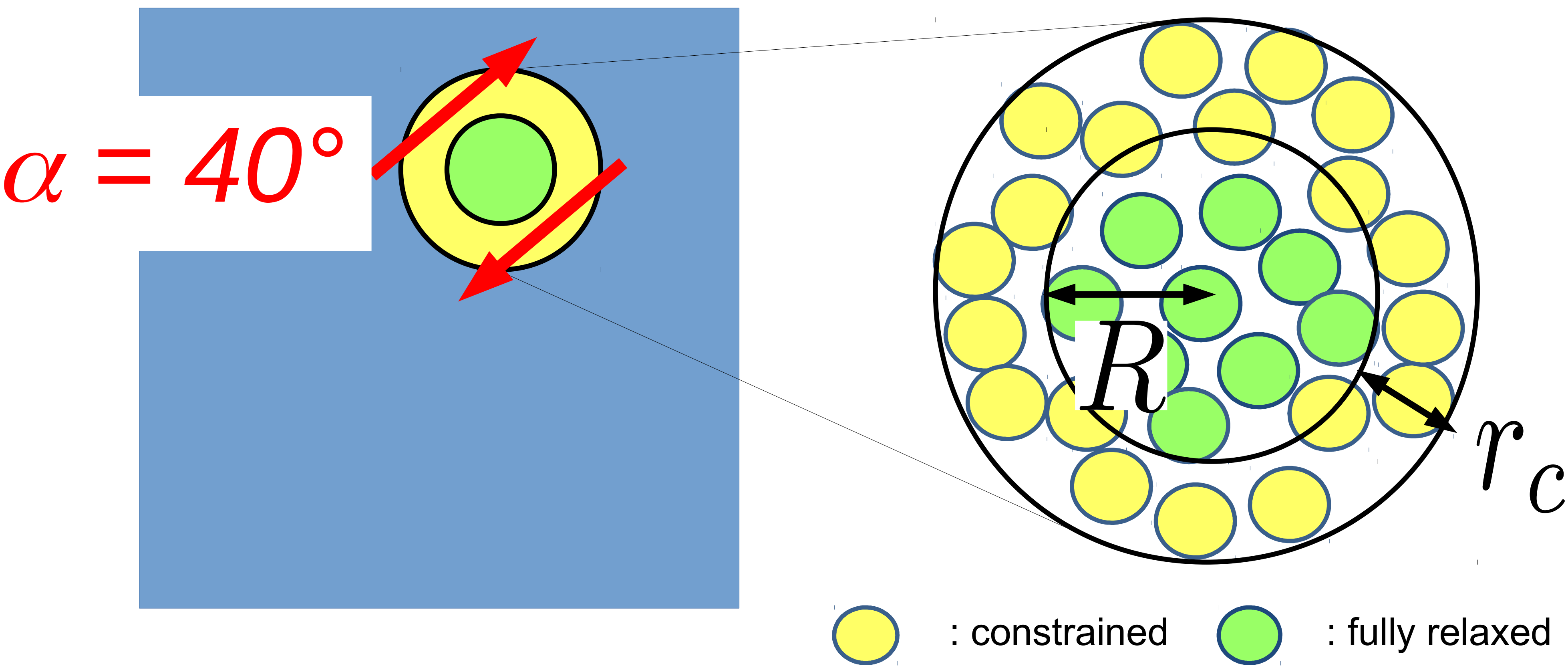
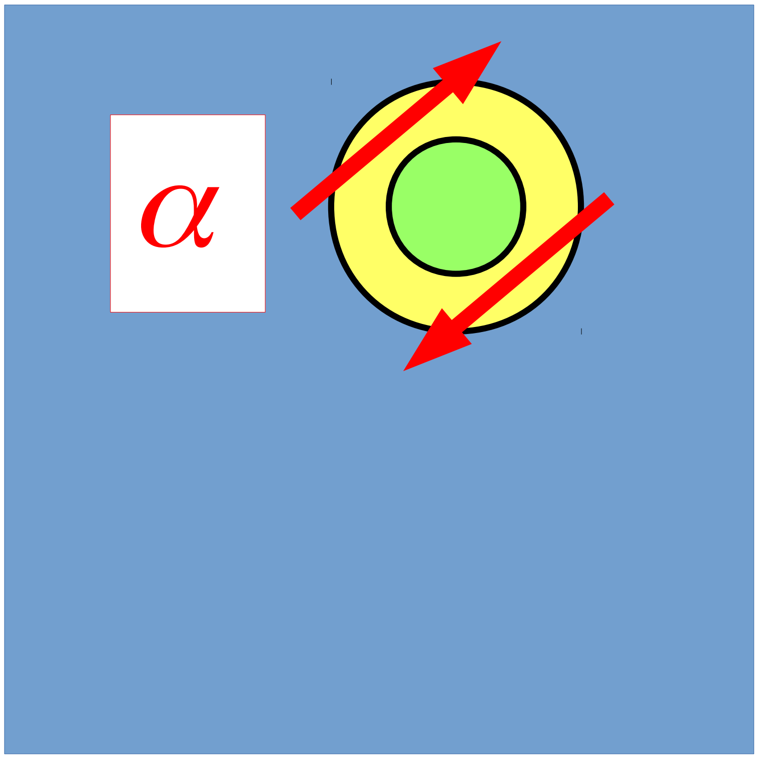


Local yield stress definition



- Local shear stress at the onset of the instability:

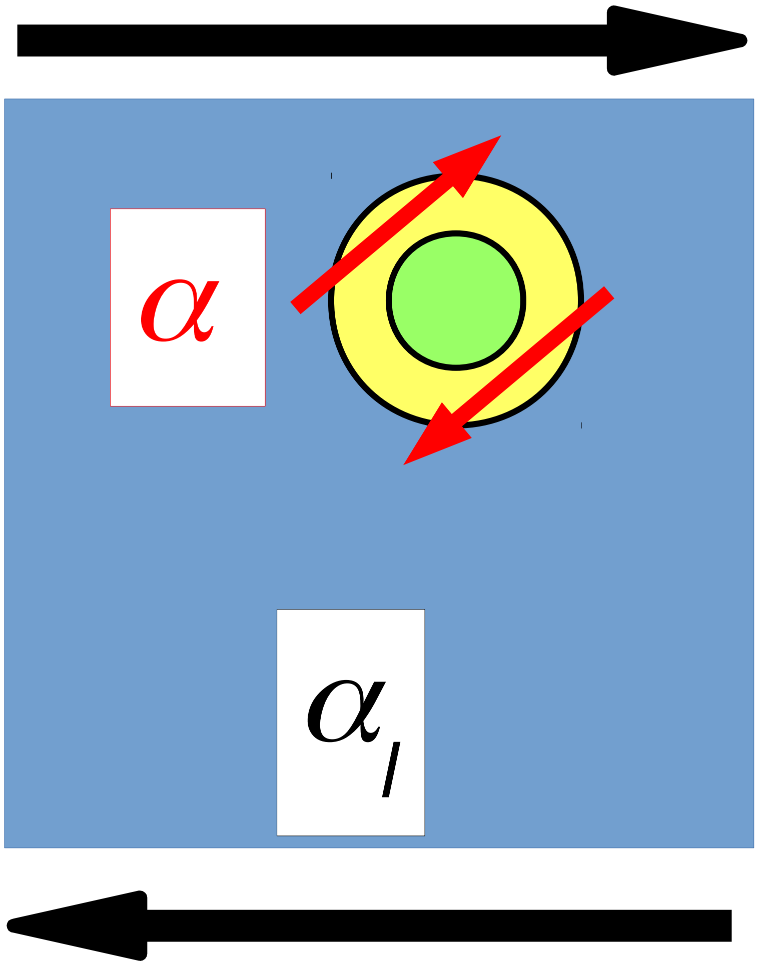
$$\tau^{\text{inst}}(\alpha)$$

- Shear stress threshold along α:

$$\tau^{c}(\alpha) = \tau^{\text{inst}}(\alpha) - \tau^{0}(\alpha)$$

where $\tau^{0}(\alpha)$ the initial stress within the as-quenched glass.

Local yield stress definition



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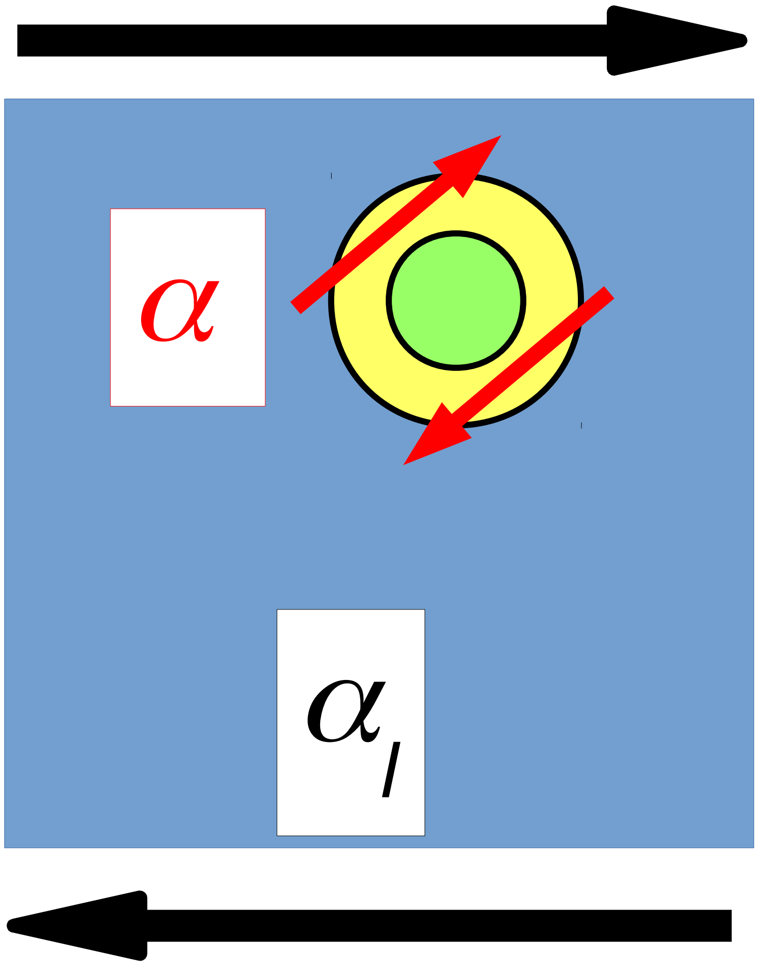
Local yield stress definition



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- Shear stress threshold along α:

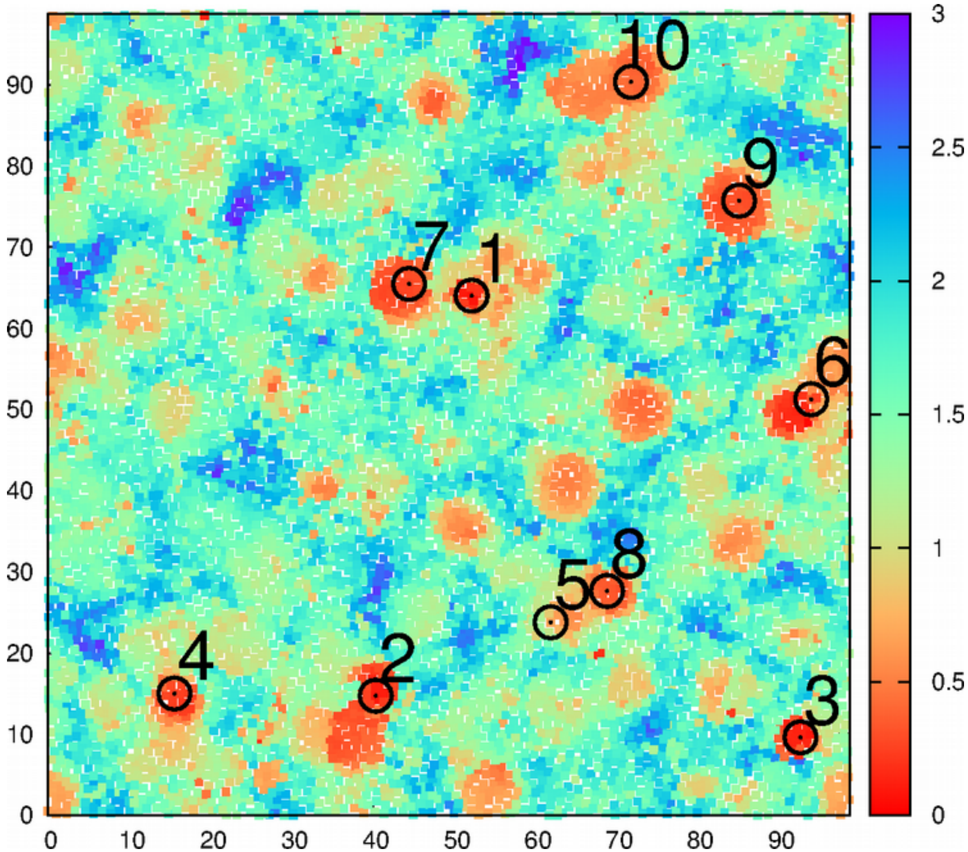
$$\tau^{c}(\alpha) = \tau^{\text{inst}}(\alpha) - \tau^{0}(\alpha)$$

where $\tau^{0}(\alpha)$ the initial stress within the as-quenched glass.

- Assuming a homogeneous elasticity, the local yield stress is defined as the minimum stress projected in the direction of remote loading α_l:

$$\tau_{y,i}(\alpha_l) = \min_{\alpha} \frac{\tau_i^c(\alpha)}{\cos[2(\alpha - \alpha_l)]} \quad \text{with} \quad |\alpha - \alpha_l| < 45^\circ$$

Results: yield stress maps

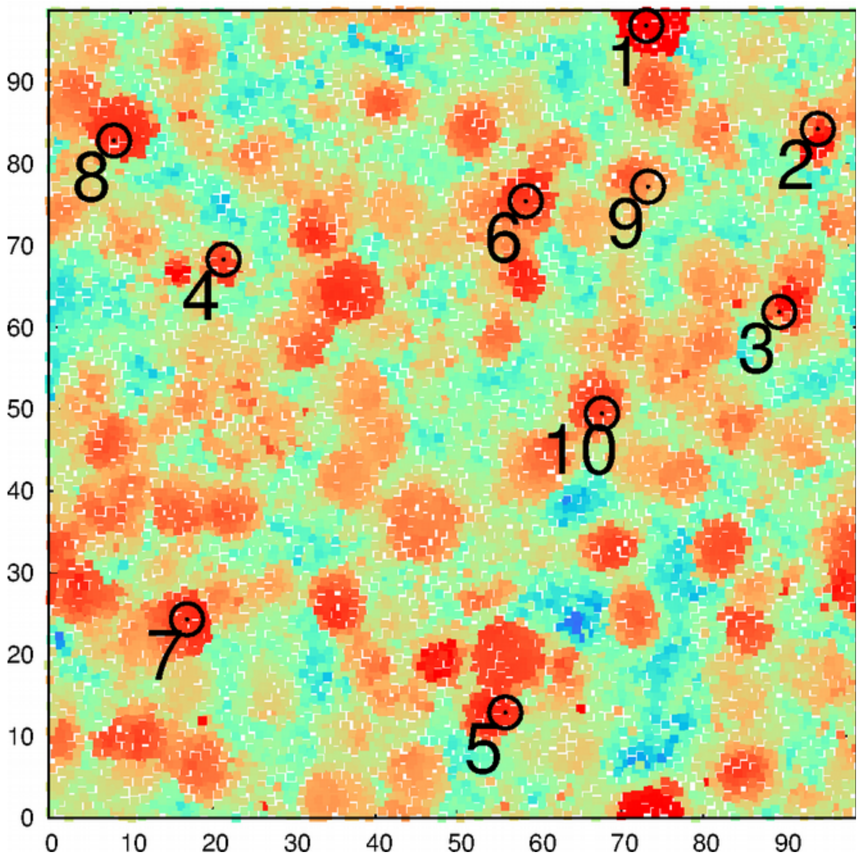


Color map: Local yield stress

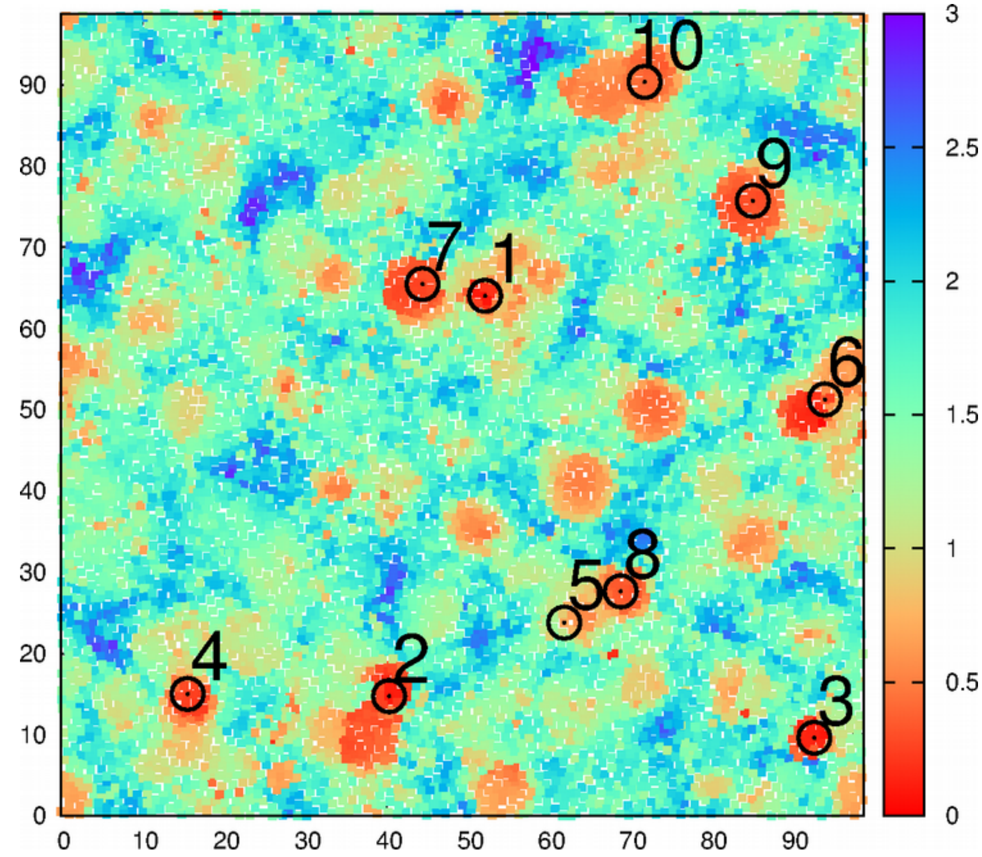
Symbols: rearrangement locations

Excellent correlation between the locations of plastic rearrangements and the low yield stresses.

Results: Quench rate effect



Fast quench

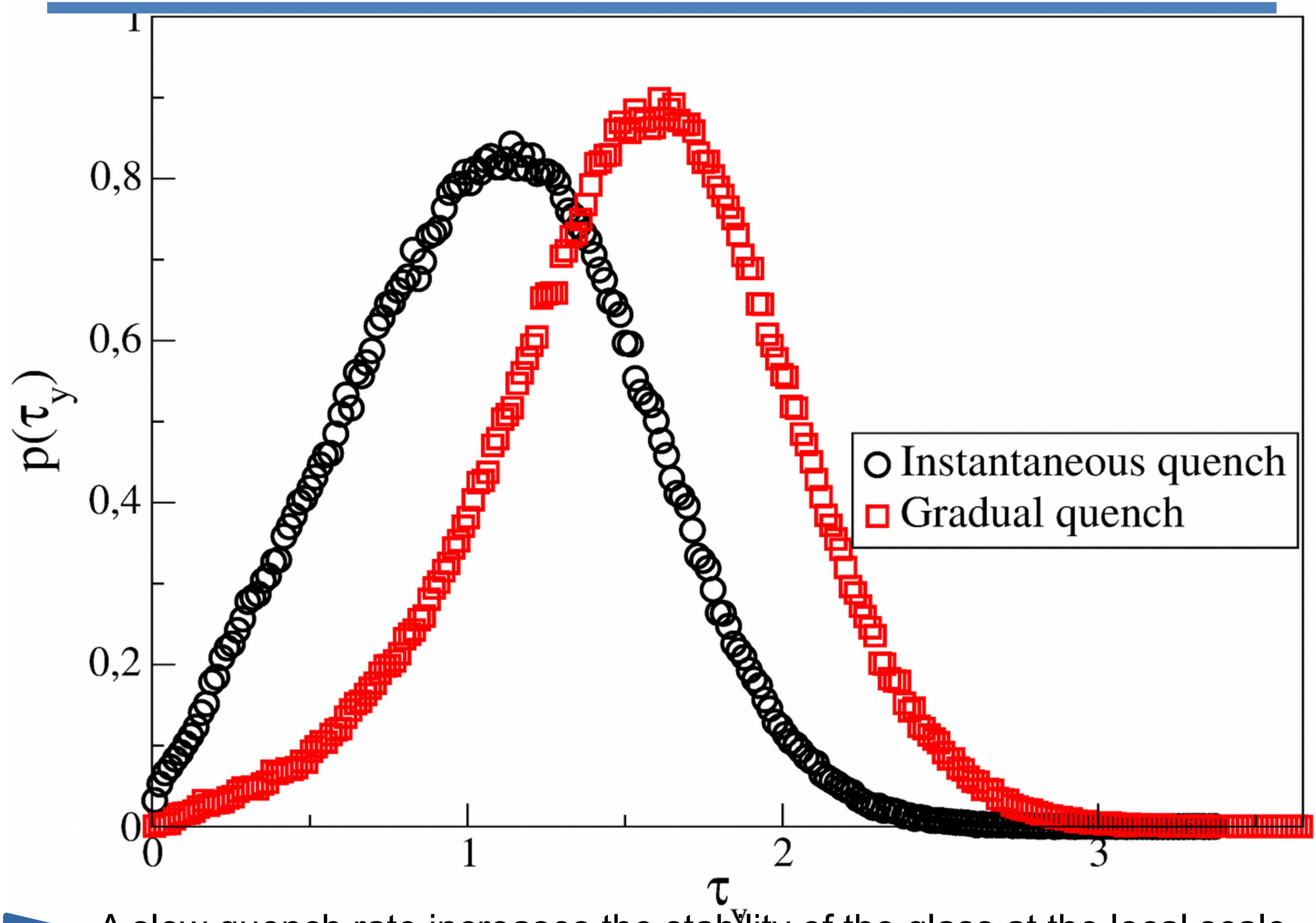


Slow quench

➡ A slow quench rate increases the stability of the glass at the local scale

S. Patinet et al PRL 2016, A. Barbot et al. PRB 2018

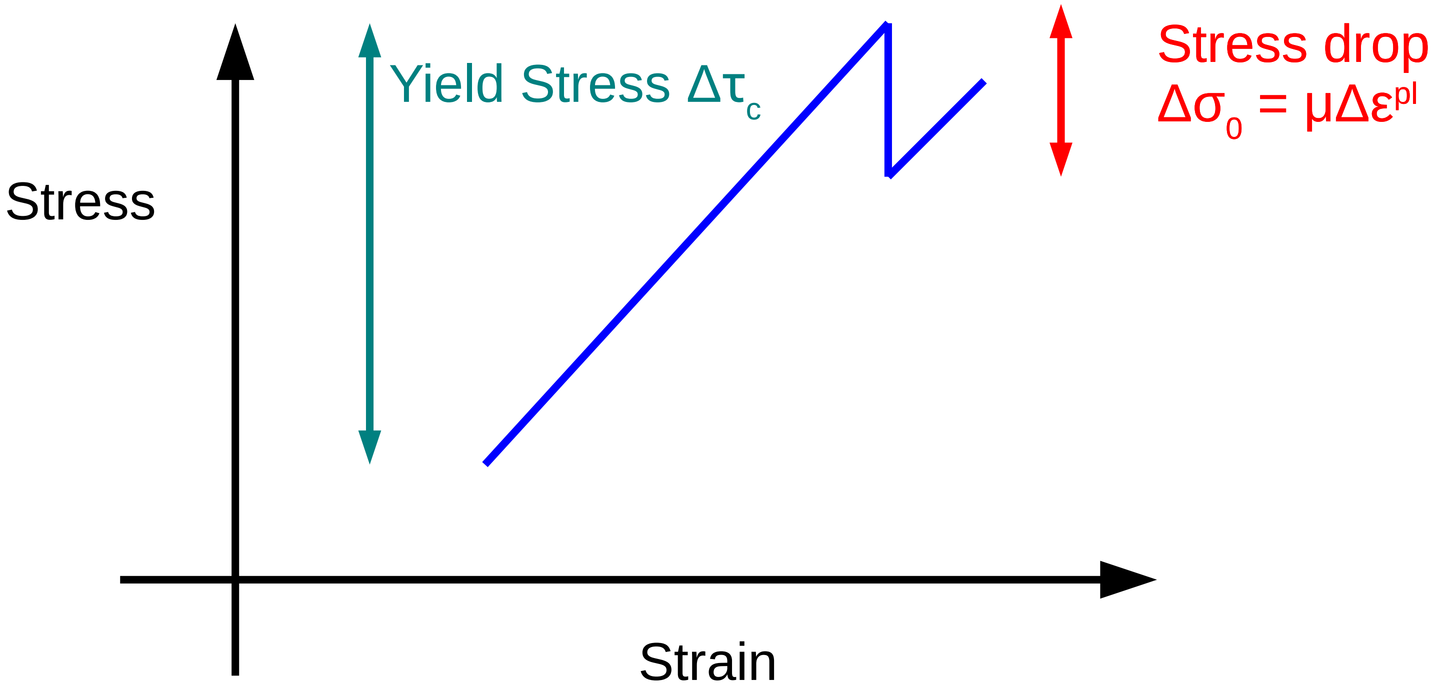
Results: Quench rate effect



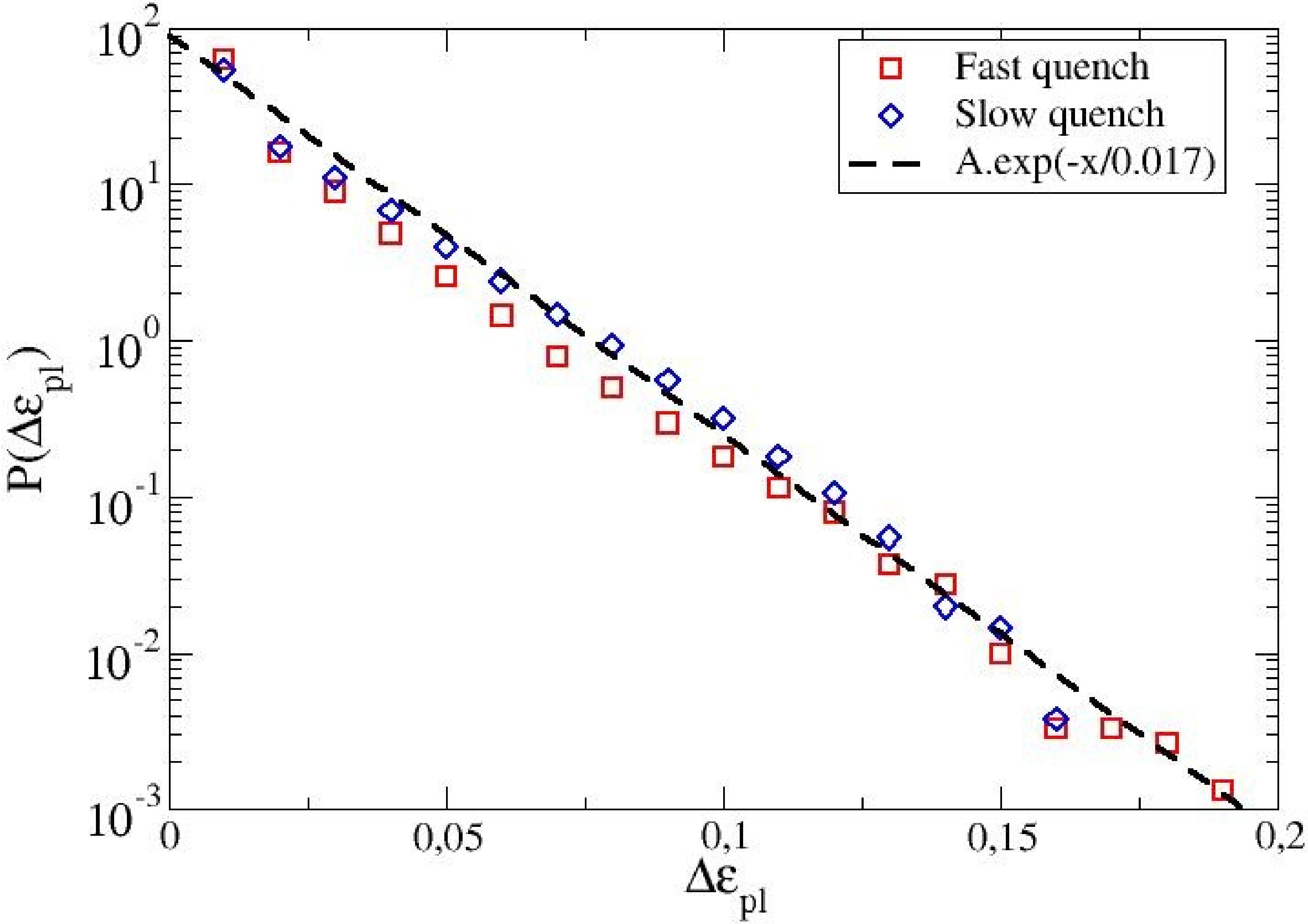
A slow quench rate increases the stability of the glass at the local scale

Plastic rearrangement : Yield stress vs stress drops

Local instability associated to a stress drop/local plastic strain :



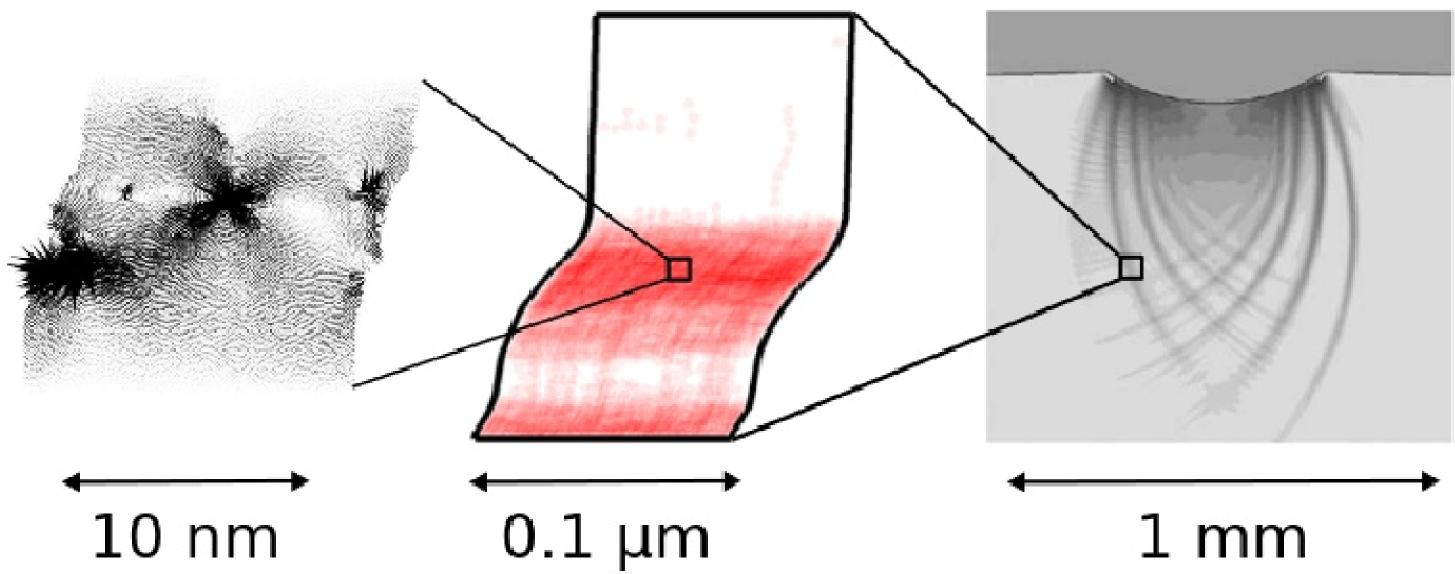
Exponential statistics of local plastic strains



S. Patinet et al PRL 2016, A. Barbot et al. PRB 2018

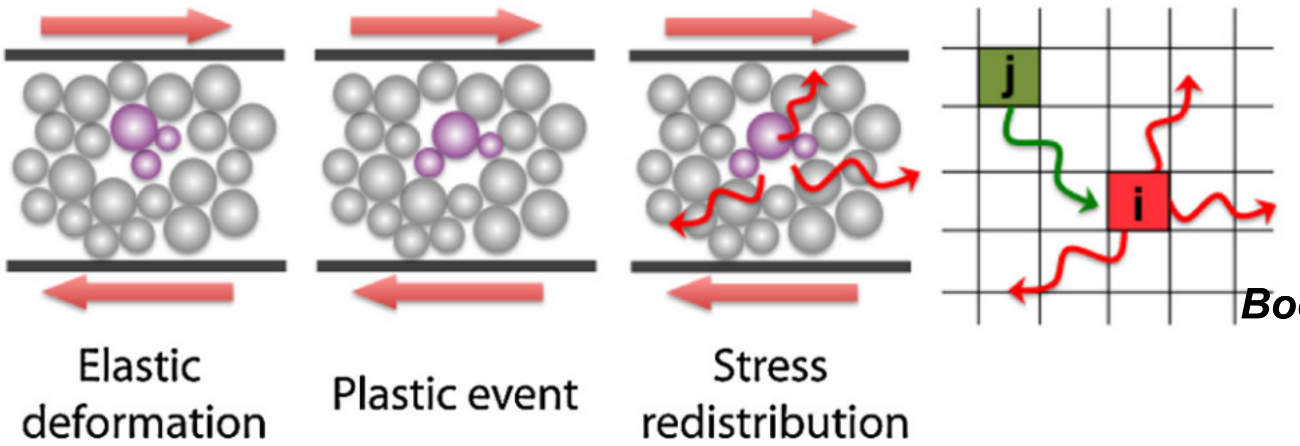
A first attempt of coarse-graining from micro to meso scale

Lattice models of amorphous plasticity



- Aim: build at mesoscopic scale a minimal model that reproduces the salient features of amorphous plasticity
- Two main ingredients:
  - Local threshold dynamics – plastic events
  - Eshelby quadrupolar elastic interaction
- Various implementations: Boston, Erlangen, Grenoble, Helsinki, Lausanne, Milano, Paris...

Mesoscopic models of amorphous plasticity



Bocquet PRL 2009

2D, scalar. Inclusions on lattice sites.

Local slips of inclusions (**threshold**-related): $\boxed{\sigma_{ij} > \sigma_{ij}^{th}}$ **disorder**

Plastic strain associated to each inclusion: $\epsilon_{ij}^{p} \rightarrow \epsilon_{ij}^{p} + \delta\epsilon^{p}$

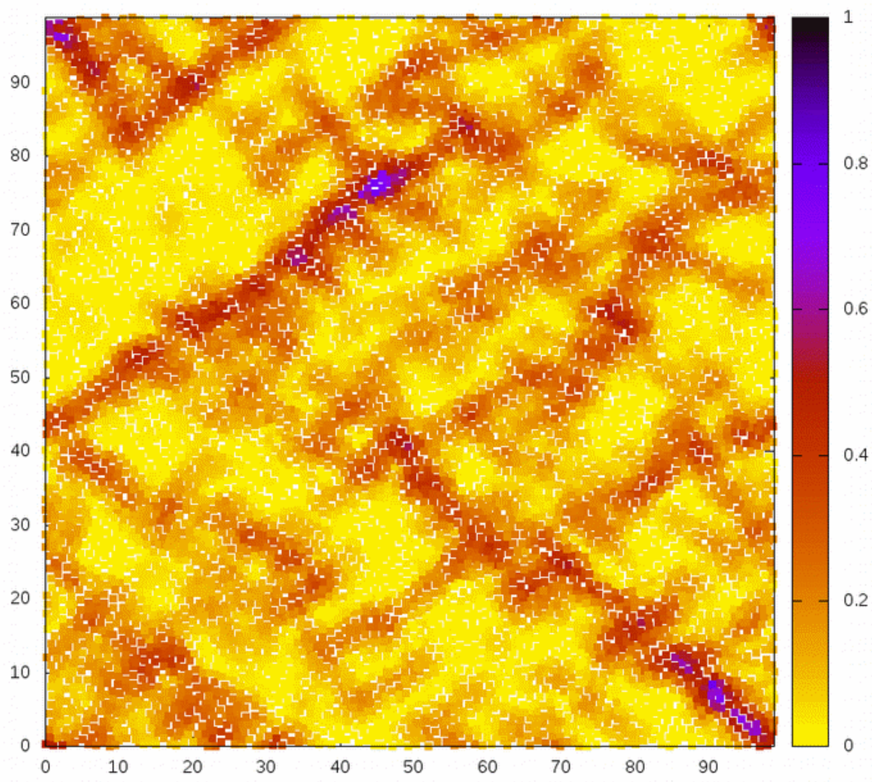
$$\sigma_{ij} \rightarrow \sigma_{ij} + G * \delta\epsilon^{p}$$

Elastic interaction between inclusions: via the **elastic kernel**

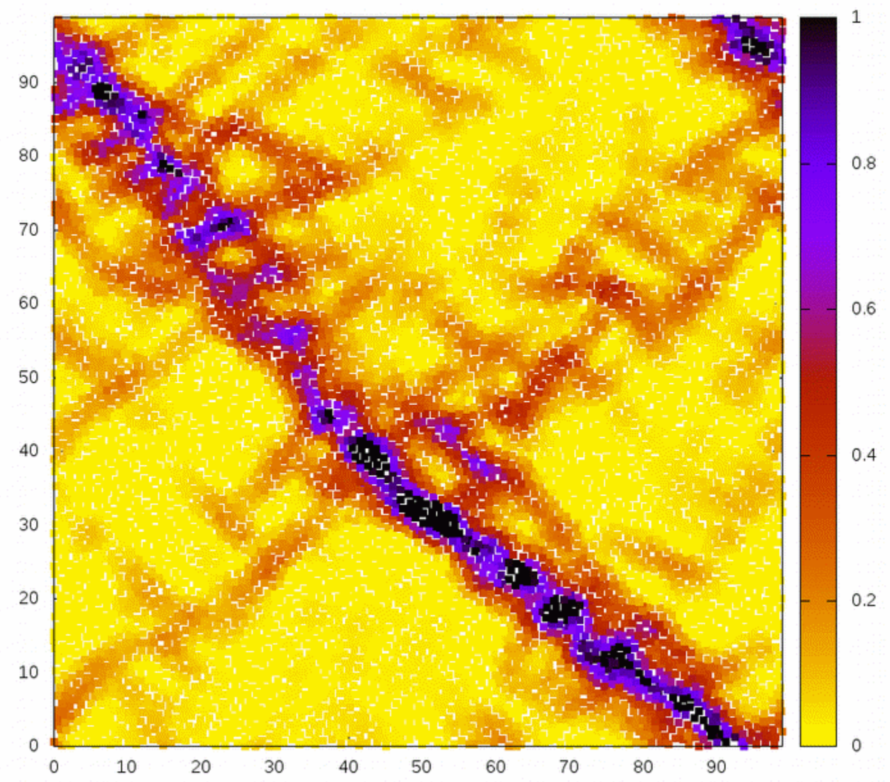
$$\boxed{G(\vec{r}) \propto \frac{\cos 4\theta}{r^2}}$$

elasticity

Shear banding depends on thermal history



Fast quench



Slow quench

Coarse-graining strategy

Naive version: glass as a disordered material

- Use mechanical properties of as-quenched glasses:
  - Elastic moduli
  - **Stationary** distributions of local yield stress :

Fast quench : $p_i(\sigma_Y) = p_r(\sigma_Y) = p^{at}_{fast}(\sigma_Y)$;

Slow quench : $p_i(\sigma_Y) = p_r(\sigma_Y) = p^{at}_{slow}(\sigma_Y)$

  - Exponential distribution of plastic increments
  - Use amplitude of local plastic increments as a tuning parameter to reproduce stress/strain curves
  - Test on other observables (localization, etc)

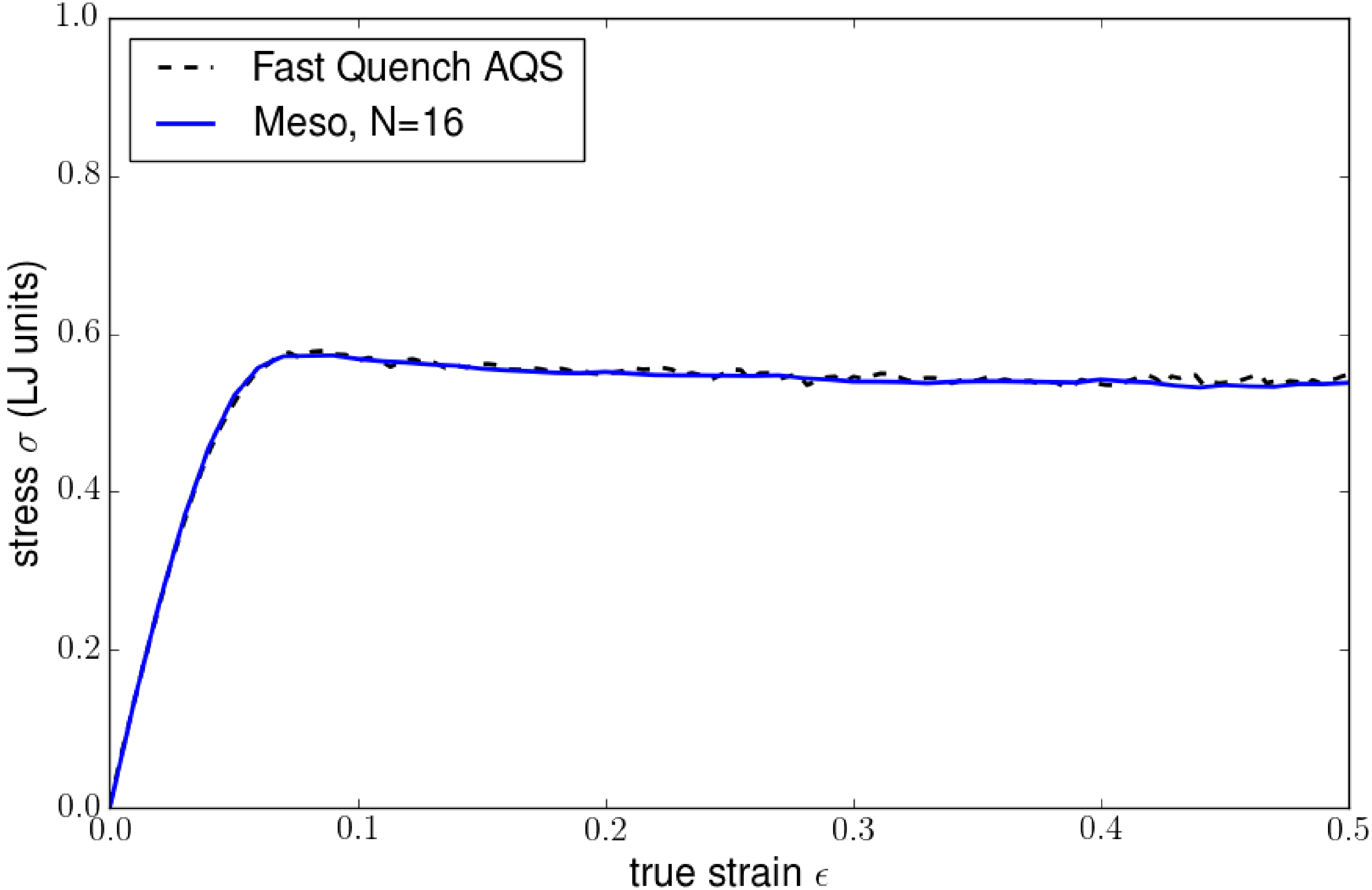
Vitreous version: glass as a mechanically aging/rejuvenating material

- Same as above but **rejuvenation**:

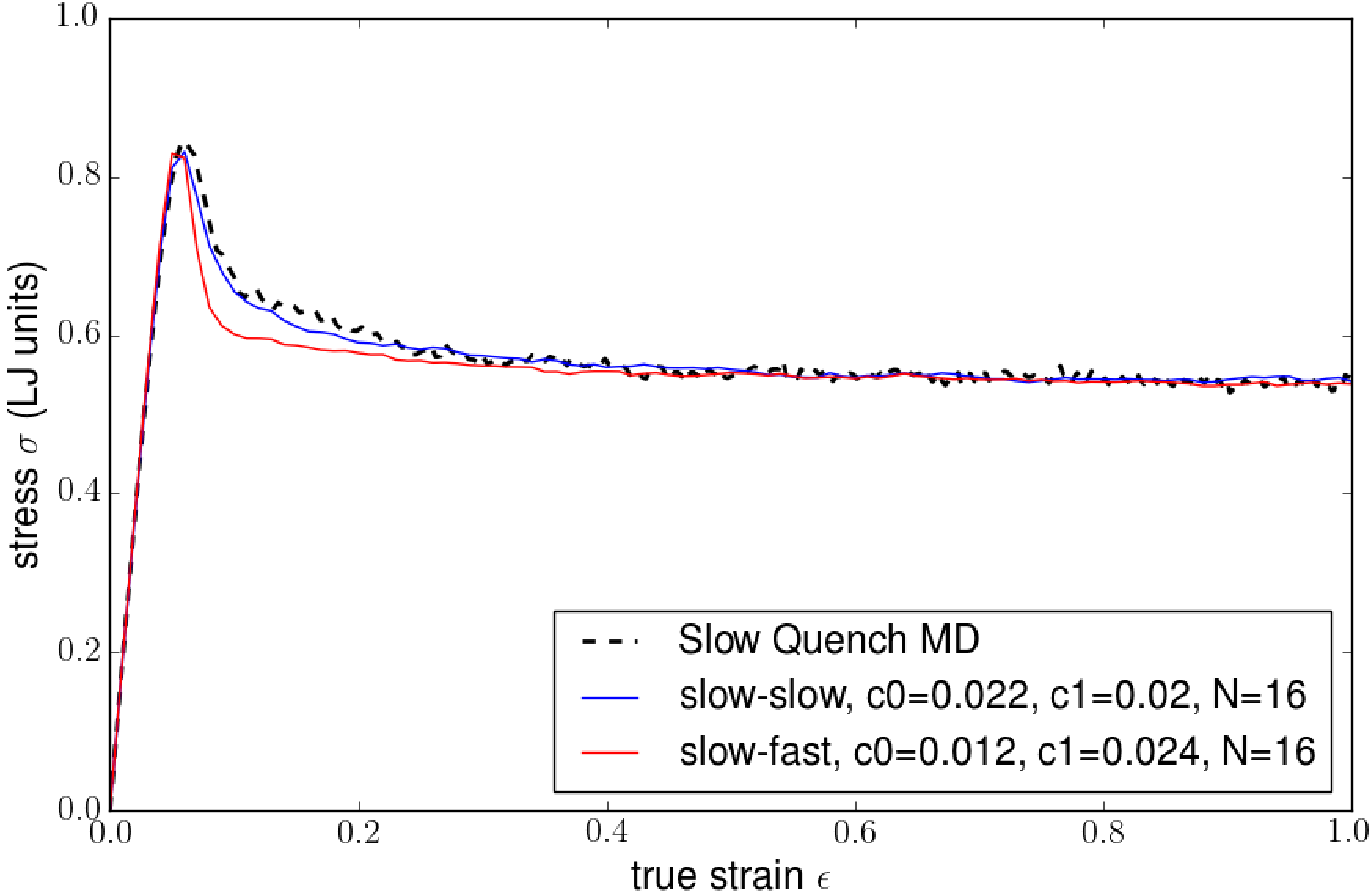
  New plastic thresholds (after rearrangements) taken from fast-quench distribution (almost invariant upon def) :

  Slow quench : $p_i(\sigma_Y) = p^{at}_{slow}(\sigma_Y)$; $p_r(\sigma_Y) = p^{at}_{fast}(\sigma_Y)$

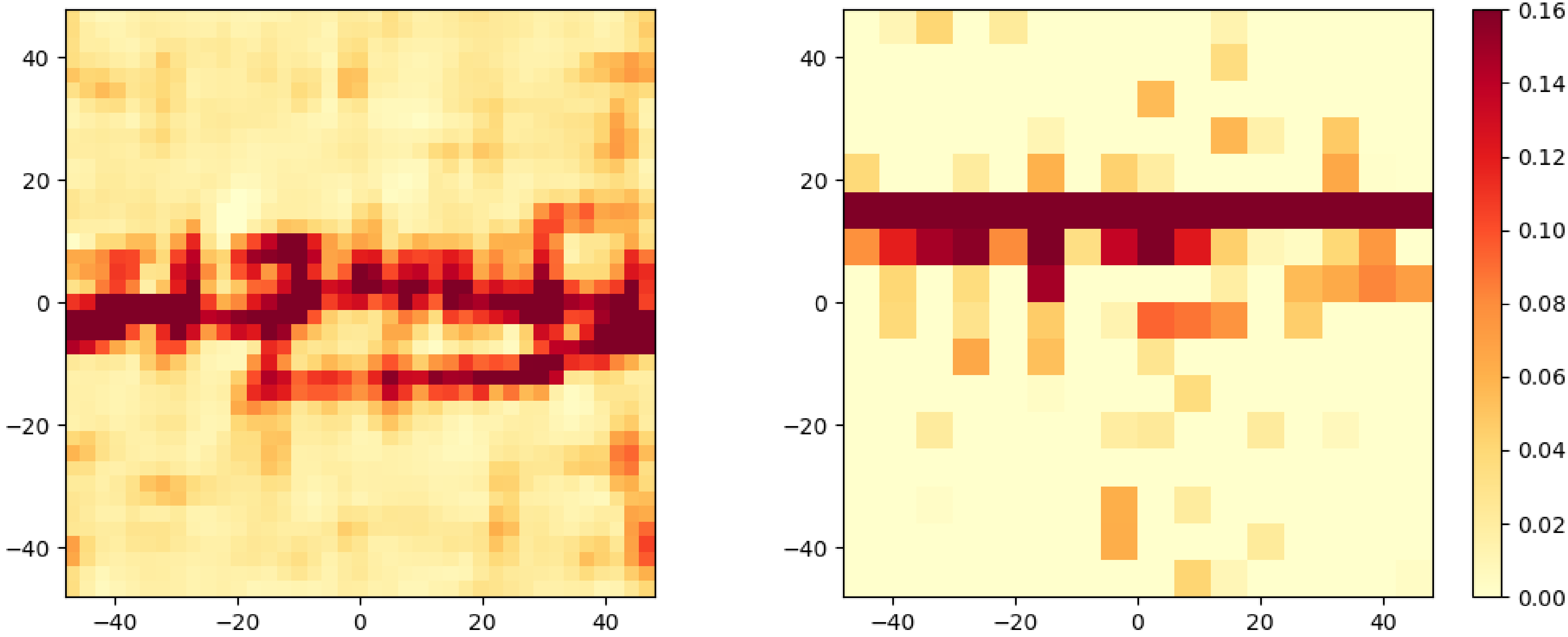
Fast quench glass : MD vs Meso



Slow quench glass : MD vs Meso

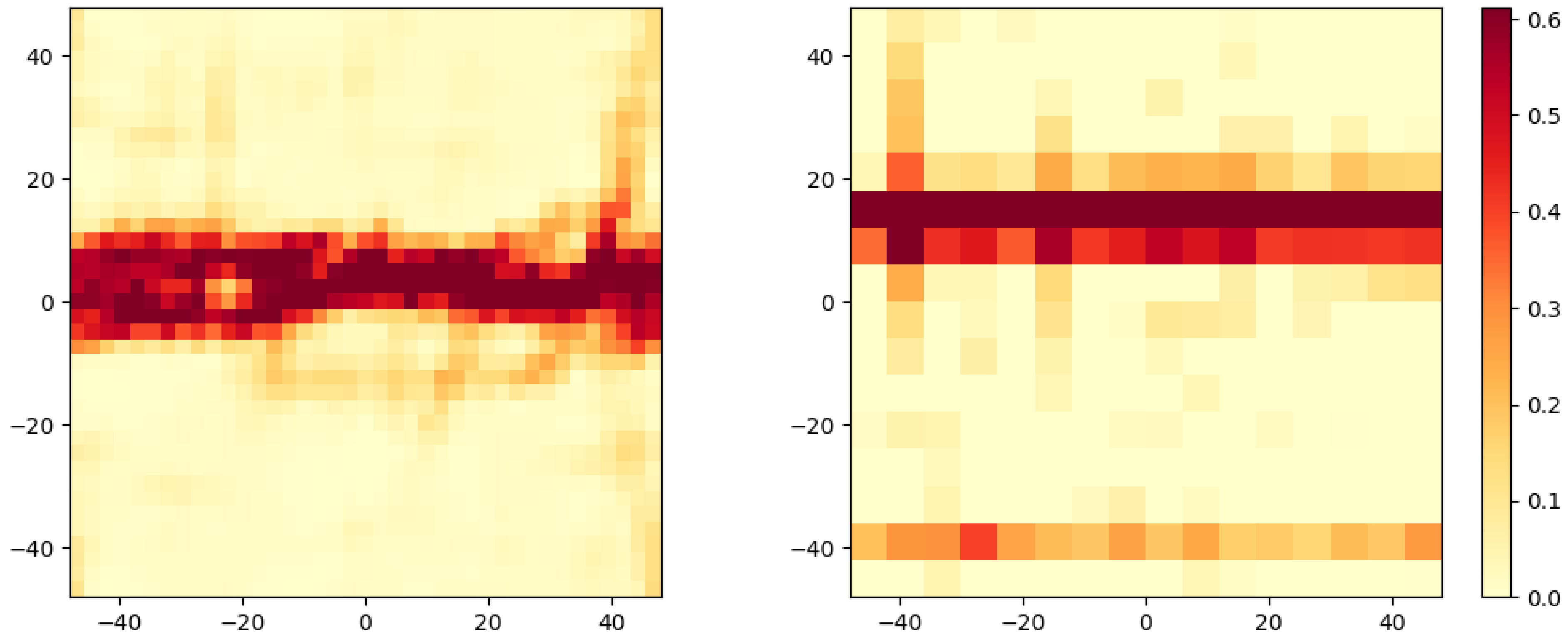


Shear-banding: MD vs Meso



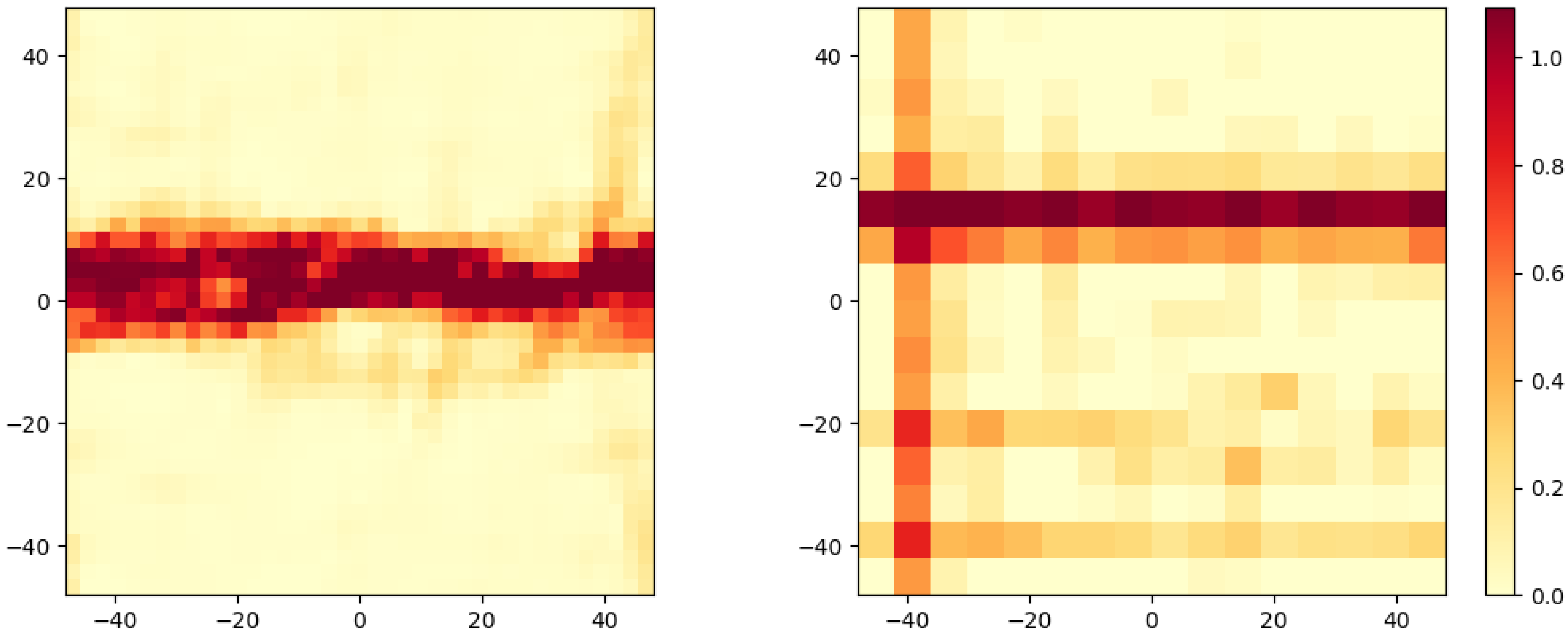
$\varepsilon_p = 0.05$

Shear-banding: MD vs Meso



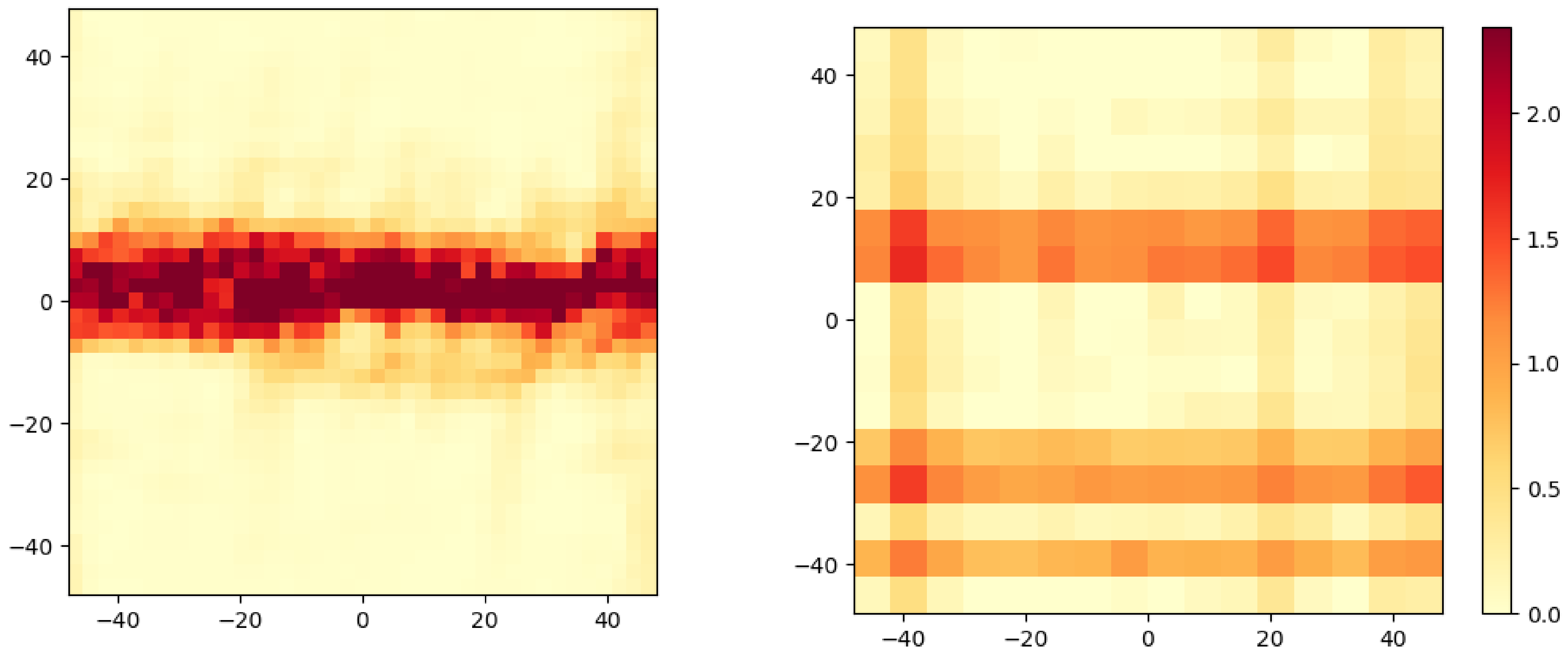
$\varepsilon_p = 0.12$

Shear-banding: MD vs Meso



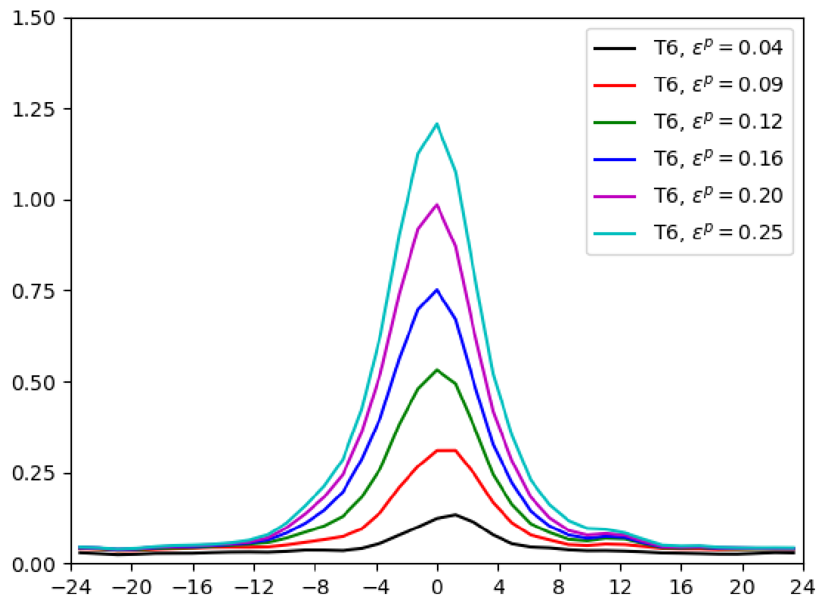
$\varepsilon_p = 0.20$

Shear-banding: MD vs Meso

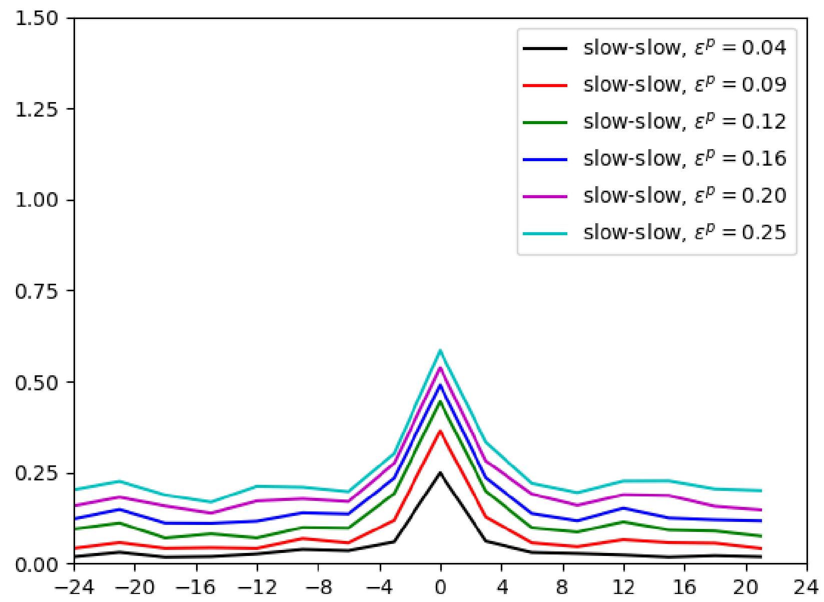


$\varepsilon_p = 0.12$

Shear-band mean profiles

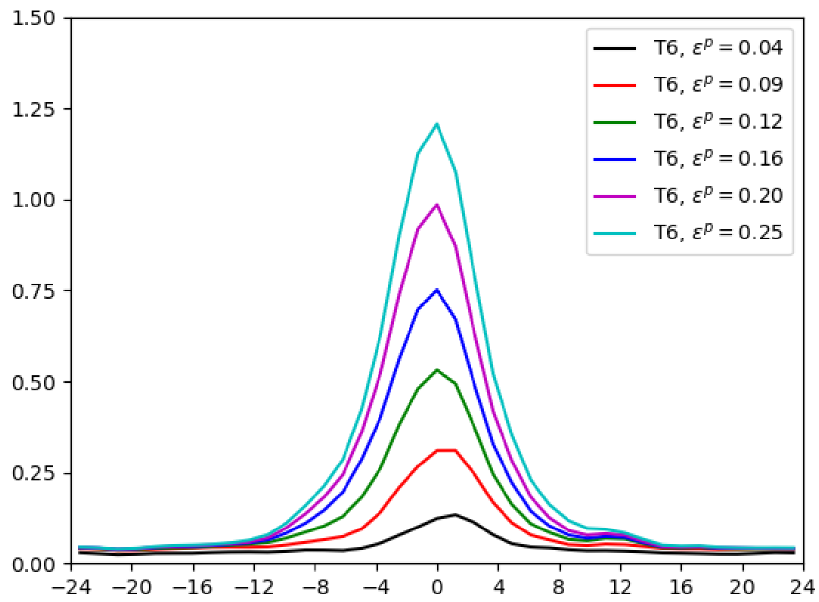


MD

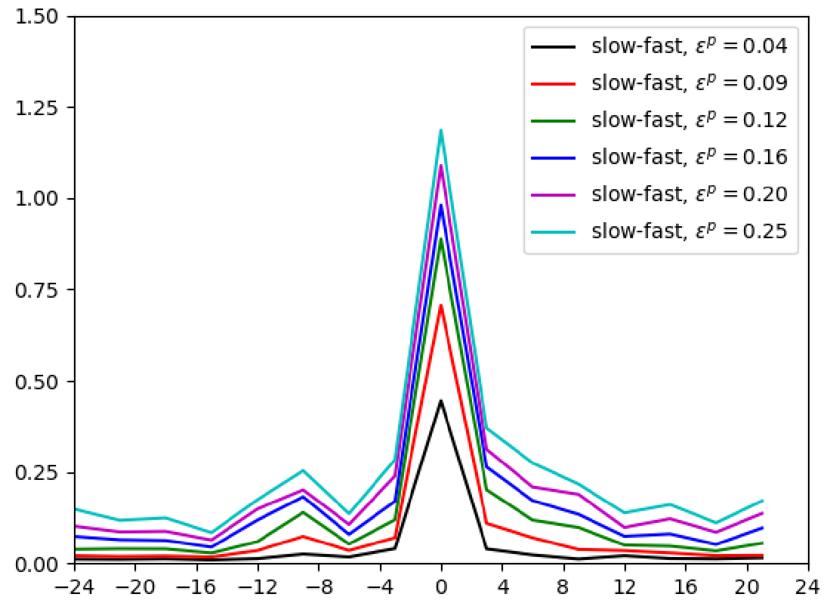


Meso with stationary distribution of thresholds

Shear-band mean profiles

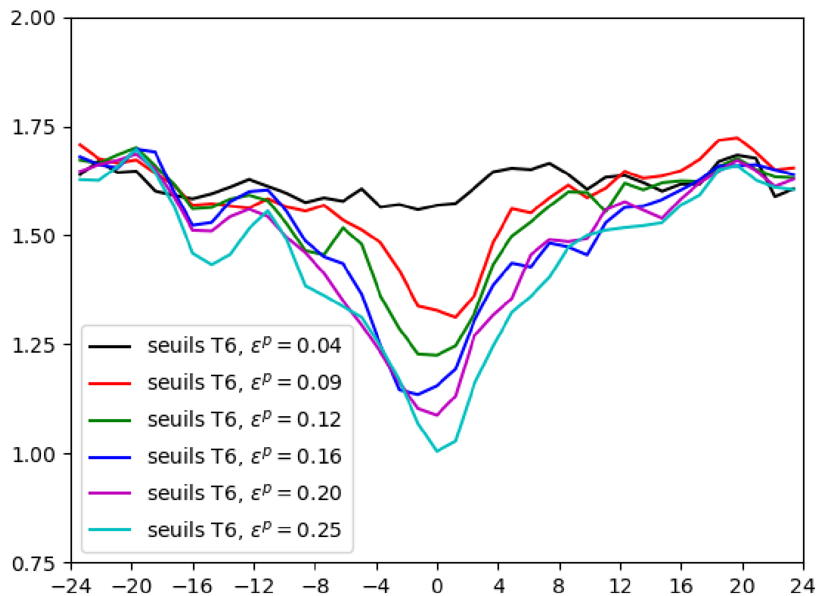


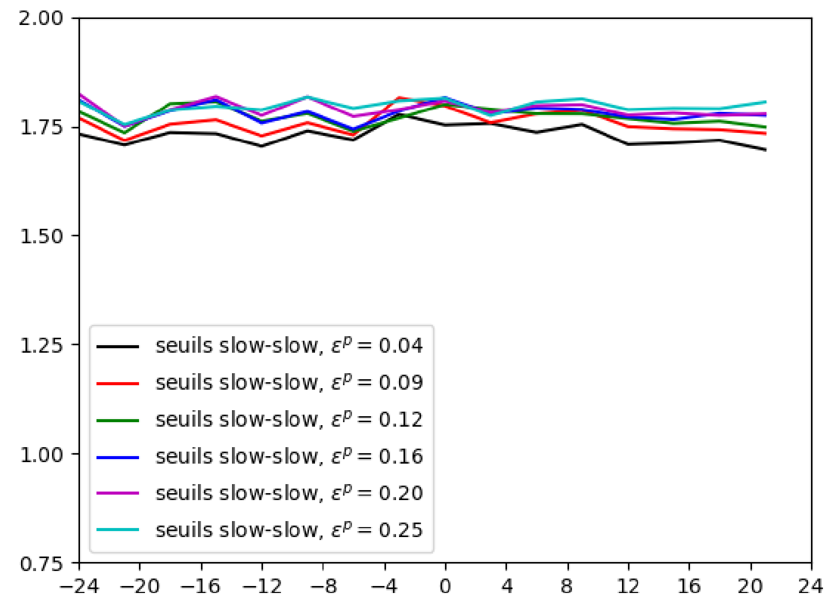
MD



Meso with rejuvenation

Yield Stress mean profiles

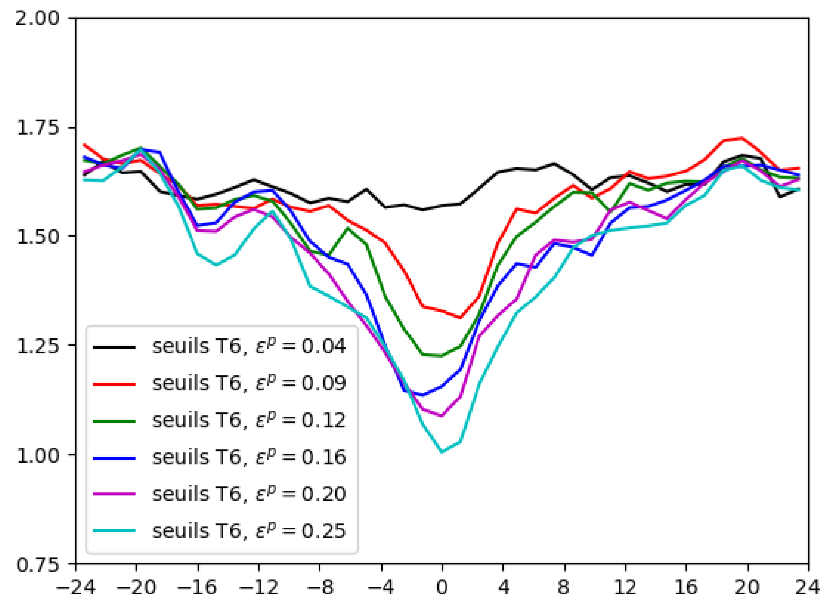




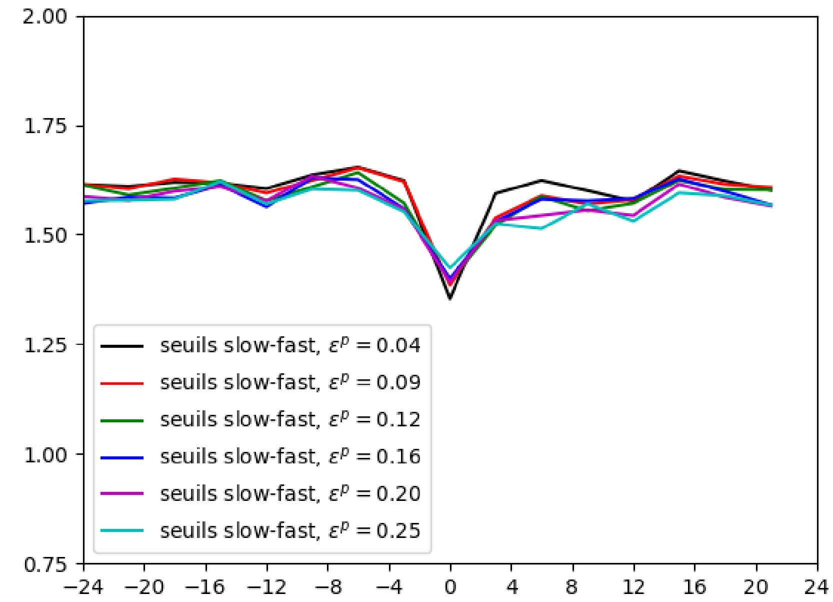
MD

Meso with stationary distribution of thresholds

Yield Stress mean profiles



MD



Meso with rejuvenation

Conclusions

- Local yield stress : A new structural/mechanical probe to study the glassy state and its plastic deformation
- Amorphous plasticity as a mechanical rejuvenation process
- Mesoscopic models with rejuvenation give semi-quantitative agreement with atomistic results

DV and S. Roux, Phys. Rev. B **84,** 134210 (2011)
Patinet et al, Phys. Rev. Lett. **117**, 045501 (2016)
Barbot et al, Phys. Rev. E **97**, 033001 (2018)
Barbot et al, *in preparation,* Tyukodi et al, *in preparation*