Irreversibility transition in mesoscopic models under cyclic shear

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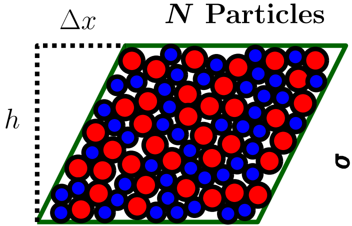
Outline

- Introduction to amorphous plasticity
- Modelling at Mesoscopic scales
- Tuning the thermal history of mesocopic model
- Aging dependence of plastic behavior upon monotonous and cyclic loading
- Transition graph characterization of the disordered landscape

Introduction: Shearing amorphous materials

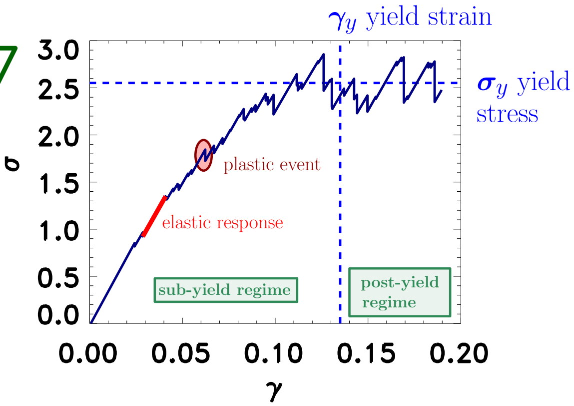
System



Shear strain:

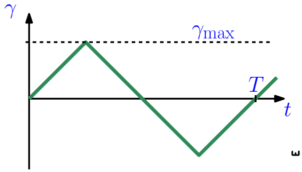
$$\gamma = \frac{\Delta x}{h}$$

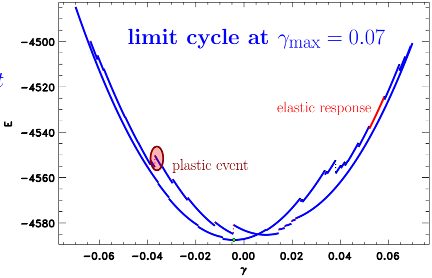
AQS Stress σ vs. Strain γ Response: monotonously increasing shear strain



Introduction: amorphous materials under cyclic shear

AQS Energy E vs. Strain γ response under cyclic shear strain





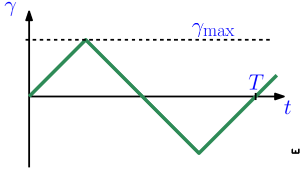
transient time t/T to cyclic response:

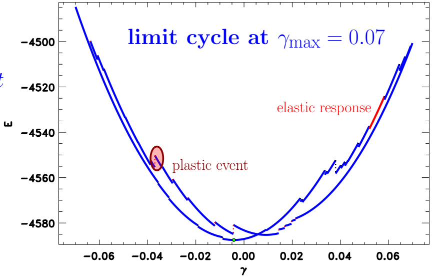
$$\lim_{\gamma_{\max}\to\gamma_y^-} \frac{t}{T} = \infty$$

(Irreversibility Transition)

- When subjected to **cyclic loading**, the system traverses the same sequence of states during each subsequent cycle: **limit cycle**.
- Depending on the strain amplitude we either converge to a limit cycle or to a **diffusive regime** marked with no existence of limit cycles.
- Status of the transition, dependence on glass preparation ?

AQS Energy E vs. Strain γ response under cyclic shear strain





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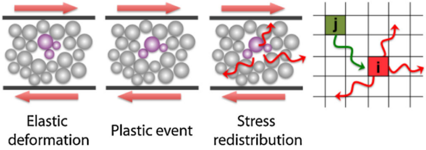
(Irreversibility Transition)

Pine, Gollub, Brady & Leshansky Nature **438** 997 2005; Corte, Chaikin, Gollub & Pine Nat. Phys. **4** 420, 2008; Keim & Arratia PRL **112** 028302 (2014); Regev, Lookman & Reichhardt PRE **88** 062401, 2013; Fiocco, Foffi & Sastry PRE **88** 020301(R), 2013; Bhaumik, Foffi & Sastry PNAS **118**, 2021; Yeh, Ozawa, Miyazaki, Kawasaki & Berthier PRL **124** 225502 (2020); Liu, Ferrero, Jagla, Martens, Rosso & Talon, JCP **156** 104902 (2022); Khirallah, Tyukodi, Vandembroucq & Maloney PRL **126** 218005 2021 . . .

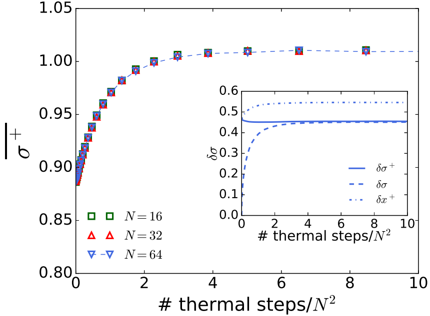
A Mesoscopic model for amorphous plasticity

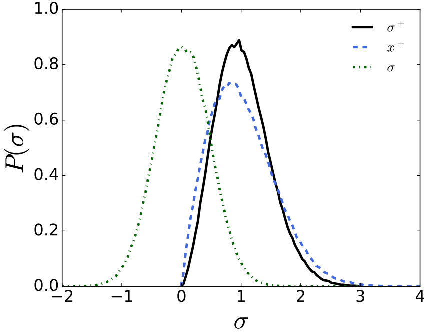


- We will use a scalar coarse-grained 2D model to study athermal quasi-statically driven sheared amorphous solids.
- We consider a square grid of *NxN* cells which interact with each other through PBCs.
- The external driving is uniform in space which can trigger local plastic events.
- A plastic slip event induces a Eshelby-like long-ranged elastic stress redistribution.

Recent review: A. Nicolas et al. Rev. Mod. Phys. 2018

Glass preparation: Mimicking instant quench from high T

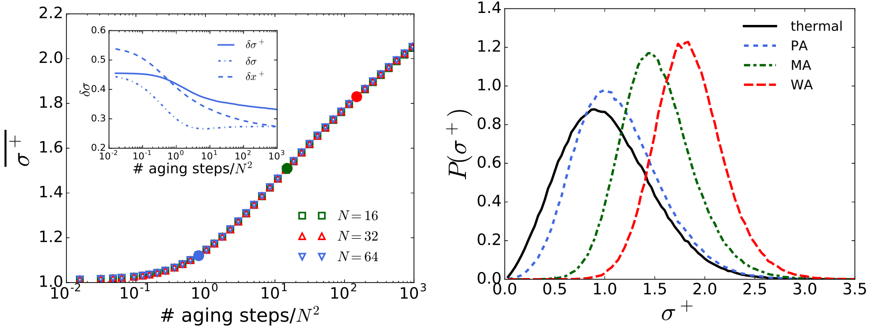




Thermal protocol: Sequence of avalanches triggered at random sites

Stationary distributions **independent** of system size.

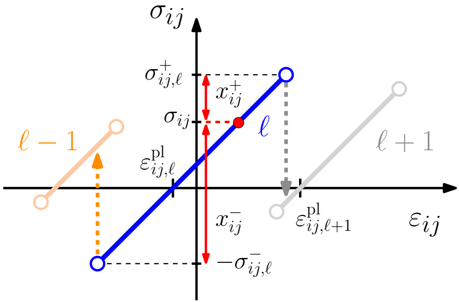
Glass preparation: Aging at vanishing temperature



Aging protocol: Sequence of avalanches triggered at extremal sites

the older the system, the harder the sites

AQS driving of amorphous solids in a quenched landscape

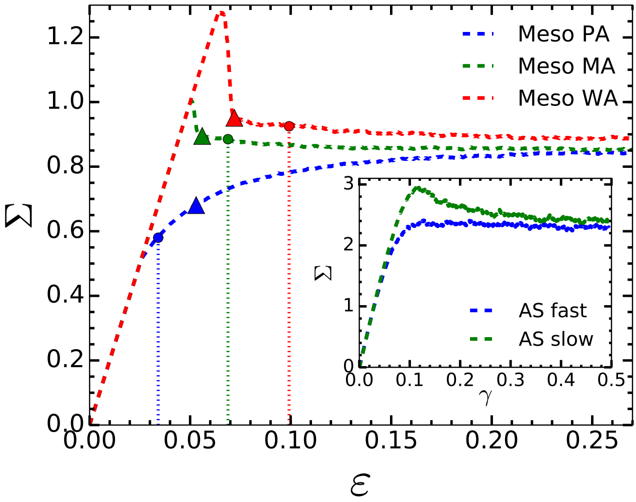


Each cell is assigned a pair of stress thresholds. One for forward and one for reverse slip direction.

A cell revisits the same pair of stress thresholds when the same plastic strain value is revisited.

The amount of local plastic strain is correlated to local stress thresholds.

Shearing the glass: Monotonous loading

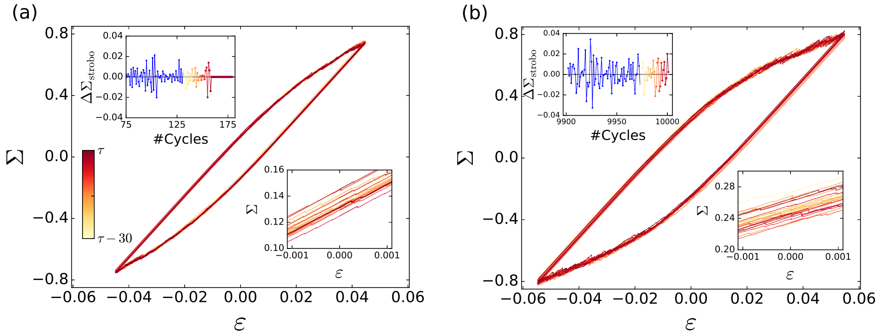


Poorly aged glass shows typical **ductile** response. As the glass is aged, stress peak emerges which gets bigger with age.

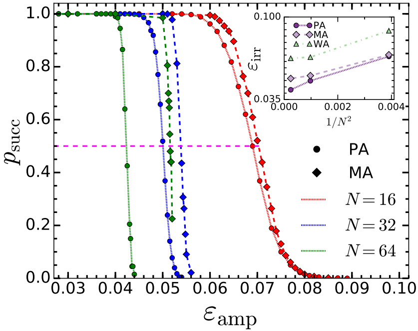
Cyclic shear: Poorly aged glass

$\varepsilon_{amp} = 0.045$, **Reversible**

$\varepsilon_{amp} = 0.055$, **Ireversible**



Cyclic shear: Irreversibility transition



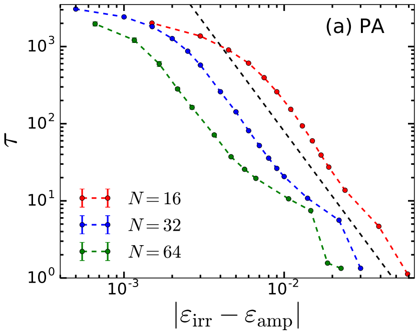
We are able to capture **limit cycles**.

We define the **irreversibility transition** as the strain amplitude at which 50 % of realisations find success in obtaining limit cycles.

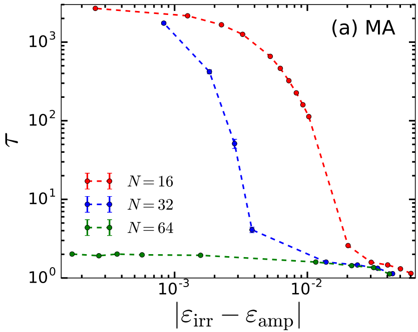
The effect of system size is felt under cyclic shear **but not** under uniform shear.

Transient duration: dependence on glass preparation

Poorly Aged

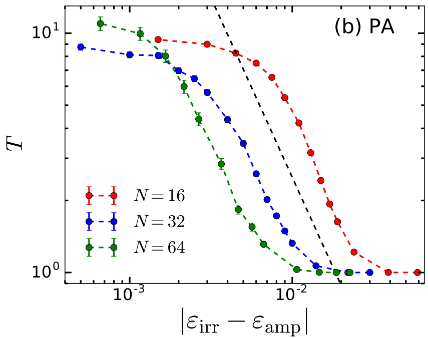


Medium Aged

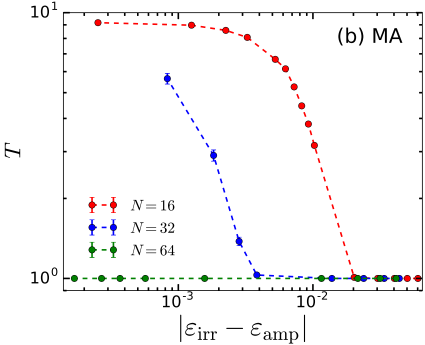


Limit periods: dependence on glass preparation

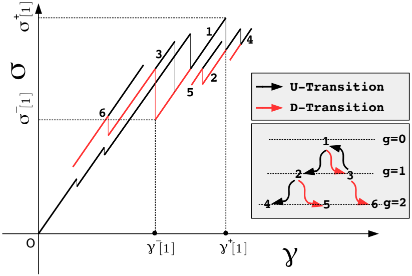
Poorly Aged

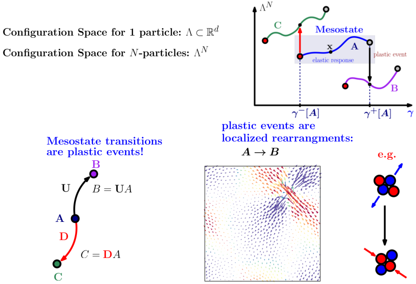


Medium Aged



Characterization of the disordered landscape *via* transition graphs



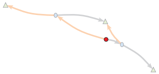


We employ a **novel technique** of representing the dynamics of sheared amorphous solids in terms of a **directed transition graph** to answer the question.

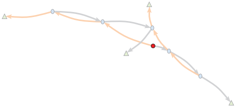
M. Mungan et al. PRL **123** 178002 (2019)

AQS graph acquisition from simulations – Generation 1

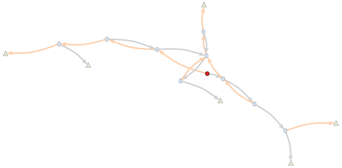
AQS graph acquisition from simulations – Generation 2



AQS graph acquisition from simulations – Generation 3



AQS graph acquisition from simulations – Generation 4



AQS graph acquisition from simulations – Generation 5

AQS graph acquisition from simulations – Generation 6

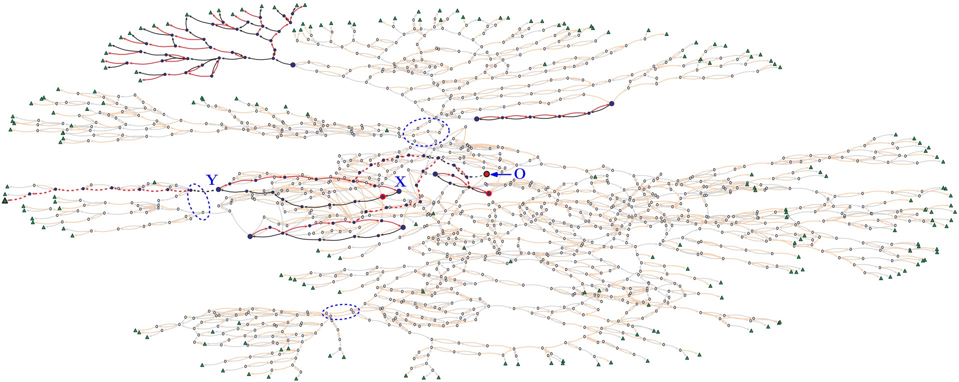
AQS graph acquisition from simulations – Generation 7

AQS graph acquisition from simulations – Generation 8

AQS graph acquisition from simulations – Generation 9

AQS graph acquisition from simulations – Generation 10

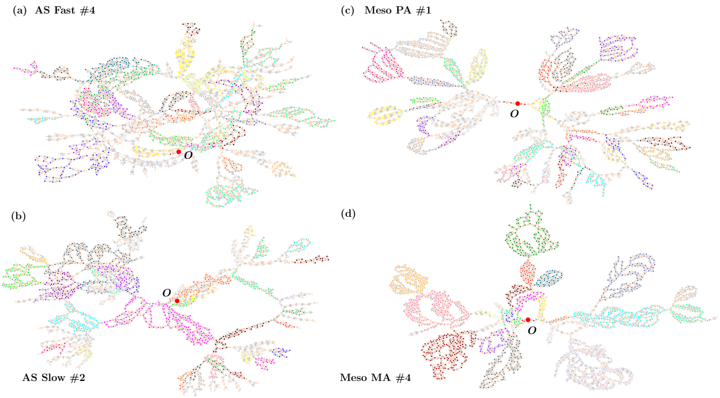
The lay of the land — $g = 25$, $\mathcal{N} = 1416$ mesostates



Degeneracy: many deformation paths lead to the same state
$\mathcal{N} = 1416 \ll 2^{26} \approx 6 \times 10^7$

Bottlenecks, tree-like regions & loops

Graph of mesostates from atomistic and mesoscale simulations



AQS dynamics $\leftrightarrow$ Graph topology

Athermal quasistatic dynamics under scalar deformations of system with many/continuous degrees of freedom can be reduced to a transition graph and thresholds.

Goal: To characterize the **topology of the AQS graph**.

In particular cyclic response to periodic shearing: **mutual reachability** as a graph property $\Rightarrow$ **strongly connected components**

Mutual Reachability and Strongly Connected Components

A pair of vertices $A, B \in \mathcal{S}$ is **mutually reachable (MR)**, if there are directed paths

$$A \to B \quad \textbf{and} \quad B \to A.$$

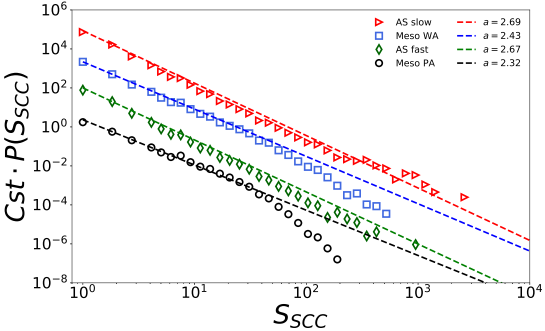
Strongly Connected Components (SCCs): Set of mutual reachable vertices

Application to shear deformation:

- **MR**: There exist sequences of plastic deformations leading from A to B **and** B to A.
- Transitions **within** an SCC are reversible.
- Transitions **between** an SCC are irreversible.

Any periodic response A_t must be confined to a single SCC

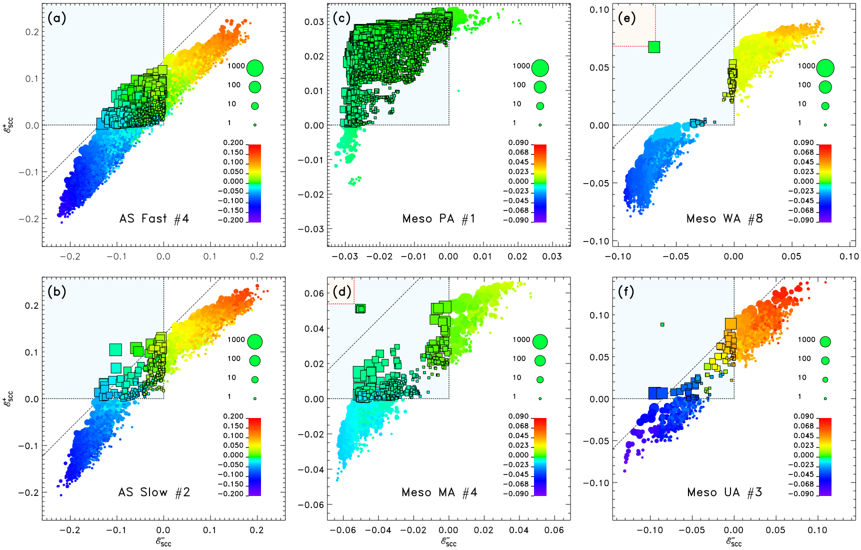
Size distribution of Strongly Connected Components (SCC)



The exponent of SCC size distribution for poorly aged glass **does not** depend on system size.

The exponent for mesoscopic models is in **reasonable agreement** with atomistic simulation.

Stability ranges of Strongly Connected Components



Conclusion

1. We use a 2-dimensional, athermal, mesoscale model for amorphous solids.

2. We proposee a glass preparation protocol and tune the aging parameter to recover ductile and brittle response under uniform shear.

3. We capture limit cycles through our model and the irreversibility transition observed under cyclic shear.

4. We compare our cycling results to that obtained through 2-dimensional atomic-scale simulations for differently aged glasses by using a novel transition graph construction.

D. Kumar et al. JCP 157, 174504 (2022)