Yielding and shear banding in amorphous solids

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Yielding versus depinning in disordered systems
ENS, Oct 22 – 24, 2018

Outline

Introduction

- Mechanical response of amorphous solids
- Oscillatory shear deformation of a model glass
- The Yielding transition
- Avalanches
- Shear banding
- Summary

P. Leishangthem
(JNCASR)

Anshul D. S. Parmar
(JNCASR/TIFR)

Saurabh Kumar
(JNCASR/Koln)

Earlier work: In Collaboration with:
Giuseppe Foffi (EPFL/Orsay)
Davide Fiocco (EPFL/Google/Frontiers)

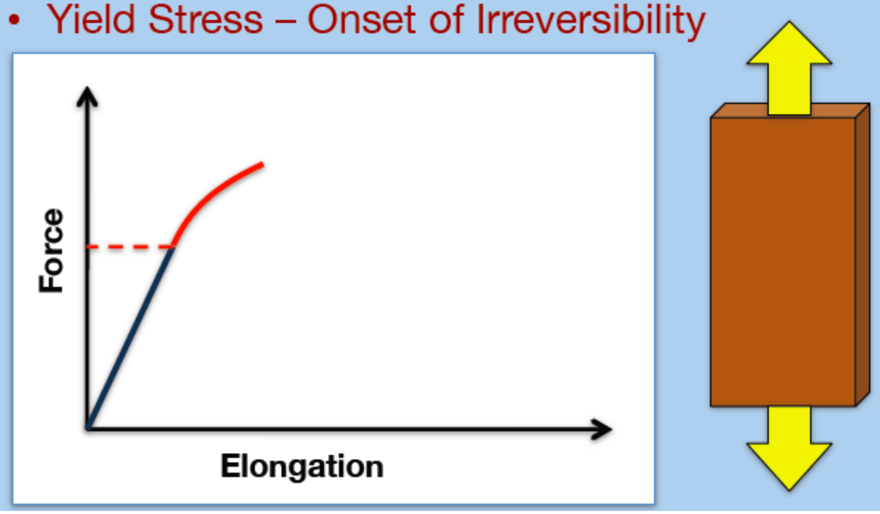
*Fiocco, Foffi, Sastry, **Phys Rev E** 88, 020301(R) (2013), **Phys Rev Lett** 112 025702 (2014),**JPCM** 27, 194130 (2015)*

*- Leishangthem, Parmar, Sastry "The yielding transition in amorphous solids under oscillatory shear deformation" **Nature Comm**. (2017)*

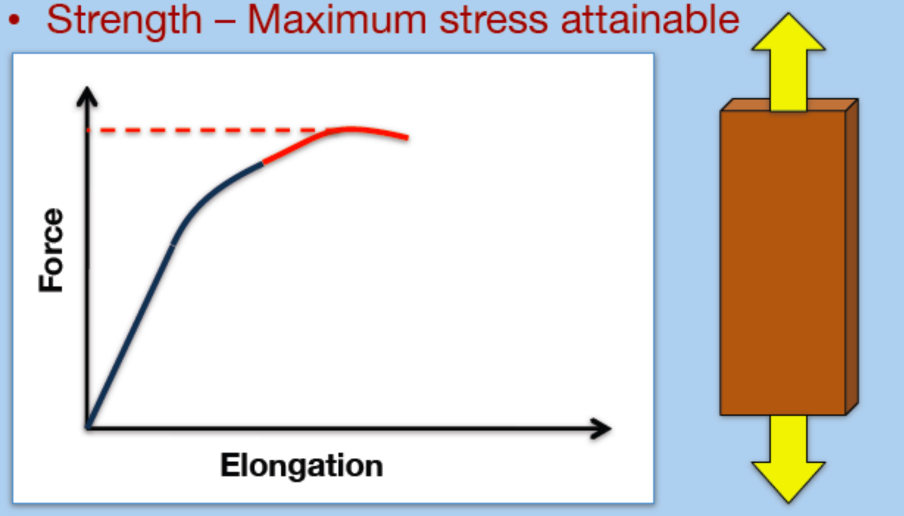
- Parmar, Kumar, Sastry. Strain localisation above the yielding point in cyclically deformed glasses. arXiv:1806.02464

Characterizing mechanical behavior of solids

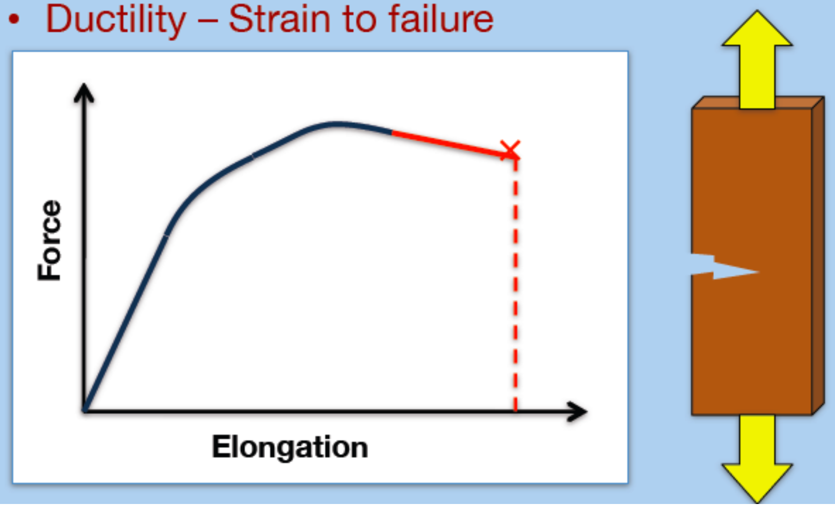
- Yield Stress – Onset of Irreversibility



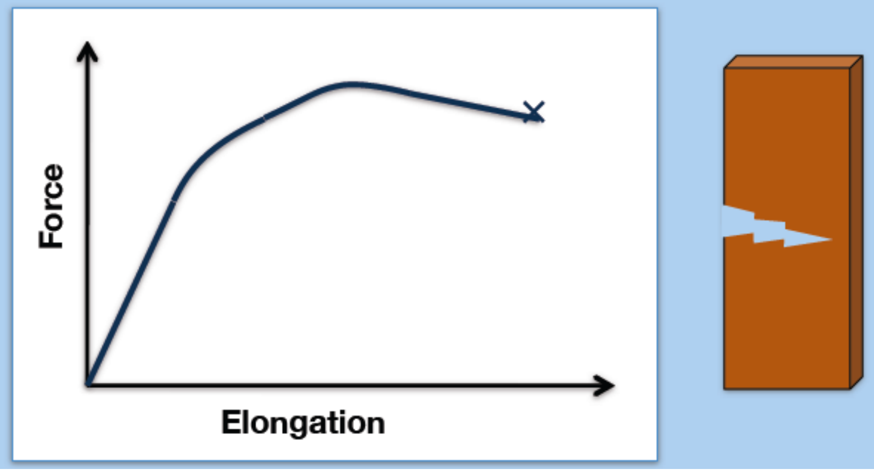
- Strength – Maximum stress attainable



- Ductility – Strain to failure



- Toughness – Energy expended per unit crack advance



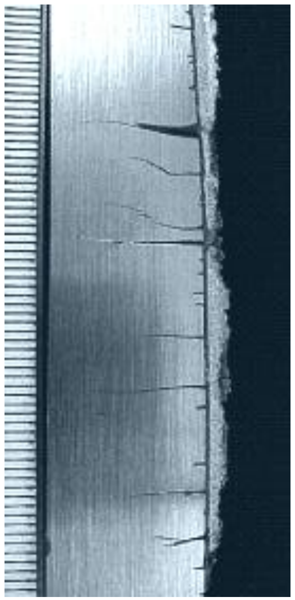
Michael Falk

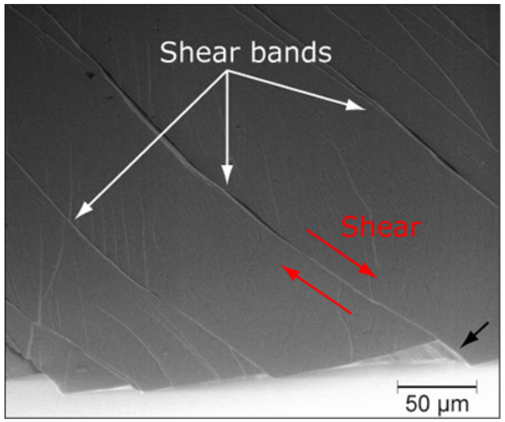
Yielding and Mechanical Failure

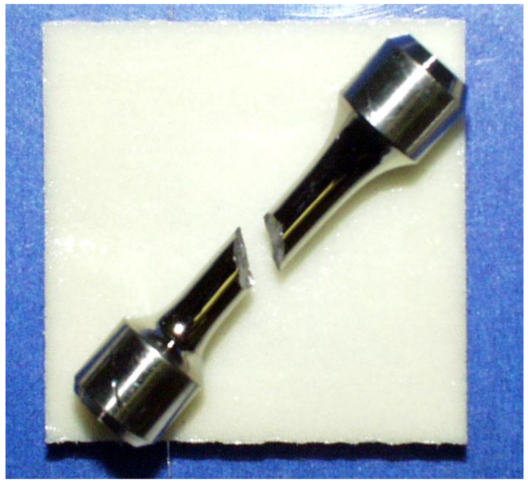
External stresses can cause (amorphous) solids to fail when deformed beyond a point of "**mechanical failure**".

Important for materials performance, and characterization.

Gorilla glass, metallic glasses, some recent important examples.

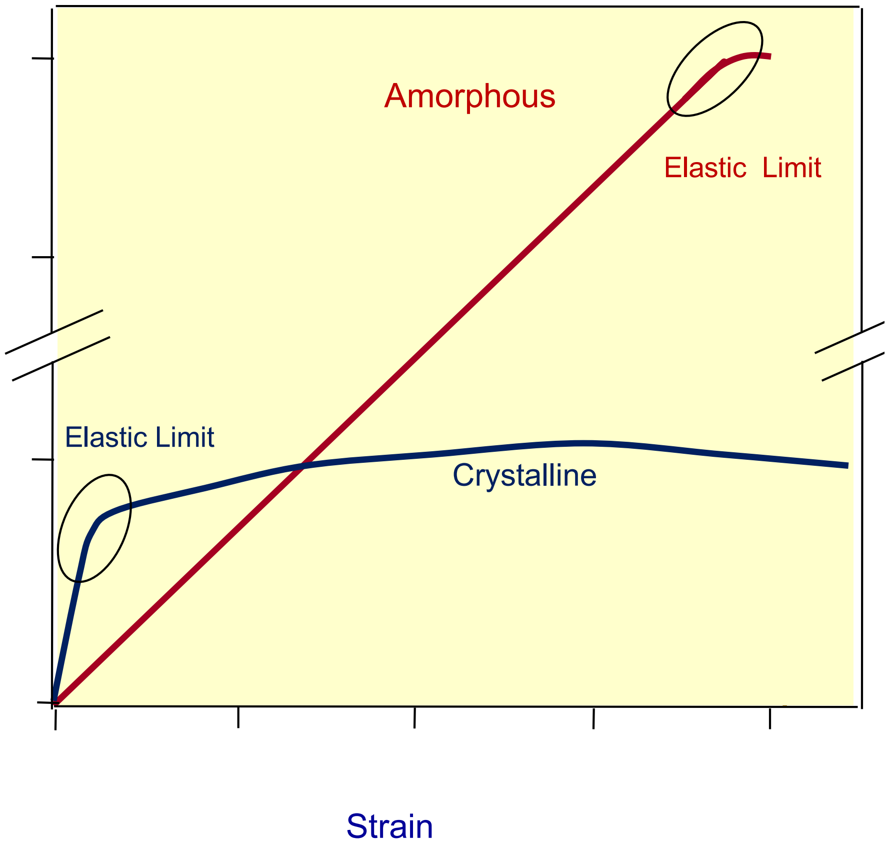


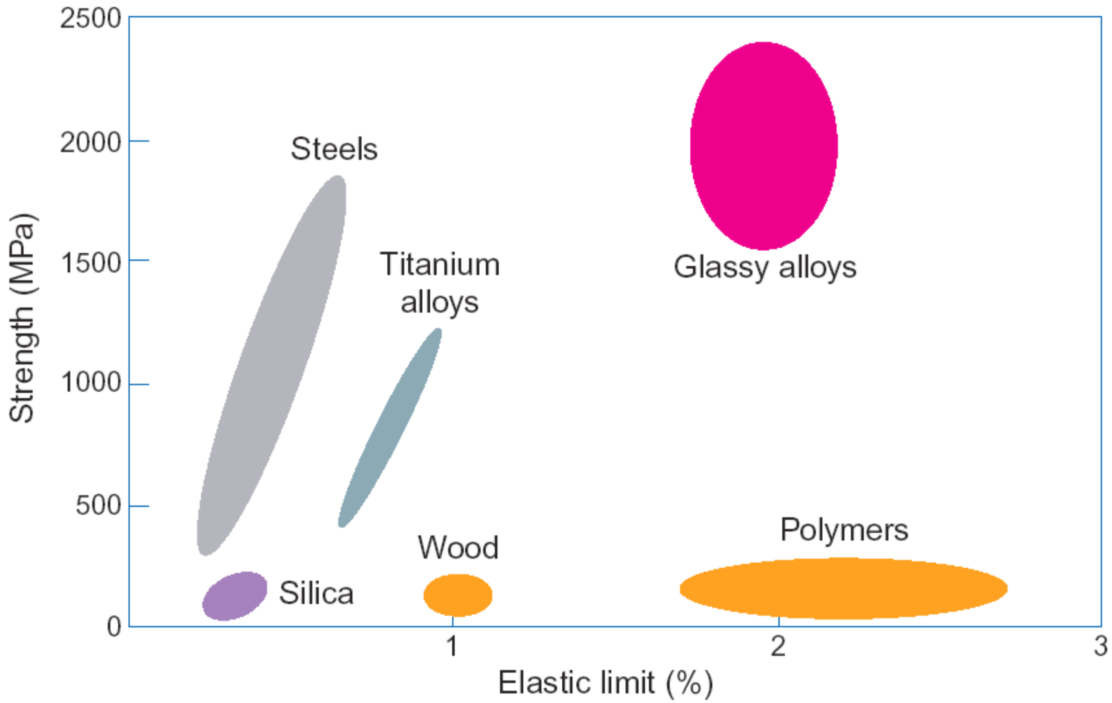




What is the microscopic description?

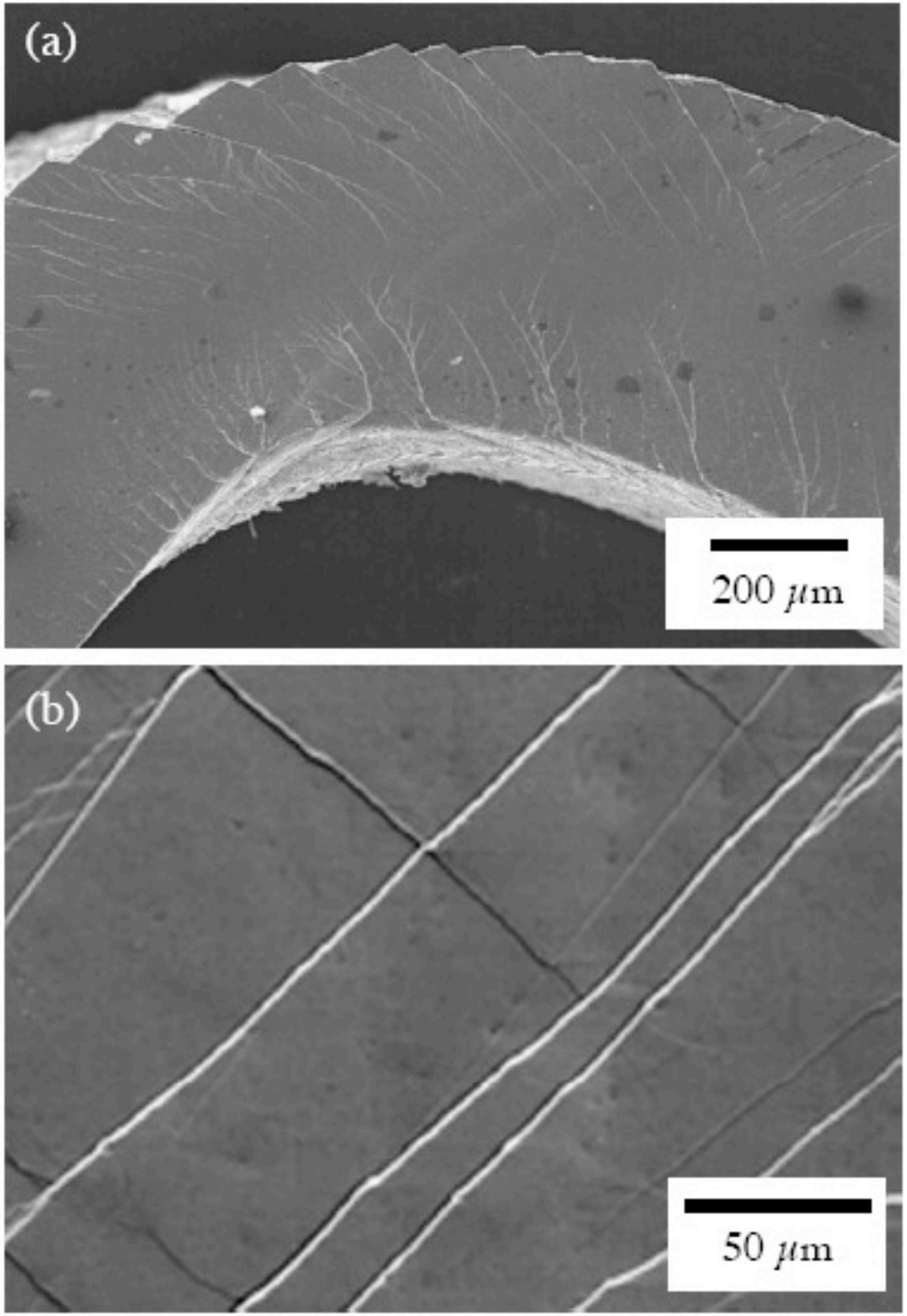
Amorphous Solids: Example - Metallic Glasses





Metallic glasses exhibit large yield strengths, and large yield strains.

Thanks: U Ramamurty



But exhibit brittle failure accompanied by shear localization (slip steps)..

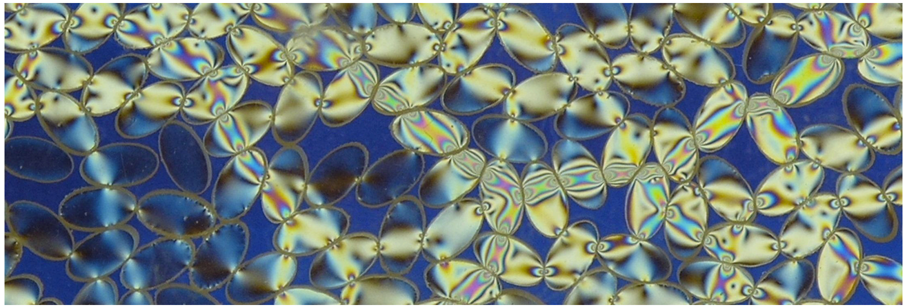
Parameters governing failure, and potentially their control, is critical for their applications.

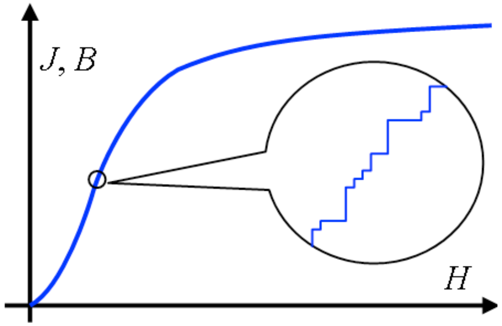
From: Schuh, Hafnagel, Ramamurty (2007)

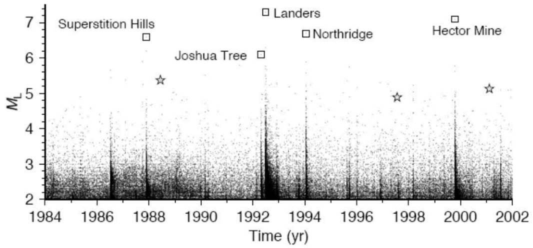
Yielding and Failure in disordered matter: Other examples

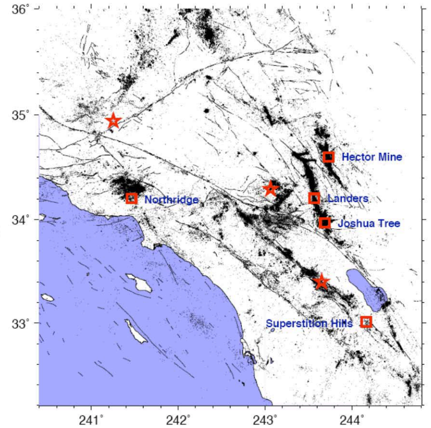
Related physics of intermittent, plastic, response in many disordered systems:

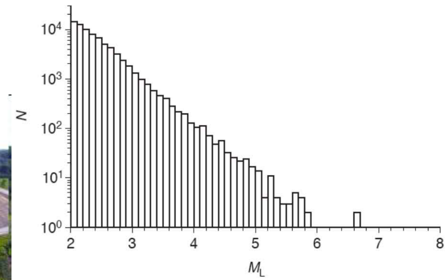
- Barkhausen noise in magnets
- Front propagation in disordered media
- Granular matter
- Landslides and avalanches
- Earth quakes

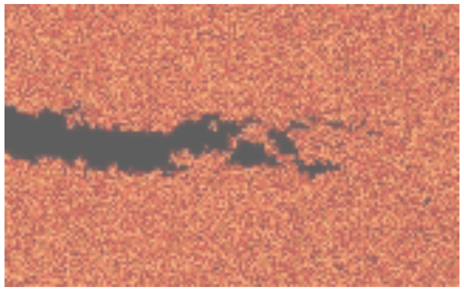










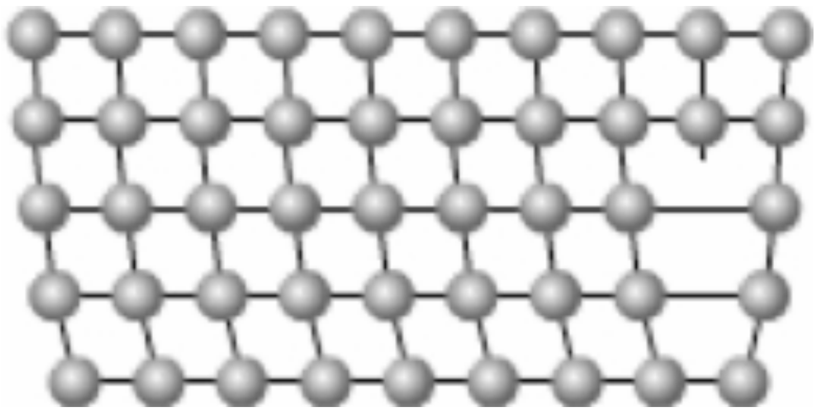


Mechanical behavior of solids

Response to mechanical stress is a fundamental characteristic of a solid.

Elastic and plastic responses – Elastic moduli, yield stress, strength of materials..

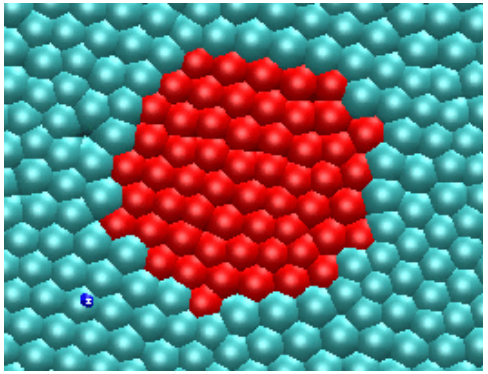
The process by which a crystalline solid responds to stress is understood in terms of the movement of dislocations – defects that are well defined and observable.



Thanks: Surajit Sengupta

The movies have been provided for teaching purposes by Professor Hideharu Nakashima (ageigz@mbox.nc.kyushu-u.ac.jp) of Kyushu University, Japan.

Mechanical behavior of amorphous solids



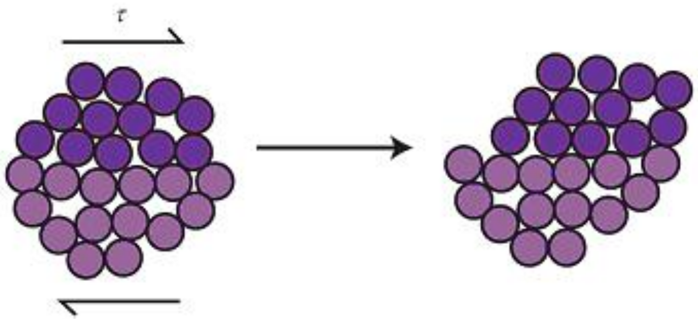
From: Peter Sollich

• Amorphous solids do not have regular translational order, and correspondingly no equivalent of dislocation defects.

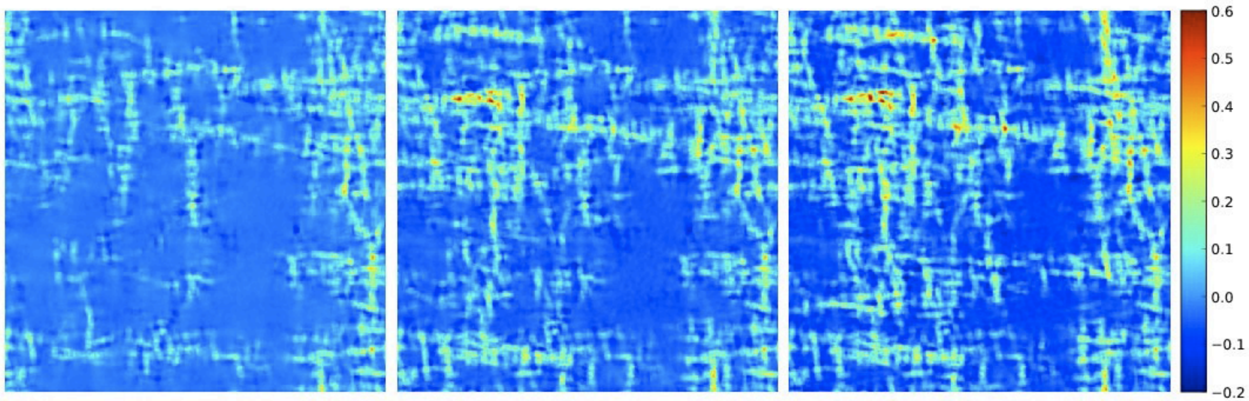
• Deformation mechanism involves localized rearrangements, and avalanches of correlated (or triggered) deformation events.

• What is the description of the transition to the state of plastic flow?

• Wide range of materials, and responses.



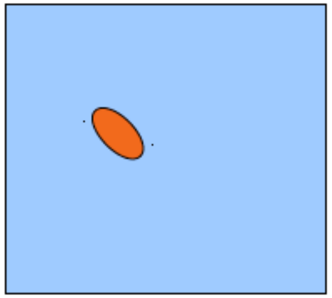
From Schuh et al 2007 [from Argon, Spaepen]

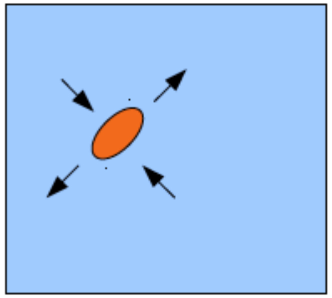


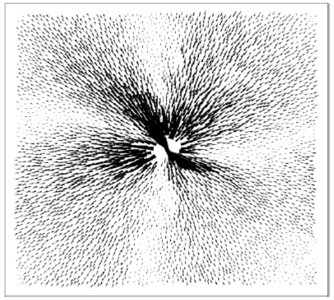
[Lemaitre, Caroli 2009]

Plastic rearrangements and interactions

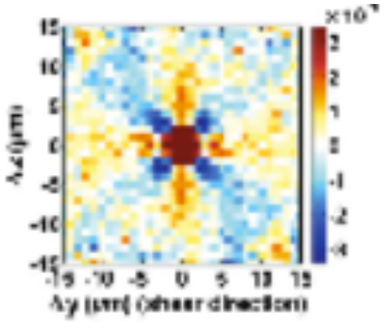
A local transformation embedded in an elastic medium leads to long range strain/stresses (Eshelby 1957), interactions:



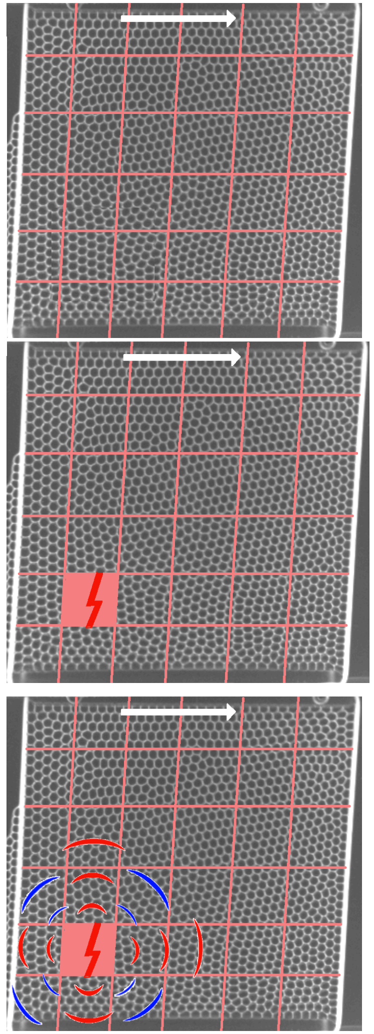




PRE 74, 016118 (2006)



Jensen et al PRE 2014



Barrat

$$G(r,r') \sim \frac{\cos(4\theta)}{|r-r'|^d}$$

Quadrupolar propagator for stress redistribution.

Observed in simulations and experiments.

Generation of stress field from a local plastic event.

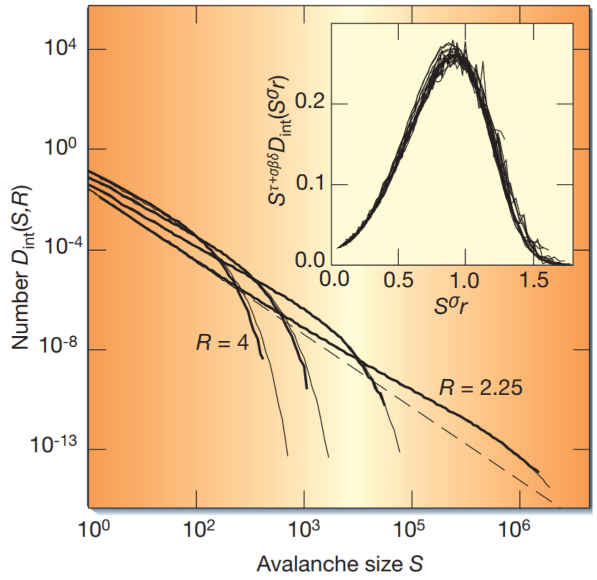
Redistributed stresses trigger other events.

Avalanches, yielding..

Crackling Noise: RFIM

Many systems crackle; when pushed slowly, they respond with discrete events of a wide range of sizes.

Examples: Earthquakes [motion of tectonic plates], candy wrapper [on crumpling] or a magnatic material under changing field.



Field on magnatic domin under an external field (H(t)):

$H(t) + \Sigma_j S_j + h_i$

h_i : a random field for each domain with variance "R".

Flipping of spins can initiate avalanches.

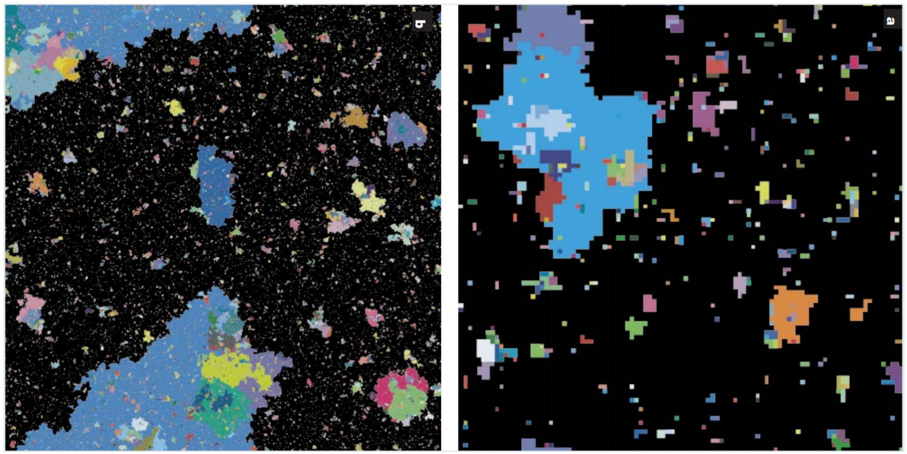
If "R" is large (or h>>J) most domains flip independently: all the avalanches are small (small popping noise).

For sufficiently large H(t): large scale avalanches.

A R – H phase diagram with a critical point.

Sethna et al Nat Rev. 2001

Cross-sections of the avalanches during the magnetization, various color: avalanches



Depinning

Depining of an interface moving in an interface (fluid, etc) a problem of broad interest.

Pinning arises from disorder. Depinning as a result of external drive.

Depinning model
$$\partial_t h(x,t) = \nu \partial_x^2 h - \partial_h V(x, h(x,t)) + f$$

- Pinning is induced by quenched disorder (V).
- Stops the motion of driven elastic manifolds for applied forces **f** below a critical value f_c.
- The avalanche size defined as the area swept by the interface in a burst.
- Avalanche size diverges at depinning.

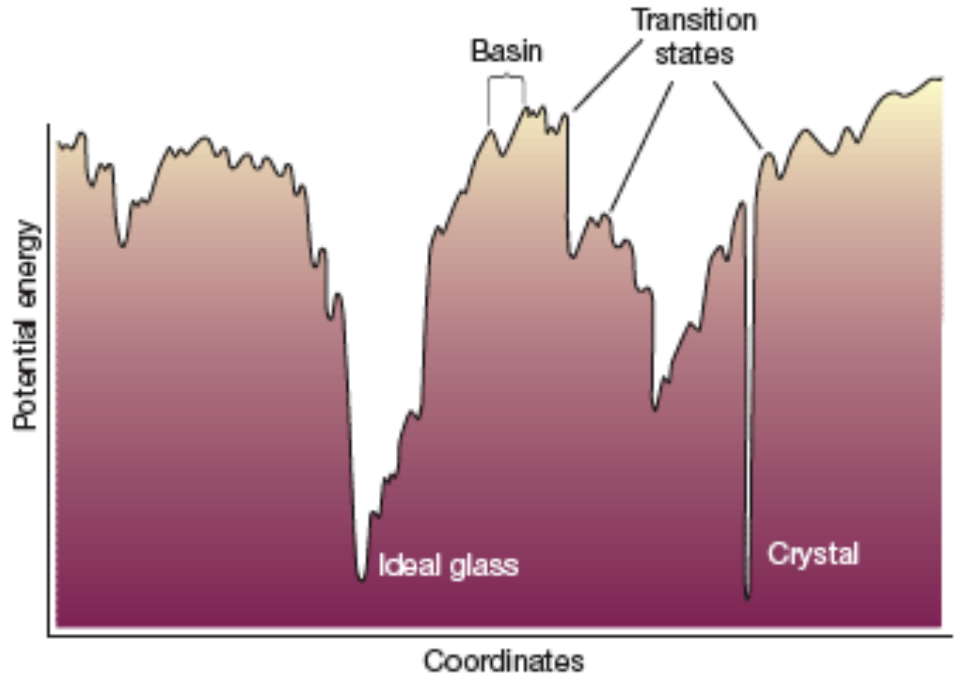
What we do: Approach and Questions

- Mechanical response to affine, shear deformations studied by analyzing the modification of the landscape, and transitions between minima, through the **AQS** (Athermal Quasi Static) protocol.
- Cyclic shear deformation of model glasses.
- Amplitude of shear deformation the only control parameter.
- Limitation: No information on the interplay between relaxation processes and instabilities triggered by deformation. But useful insights obtained.
- Simulations done also at finite shear rate and temperatures for comparison.

Focus for this talk:

The Yielding Transition.

Shear banding.



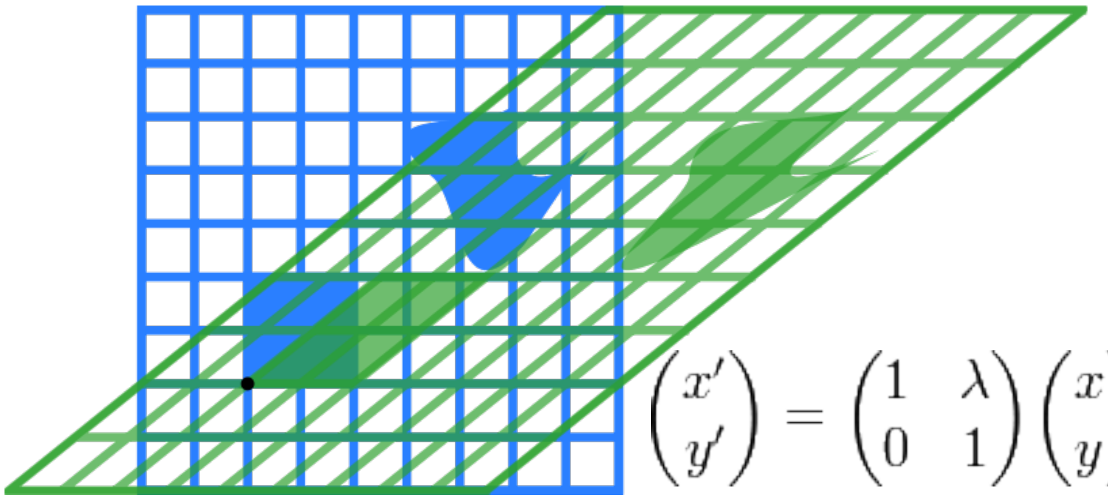
Questions/Issues

- The character of avalanches before yielding and after yielding.
- The nature of the yielding transition. Is it a sharply defined transition?
- Strain localization above yielding.
- Relaxation/annealing effects under cyclic loading.

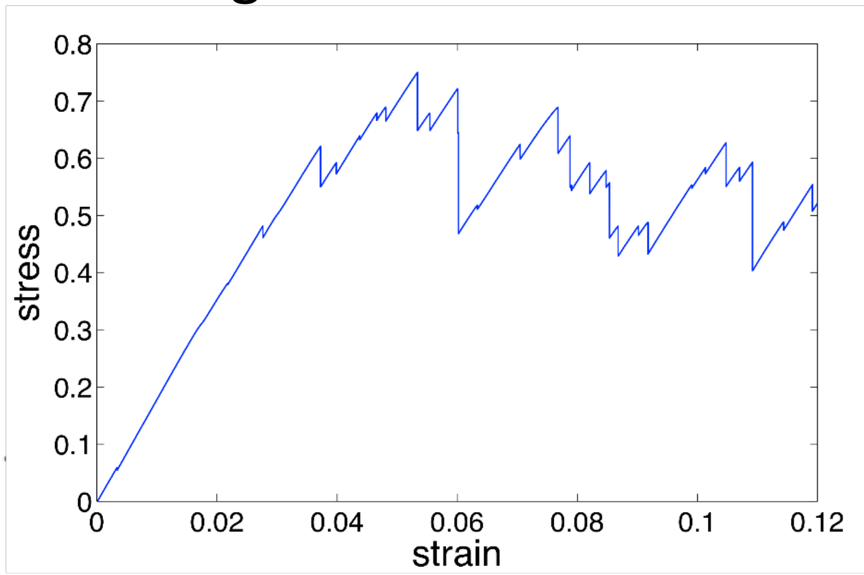
Computer simulations of deformation of model glasses in search of some answers

Athermal Quasi Static Deformation

1. Subject energy minimum structures to shear deformation.
2. Minimize the resulting deformed structure subject to suitable (Lees-Edwards) boundary conditions.
3. Deformation strain increased quasi-statically.
4. The procedure produces a sequence of configurations that are always energy minima.
5. Continuous change of energies interrupted by discontinuous change.
6. Discontinuous changes correspond to rearrangements.

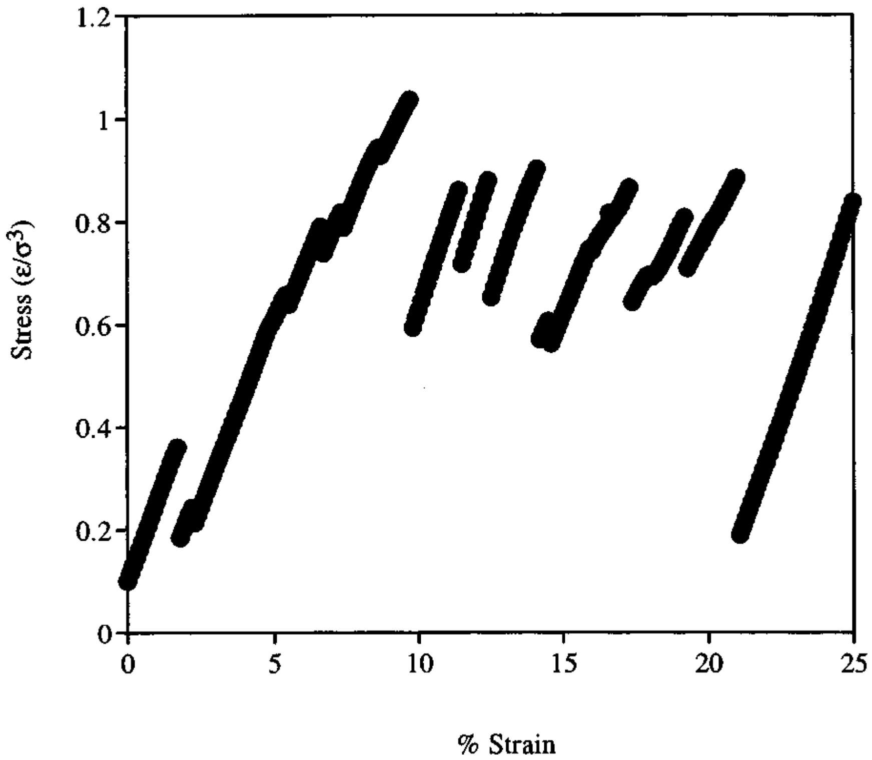


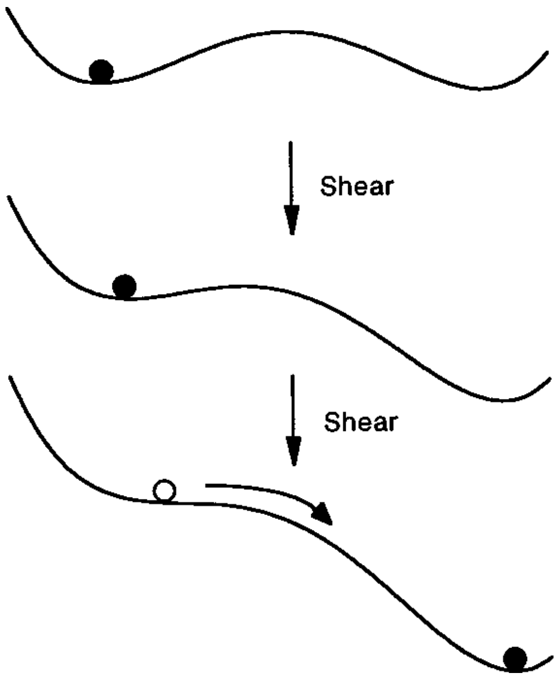
$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} 1 & \lambda \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$



Mechanical deformation of model glasses

Discontinuous changes in stress from destabilization of minima.



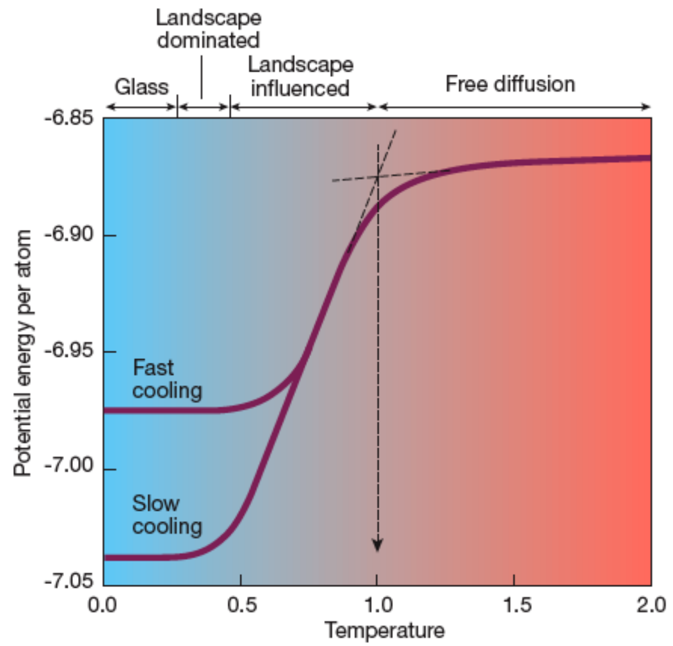


Malandro and Lacks 1999

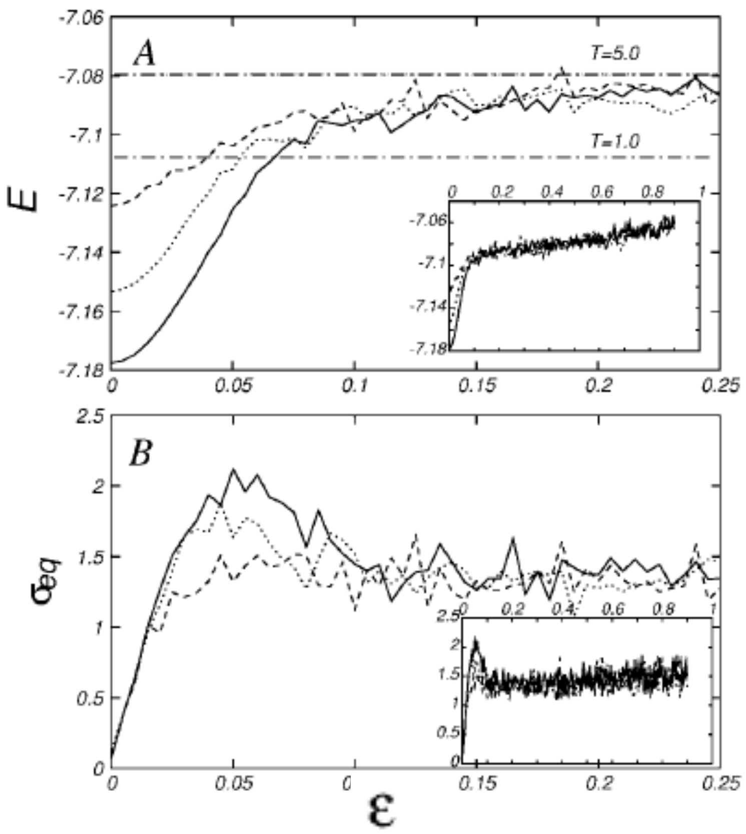
Mechanical deformation leading to yielding..

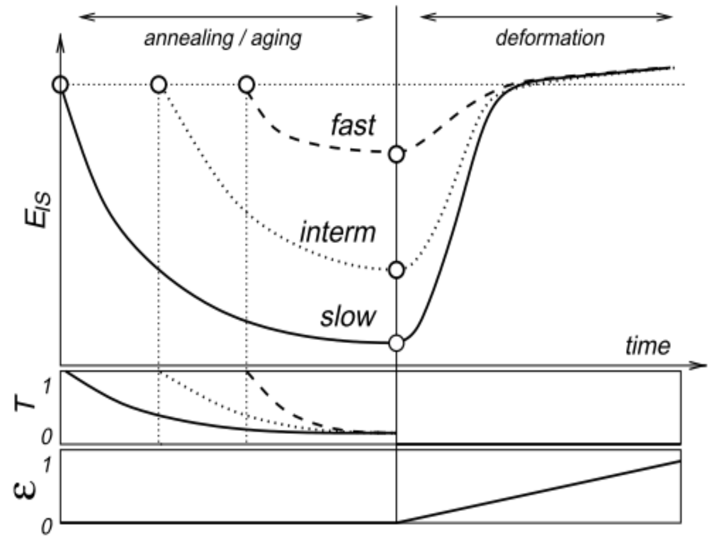
Early studies:

1. Deeper energy minima are sampled at lower temperatures.
2. Upon shearing, the energy of the minima rises to those at very high temperatures.
3. Deformation induced 'rejuvenation'



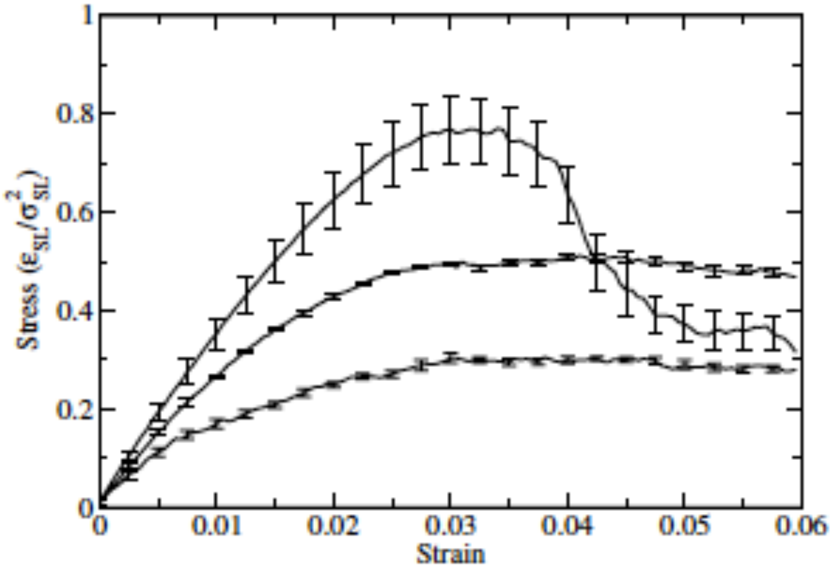
Sastry et al Nature 1998





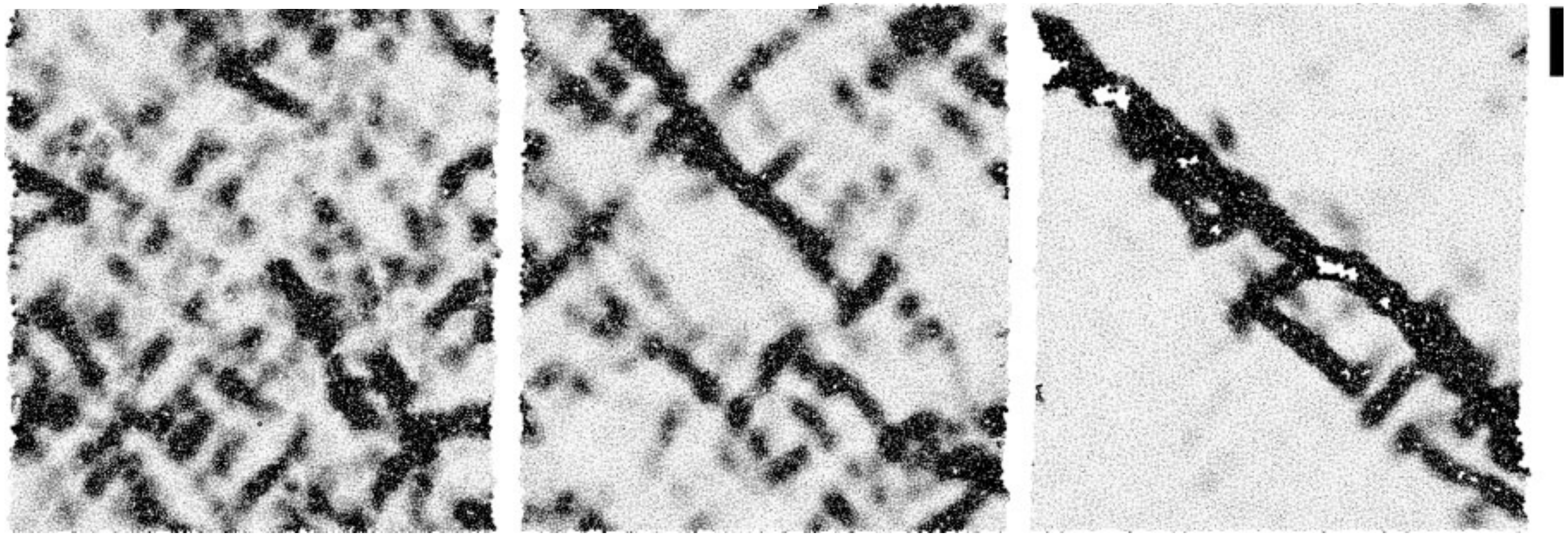
Utz, Debenedetti and Stillinger and Utz, 2000

Strain Localization



Strain localisation depends on degree of structural relaxation prior to shear deformation.

Shi and Falk (2005)

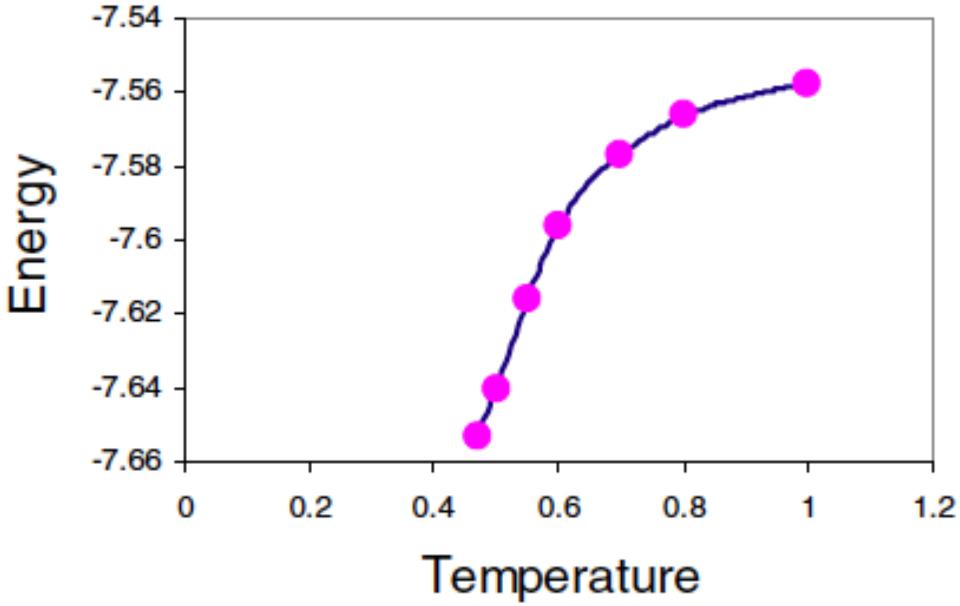


Related: Transient shear bands in flow (Srivastav et al 2016, Vasisht et al 2017)

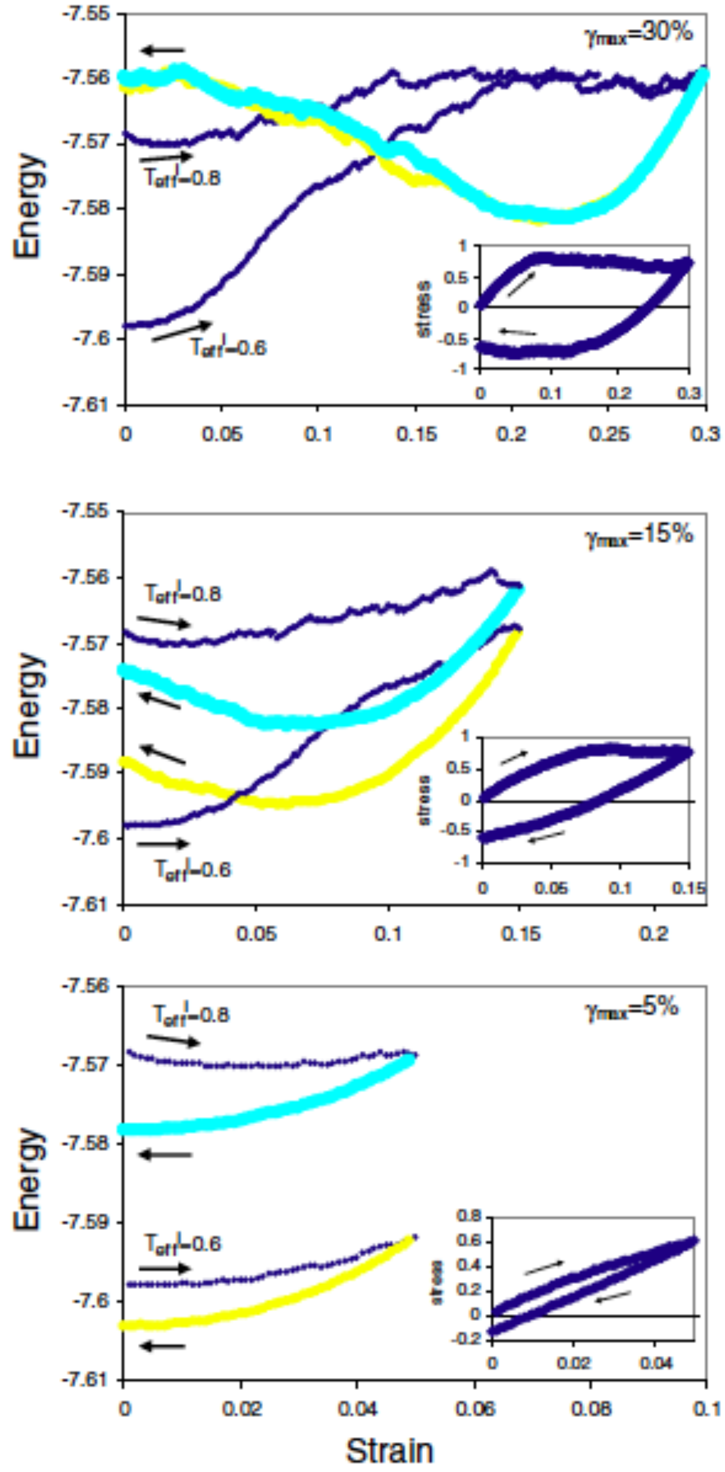
Somewhat more complicated picture when a forward and back cycle of strain is applied:

The nature of change (aging or rejuvenation) depends on amplitude of strain and the initial state..

What happens if this cycle is repeated?



Lacks and Osborne, PRL 2004.



Cyclic Deformation: Schematic

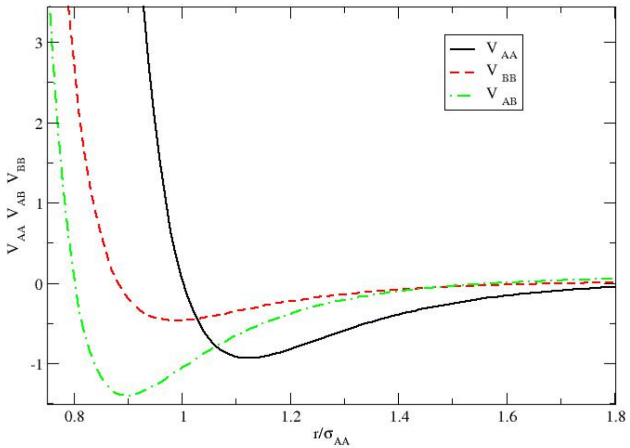
Shear deformation modifies the potential energy landscape and destabilizes the system, eventually leading to irreversible rearrangements.

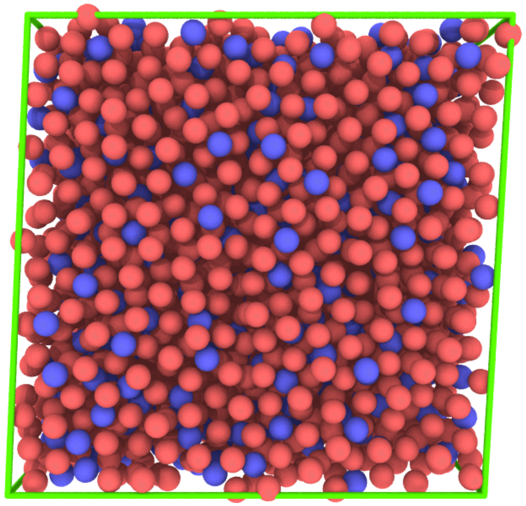
How does such deformation modify the properties of the glasses?

Simulations of oscillatory strained binary Lennard-Jones (LJ) solids

Kob-Andersen binary glass forming model liquid.
(Constant Volume AQS)

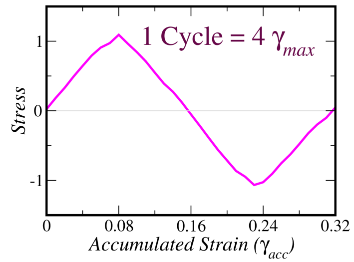
$$\phi_{ij}(r) = 4\epsilon_{ij}\left(\frac{\sigma_{ij}^{12}}{r^{12}} - \frac{\sigma_{ij}^{6}}{r^{6}}\right)$$





$0 \rightarrow \gamma_{max} \rightarrow 0 \rightarrow -\gamma_{max} \rightarrow 0$

Different system sizes: 2000, 4000, 8000, 16000, 32000, 64000, 128000 and 256000.



Two starting temperatures: **1** (poorly) & **0.466** (well annealed glass)

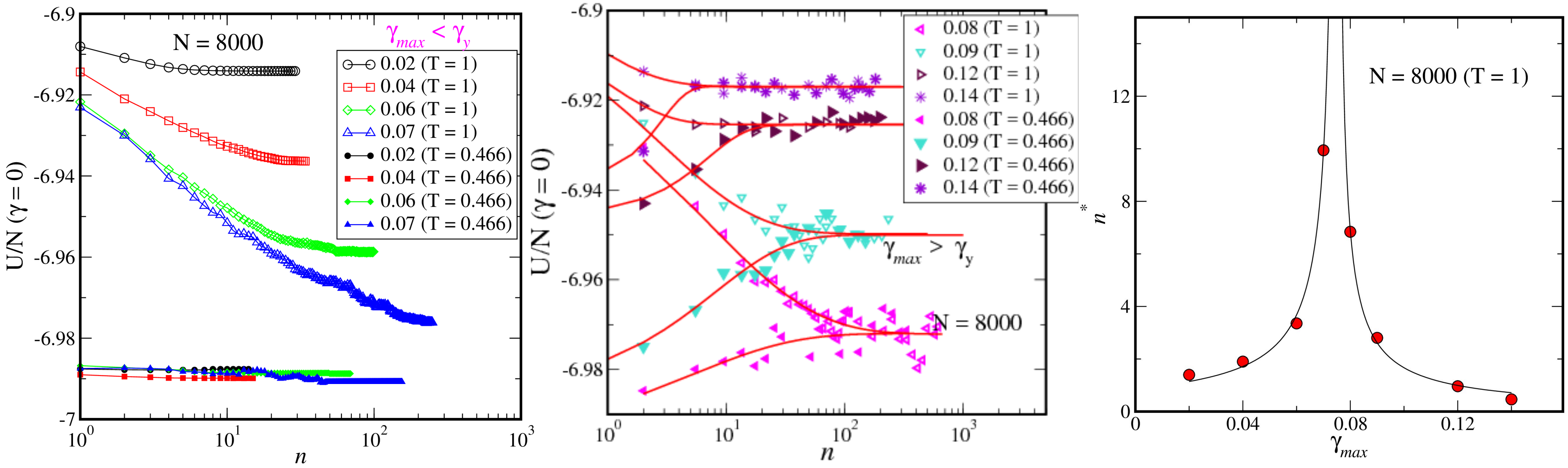
Cyclic shear for range of γ_{max} values with strain step $d\gamma = 2\times10^{-4}$.

Each $\gamma = 0$ configuration labeled with the *accumulated* strain $\gamma_{acc} = \sum d\gamma$

These **stroboscopic** configurations were used to compute various quantities, i.e. energy, MSD etc …

Potential Energy vs. Cycle Number

The potential energy per particle reaches a plateau that
(a) Depends on γ_{max} **only** at large values of γ_{max}.
(b) Depends on γ_{max} and initial state for small γ_{max}.



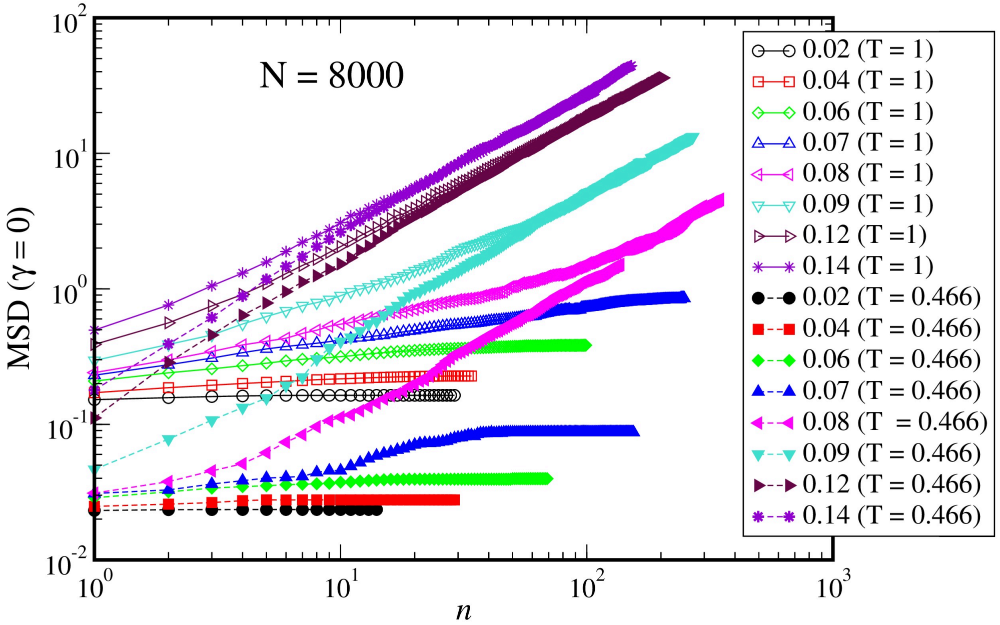
- Aging/rejuvenation depends on strain amplitude and initial annealing on the glasses.
- Relaxation to the steady state **becomes more sluggish as γ_y is approached.**

Change in behavior across a critical strain amplitude γ_c

Mean Squared Displacement vs. Cycle #: Diffusion Coefficient

Depending on γ_{max} systems are either diffusive or non-diffusive.

In the diffusive regime, asymptotic slopes depend only on γ_{max}.



$$\mathrm{MSD} = D\gamma^*_{acc}$$

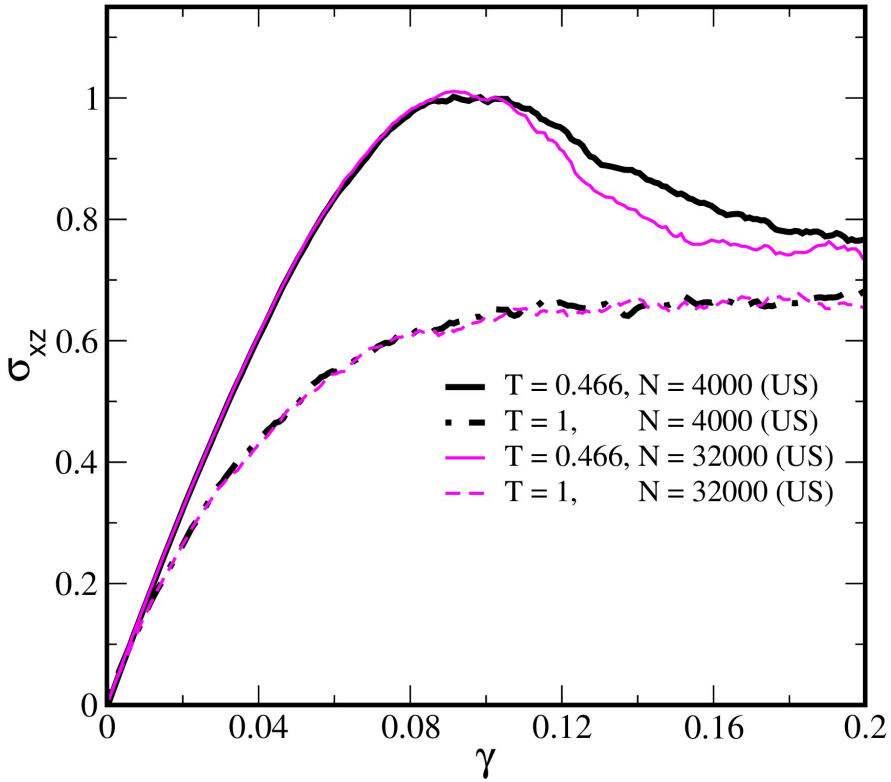
The diffusion coefficient vanishes below a finite value of γ_{max}

[How? Will be addressed later]

Critical γ_{max} a function of system size… but approach finite value asymptotically.

Non-equilibrium transition from localized to diffusive regimes!

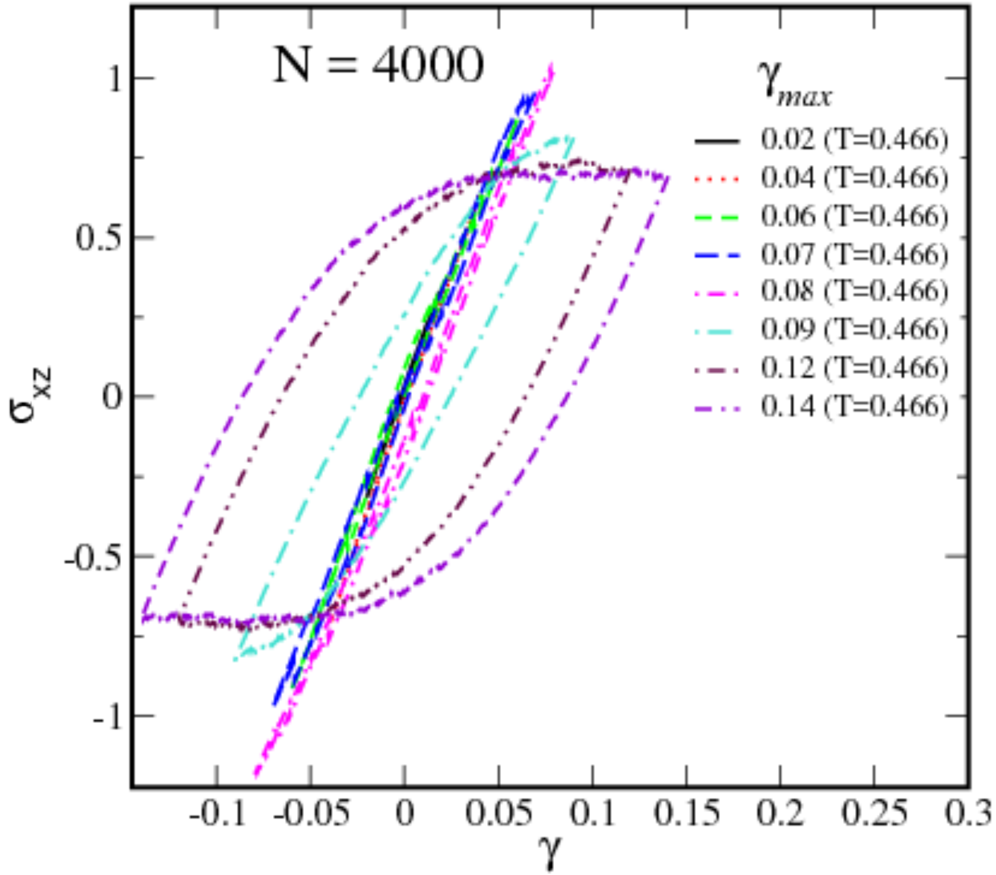
Yielding
Uniform Shear



There is **no sharp point** to identify from uniform shearing.

Significant **sample** (annealing) **dependence**.

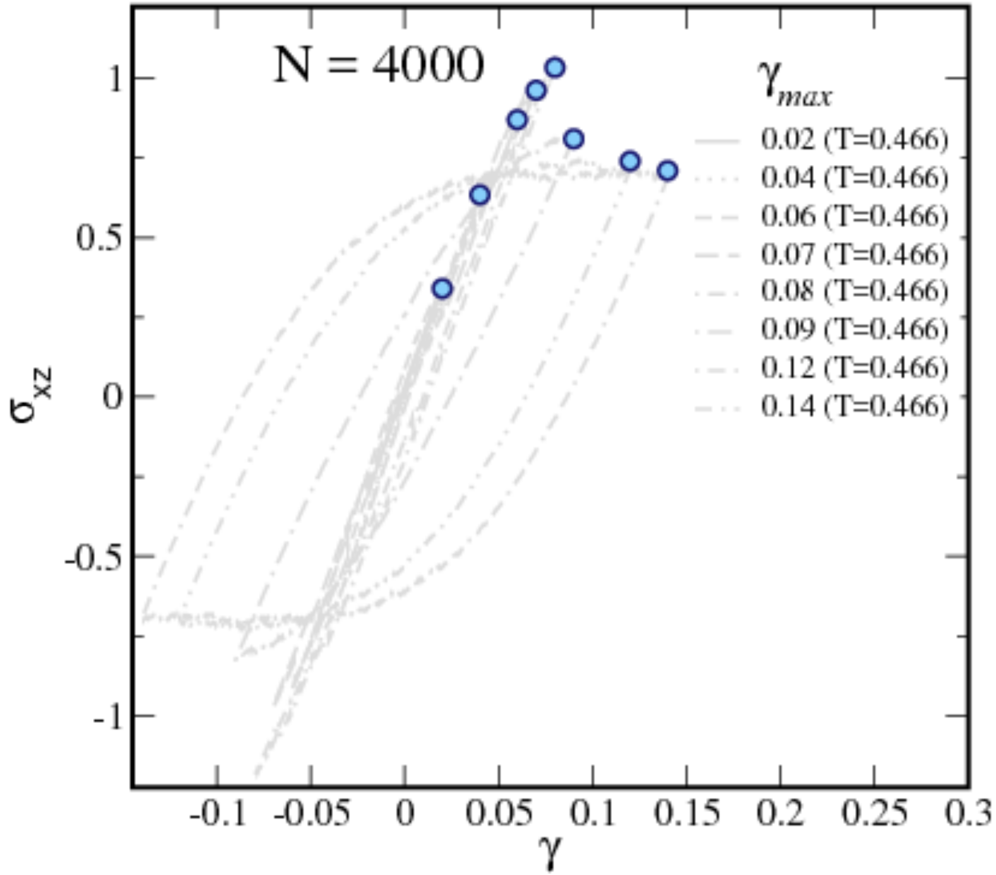
Yielding: Oscillatory shear



Oscillatory shear provides a better characterization of the transition.

We focus on maximum stress during cyclic shear..

Yielding: Oscillatory shear



Oscillatory shear provides a better characterization of the transition.

We focus on maximum stress during cyclic shear..

In **uniform shearing** (US), there is a clear difference in the stress-strain curves depending on the prior annealing of the glasses.

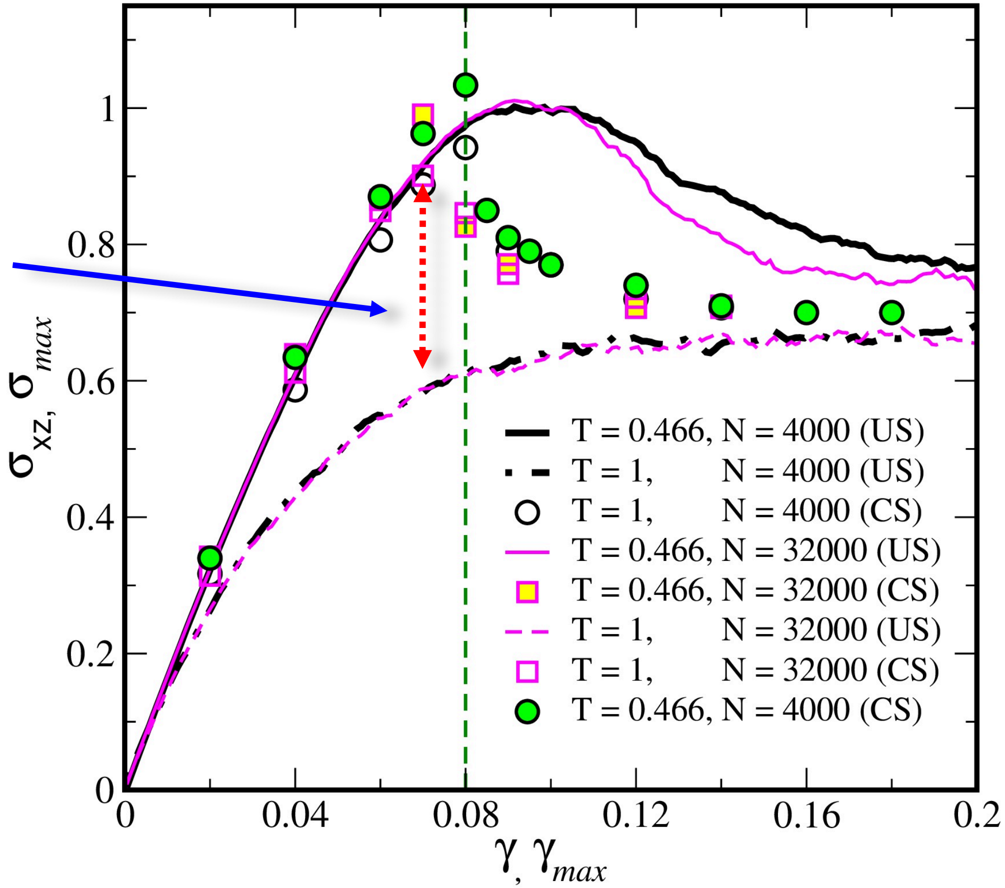
For **cyclic shear** (CS) qualitatively the same behavior regardless of initial sample conditions.

A sharply defined, discontinuous yielding transition.

work hardening !!

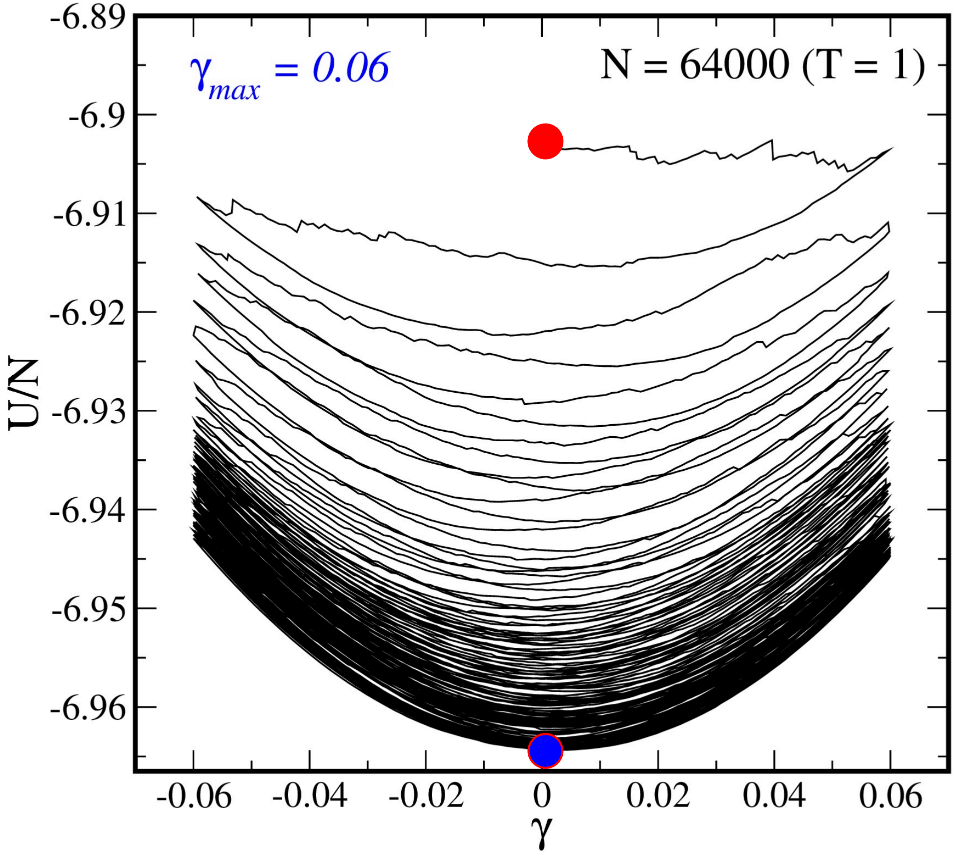
Oscillatory shear provides clear signature of yielding.

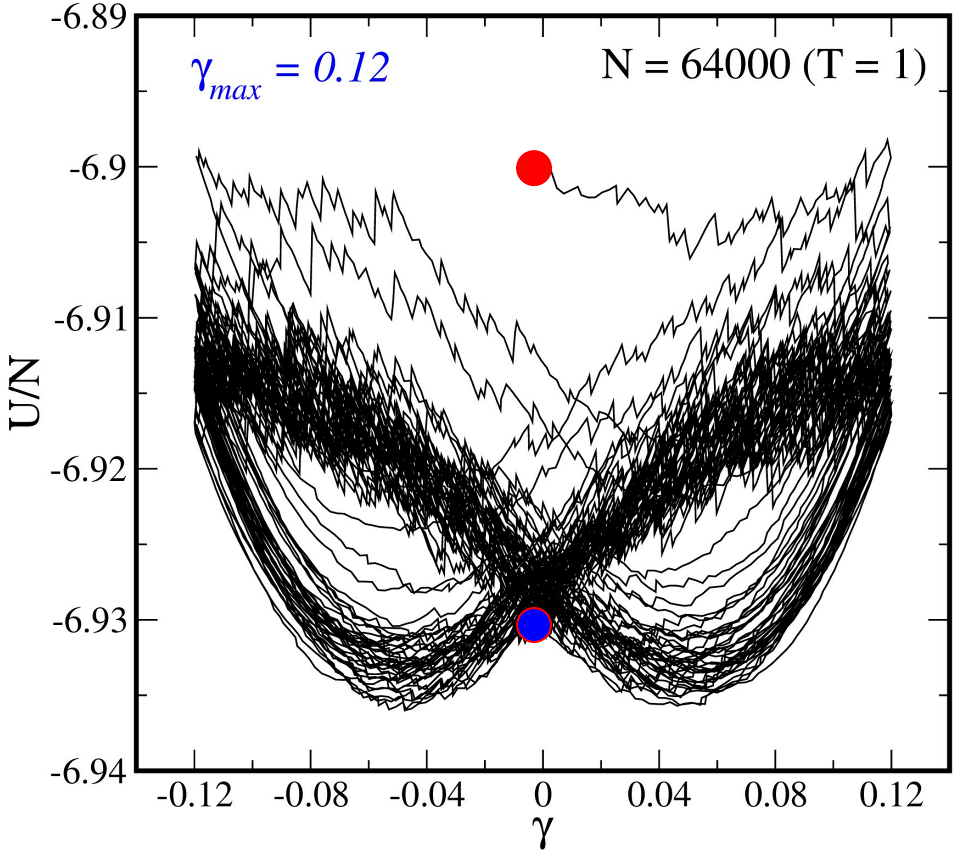
Pointers for thermo-mechanical processing of metallic glasses?



Ref: Jaiswal et al 2016, Parisi et al 2017, Osawa et al 2018, Popovic et al 2018..

Evolution of energy with cycles

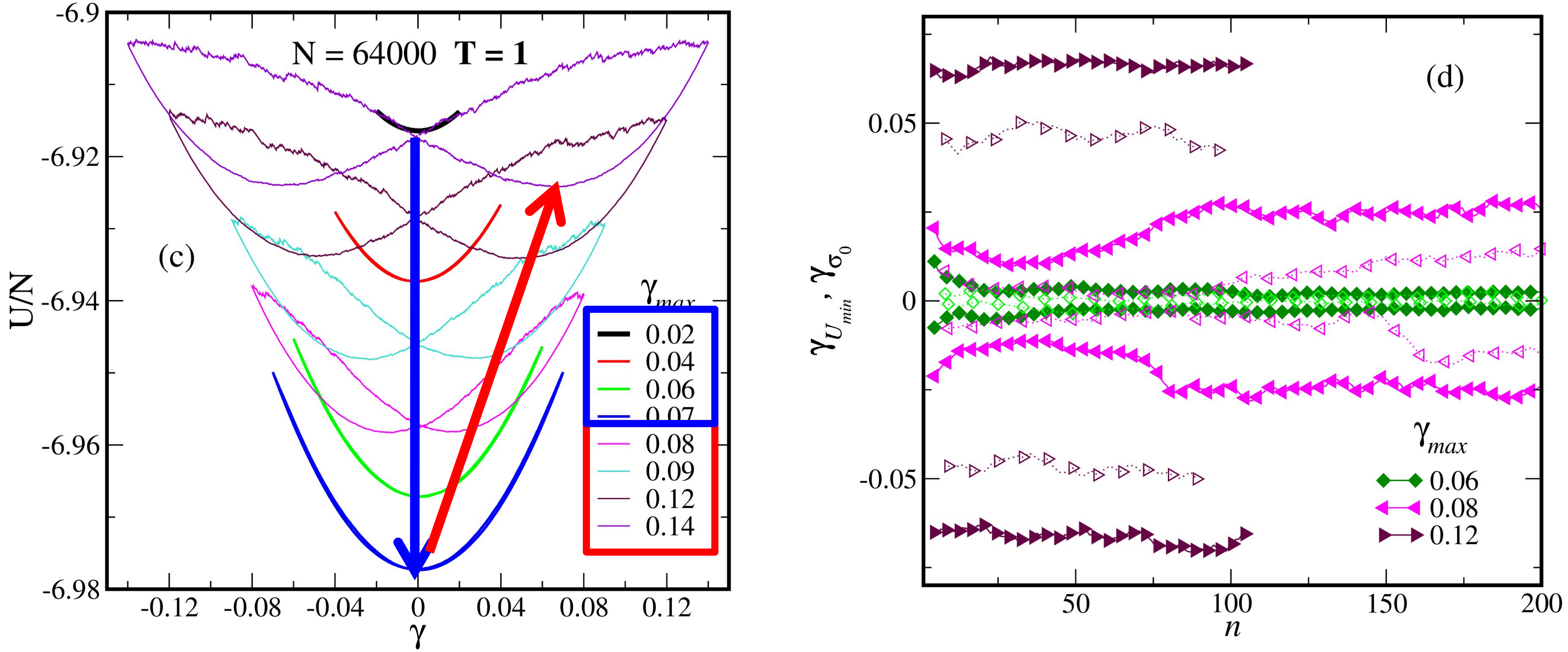




•For γ_{max} = 0.06 (i.e. $\gamma_{max} < \gamma_y$) the energy approaches to a single minimum at γ = 0, but

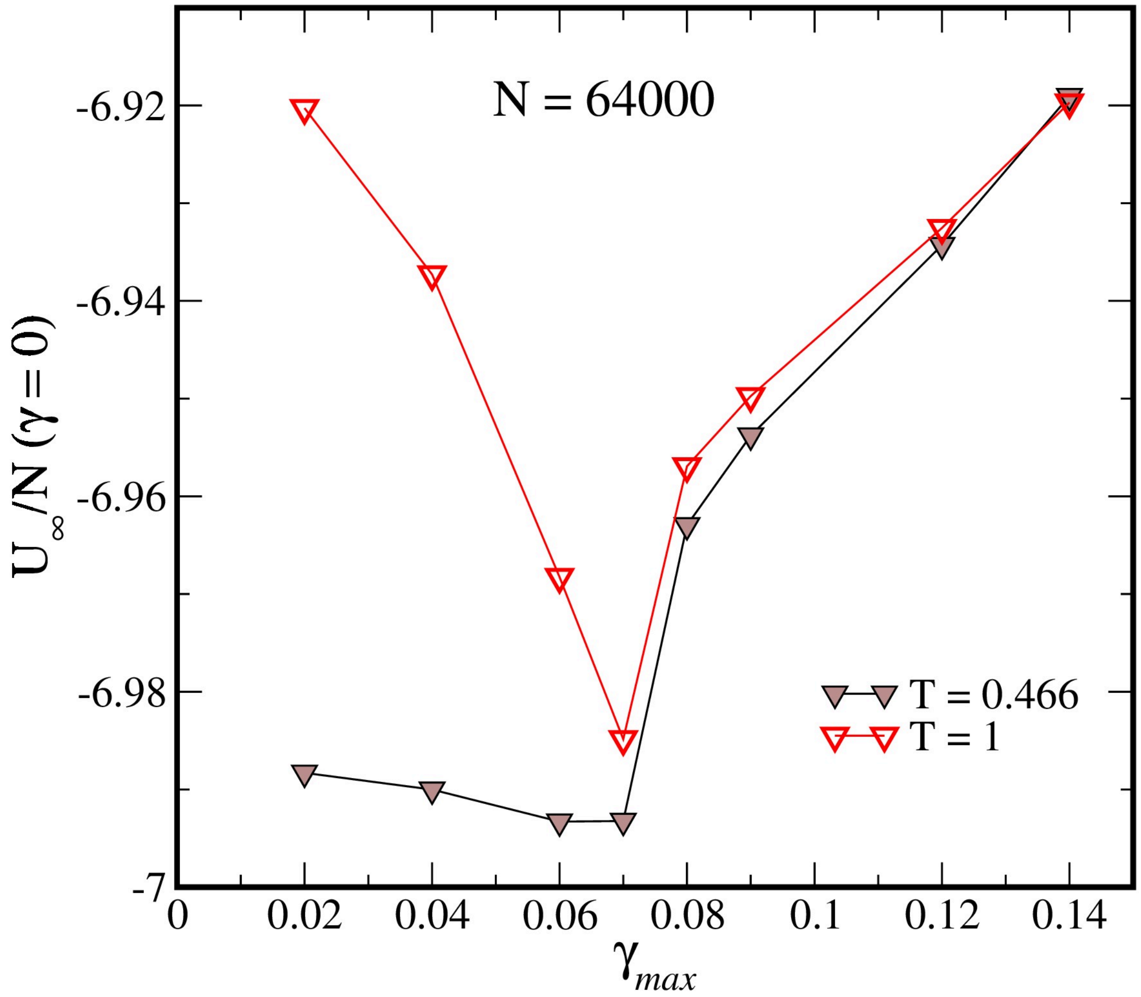
•Energy bifurcates into two minima (for γ_{max} = 0.12 (i.e. $\gamma_{max} > \gamma_y$)) at finite strain.

Evolution of energy with cycles



- Energy vs. strain in the steady states, displaying a bifurcation in the strain corresponding to minima in energy at the yielding transition between γ_{max} = 0.07 and 0.08.
- Evolution of strain values for energy minimum and zero-stress states indicate transition.

Asymptotic energy *vs.* strain amplitude

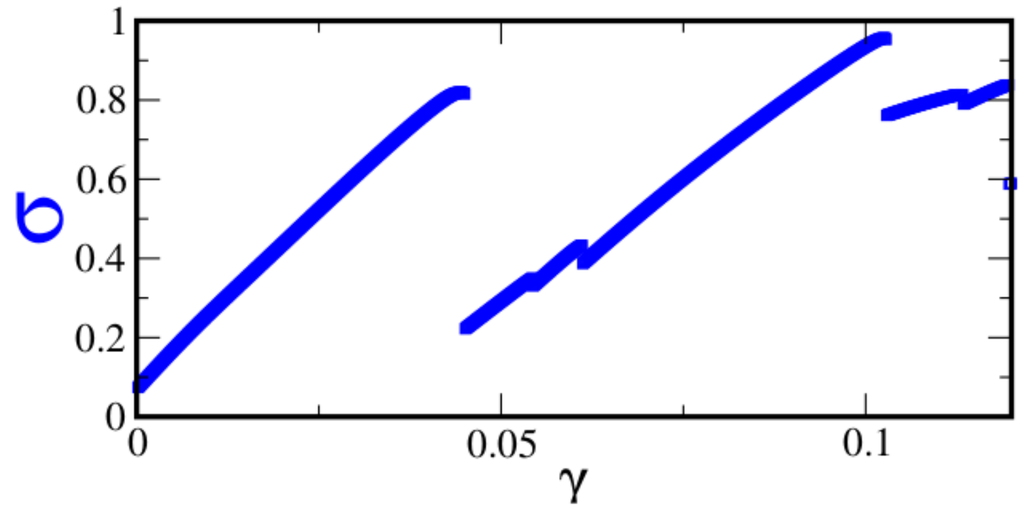


Better annealing close to the transition.

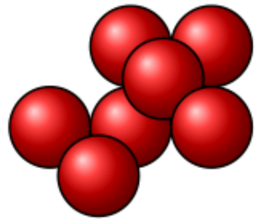
What is the nature of the energy increase beyond the yielding transition?

Energies of stroboscopic configurations decrease with γ_{max} till the yield strain is reached, after which they increase with γ_{max}.

Avalanches



Plastic Instabilities:



Stress Released

Energy Dissipated

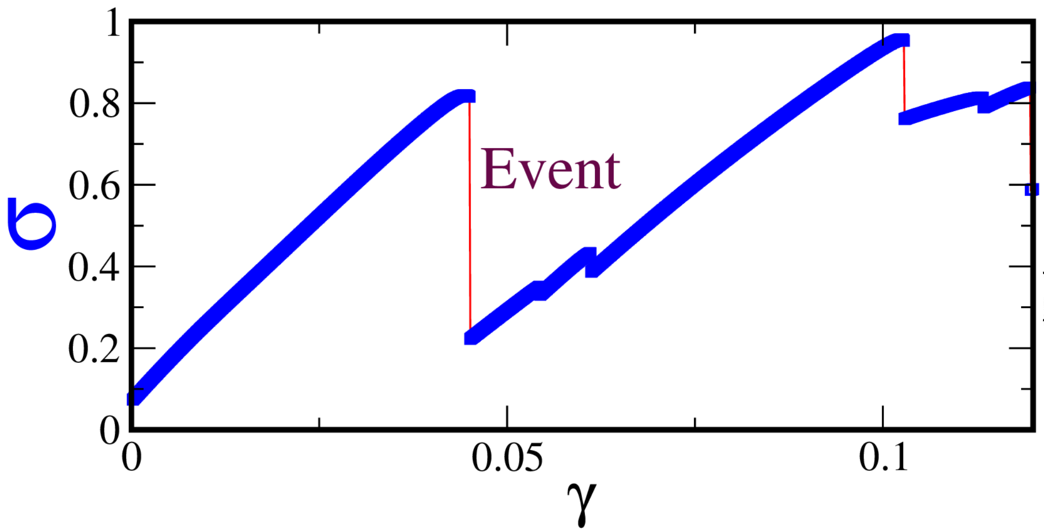
Clusters of Active Particles

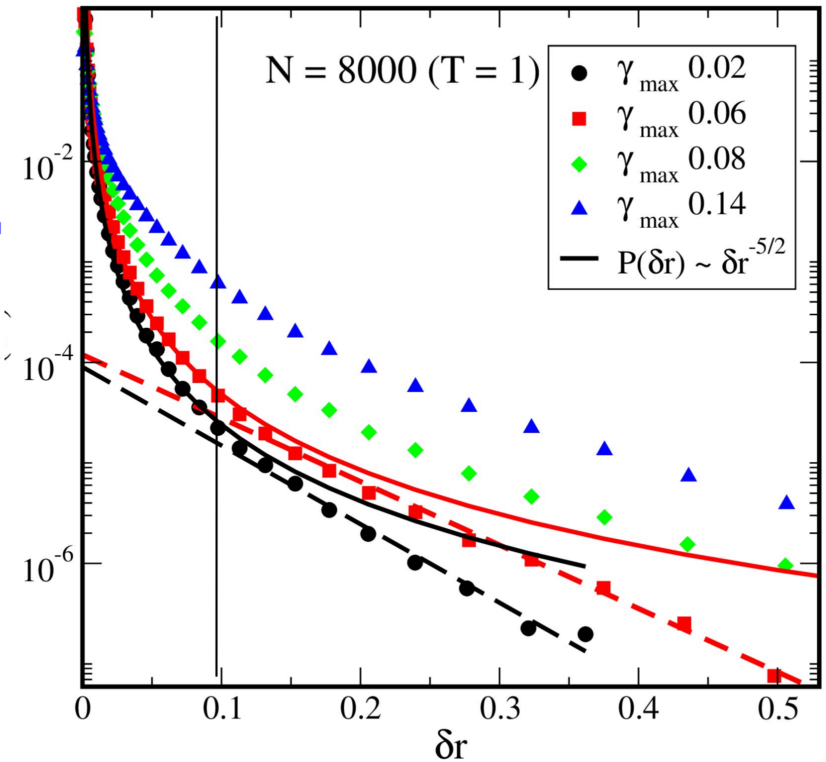
Avalanches

Definitions:

Active particles: Particle is active if moved beyond $0.1\sigma_{AA}$ cutoff in the event.

Clusters: Active particles with connectivity of $1.4\sigma_{AA}$ (the first coordination shell)





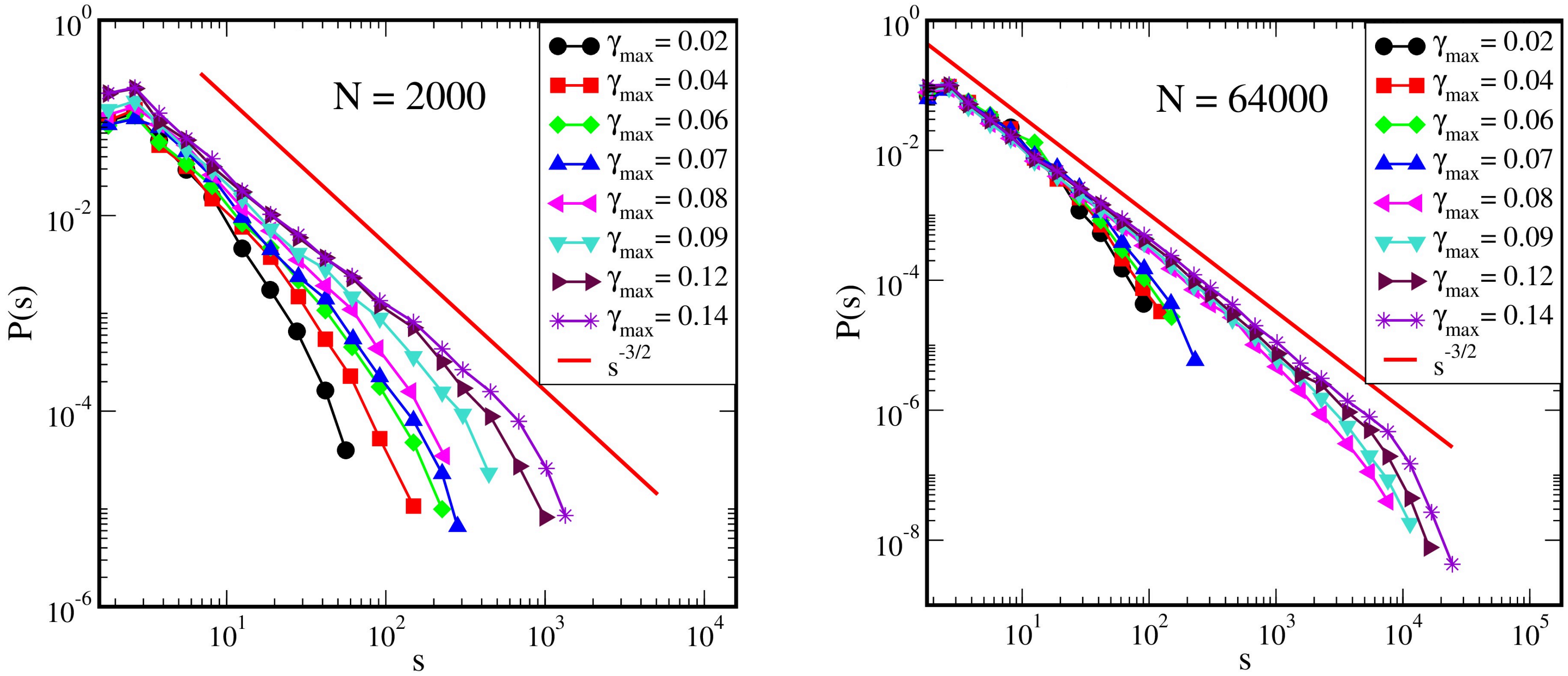
We study statistics of:

(a) **Cluster sizes** (b) **Energy drops**

How do events (avalanches) evolve with amplitude of strain?

Do they capture the approach to the yielding transition?

Distributions of Avalanche Sizes



- For N = 2000 displaying a power law with a cutoff that grows with γ_{max} but **does not indicate sharp changes** at yielding.
- For N = 64000 displaying a **sharp increase** in the cutoff size across the yielding transition. Power law regime with power 3/2.

System size effects are important!!

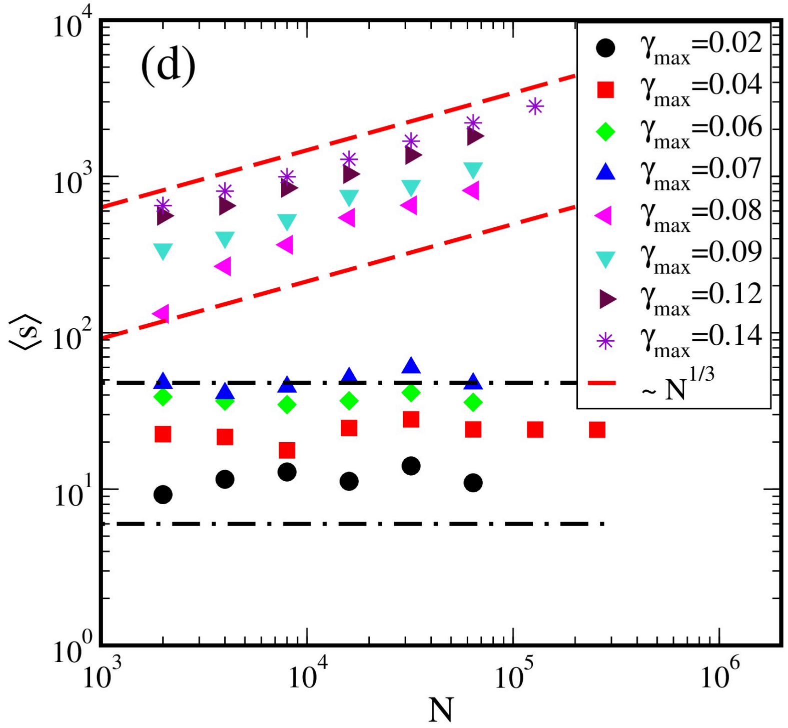
Avalanche size *vs.* Strain Amplitude System Size Effects

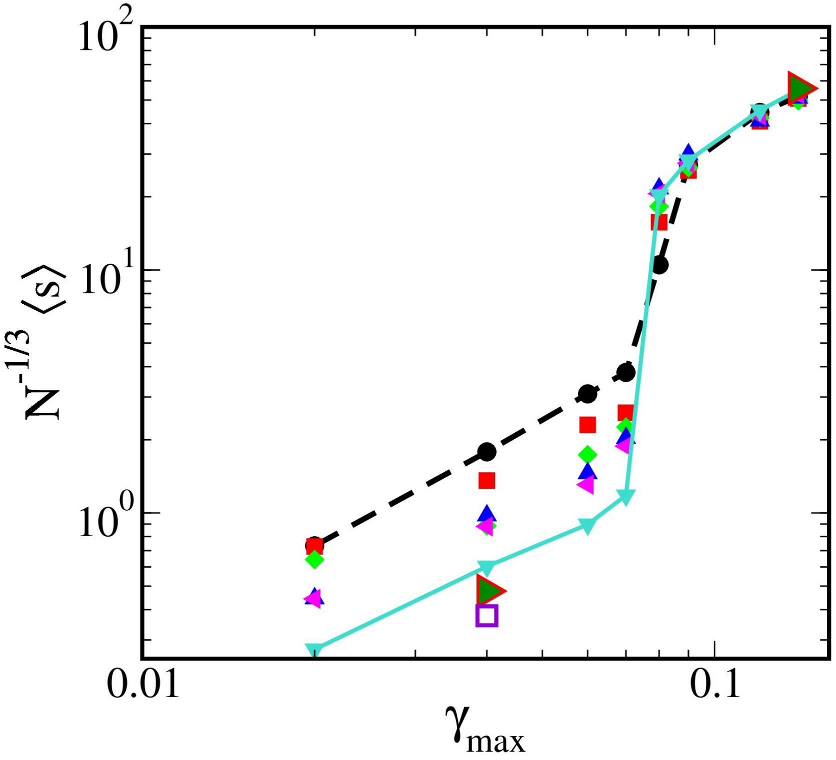
Above the yield point mean avalanche size shows clear size dependence ~ $N^{1/3}$

Consistent with uniform shear results for the case of plastic flow states.
[Lerner and Procaccia 2009]

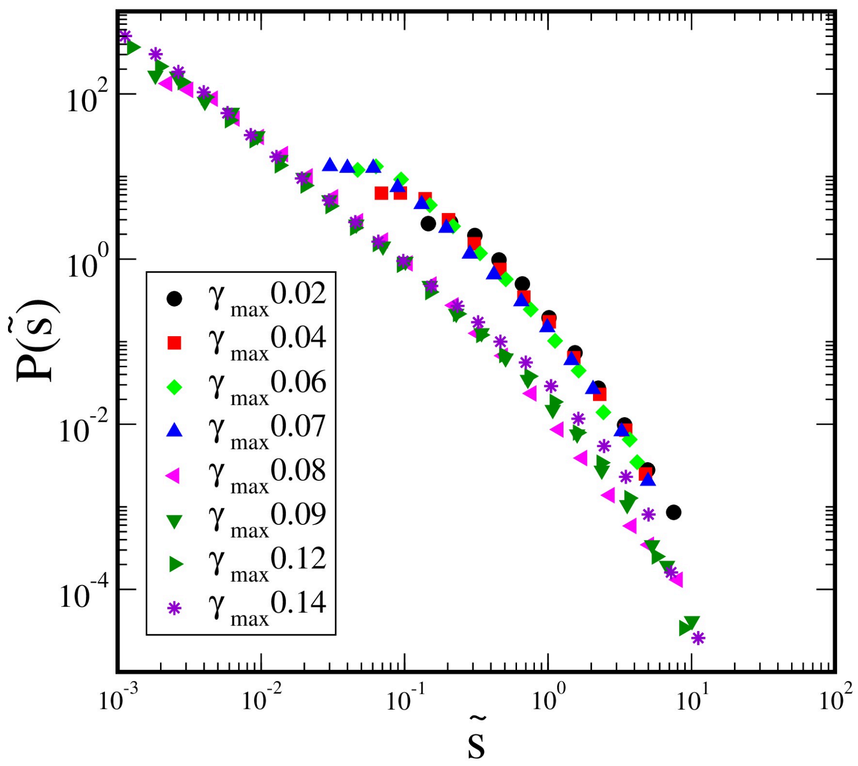
Below the yield point, avalanche sizes show **weak system dependence** that saturate.

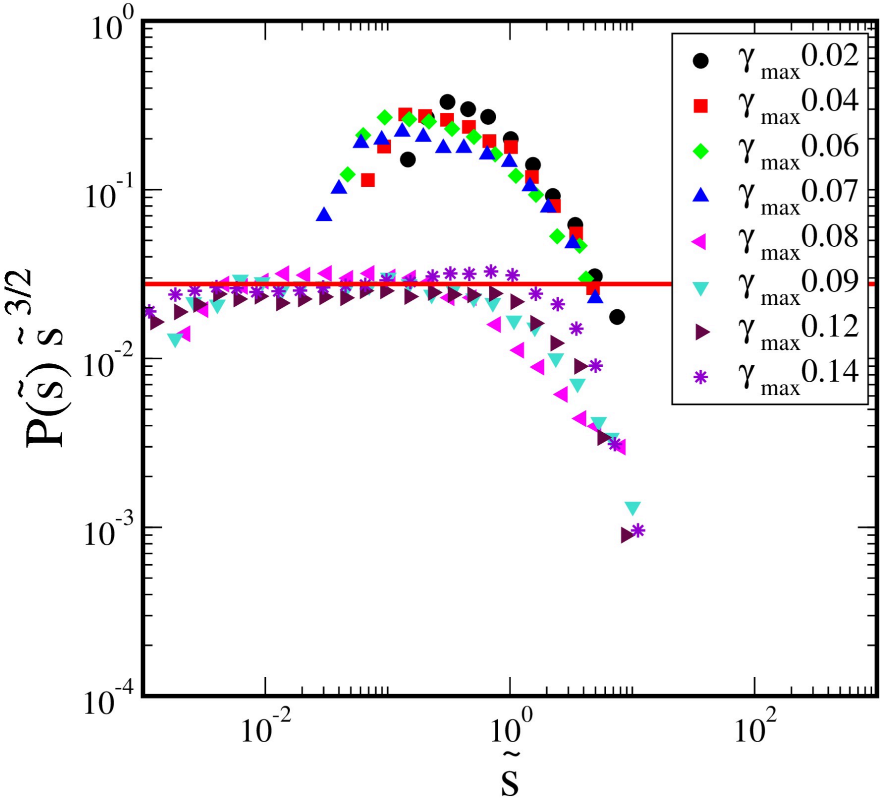
Mean Cluster Sizes Vs. N





Scaled distributions





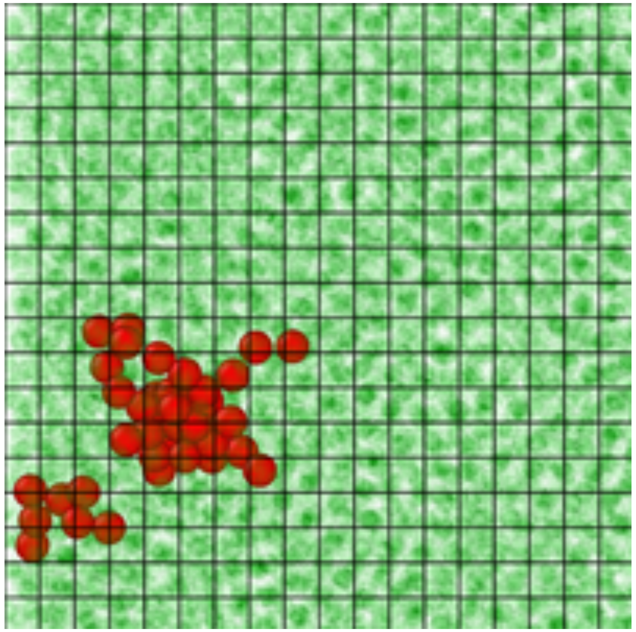
- Scaled cluster size (= s/<s>) distributions exhibit data collapse separately for $\gamma_{max} < \gamma_y$ and $\gamma_{max} > \gamma_y$.

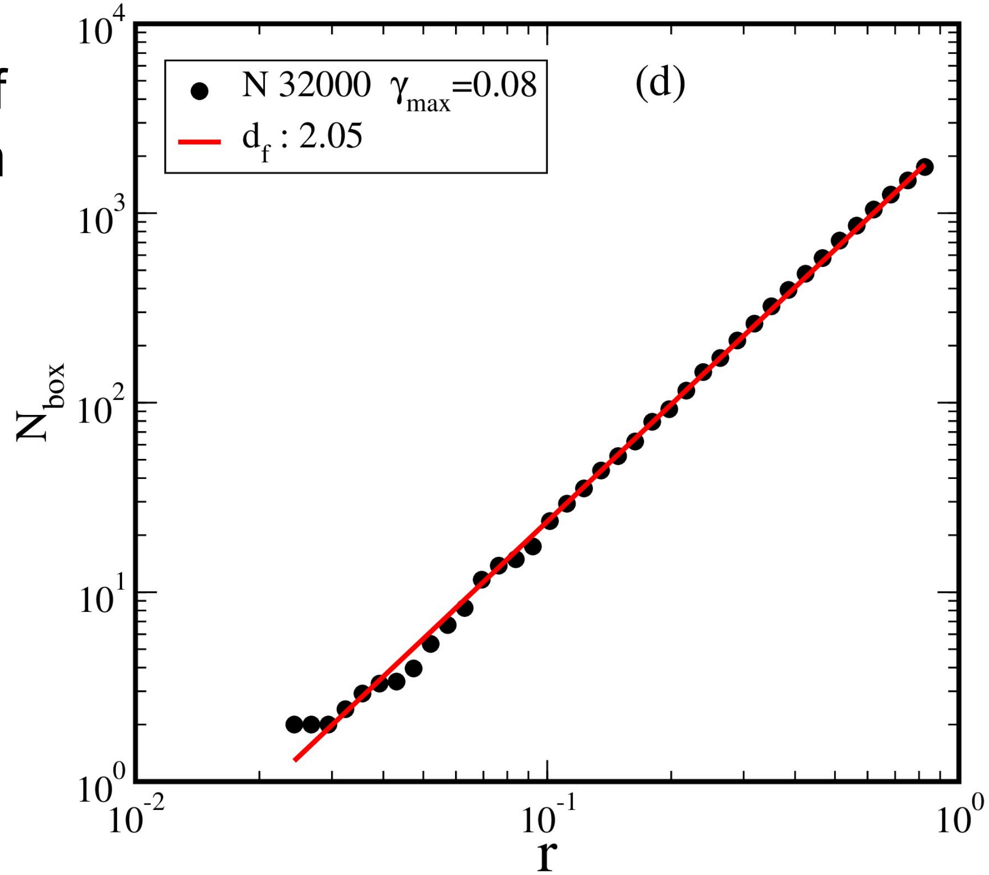
- Distributions for $\gamma_{max} < \gamma_y$ do not display a power law regime, whereas $\gamma_{max} > \gamma_y$ do.

Qualitatively different avalanche distributions!

Fractal dimension

Fractal dimension of the clusters of the "active particles" estimated from box counting.





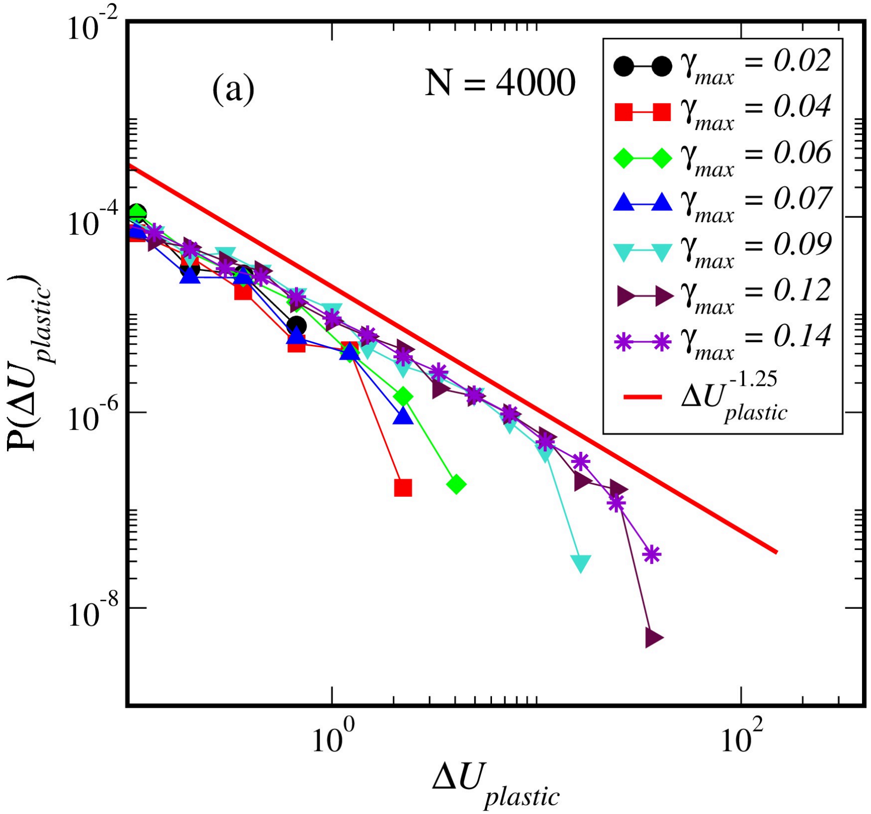
A log-log plot of the number of occupied boxes (N_{box}) is shown vs. the magnification r.

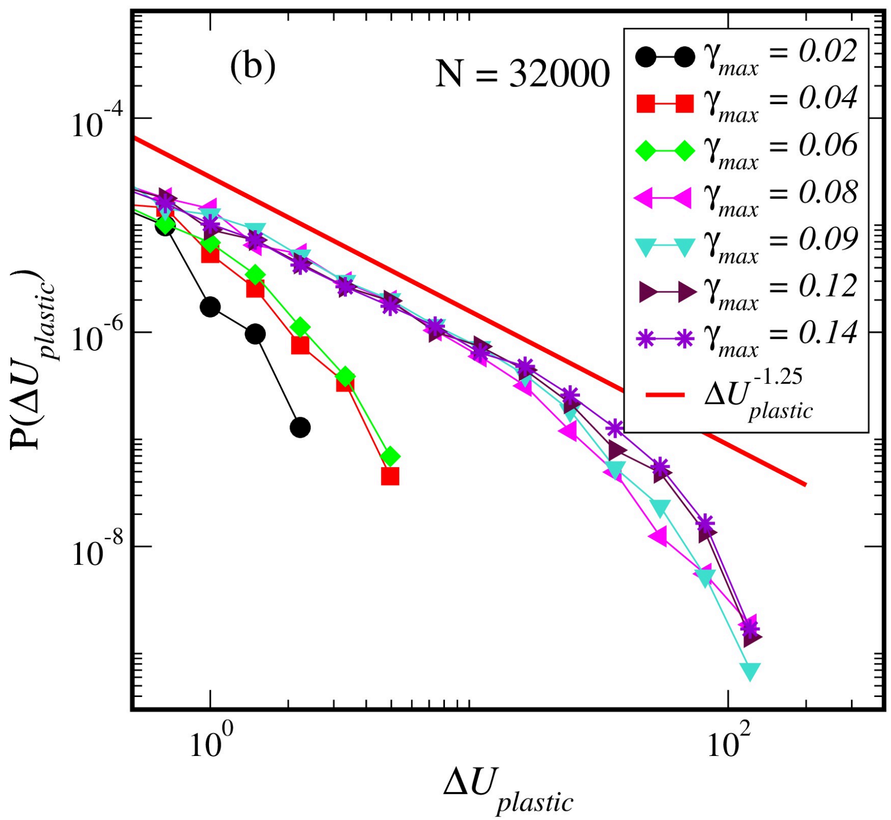
The slope results in an estimated fractal dimension $d_f \sim 2$.

Not consistent with size scaling exponent of 1.

Anisotropies? [Maloney & Robbins PRL 2009]

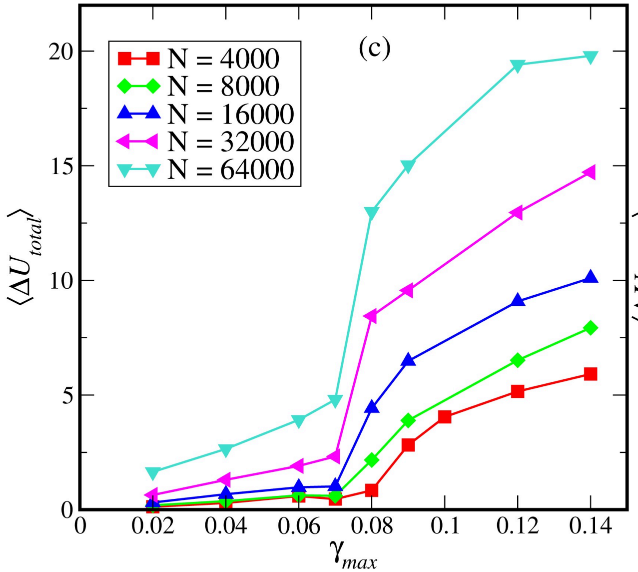
Avalanche: Energy drops

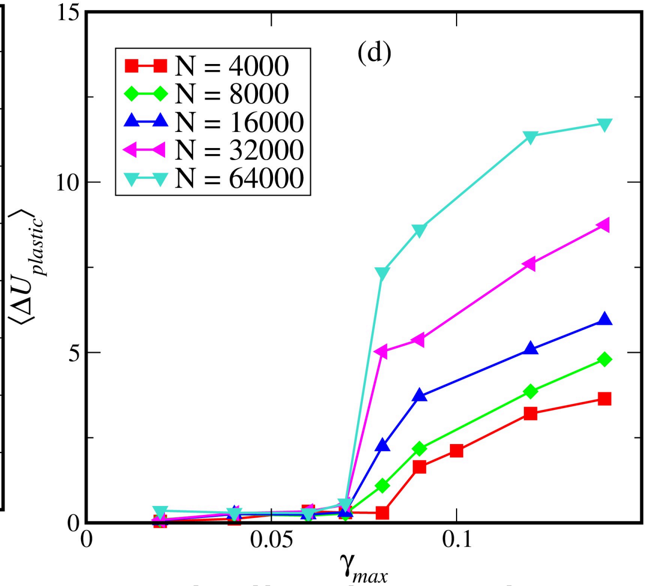


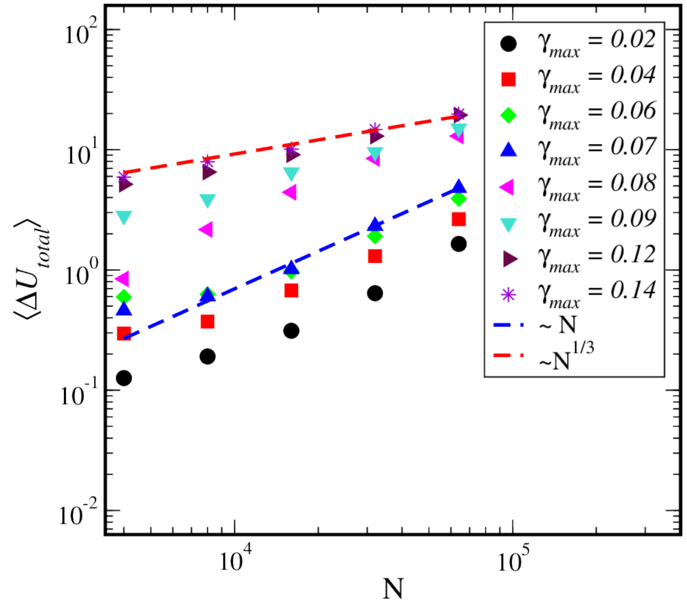


Energy drops distribution shows power law distribution with cutoff and the cutoff increases with γ_{max}.

Avalanche: Energy drops

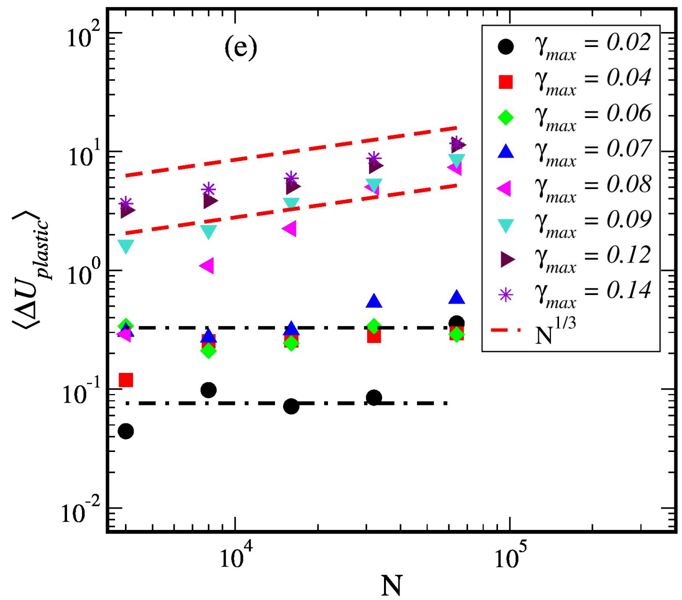






- Mean energy drops vs. γ_{max}, indicating a sharp change at γ_y.

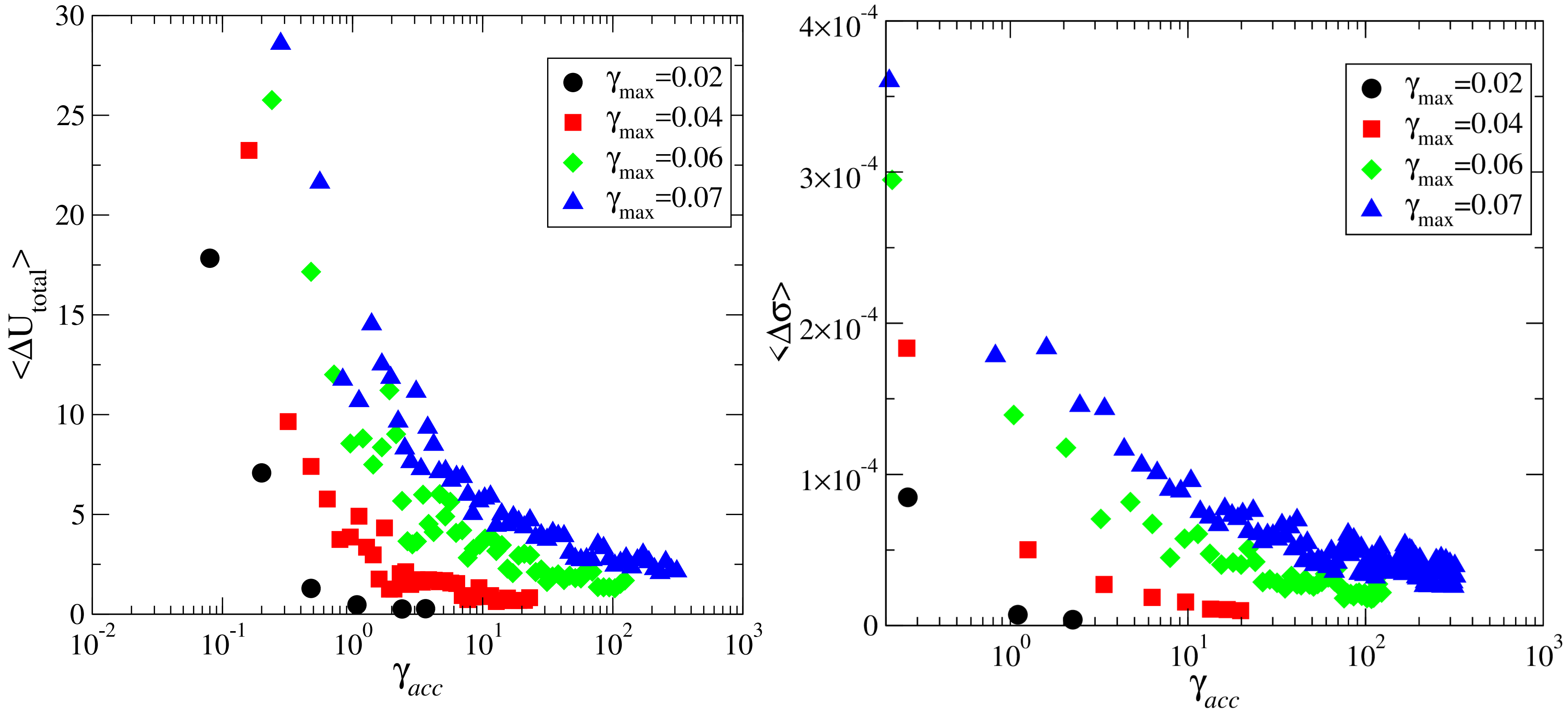
- Mean energy drops considering only plastic regions show no system size dependence below γ_y .
- Mean energy drop (plastic component) vs. system size N shows no significant size dependence for $\gamma_{max} < \gamma_y$ but a clear $N^{1/3}$ dependence above.



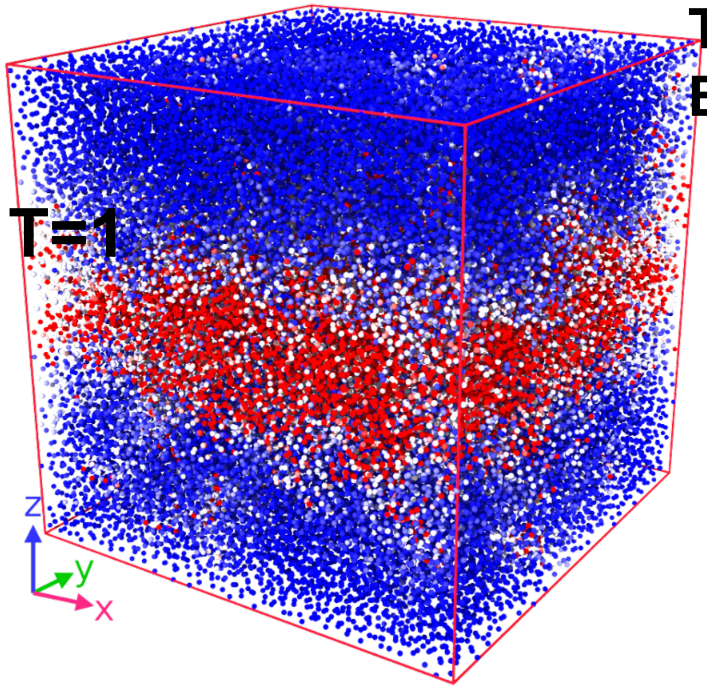
Avalanches during the transient

Although the avalanche sizes are small below yield in the steady state. Large organizations occur during the transient.

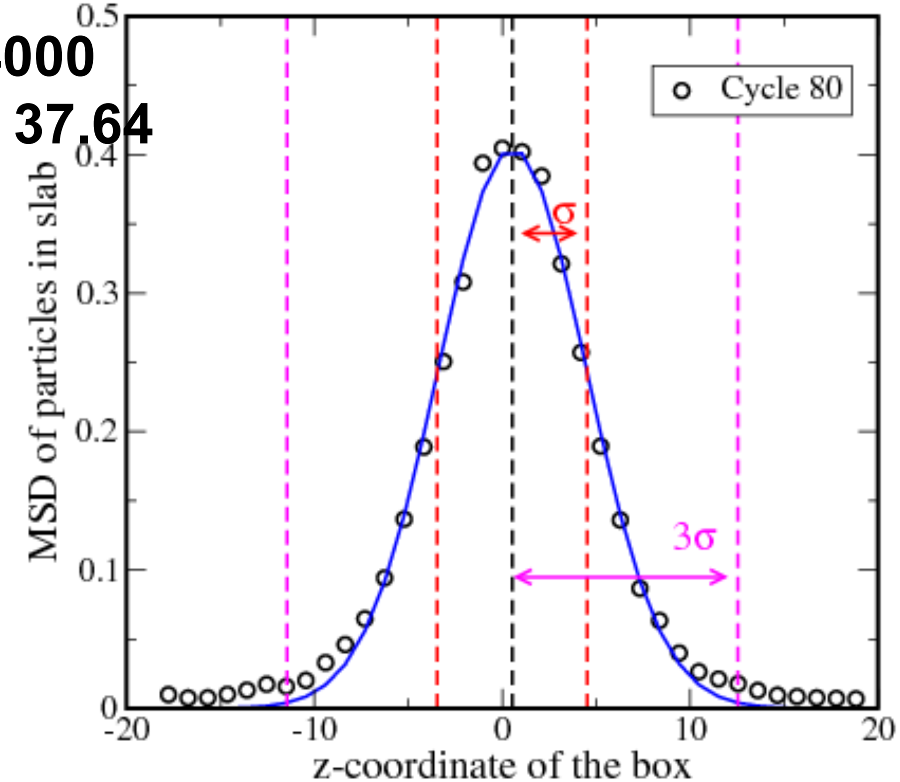
Larger and longer lived for larger strain amplitudes.



Shear Banding



T=1, N=64000
Box size= 37.64



- A configuration from the steady states for γ_{max}=**0.09**.
- Color code: MSD values

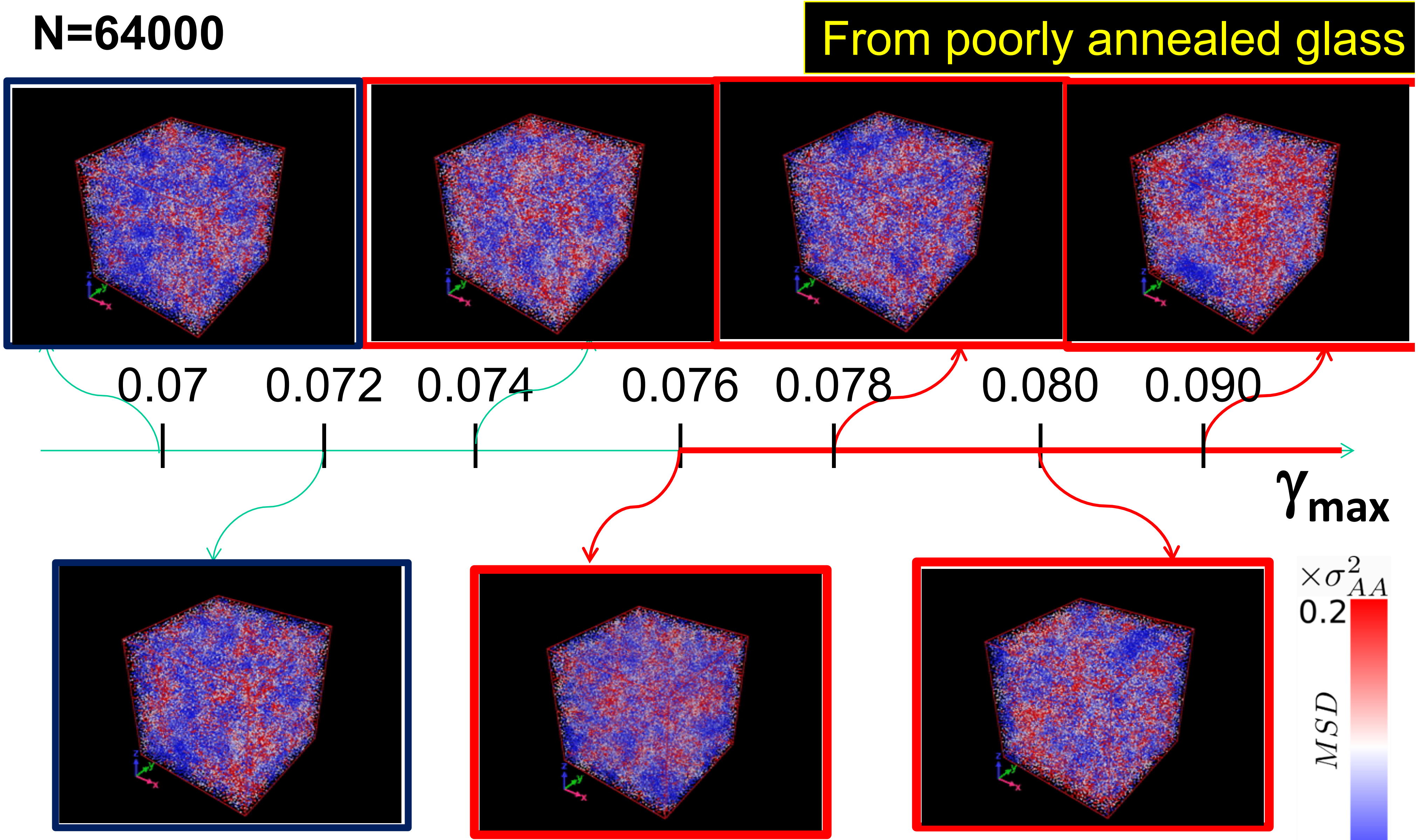
- The slabwise MSD of particles as function of the height of the band.

Yielding is accompanied by the formation of shear bands.

Displacements per cycle, energy etc indicate presence of shear bands ~ 20 particle diameter!

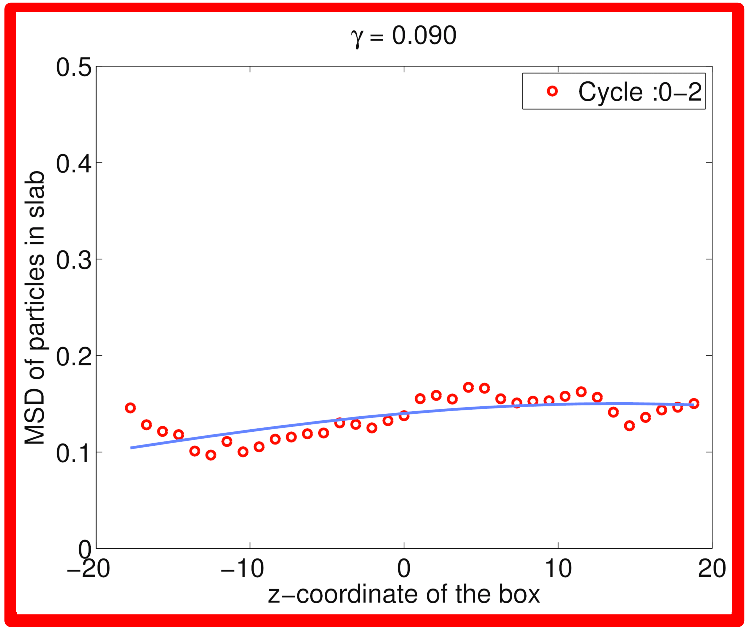
Probed by different initializations (from liquid/poorly annealed glass, strain amplitude below (.07), above (.08) yield value).

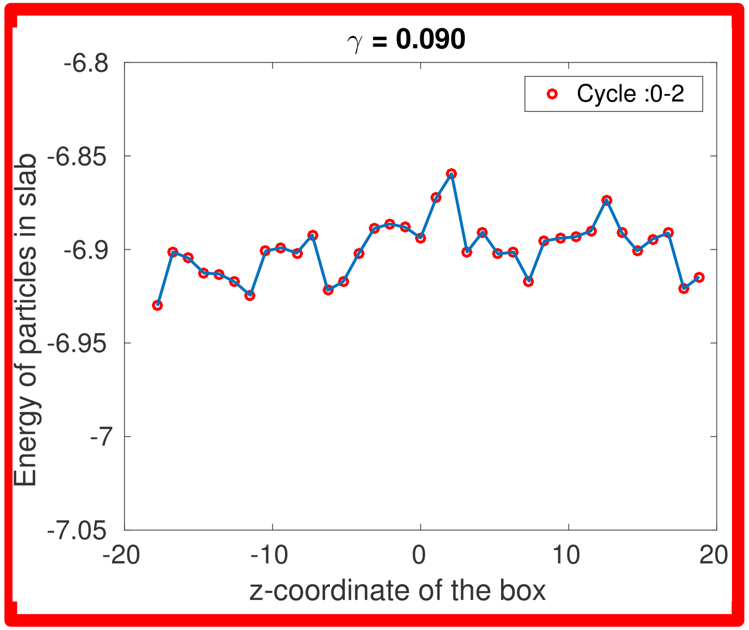
Across the yielding transition

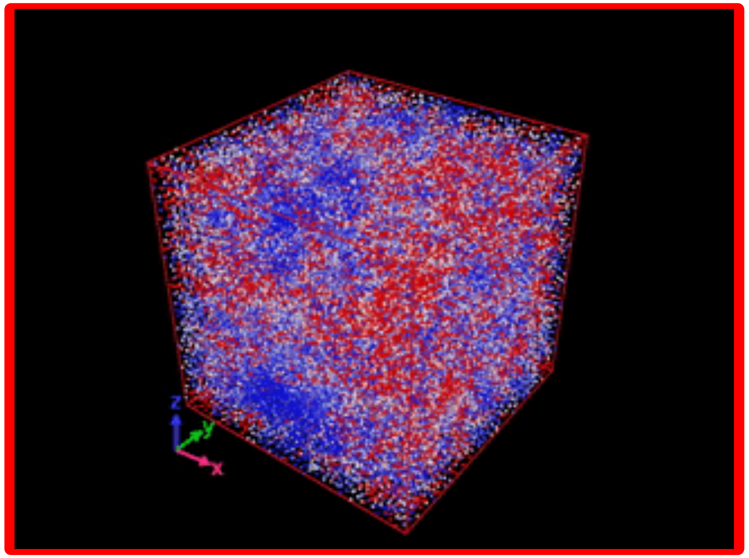


Shear bands are present in the steady states for strain amplitudes above yielding value ~ 0.07

Evolution towards steady states



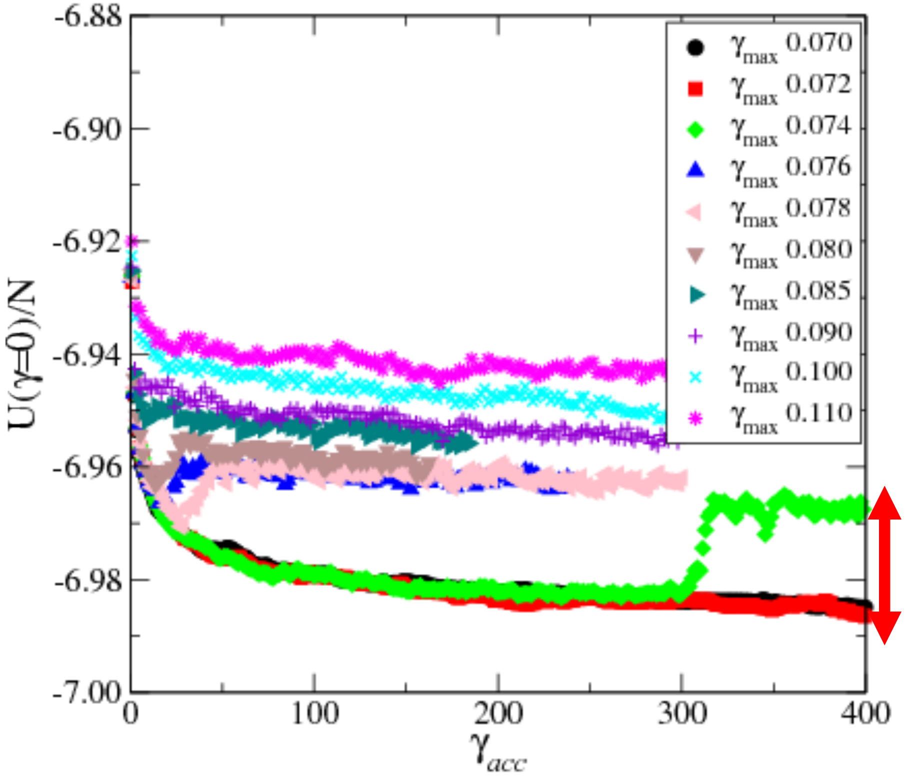


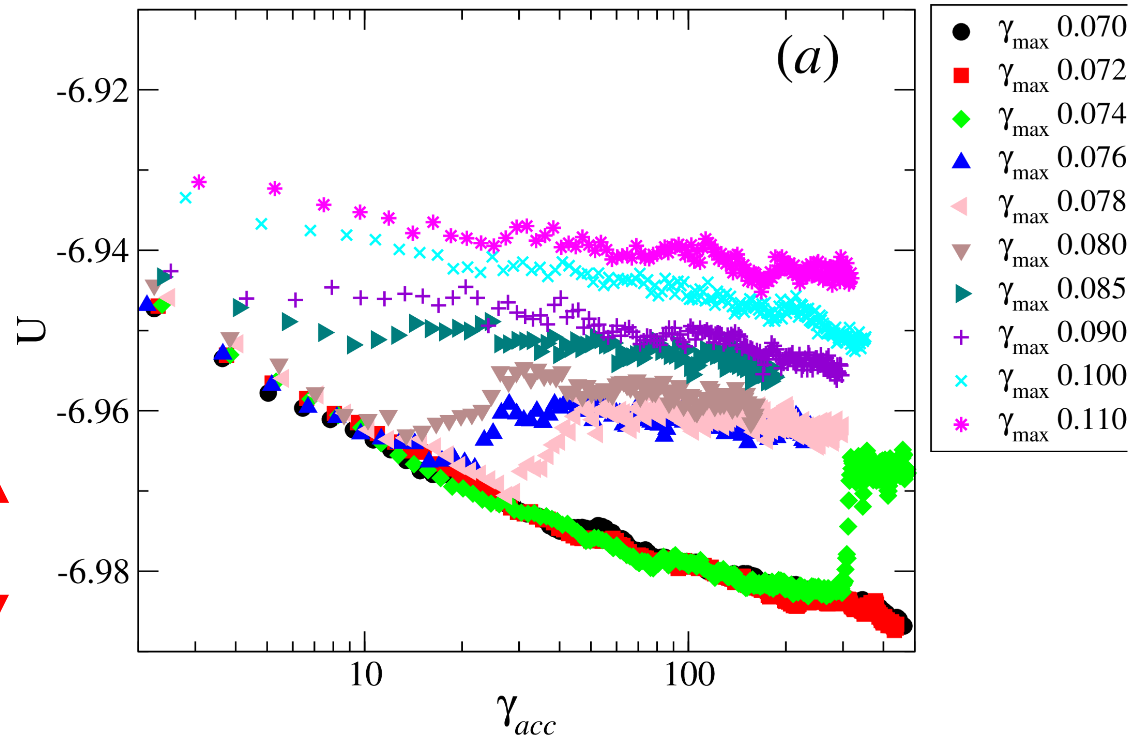


- Shear bands are present in the steady states.
- The energy and MSD profile changes in the presence of the shear band.

γ_{max}=0.09

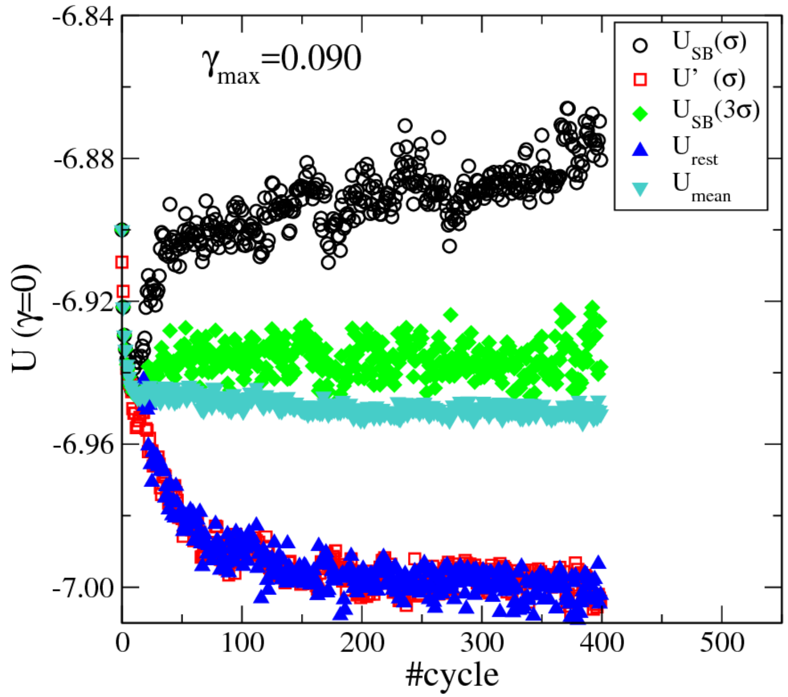
Evolution towards steady states

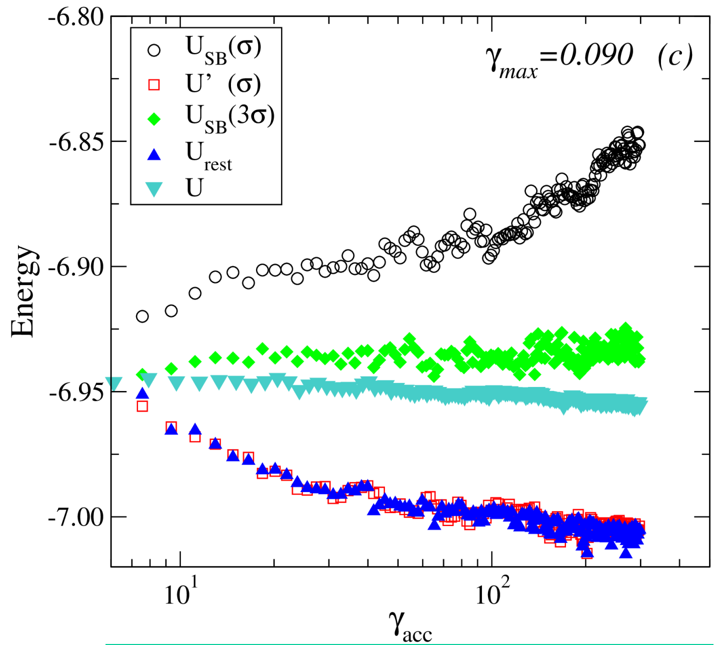




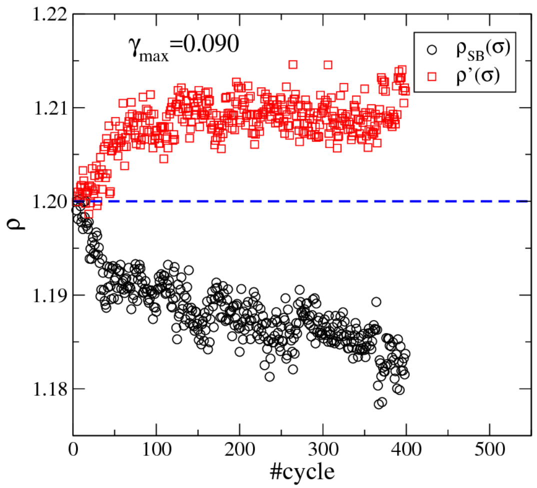
- Energies show monotonic change with cycles below yielding.
- Logarithmic relaxation!
- Abrupt change when yielding (and shear banding) happens.

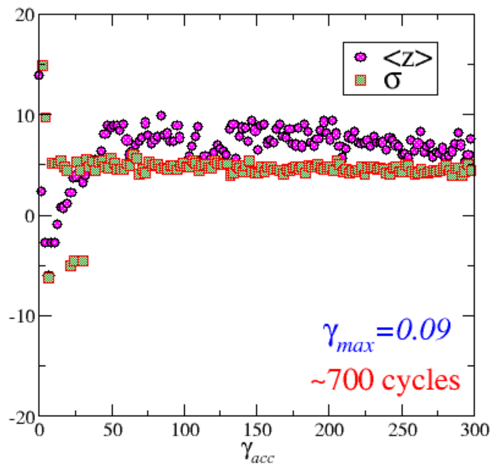
Evolution towards steady states





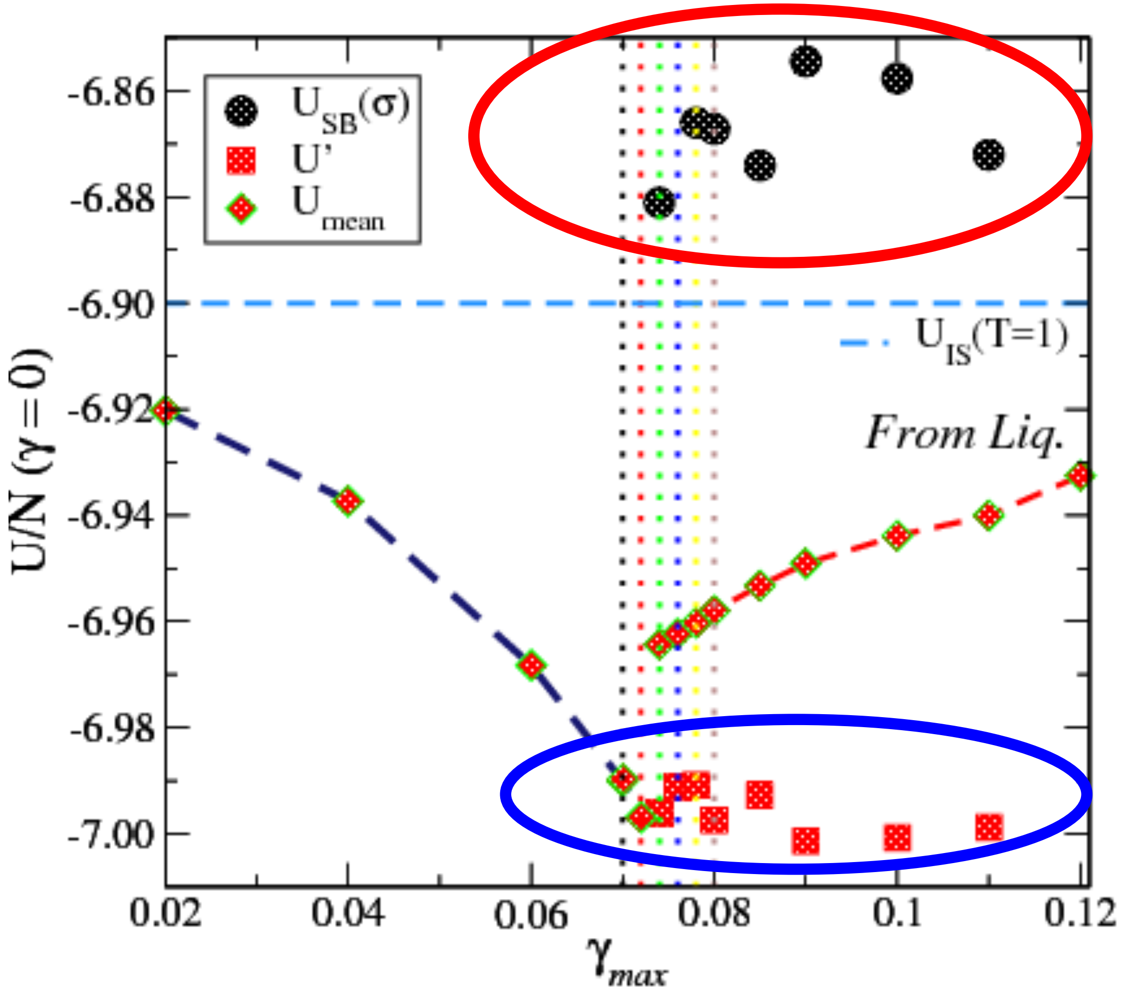
Shear band γ_{max}=0.09





- The energy and mobility of the particles in the shear band are higher than particles outside the shear band.
- The shear band is “fluid like”, and density of the band is less than the bulk of the system.
- Shear bands are mobile but the width is stationary.

Annealing above Yielding



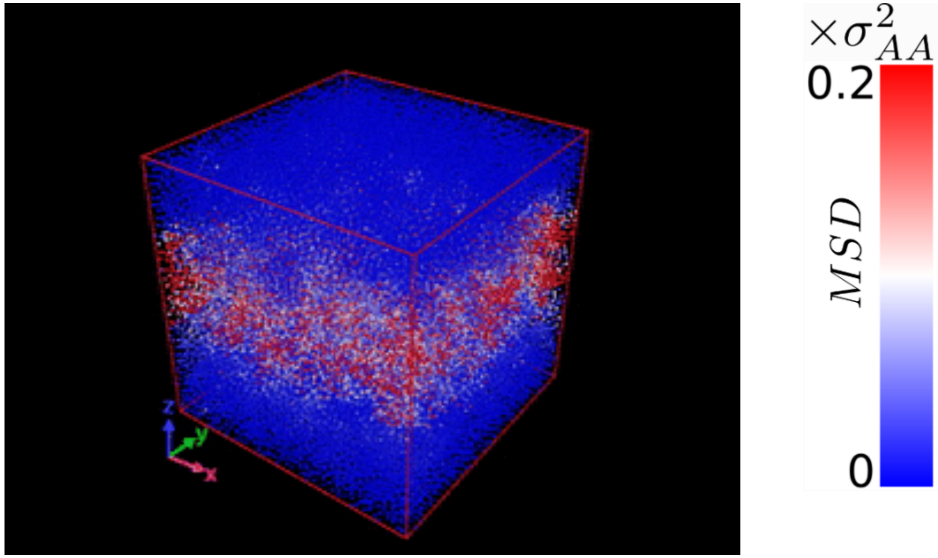
Energy in shear band ~ highest temperature glasses.

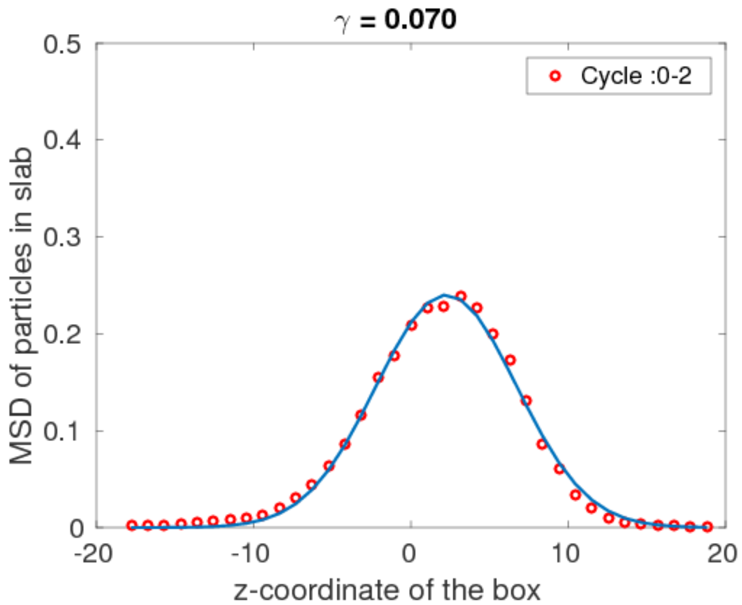
Finite jump in the mean energy.

Continued annealing outside the shear band

- Particle in the shear band access energies at the "top of the landscape"
- **The rest of the system continues to be annealed beyond yield point.**
- Location of yielding point exhibits some initial condition dependence.

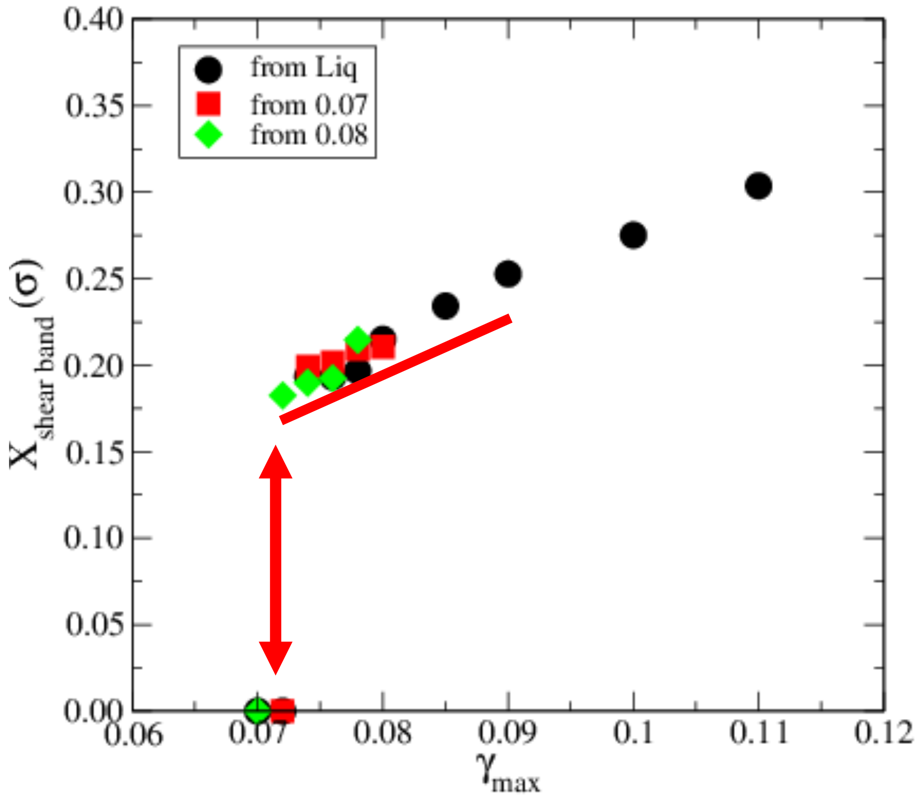
Vanishing shear band
From γ_{max} = 0.08, @ γ_{max} =0.07

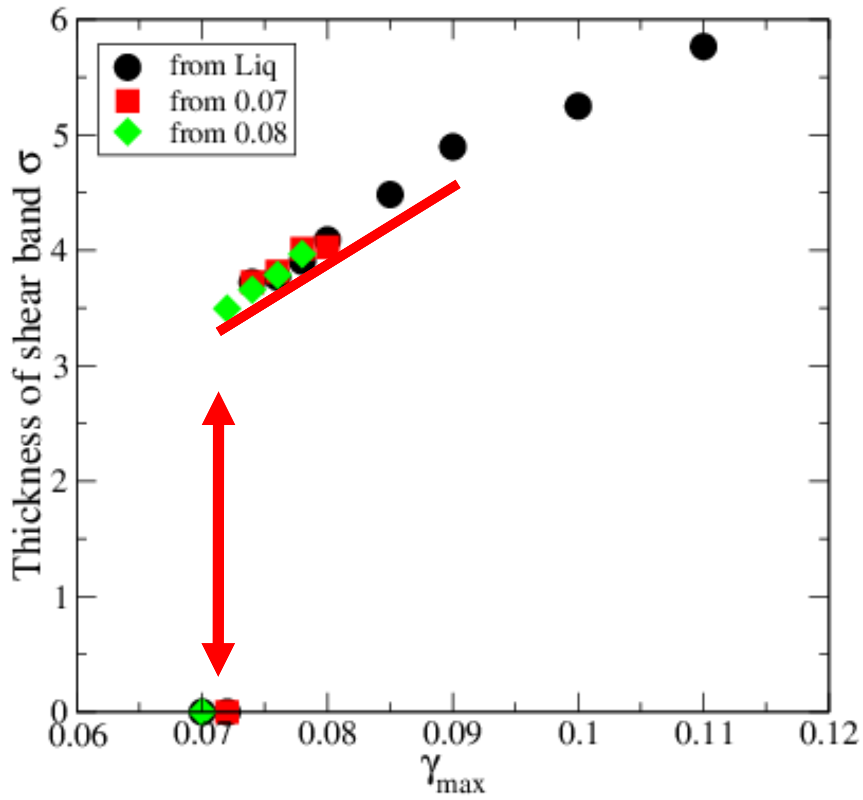




The shear band vanishes after a large number of strain cycles at smaller amplitude.

Characteristics of the shear band





The **fraction** of the particles, **width** of the shear band changes in **discontinues manner** at the critical amplitude.

γ^{c}_{max}

0.074

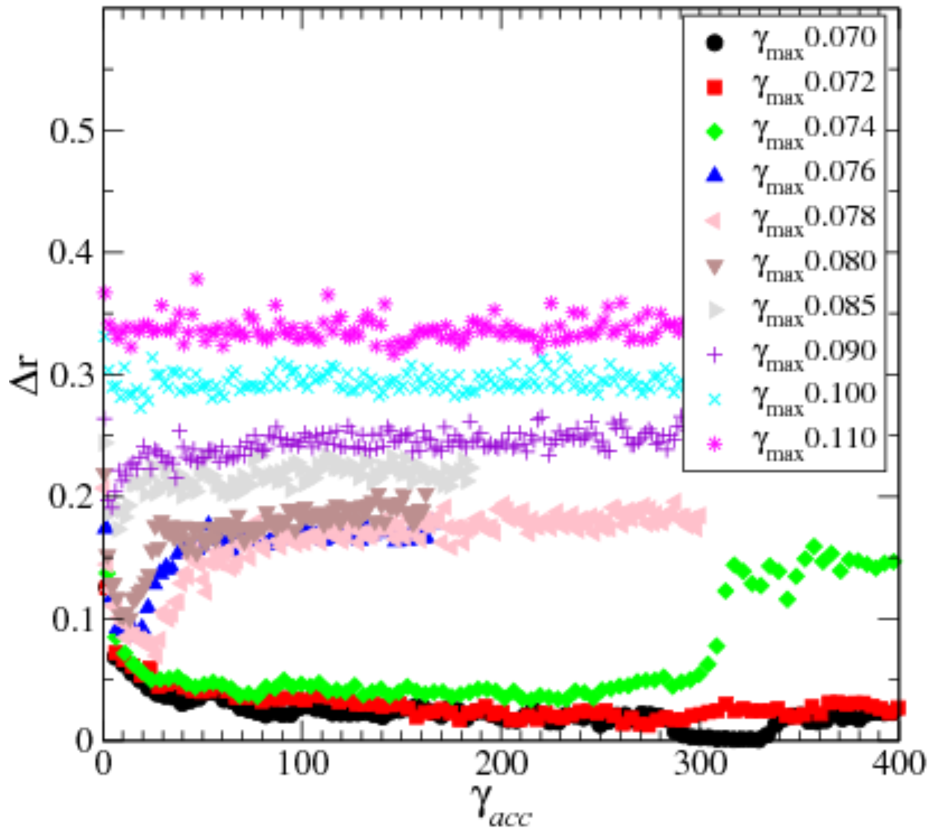
0.072

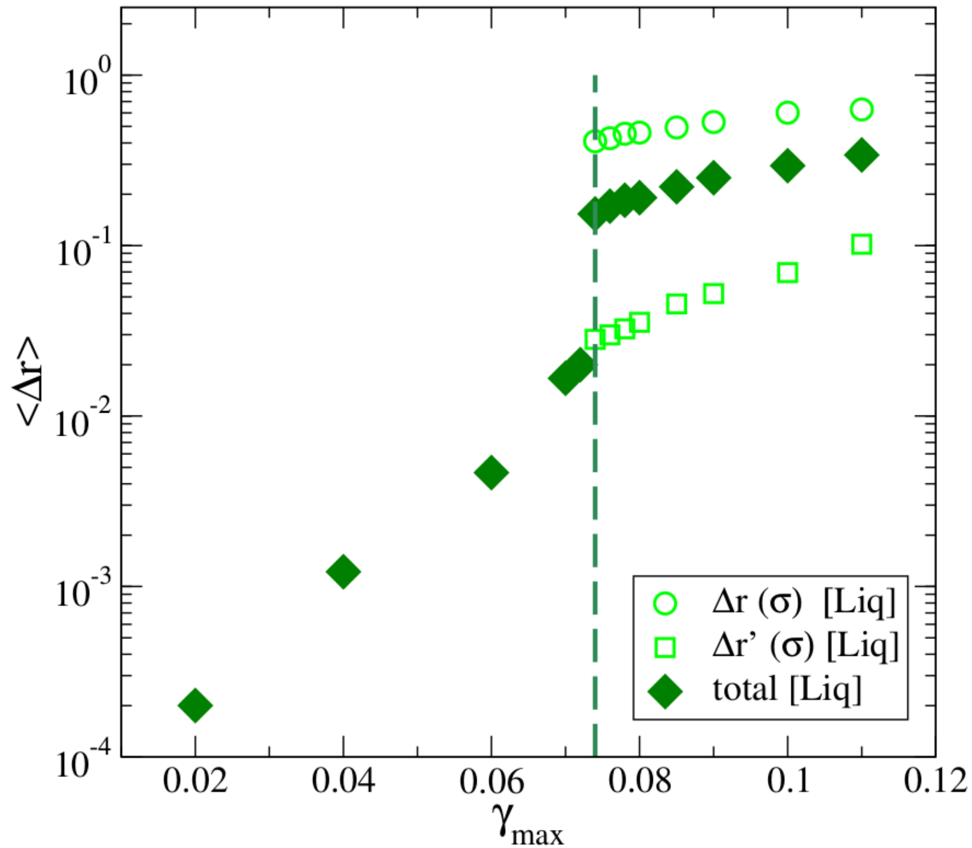
How does diffusivity change?

Microscopic dynamics associated with shear banding

The average particle displacement after one deformation cycle: j is the index of cycle.

$$\Delta r = \frac{1}{N} \sum | \vec{r}\,(j+1) - \vec{r}\,(j) |$$



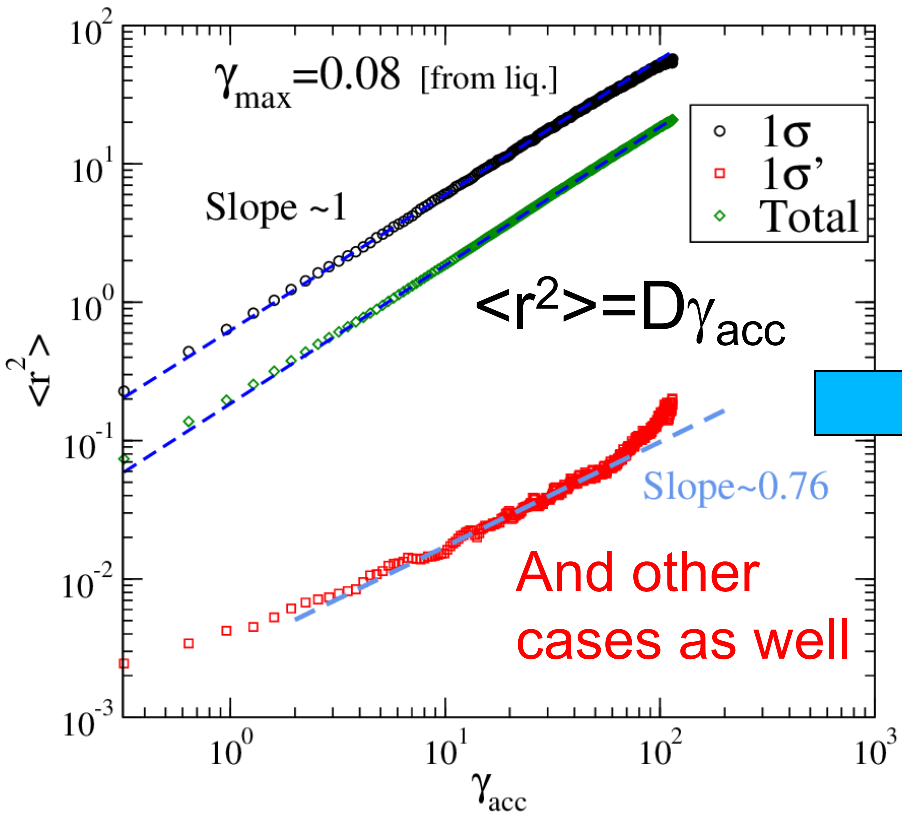


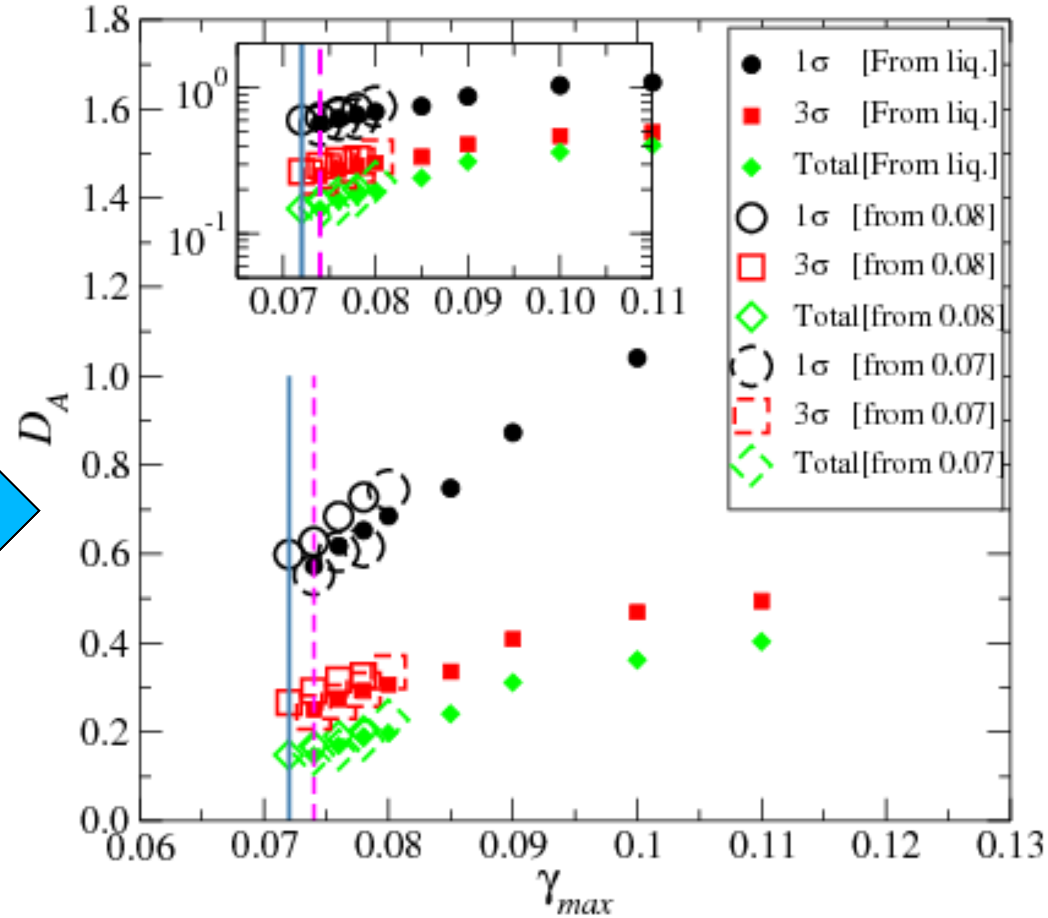
Across the yielding transition, the averaged particle displacement changes in a discontinuous manner.

Outside the shear band and below yielding, movement finite but very small.

Characteristics of the shear band - Diffusivity

The diffusion of total system, most mobile particles(1σ), the shear band (3σ) and least mobile particles $(3\sigma')$ estimated.





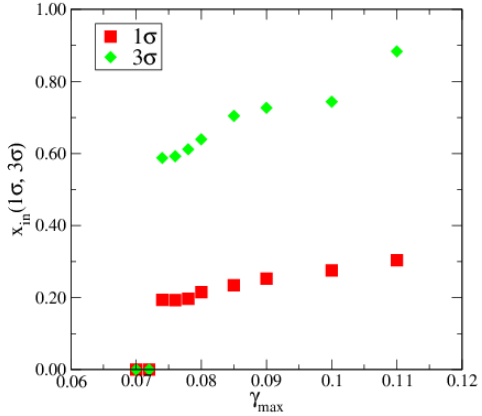
The **diffusion coefficient** changes in **discontinues manner** at the yielding strain amplitude.

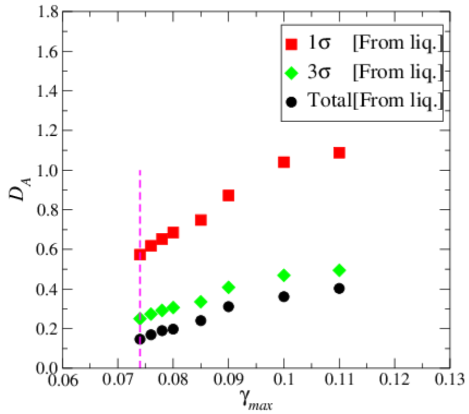
Sub-diffusive behaviour outisde the shear band.

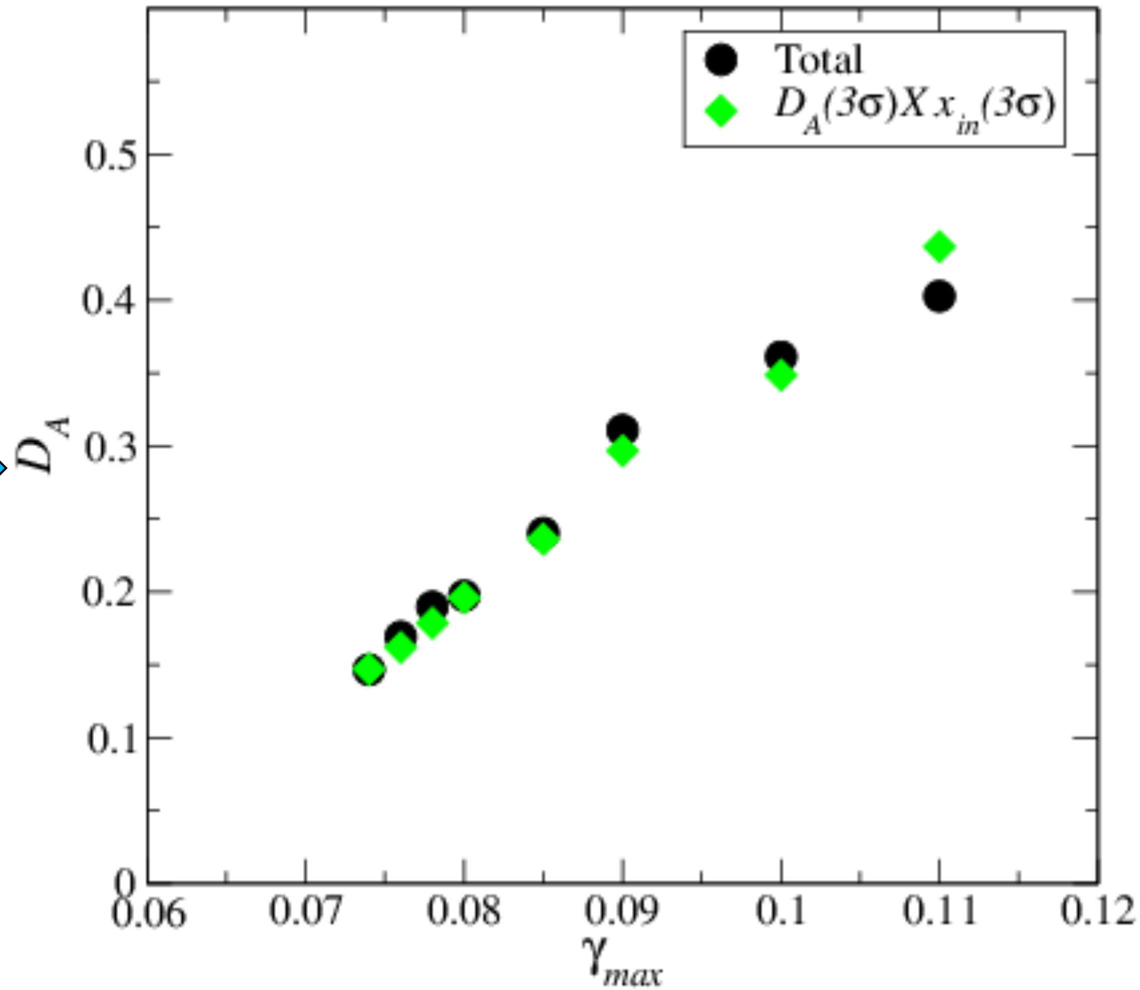
γ^c_{max}
0.074
0.072

Characteristics of the shear band - Diffusivity

Above the yielding transition, the finite diffusion is an outcome of the shear band.







The **diffusion coefficient** of the mobile particles changes in **discontinues manner** at the critical amplitude.

Finite Temperature and Shear Rates

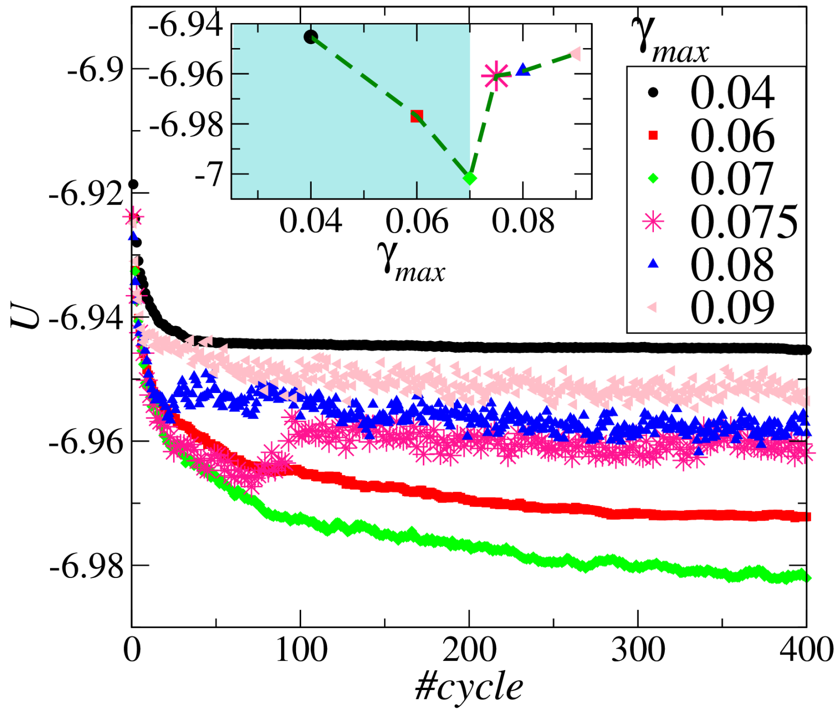
What happens if we go beyond the AQS limit?

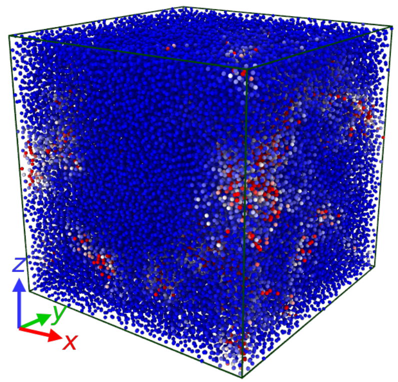
We perform shear deformation at finite strain rates and temperatures.

The system is sheared (*via* SLLOD) at range of temperatures 0.01, 0.1, at strain rate 10^{-5} and varying amplitudes (γ_o).

$$\gamma(t) = \gamma_o \sin(\omega T)$$

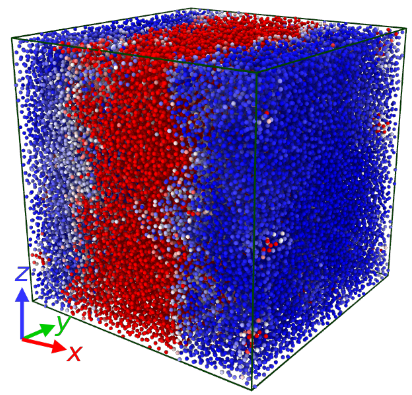
The picture does not change.





γ = 0.07

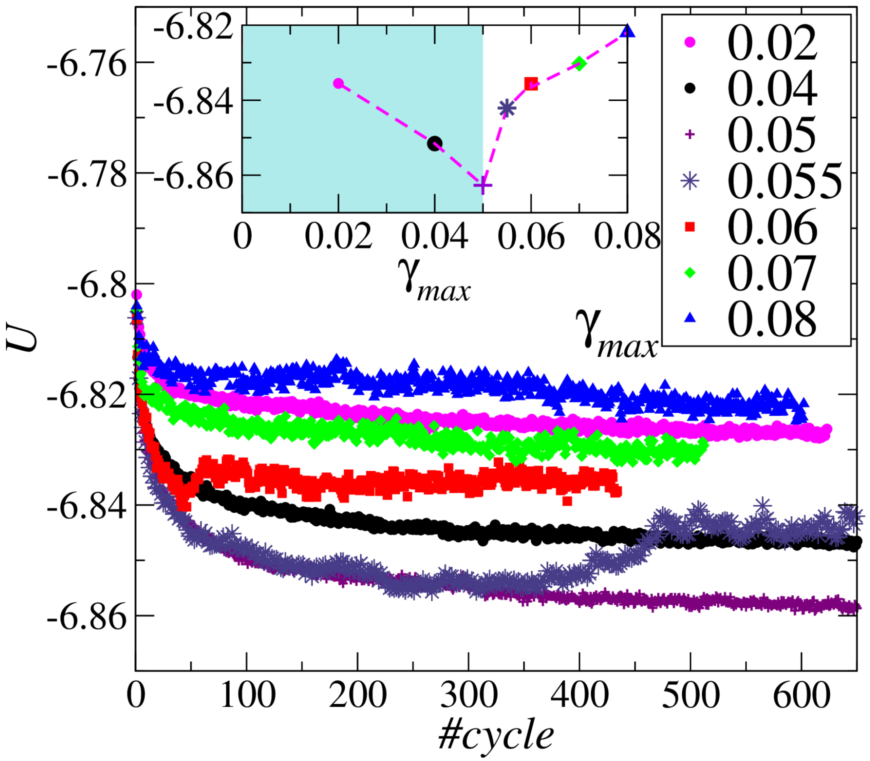
γ = 0.075

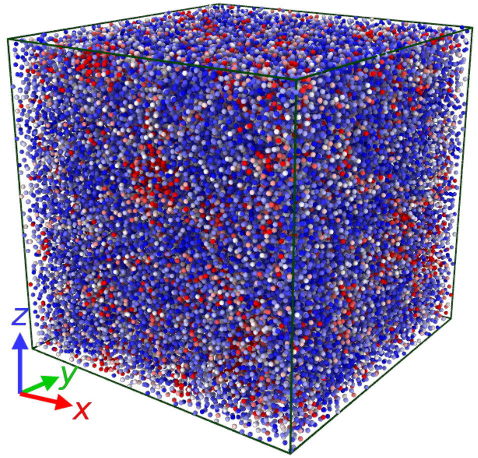


T = 0.001

Finite Temperature and Shear Rates

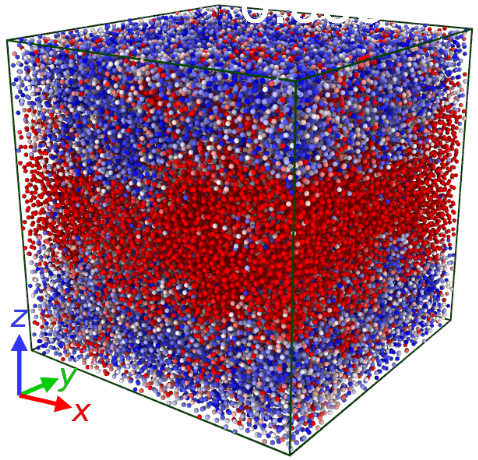
T = 0.1





γ = 0.05

γ = 0.055

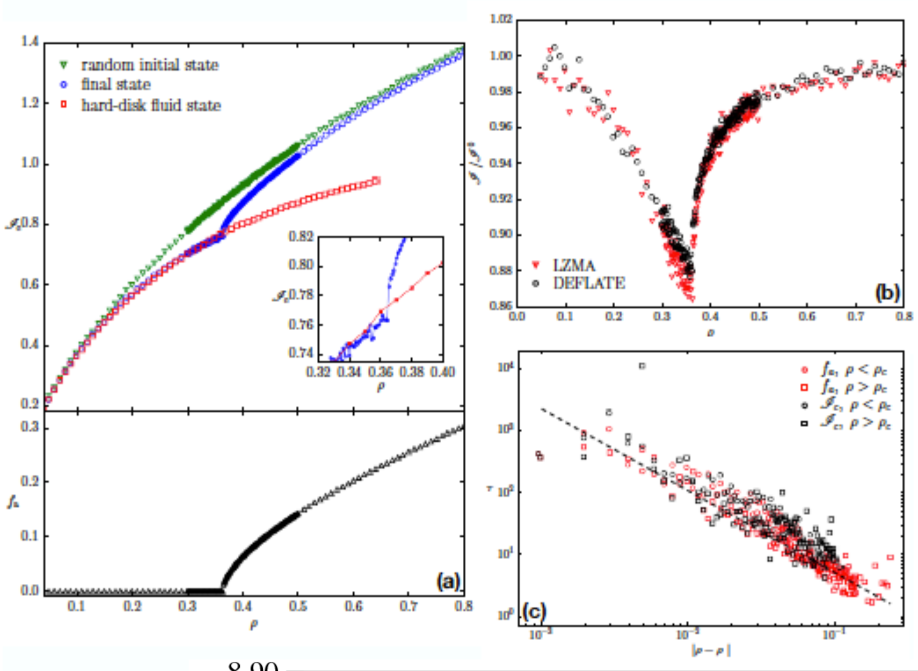


At a higher temperature, shear banding still present, but more fluctuations.

Lower yield strain amplitude.

Entropic characterization of the yielding

Recent interest in information measures
In driven systems (CID Martiniani et al 2017)

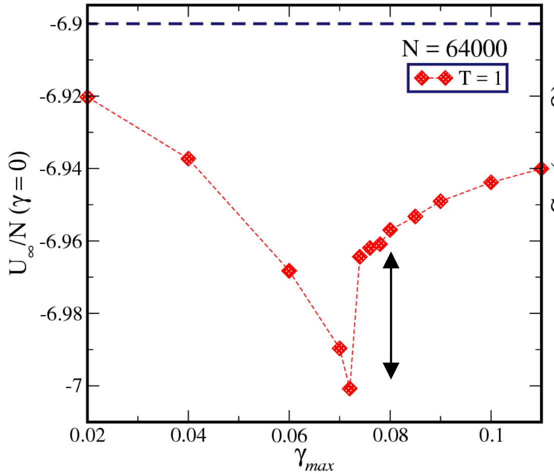


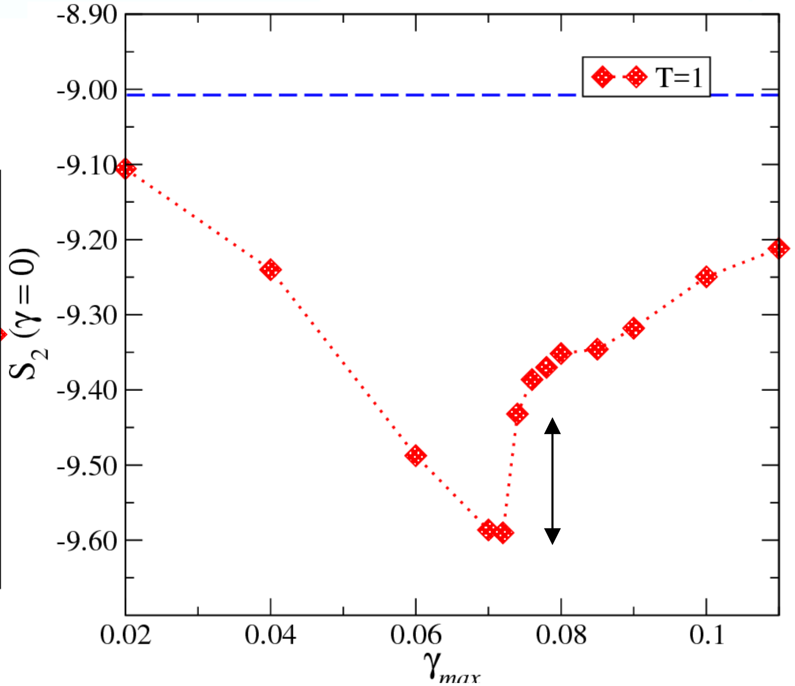
How about conventional structure based entropy? Pair excess entropy (S_2) for a binary system:

$$\frac{S_2}{k_B} = -2\pi\rho \sum_{\alpha,\beta} x_\alpha x_\beta \int_0^\infty \{g_{\alpha\beta}(r)\ln g_{\alpha\beta}(r) - [g_{\alpha\beta}(r) - 1]\} r^2 dr,$$

$g_{\alpha\beta}(r)$ is the pair correlation function for various components

The S_2 and total energy jumps across the yielding amplitude.

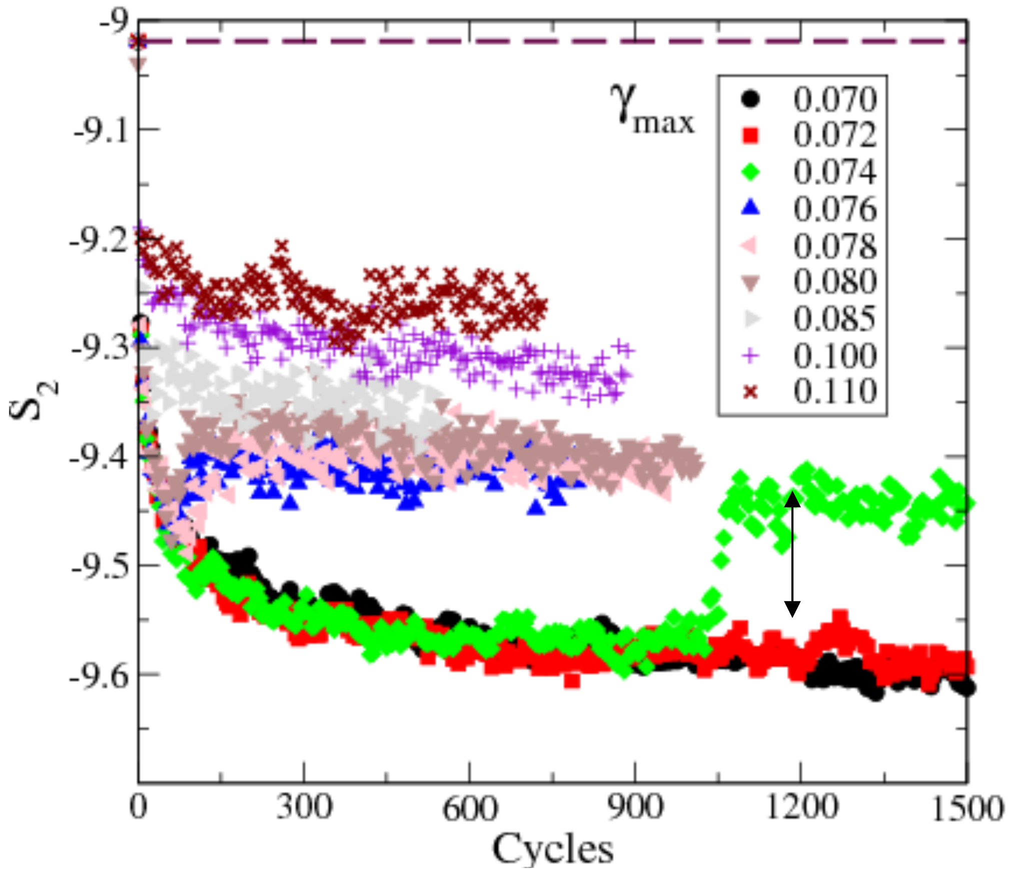


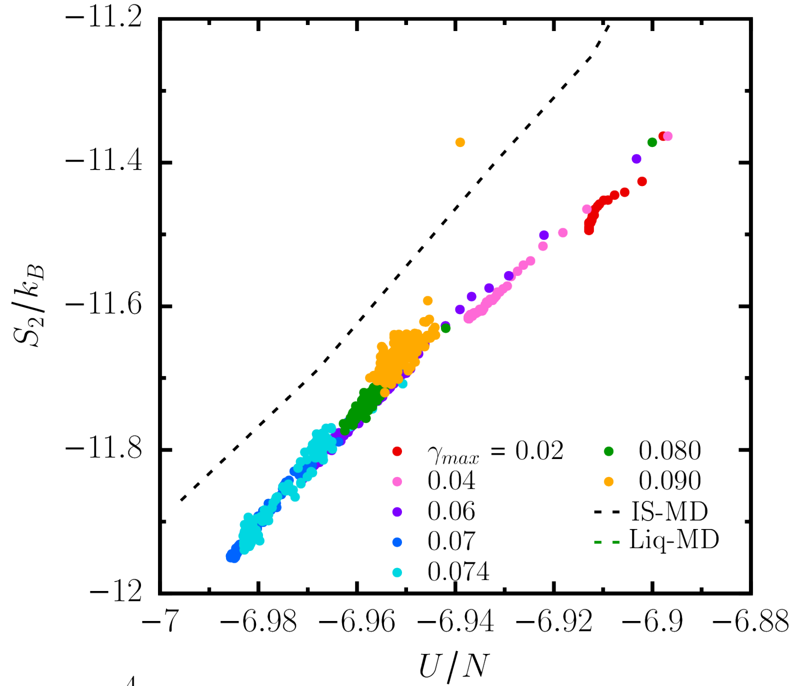


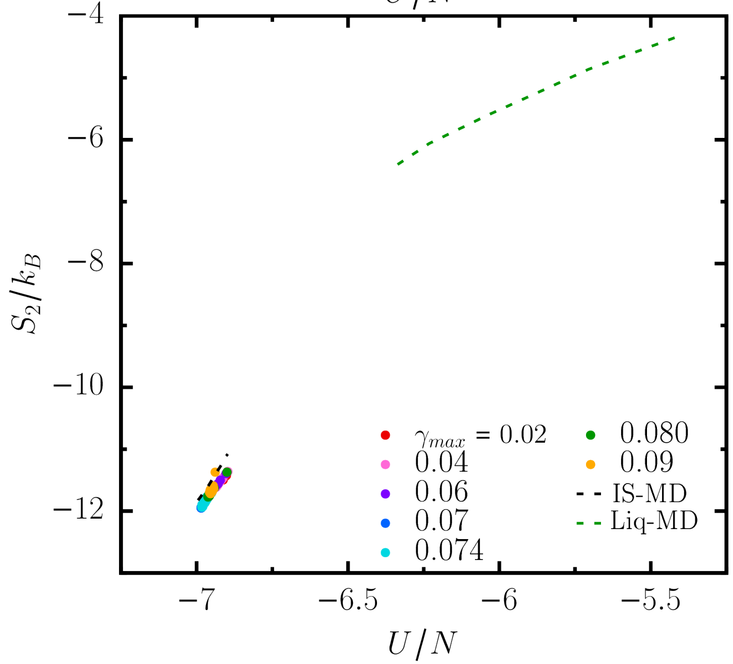
Arun Bupathy

Entropic characterization of the yielding

- S_2 tracks the energy of the inherent structures.
- Close to relation found in T dependence for the liquid, but not the same.







Annealing Effects are Important

Many past studies argue for a role of annealing (variously, relaxation, aging etc..) in the phenomenon of shear banding:

Pulled front/STZ: Alix-Williams and Falk 2018
SGR model: Fielding et al 2016
Elasto-plastic model: Martens et al, 2010
Analytic theory for avalanches: Dahmen et al 2009

In many cases what is discussed is shear banding in flow.

Transient vs permanent shear bands.

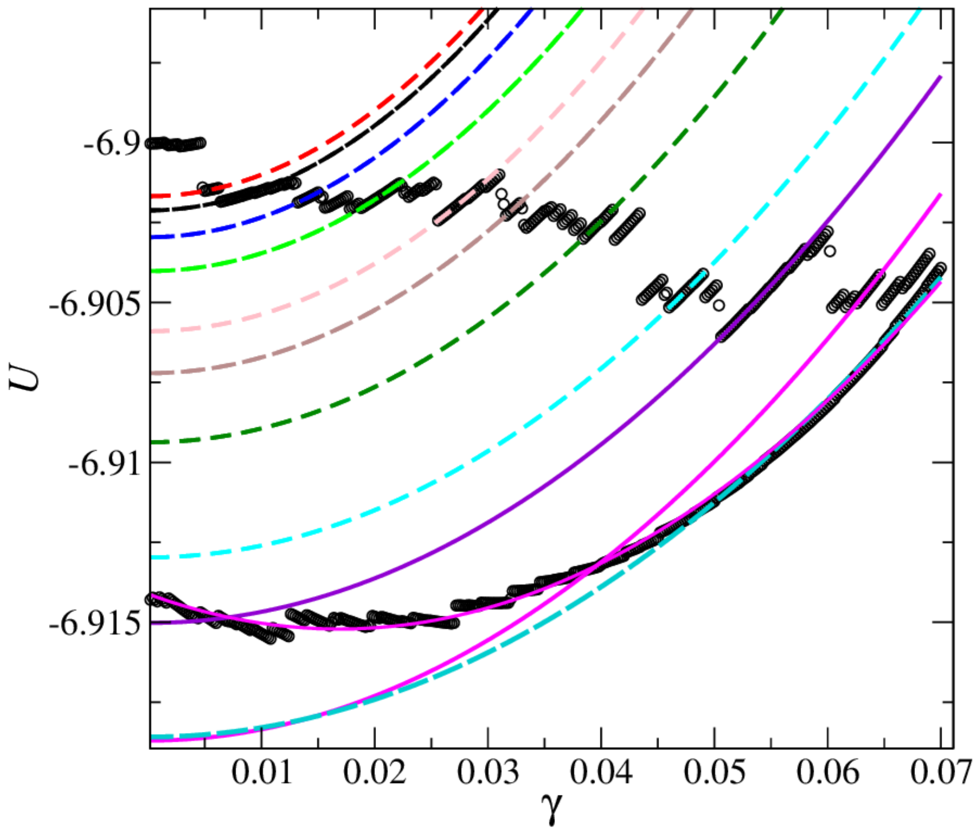
Incorporation of annealing effects in cyclic deformation (e.g. SGR model) leads to shear banding in the sense that is discussed here.

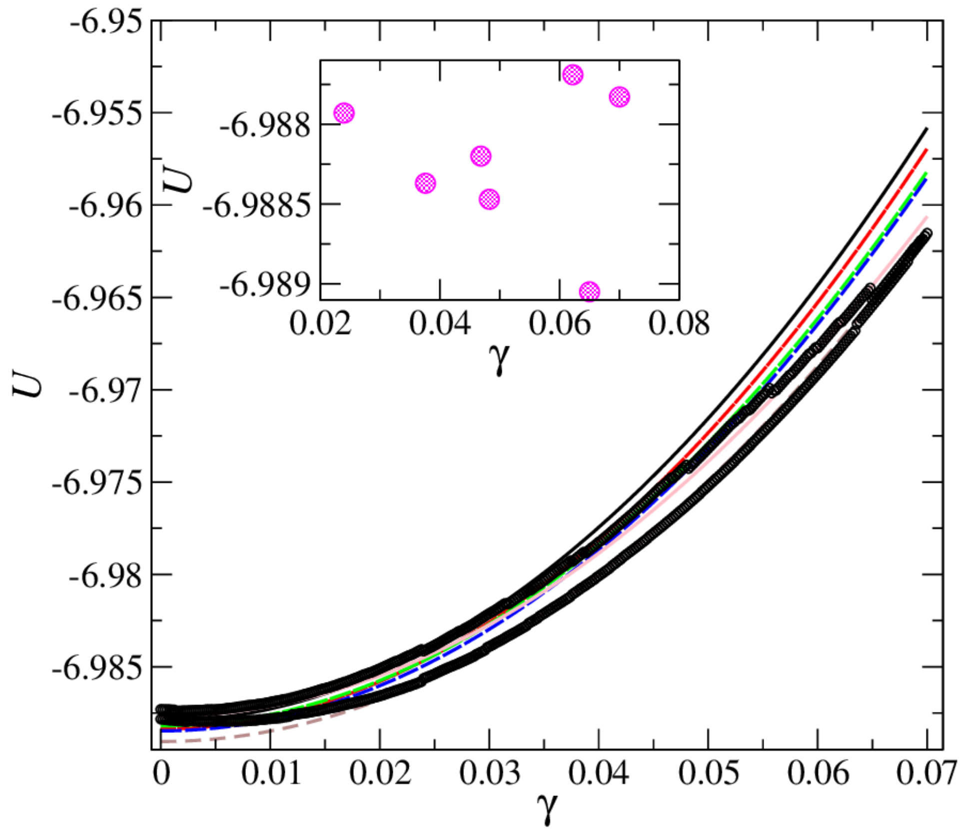
Annealing Effects under uniform shear

Do annealing effects play a role in yielding under uniform shear?

For poorly annealed glasses, they clearly do. Energy decreases as the system is sheared.

Even when it doesn't obviously, one must consider energy when the system is unloaded.

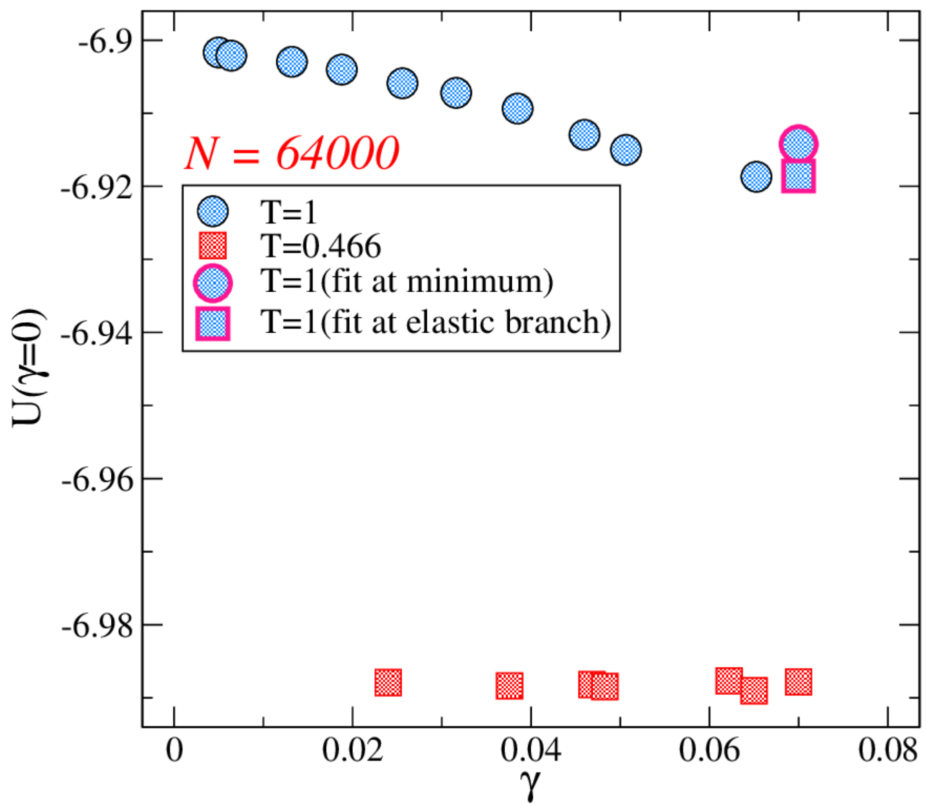




Annealing Effects under uniform shear

A harmonic extrapolation back to zero strain reveals that a uniformly sheared glass anneals as a function of strain.

Preliminary analysis.



Ref: Dubey et al 2016

Summary

The yielding transition appears as a sharp transition associated with an abrupt divergence of the sizes of avalanches, at the yielding transition, for cyclic deformation.

At variance with descriptions predicting divergences upon approach to the transition.

Strong and significant annealing effects before and after the yielding transition.

Annealing under cyclic deformation an interesting phenomenon to understand better.

The role of annealing not prominently treated in approaches to understanding yielding, but various threads in the literature which acknowledge its role.

Observation of shear banding above the yielding point. How do we understand them? Role of annealing. Connection to shear banding in flow.

Description of yielding as a mechanical instability. Integrating with other aspects of glass physics?