Yielding and Shear Banding in Amorphous Solids under Oscillatory Shear Deformation

Srikanth Sastry

Jawaharlal Nehru Centre for Advanced Scientific Research

Bengaluru, India

Non-linear mechanics and rheology of dense suspensions: nanoscale structure to macroscopic behavior

KITP

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Outline

Introduction

- ✧ Mechanical response of amorphous solids
- ✧ Oscillatory shear deformation of a model glass
- ✧ Non-equilibrium transition under cyclic deformation
- ✧ The Yielding transition
- ✧ Avalanches
- ✧ Shear banding
- ✧ Summary

P. Leishangthem
(JNCASR)

Anshul D. S. Parmar
(JNCASR/TIFR
Hyderabad)

Saurabh Kumar
(JNCASR/Koln)

Arunkumar
Bupathy
(JNCASR)

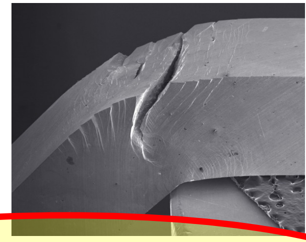
Earlier work: In Collaboration with:
Giuseppe Foffi (EPFL/Orsay)
Davide Fiocco (EPFL/Google)

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

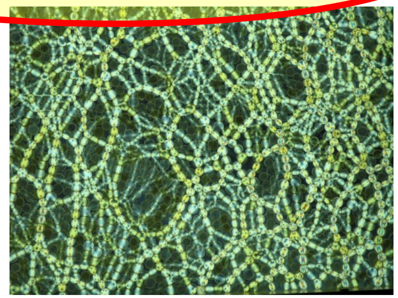
*Leishangthem, Parmar, Sastry "The yielding transition in amorphous solids under oscillatory shear deformation" **Nature Comm**. (2017) **+ Ongoing work***

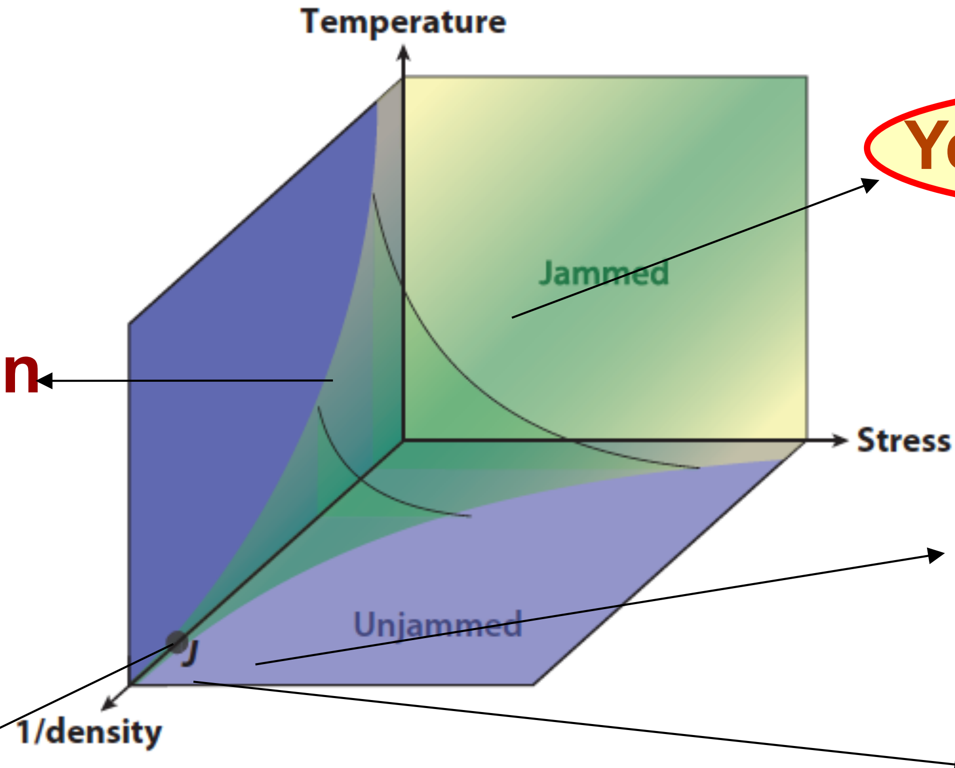
Jamming Phase Diagram

Liu, Nagel (1998)



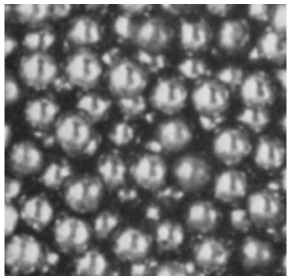
Yeilding Transition





Glass Transition

Shear Jamming



Jamming Transition

Shear Thickening

Jamming Phase Diagram: Different routes to undergo a transition between rigid and flowing states.

Emergence/loss of rigidity in disordered matter.

Transitions out of equilibrium in character, in different ways.

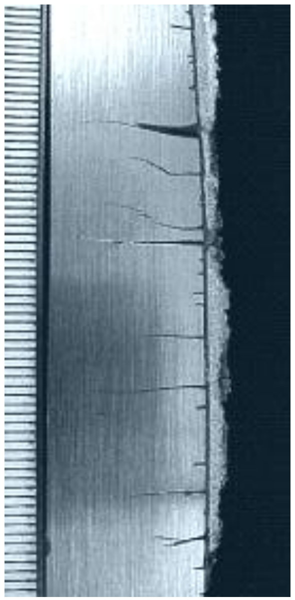
Yielding – Rigid to flowing state under external driving.

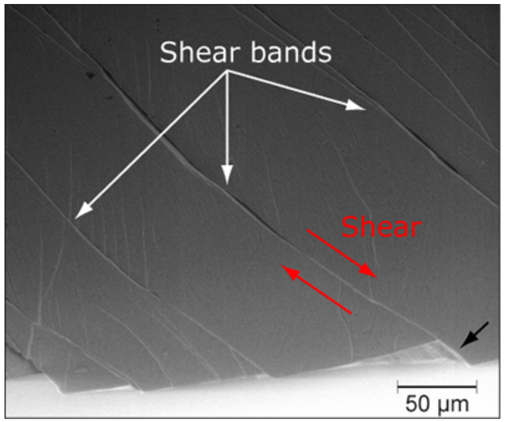
Yielding and Mechanical Failure

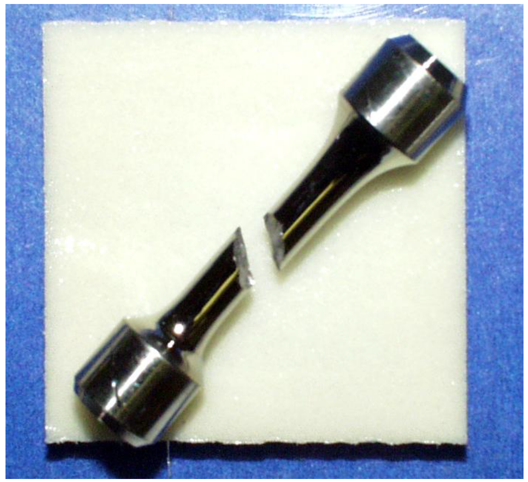
External stresses can cause (amorphous) solids to fail when deformed beyond a point of "**mechanical failure**".

Important for materials performance, and characterization.

Gorilla glass, metallic glasses, some recent important examples.

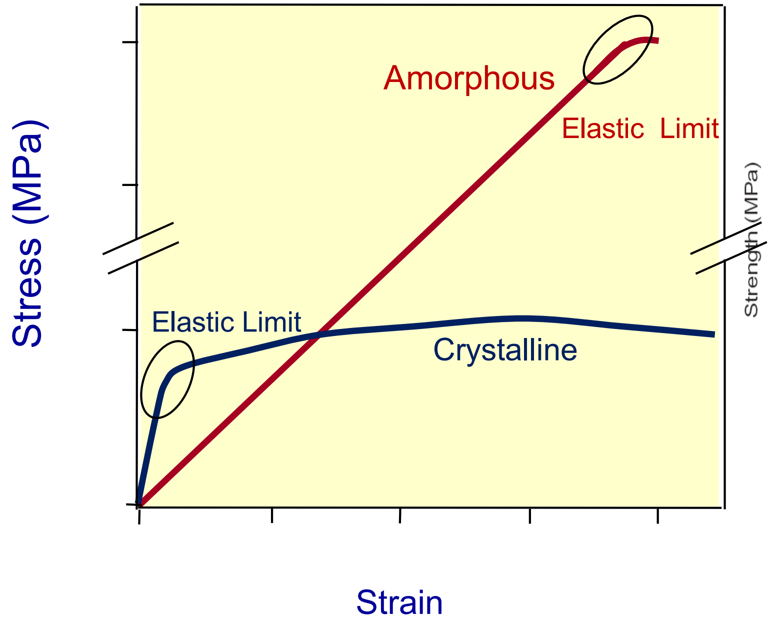


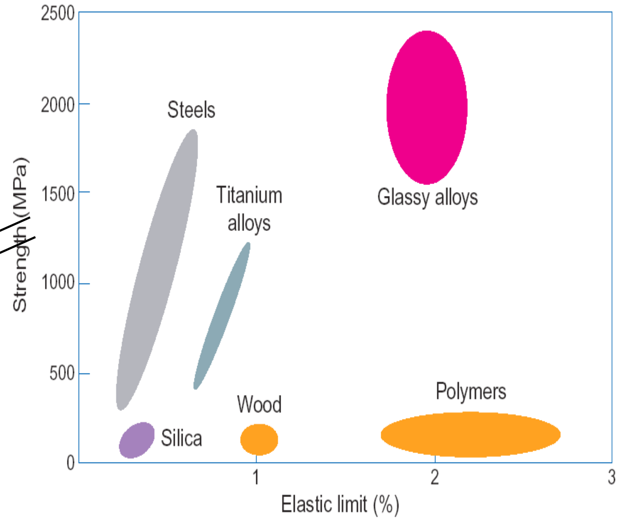


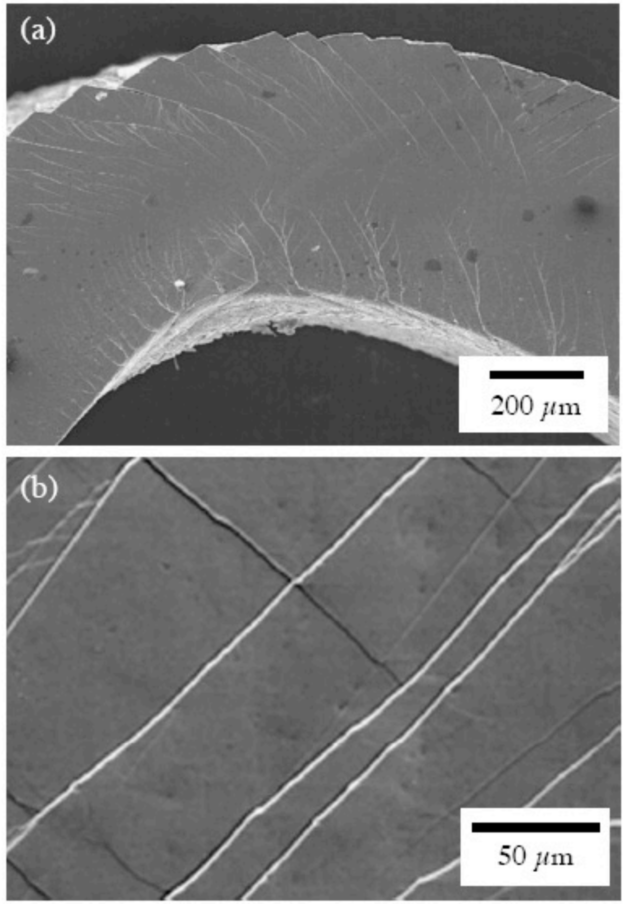


What is the microscopic description?

Example - Metallic Glasses







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

From: Schuh, Hafnagel, Ramamurty (2007)

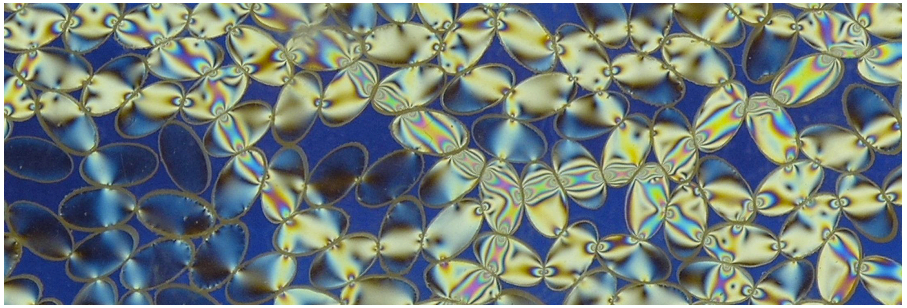
But exhibit brittle failure accompanied by shear localization (slip steps)..

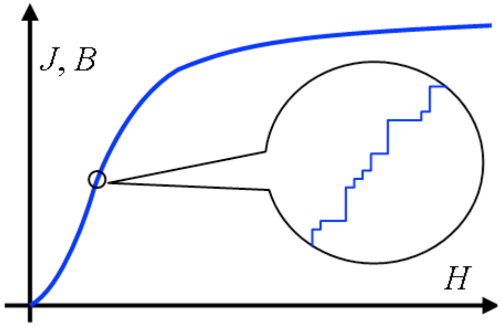
Parameters governing failure, and potentially their control, is critical for their applications.

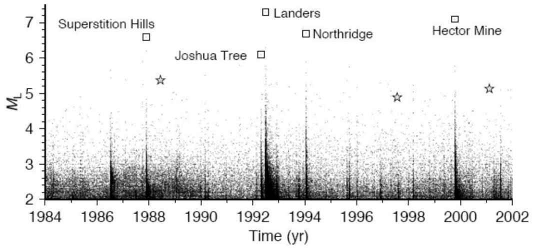
Yielding and Failure in disordered matter: Other examples

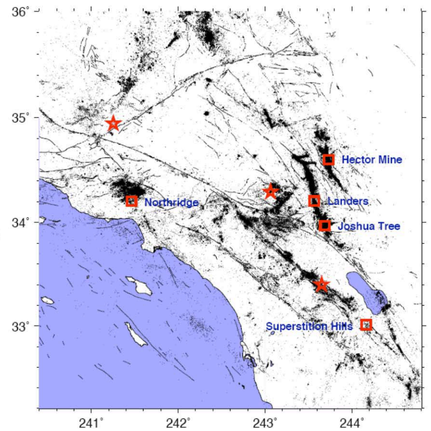
Related physics of intermittent, plastic, response in many disordered systems:

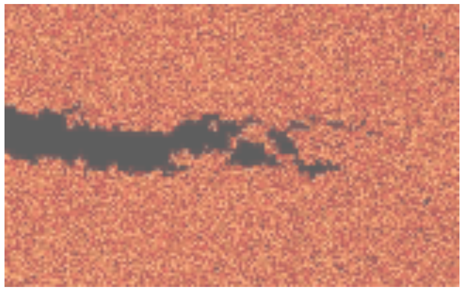
- Barkhausen noise in magnets
- Front propagation in disordered media
- Granular matter
- Landslides and avalanches
- Earth quakes

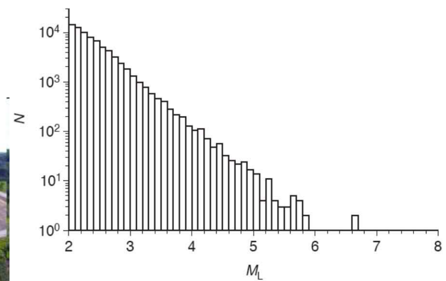








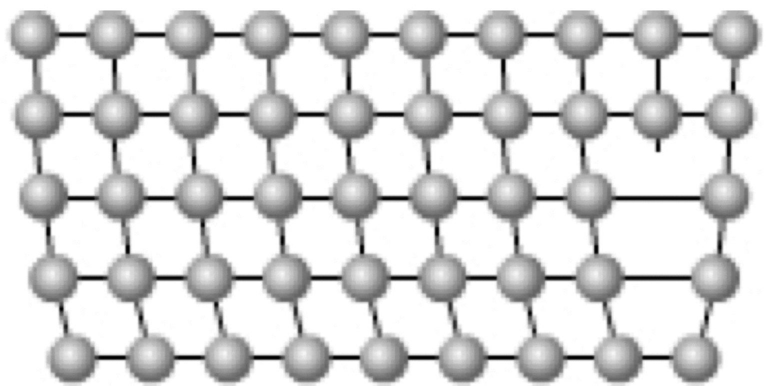




Mechanical behavior of solids

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

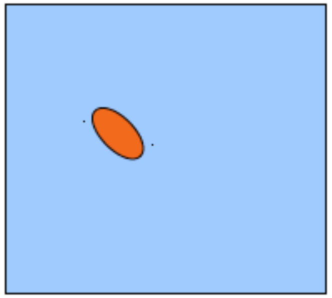
The movies have been provided for teaching purposes by Professor Hideharu Nakashima (ageigz@mbox.nc.kyushu-u.ac.jp) of Kyushu University, Japan.

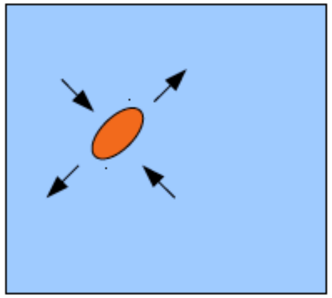
- **Amorphous solids** do not have regular translational order, and correspondingly no equivalent of dislocation defects.

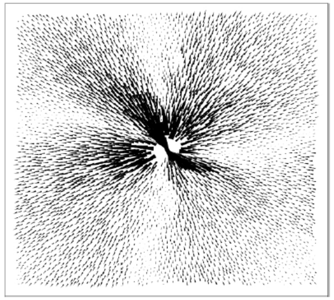
- Deformation mechanisms involve localized rearrangements, and avalanches of correlated (or triggered) deformation events.

Plastic rearrangements and interactions

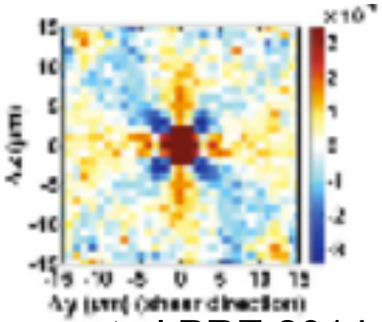
A local transformation embedded in an elastic medium leads to long range strain/stresses (Eshelby 1957), interactions:



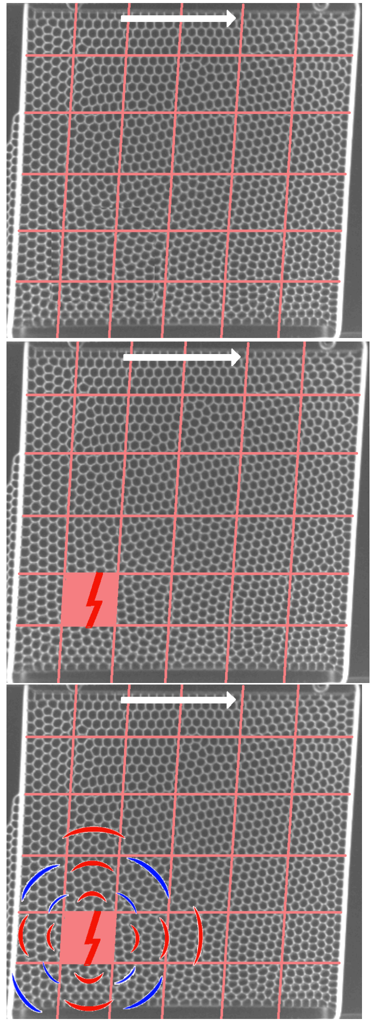




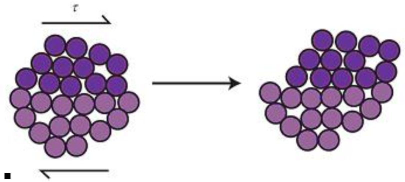
PRE 74, 016118 (2006)



Jensen et al PRE 2014

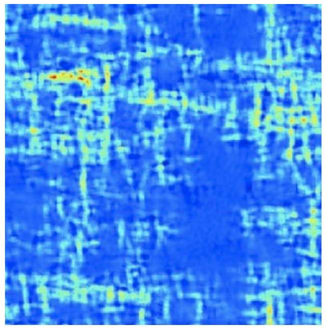


$$G(r, r') \sim \frac{\cos(4\theta)}{|r - r'|^d}$$



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..?

From Schuh et al 2007 [from Argon, Spaepen]
[Lemaitre, Caroli 2009]

Barrat

Questions/Issues

- The nature of plastic deformation events in sheared amorphous solids.
- The nature of interactions between localized events that lead to *avalanches* of correlated reorganization.
- The character of avalanches before yielding and after yielding.
- The nature of the yielding transition. Is it a sharply defined transition?
- Comparison to other transitions in driven disordered systems.
- Connection to the physics of the glass and jamming transitions?

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

What we do: Approach and Questions

1. Energy landscape picture of configuration space.

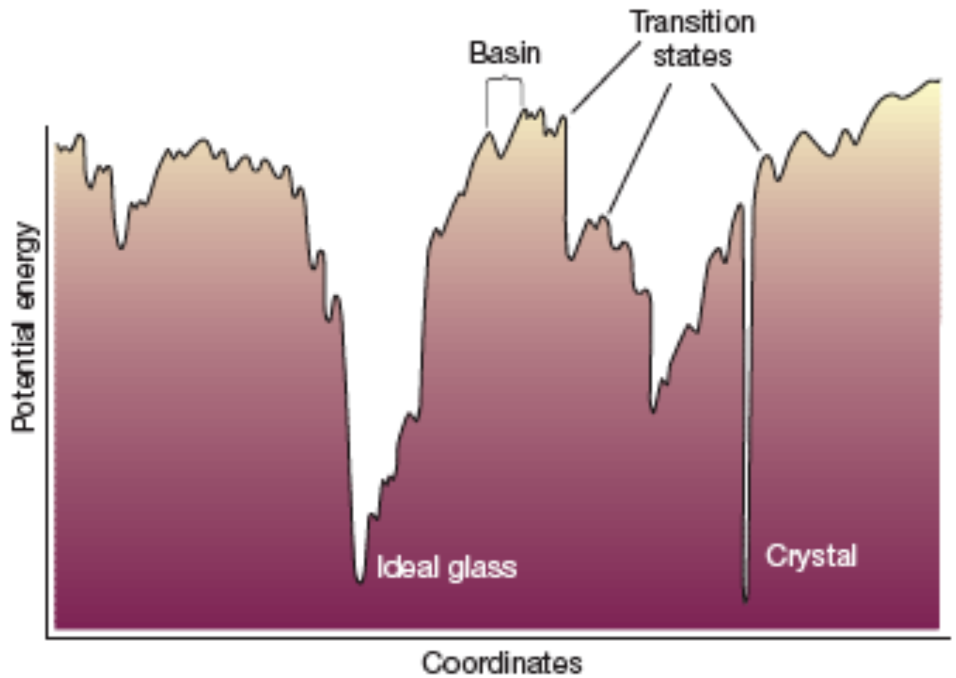
- Mechanical response to affine, shear deformations studied by analyzing the modification of the landscape, and transitions between minima, through the **AQS** (Athermal Quasi Static) protocol.
- Limitation: No information on the interplay between relaxation processes and instabilities triggered by deformation.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

Focus for this talk:

Nonequilibrium transition to ergodic state triggered by the cyclic shear deformation.

The Yielding Transition.

Shear bands.



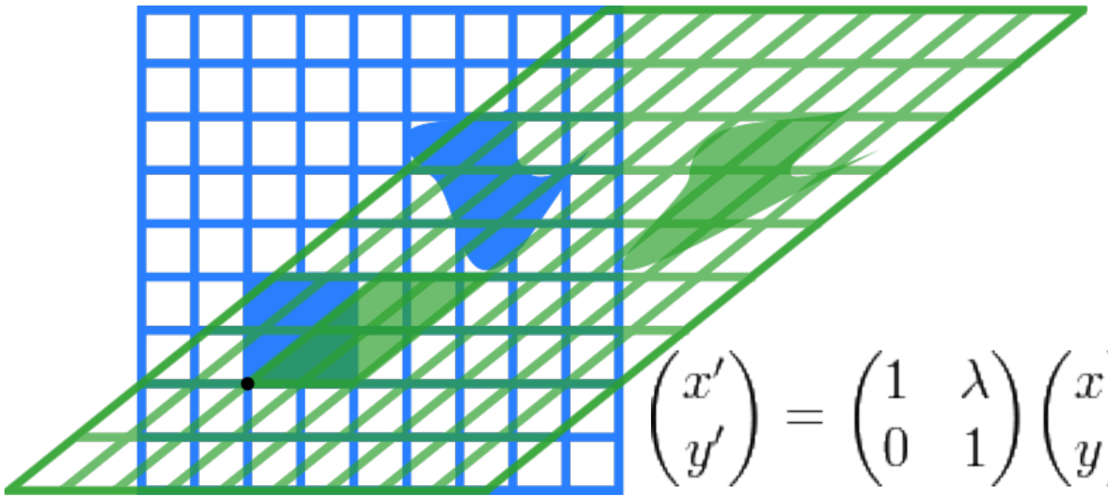
Energy landscape picture: Schematic

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

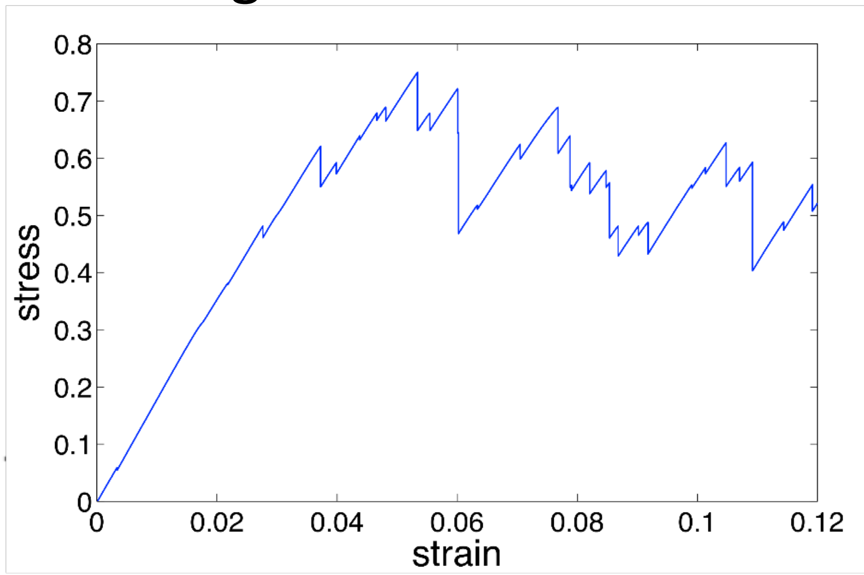
How does such deformation modify the properties of the glasses?

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.



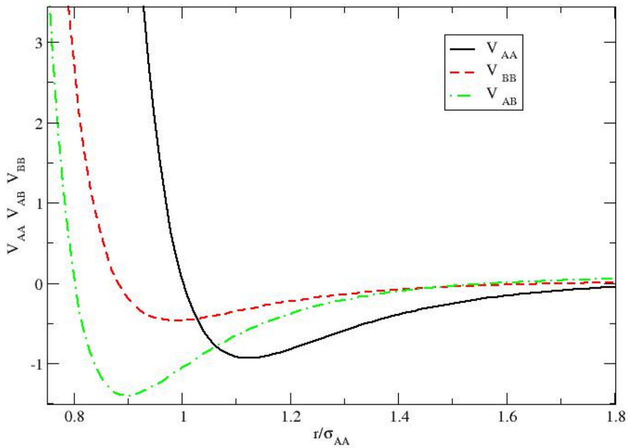
$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} 1 & \lambda \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}.$$

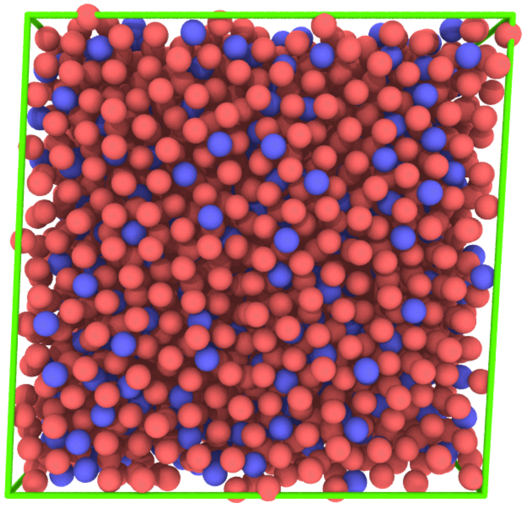


Simulations of oscillatory strained binary Lennard-Jones (LJ) solids

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

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

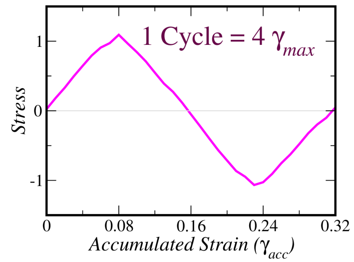




$0 \rightarrow \gamma_{max} \rightarrow 0 \rightarrow -\gamma_{max} \rightarrow 0$

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

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



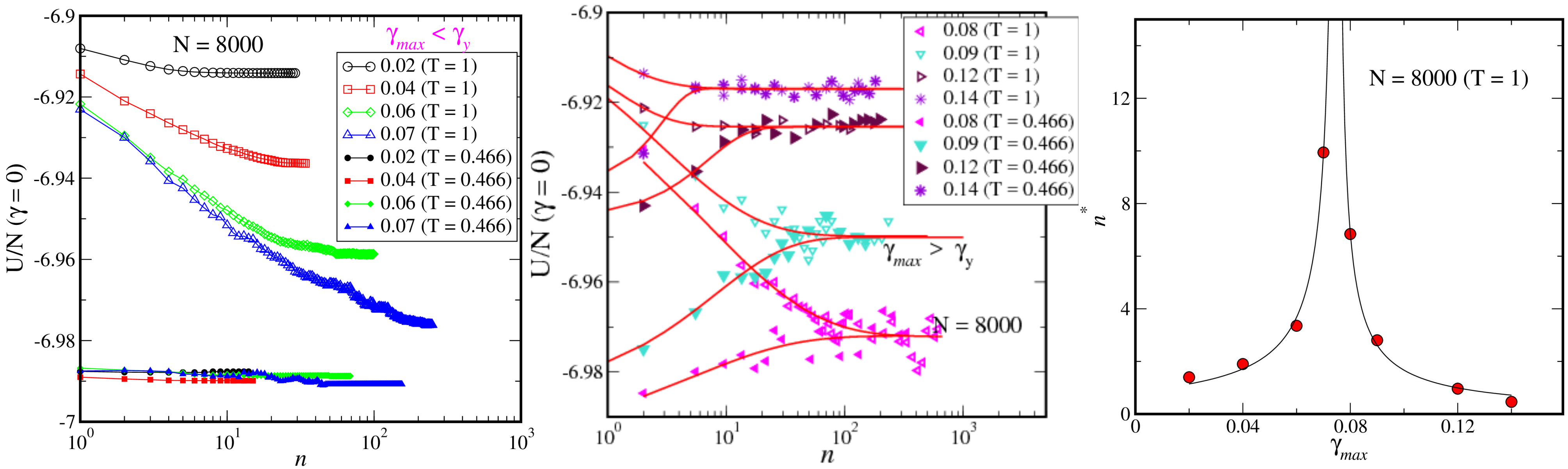
Cyclic shear for range of γ_{max} values with strain step $d\gamma = 2\times10^{-4}$.

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.**

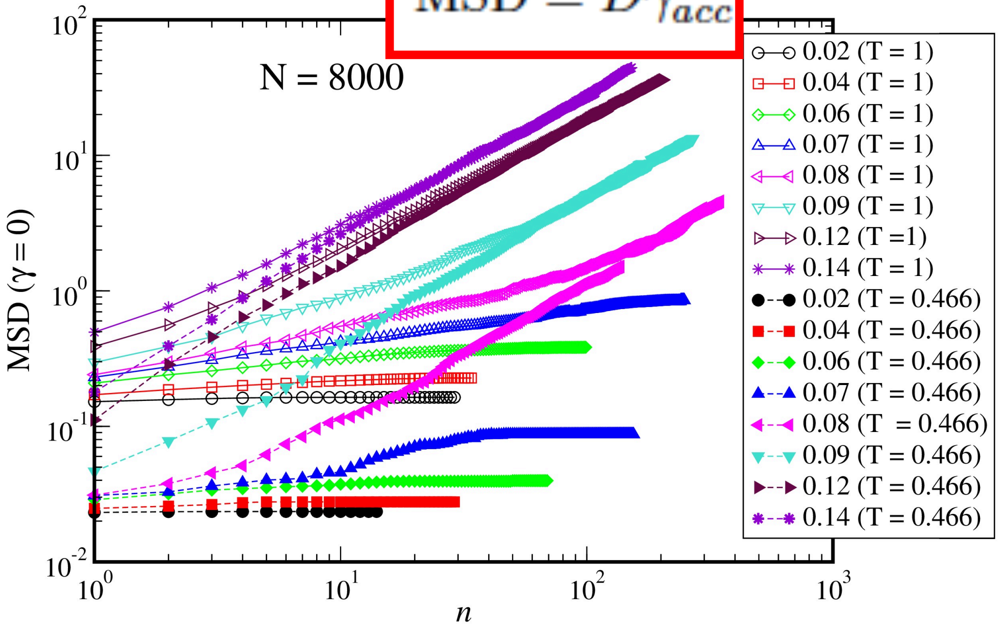
Change in behavior across a critical strain amplitude γ_c

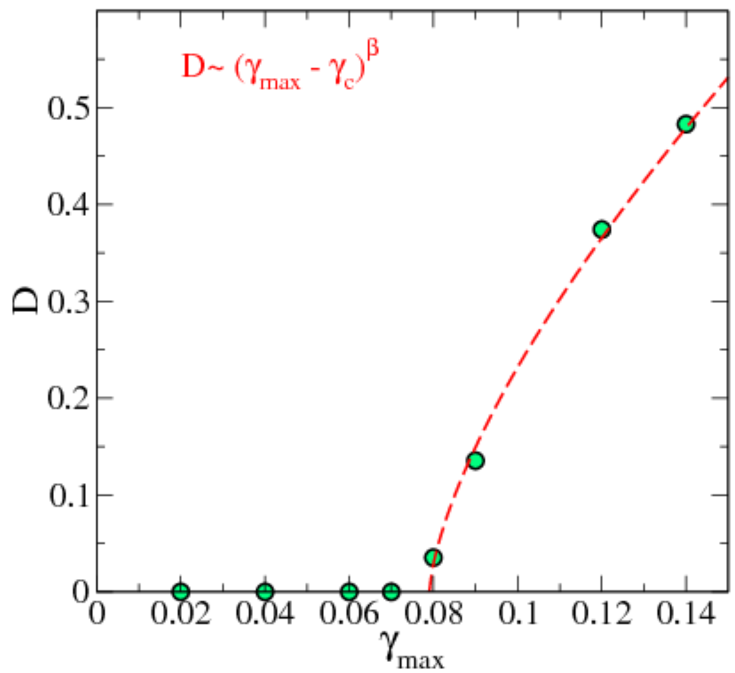
Mean Squared Displacement vs. Cycle #: Diffusion Coefficient

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

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

$$\mathrm{MSD} = D\gamma_{acc}^{*}$$



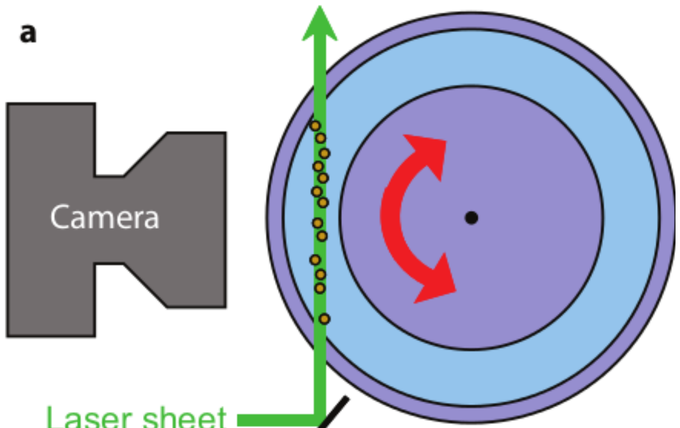


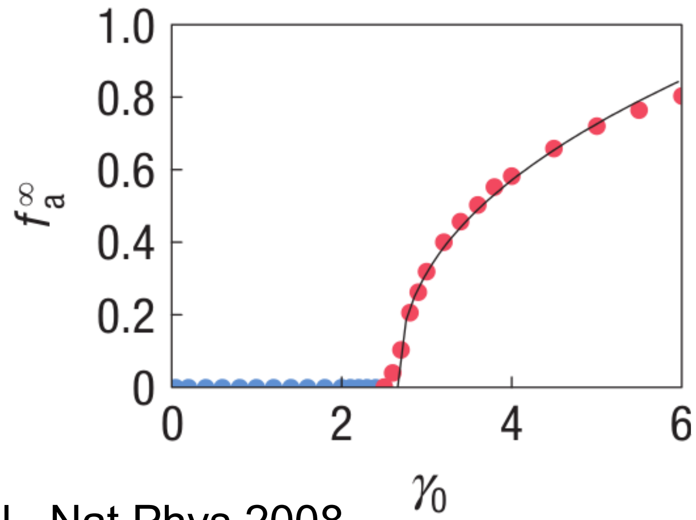
- The diffusion coefficient vanishes below a finite value of γ_{max} [How?]
- Critical γ_{max} a function of system size… but approach finite value asymptotically.

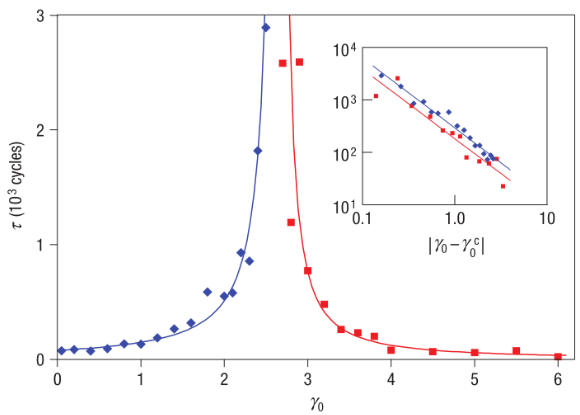
Non-equilibrium transition from localized to diffusive regimes!

Non-equilibrium phase transitions

The behavior seen in our system is similar to that observed in experiments dealing with colloids immersed in a viscous fluid subject to oscillatory deformation.







Pine et al Nature 2005 Corté et al., Nat Phys 2008

After a full oscillation, colloids in the cylinder return to the starting point or move a little. Those that move are named "active".

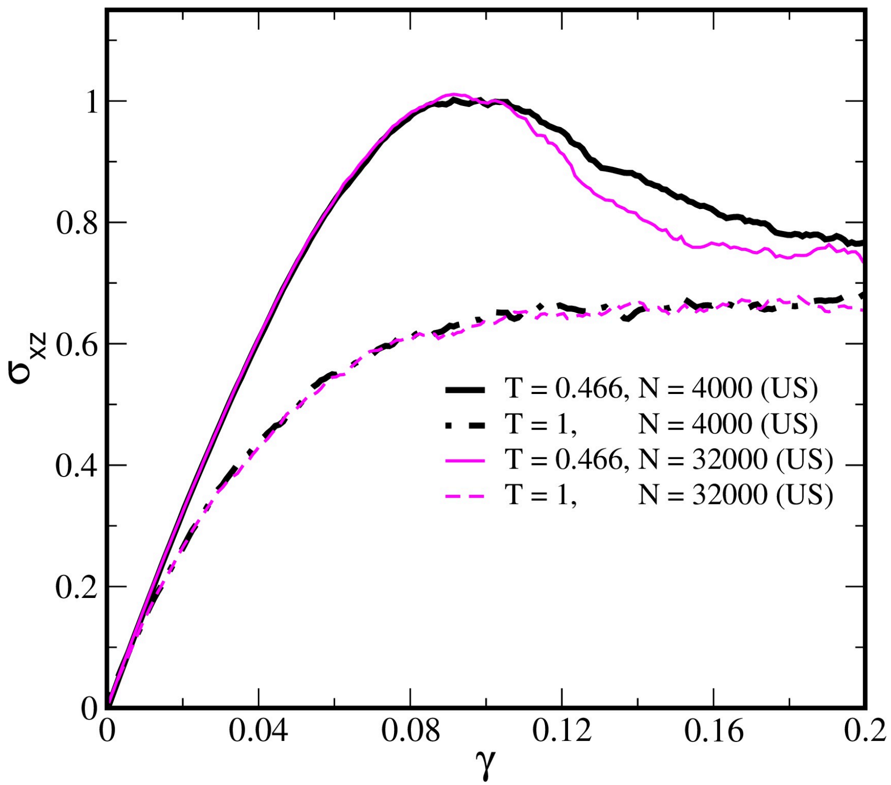
The fraction of active particles, and the time to reach steady states indicate a absorbing to ergodic state transition.

Interpreted as a non-equilibrium phase transition, possibly in the same universality class of directed percolation with a conserved order parameter (C-DP). [Menon and Ramaswamy 2009].

Are these different systems exhibiting the same behavior?

Yielding
Uniform Shear

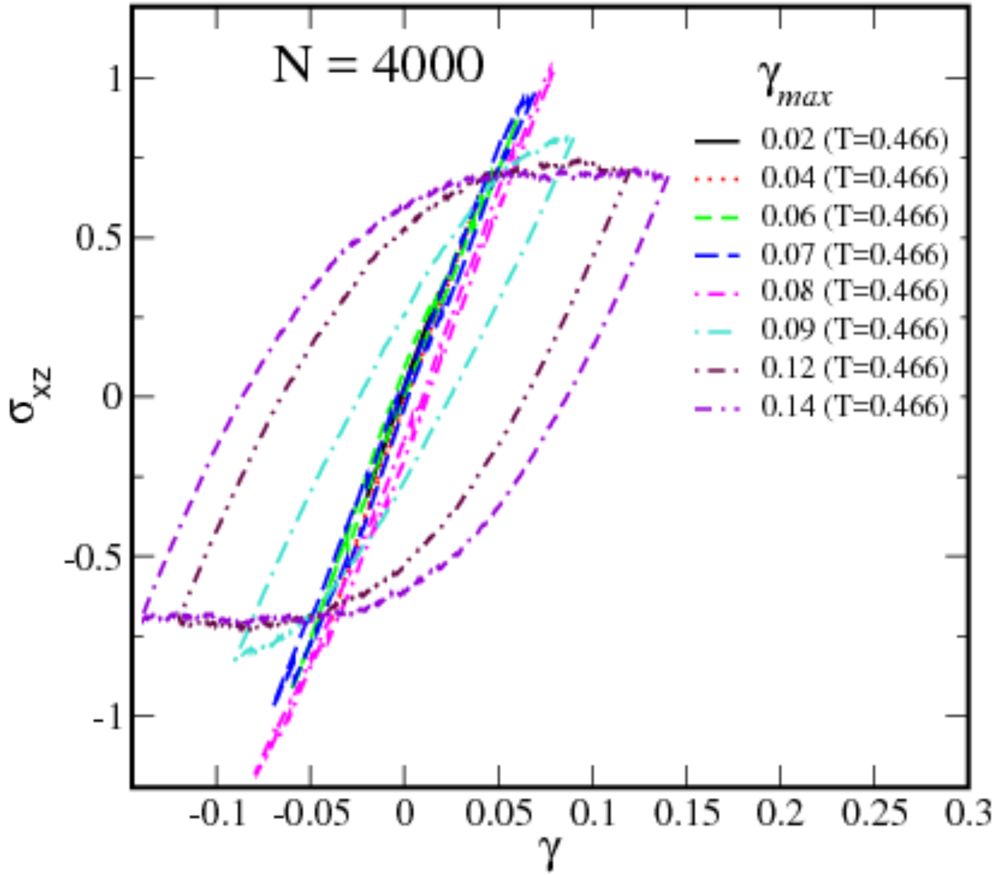
Does the non-equilibrium transition correspond to yielding?



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

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

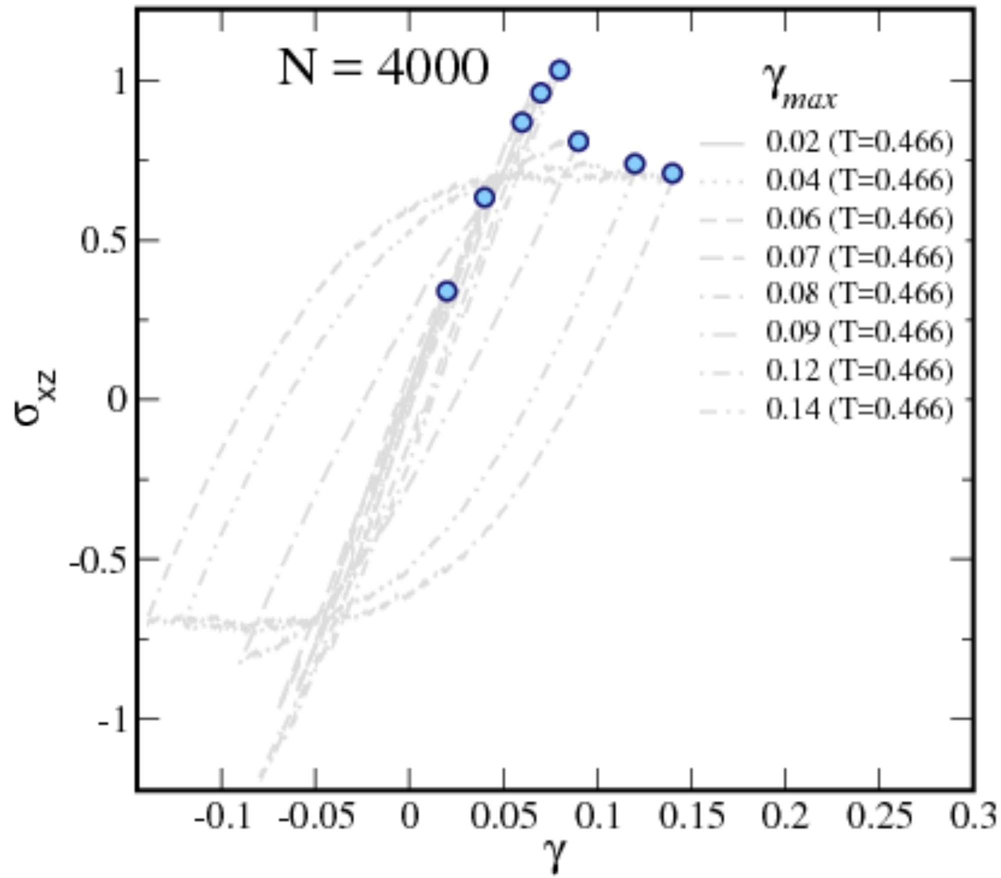
Yielding: Oscillatory shear



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.

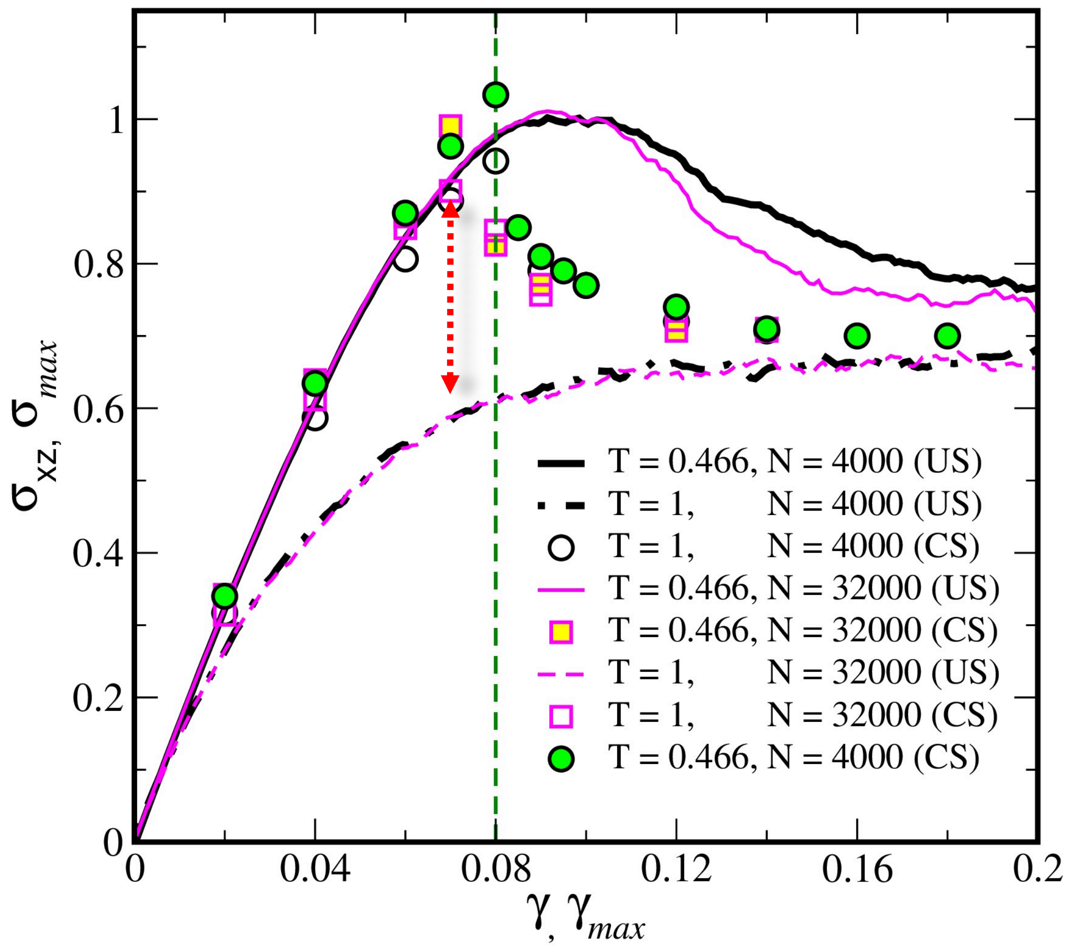
We focus on maximum stress during cyclic shear..

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

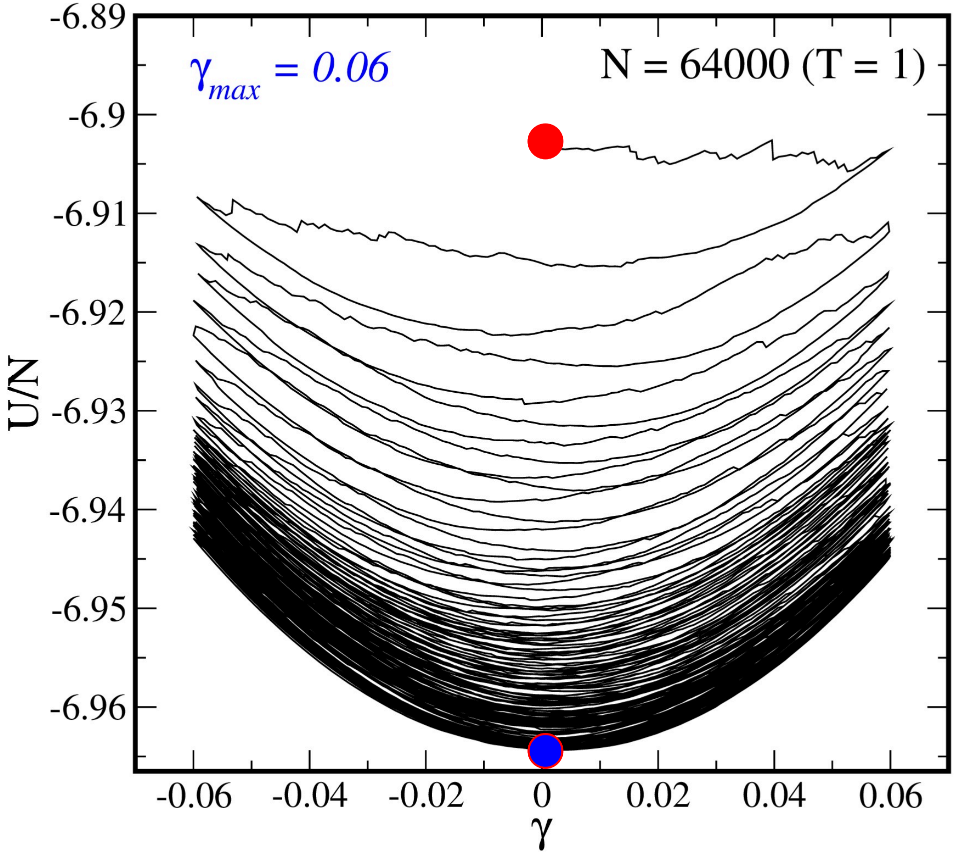
- For **cyclic shear** (CS) they fall on the same curve (more or less) irrespective of the initial (sample) conditions.

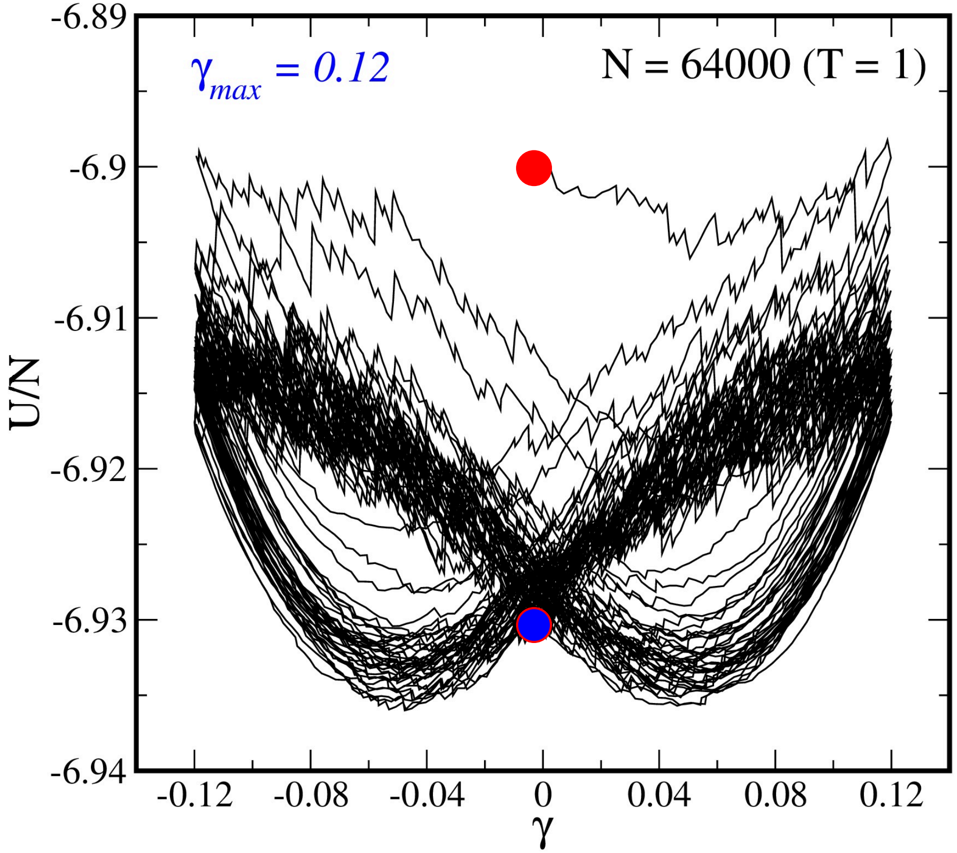
Oscillatory sheared states better for characterizing yield.

Pointers for thermo-mechanical processing of glasses?



Evolution of energy with cycles

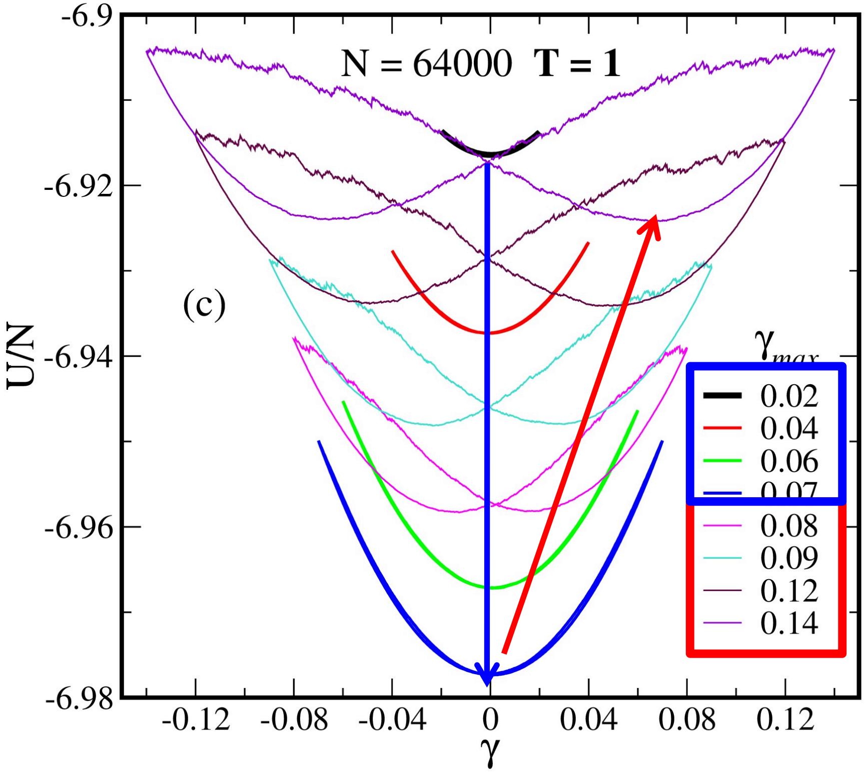


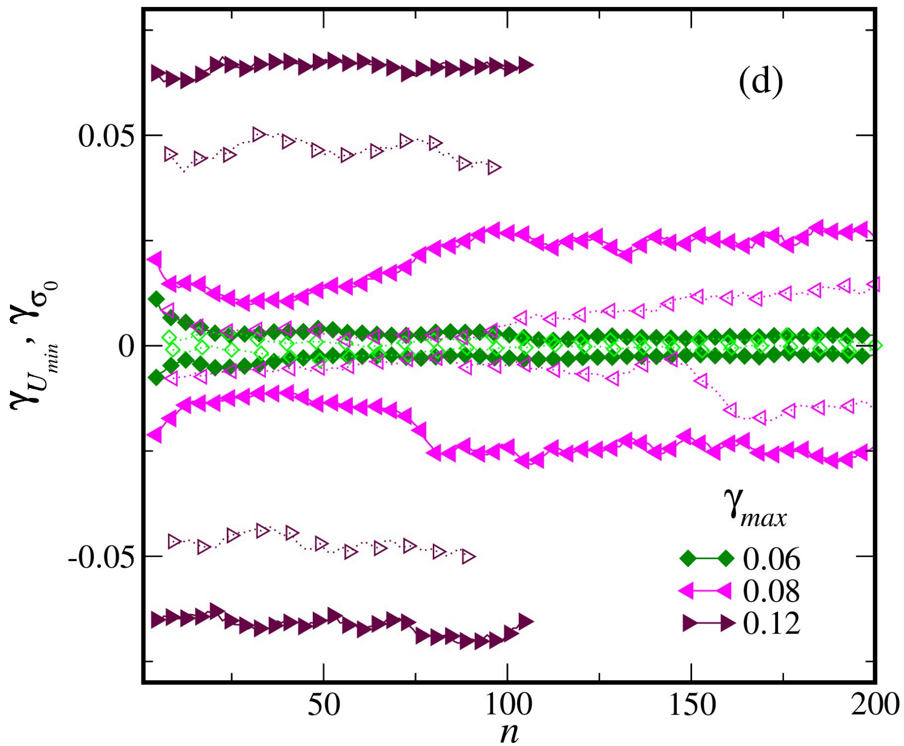


- For γ_{max} = 0.06 (i.e. $\gamma_{max} < \gamma_y$) the energy approaches to a single minimum at γ = 0, but
- **Energy bifurcates** into two minima (for γ_{max} = 0.12 (i.e. $\gamma_{max} > \gamma_y$)) at finite strain.

Indicates emergence of plasticity.
A hallmark of the transition!

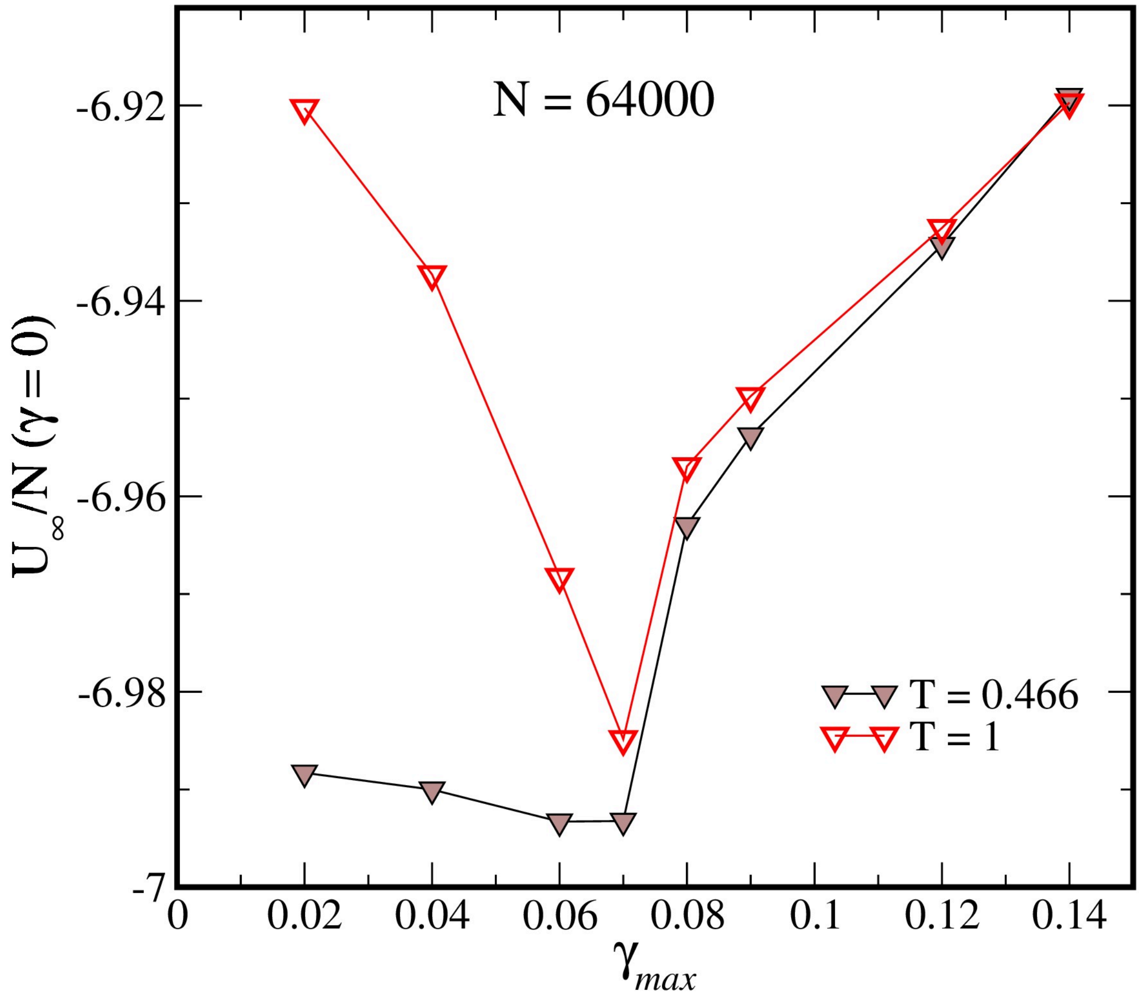
Evolution of energy with cycles





- 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

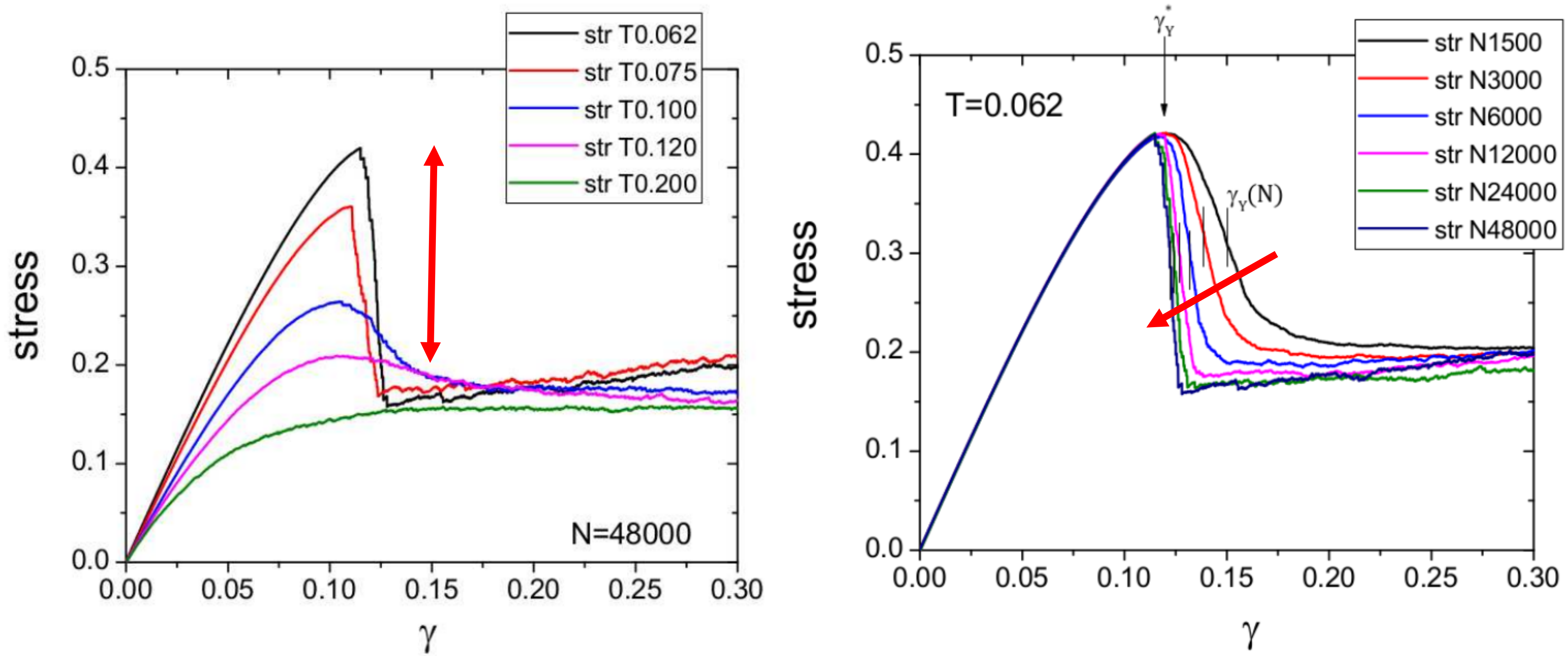


Better annealing close to the transition.

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}.

Uniform Shear: Ultrastable glasses



Ultra stable glasses shows sharp change in the yielding behavior.

Discontinuous change at yielding similar to cyclic shear, resulting in both cases from better annealing.

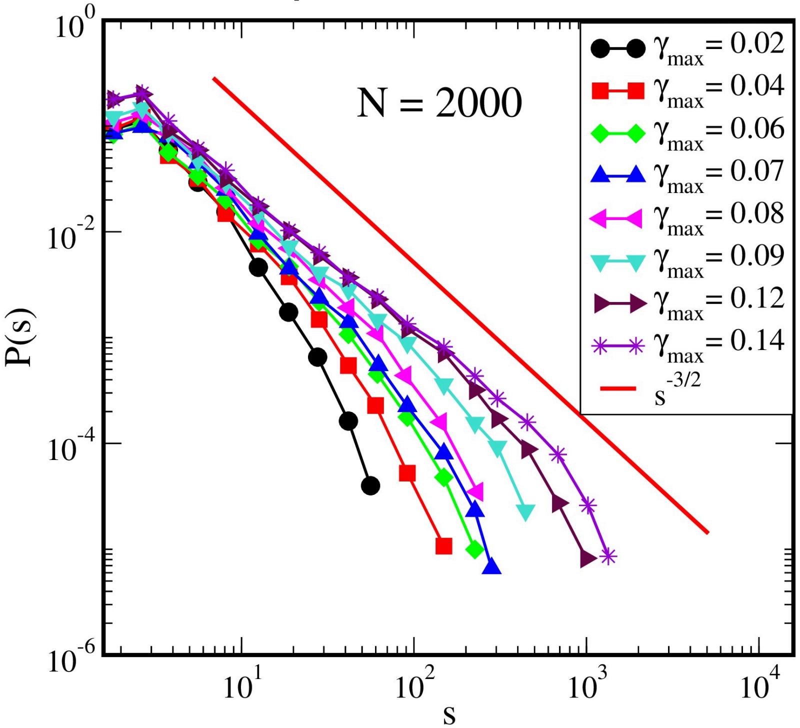
M. Ozawa and L. Berthier

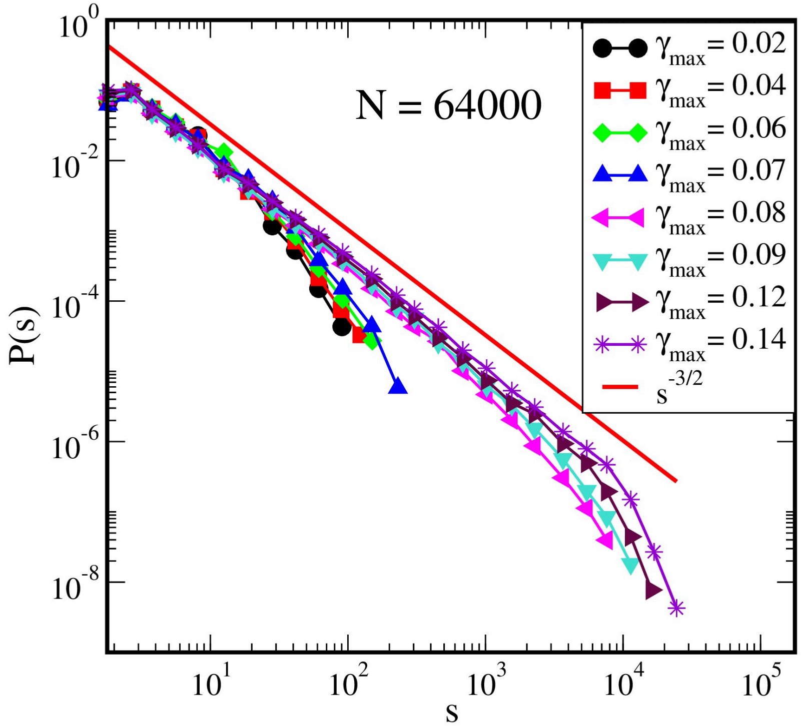
Distributions of Avalanche Sizes

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)





- 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

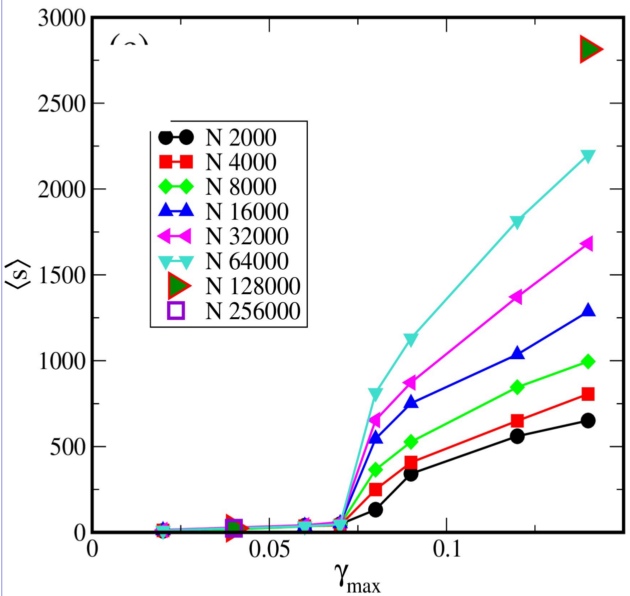
Above the yield point mean avalanche size shows clear size dependence ~ $N^{1/3}$

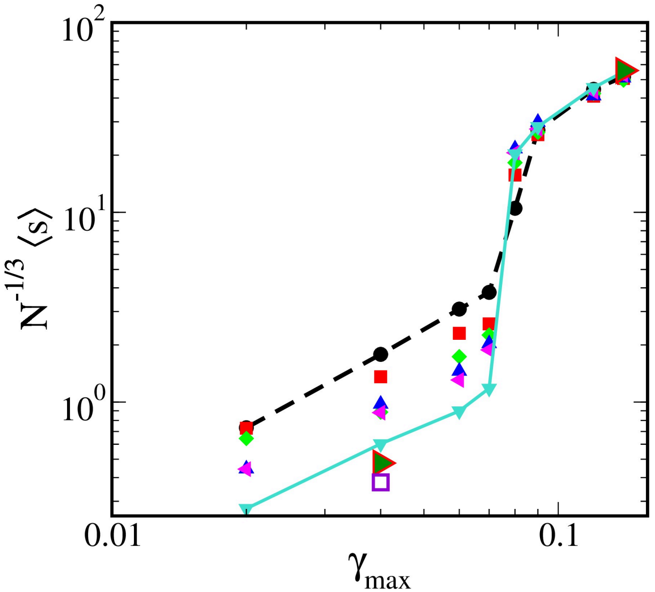
Consistent with uniform shear results for the case of plastic flow states.

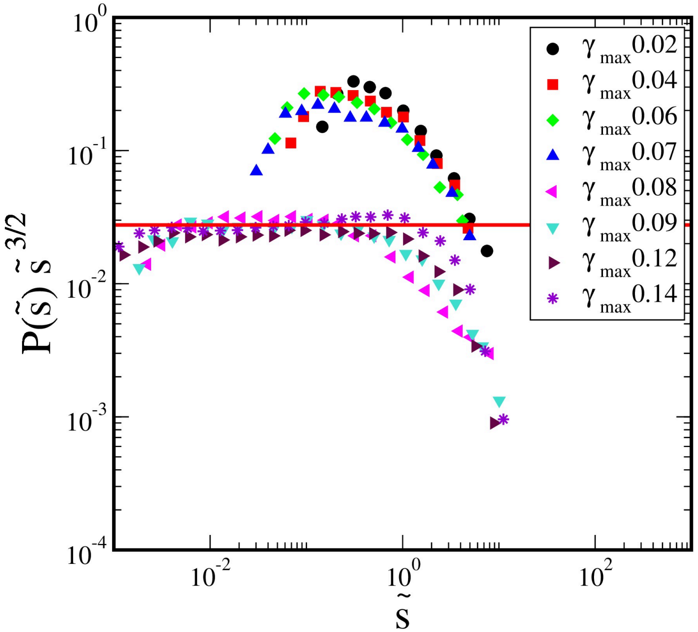
Below the yield point, avalanche sizes remain finite and do not show **dependence on system size.**

Scaled cluster size (= s/<s>) distributions for $\gamma_{max} < \gamma_y$ do not display a power law regime, whereas for $\gamma_{max} > \gamma_y$ they do.

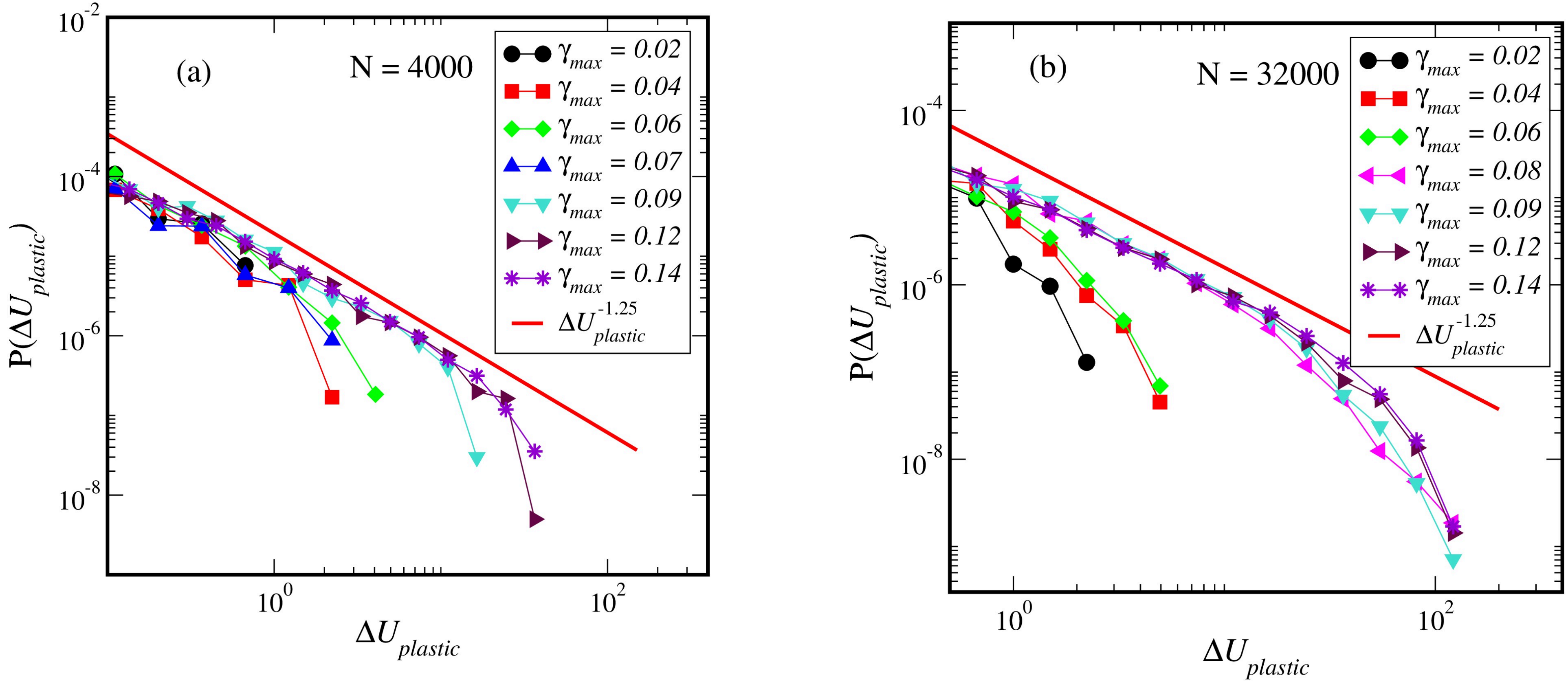
Qualitatively different avalanche distributions!





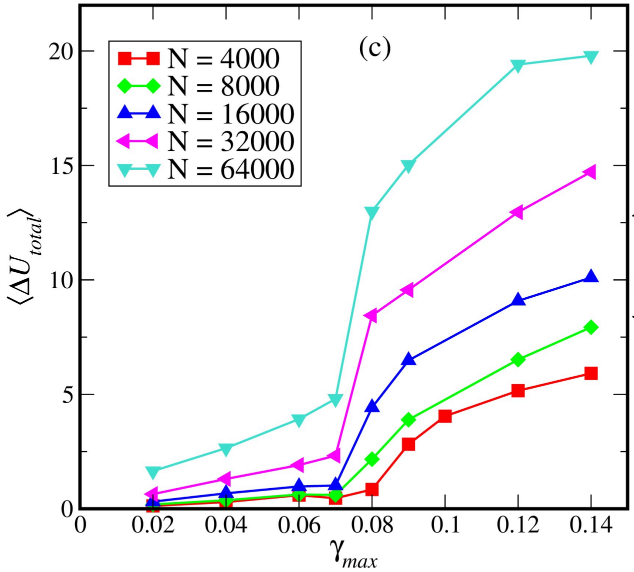


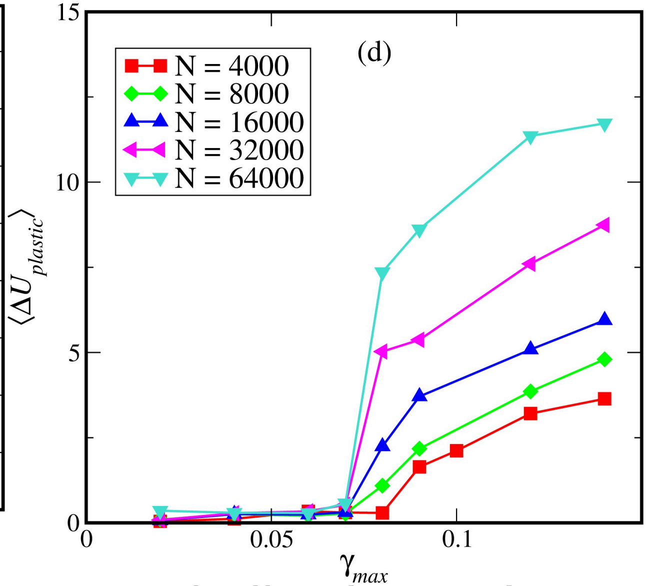
Avalanche: Energy drops

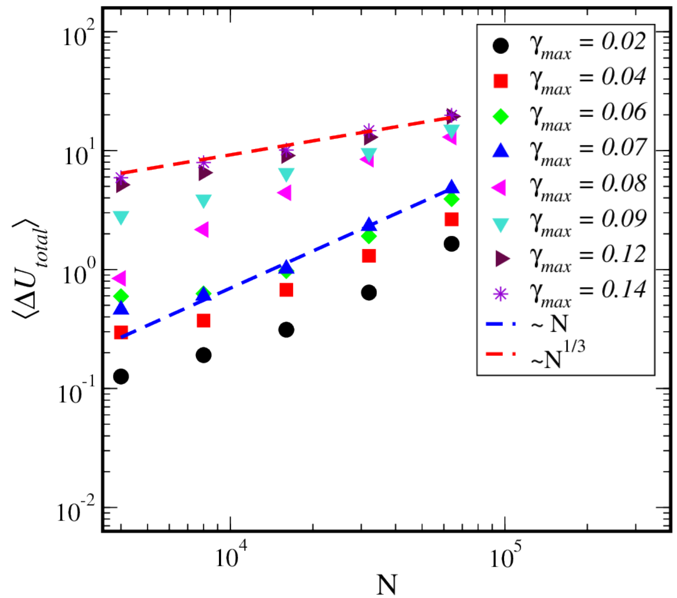


Energy drops distribution shows power law distribution with cutoff and the cutoff increases with γ_{max}.

Avalanche: Energy drops

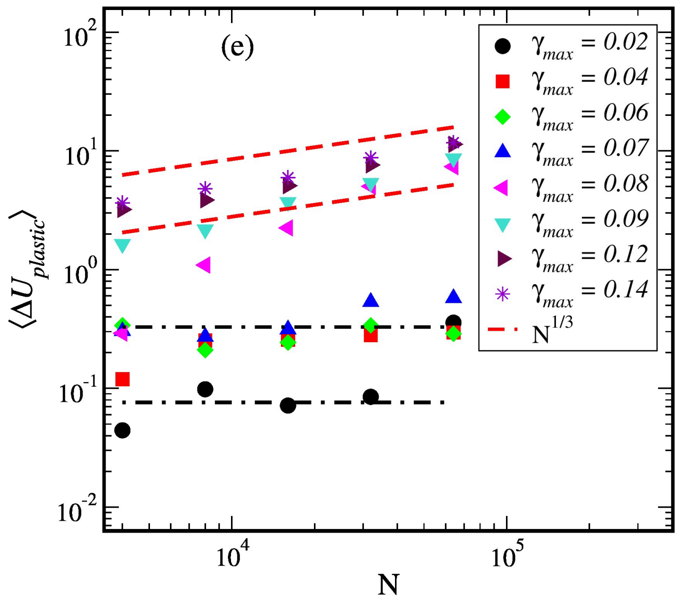




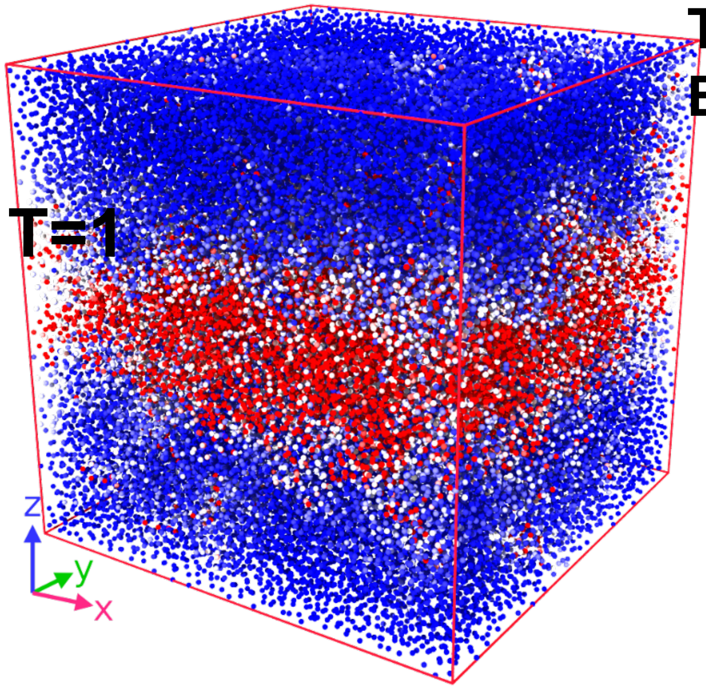


- Mean energy drops vs. γ_{max}, indicating a sharp change at γ_y.

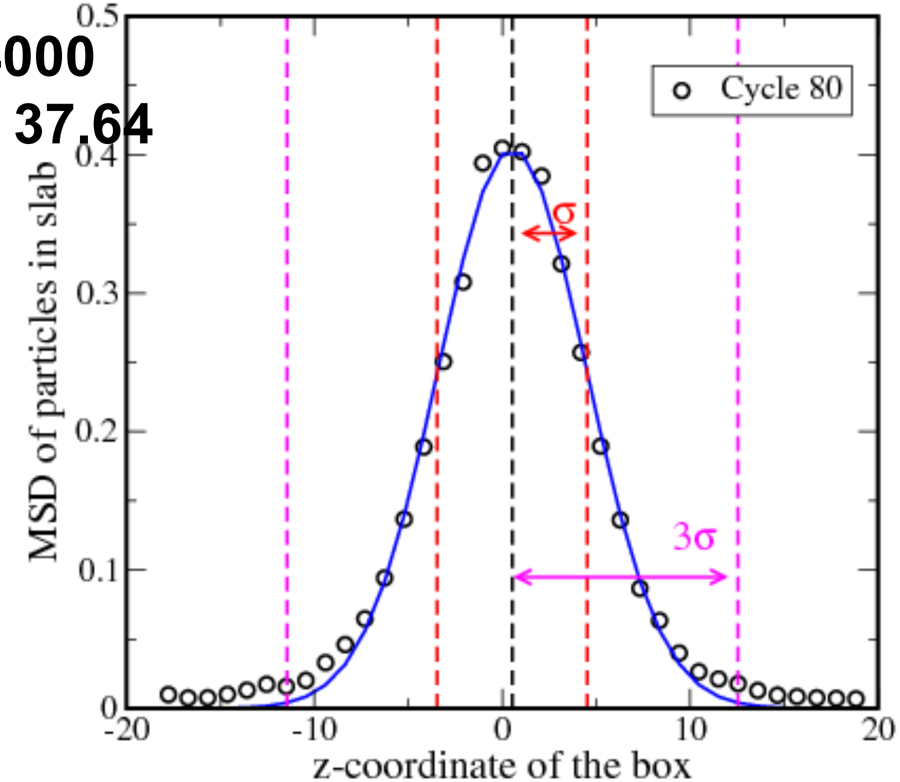
- Mean energy drops considering only plastic regions show no system size dependence below γ_y .
- Mean energy drop (plastic component) vs. system size N shows no significant size dependence for $\gamma_{max} > \gamma_y$ but a clear $N^{1/3}$ dependence above.



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

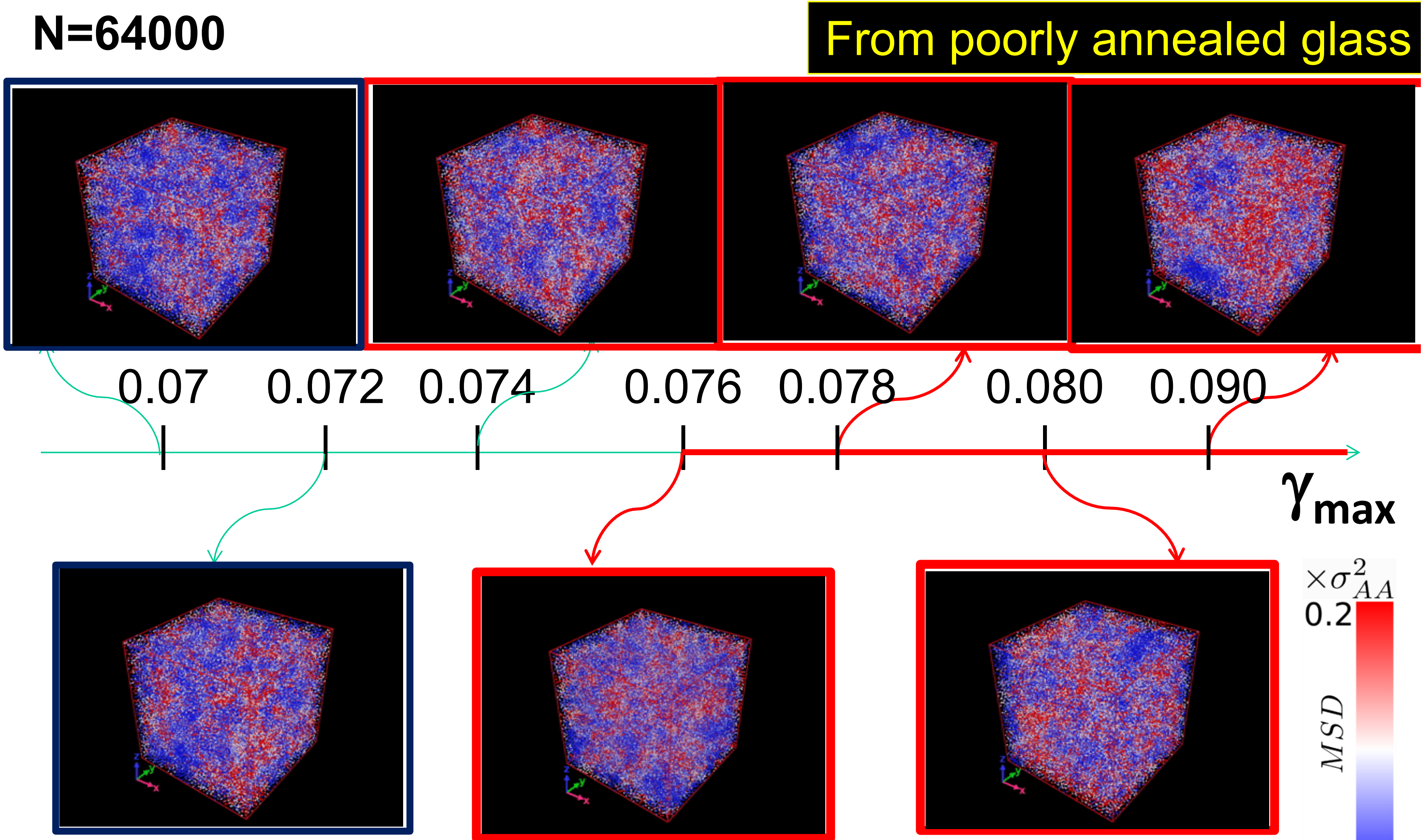
- The slabwise MSD of particles as function of the height of the band.

Yielding is accompanied by the formation of shear bands.

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

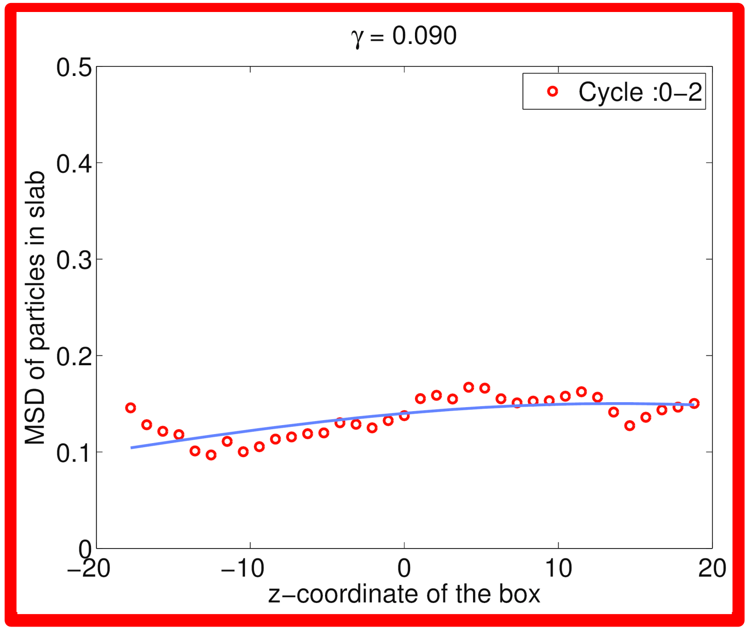
Probed by different initializations (from liquid/poorly annealed glass, strain amplitude below (.07), above (.08) yield value).

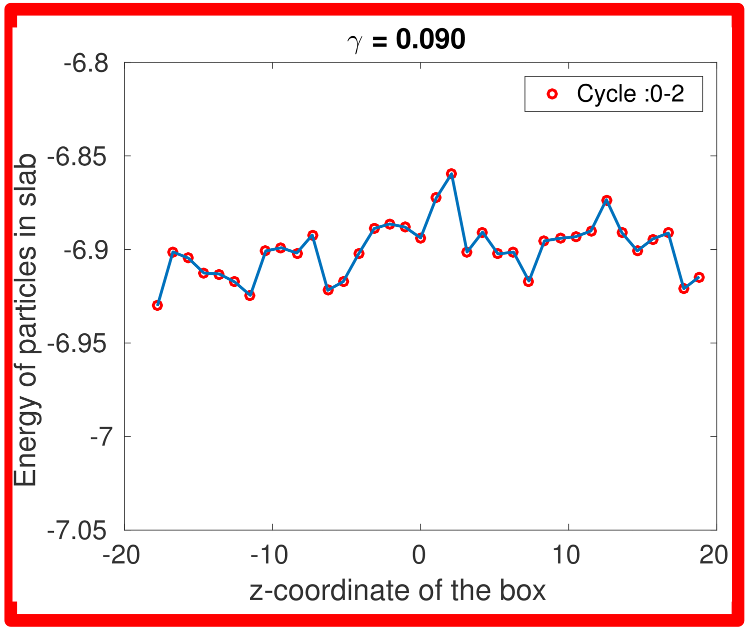
Across the yielding transition

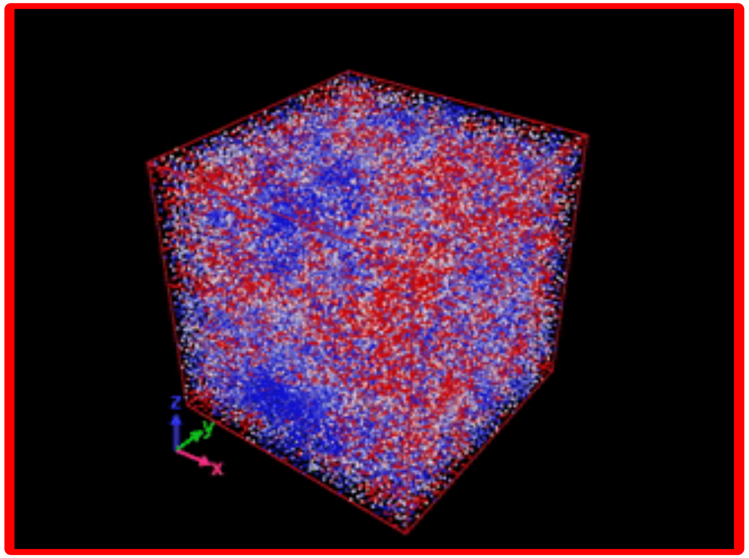


Shear bands are present in the steady states for strain amplitudes above yielding value ~ 0.07

Evolution towards steady states



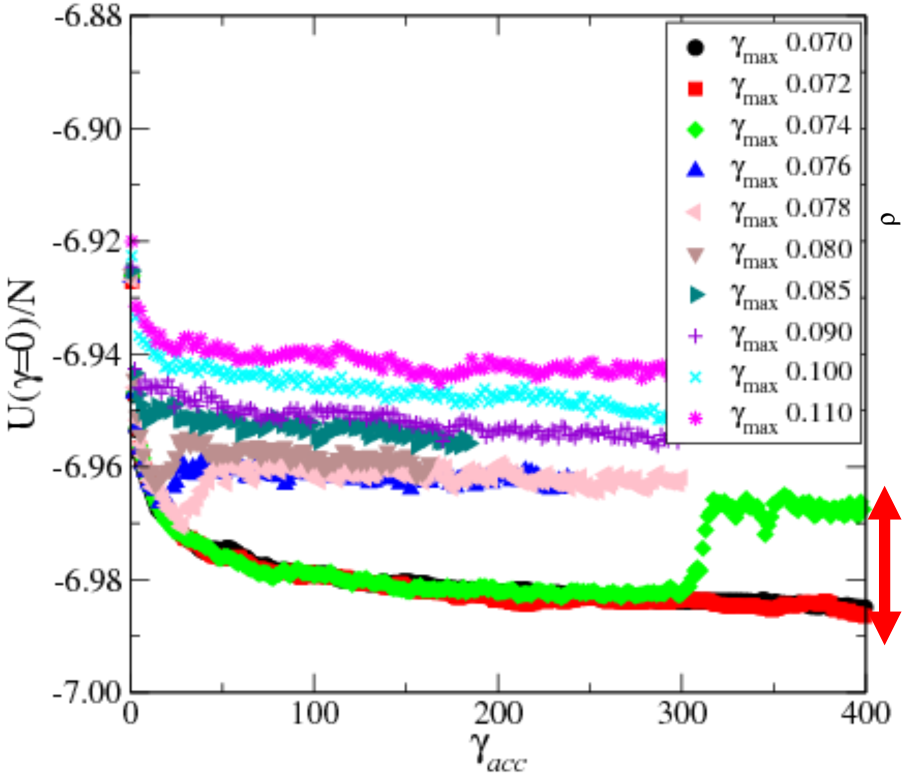


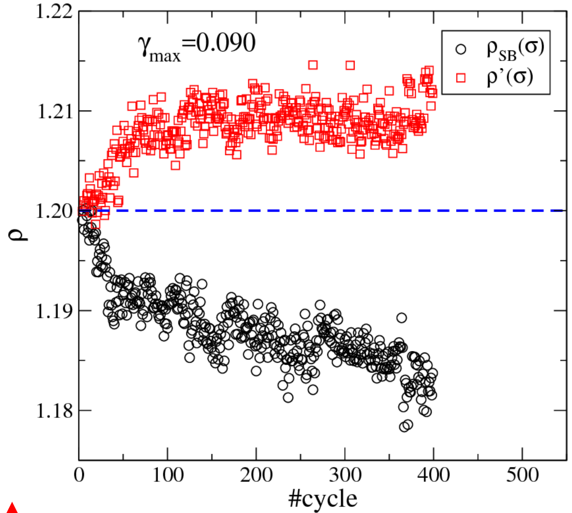


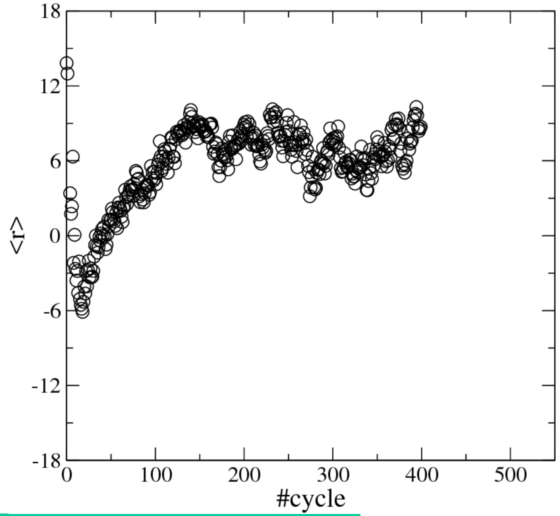
- Shear bands are present in the steady states.
- The energy and MSD profile changes in the presence of the shear band.

γ_{max}=0.09

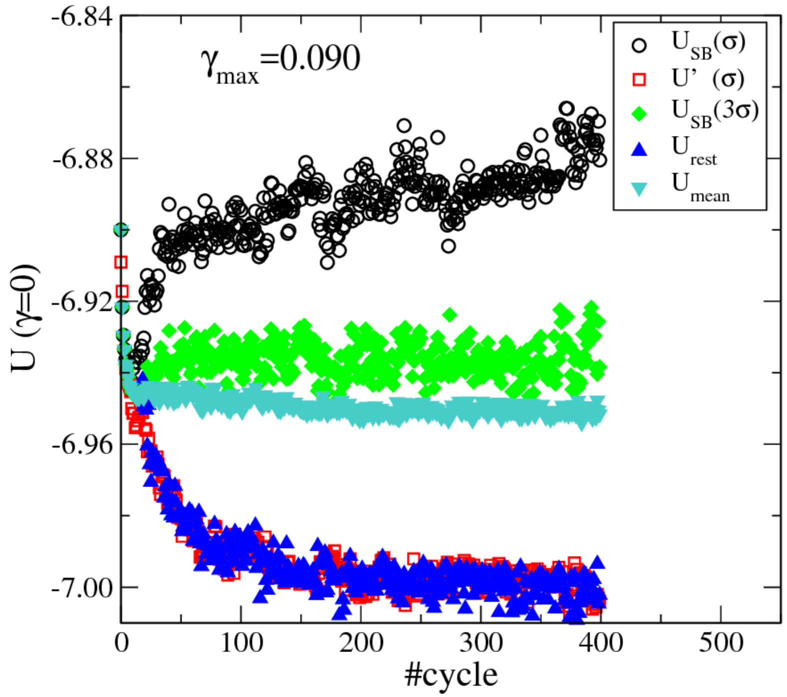
Evolution towards steady states





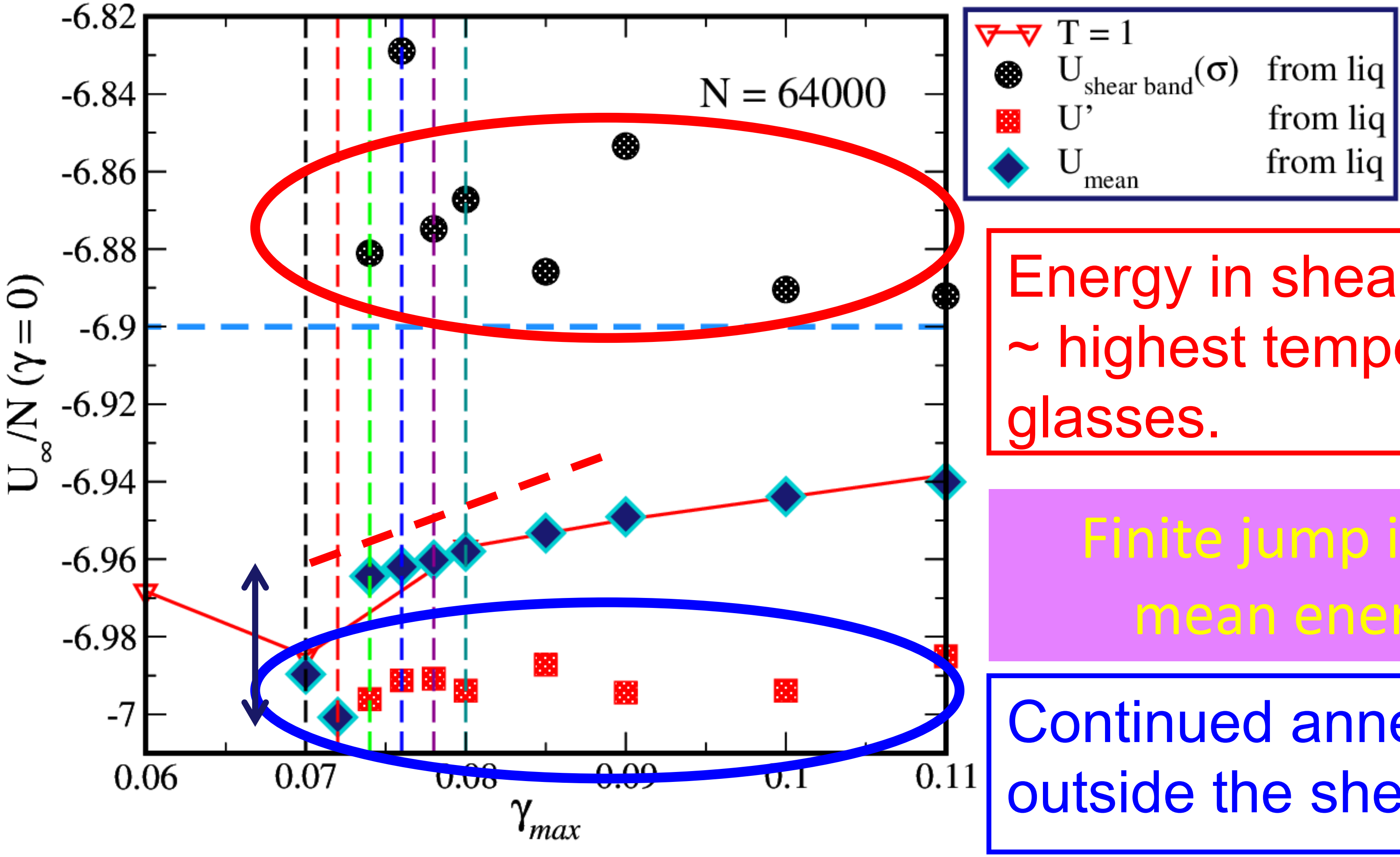


Shear band γ_{max}=0.09



- 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.

Annealed regime above Yielding



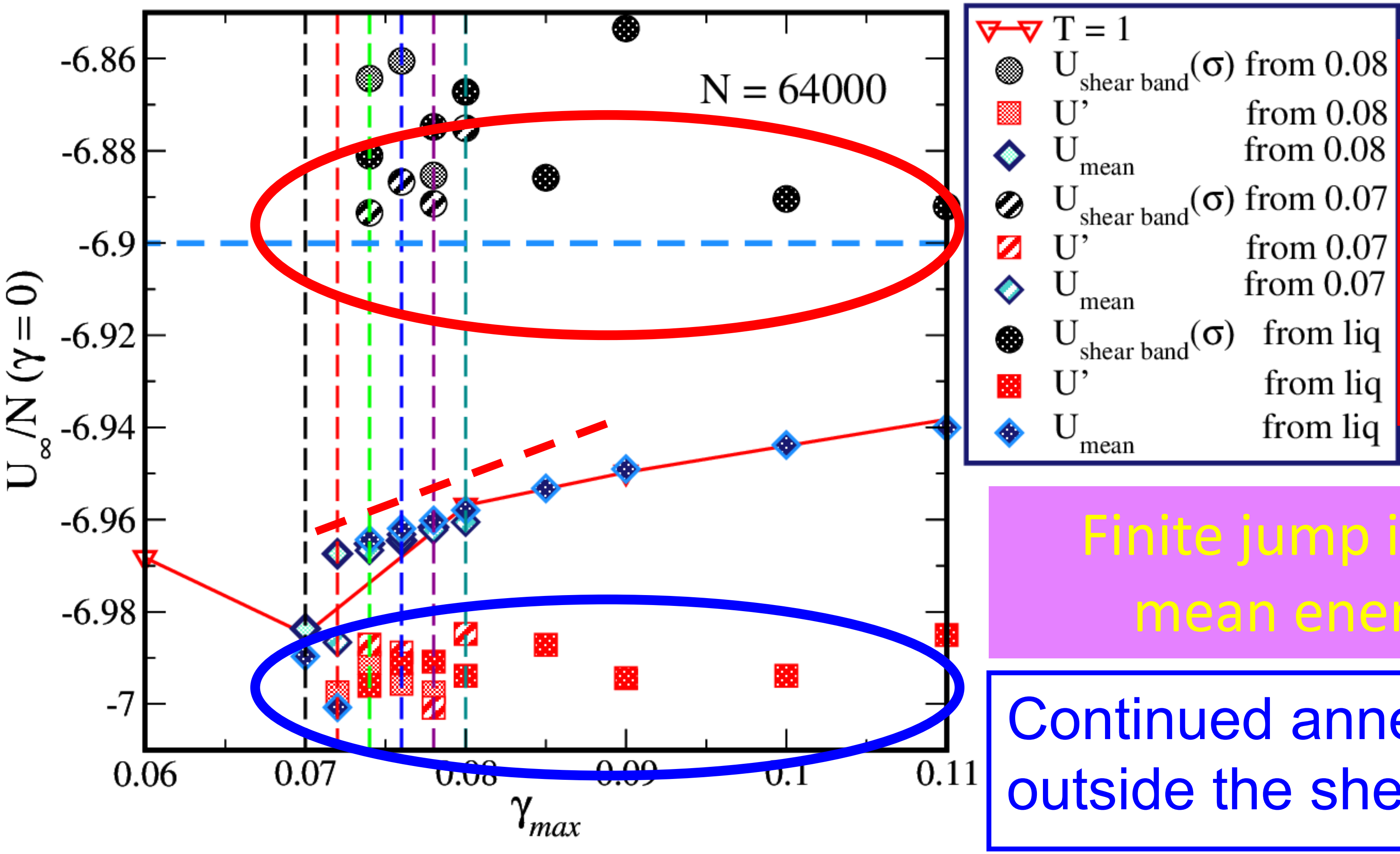
Energy in shear band ~ highest temperature glasses.

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 hysteresis/initial condition dependence.

Annealed regime above Yielding- various cases



Energy in shear band ~ highest temperature glasses.

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- Particle in the shear band access energies at the "top of the landscape"
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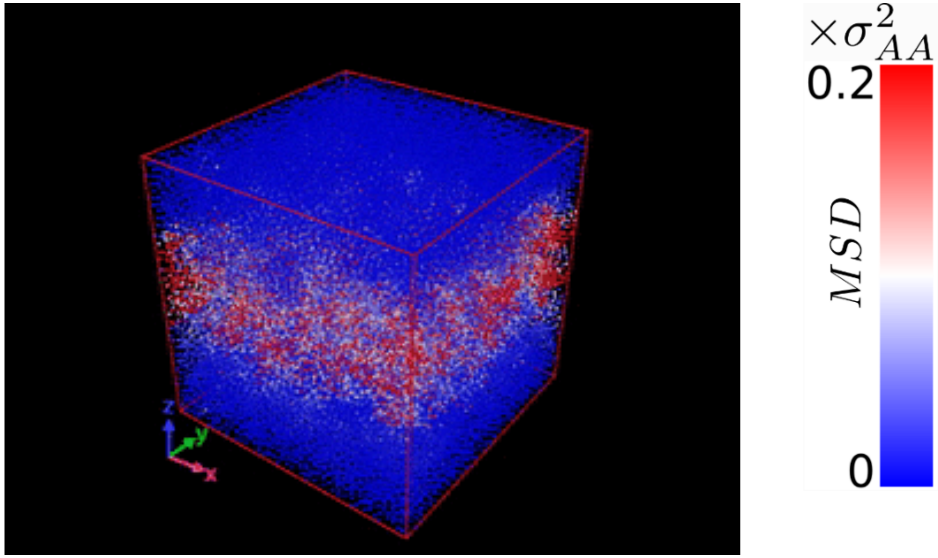
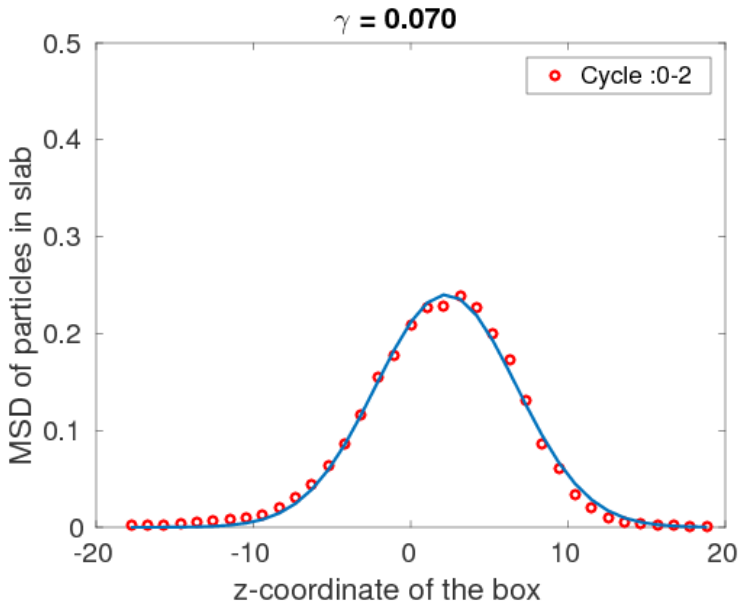
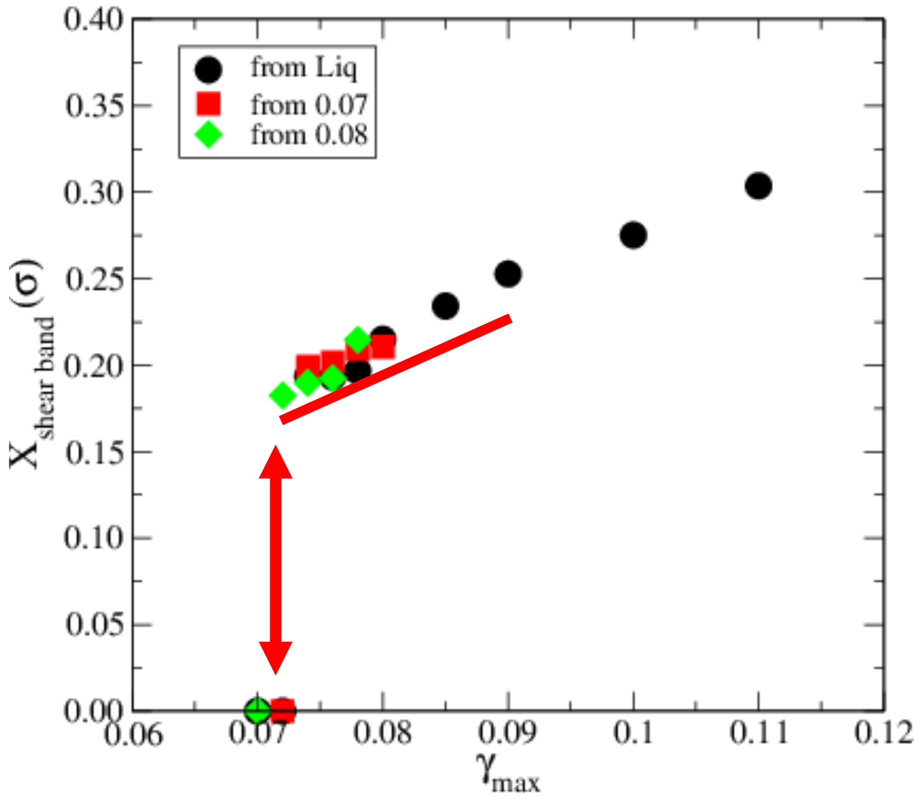
Vanishing shear band
From γ_{max} = 0.08, @ γ_{max} =0.07

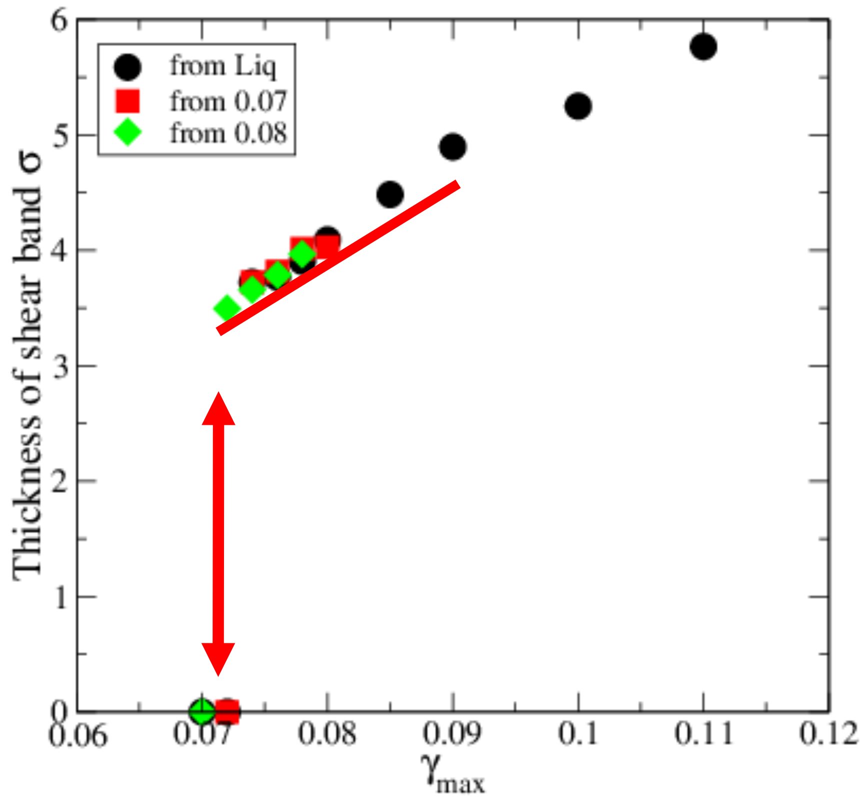




The shear band vanishes after a large number of strain cycles at smaller amplitude.

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

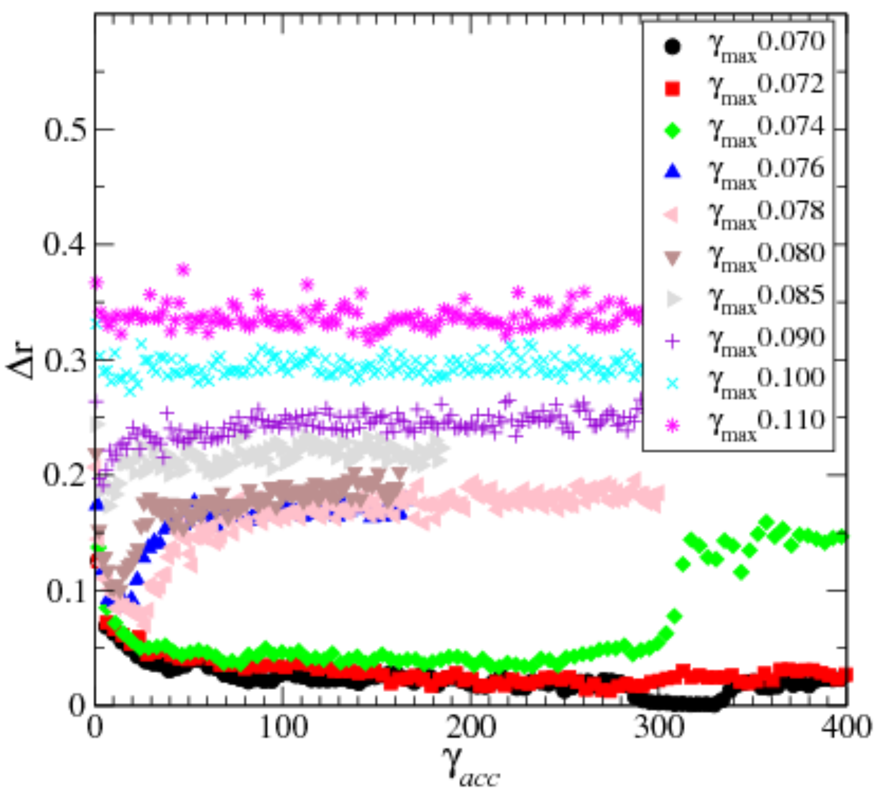
0.072

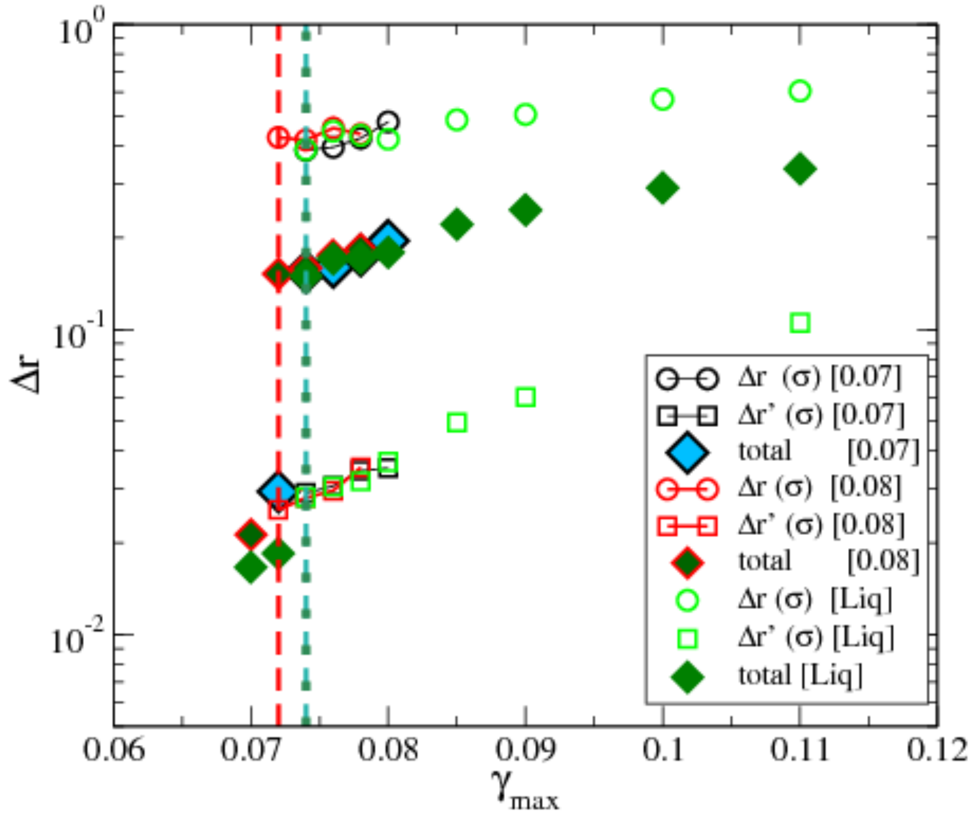
How does diffusivity change?

Sharp transition in microscopic dynamics

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

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

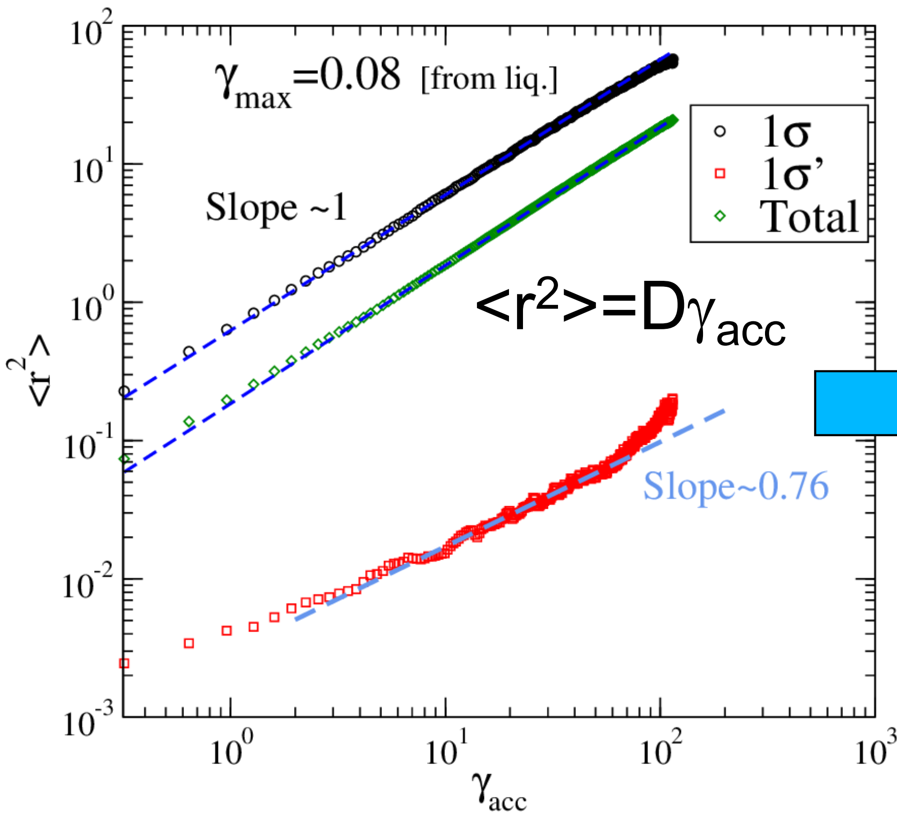


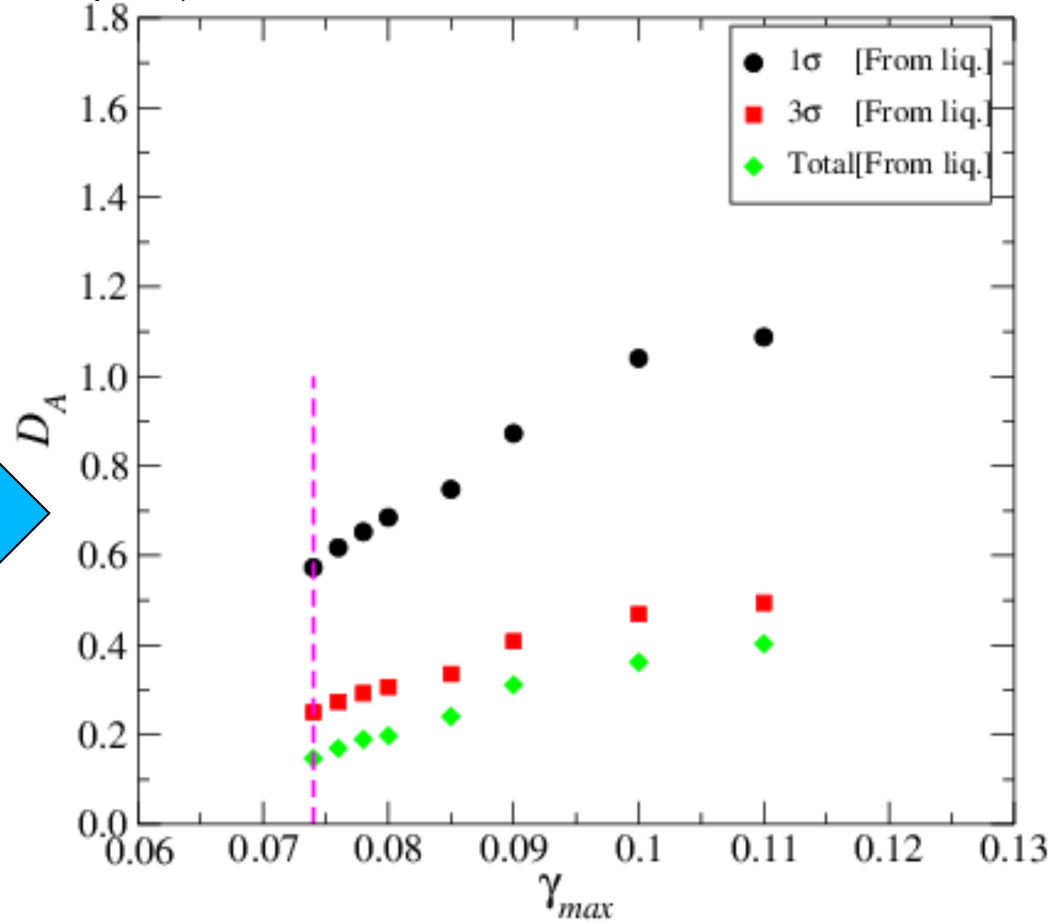


Across the yielding transition, the averaged particle displacement changes in a discontinuous manner.

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.

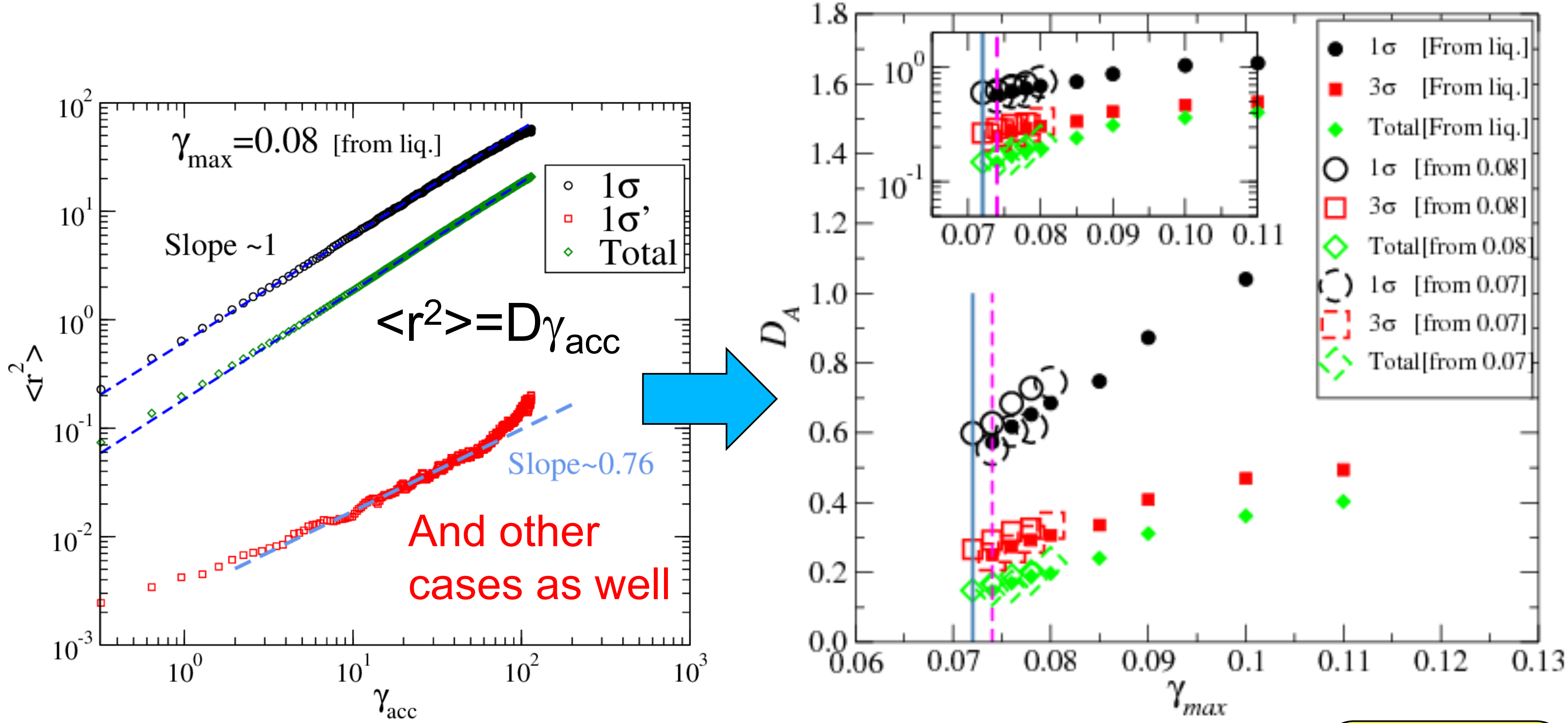




The **diffusion coefficient** changes in **discontinues manner** at the yielding strain amplitude.

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.

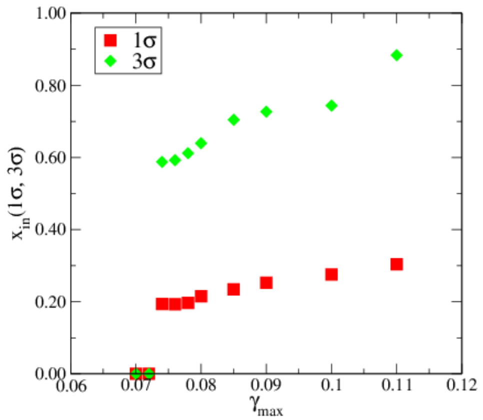
γ^c_{max}

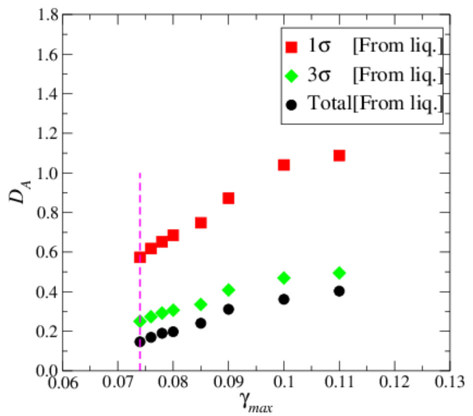
0.074

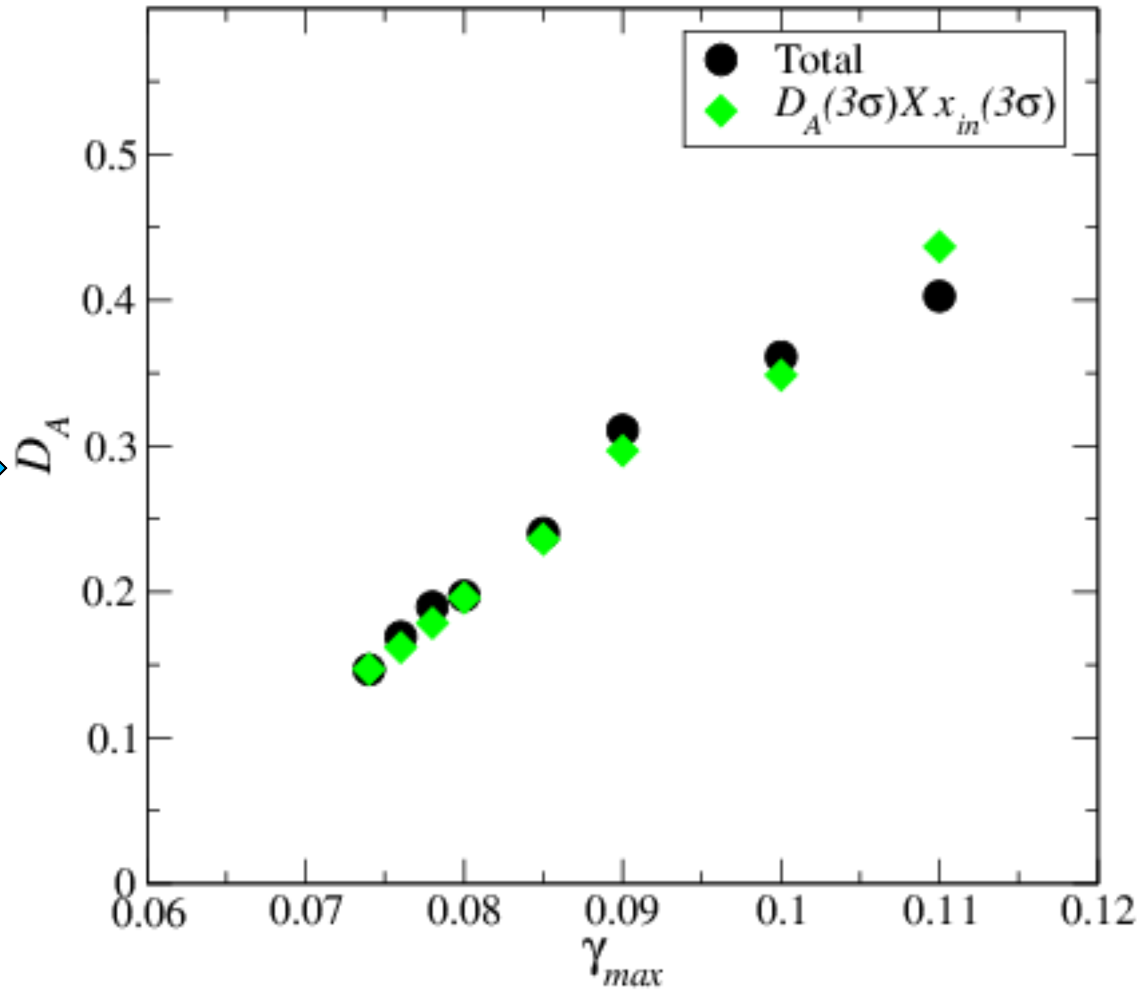
0.072

Characteristics of the shear band - Diffusivity

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



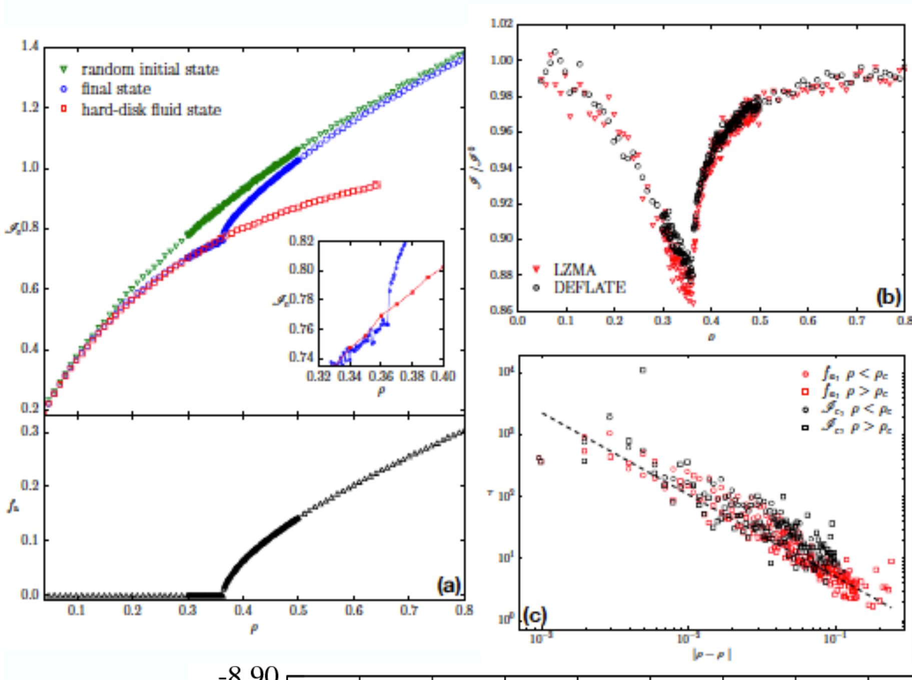




The **diffusion coefficient** of the mobile particles changes in **discontinues manner** at the critical amplitude.

Entropic characterization of the yielding

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

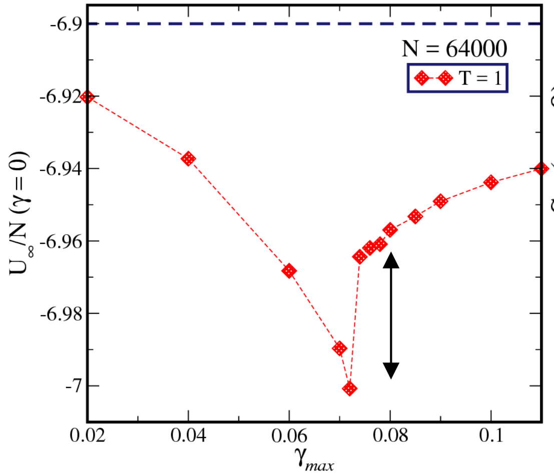


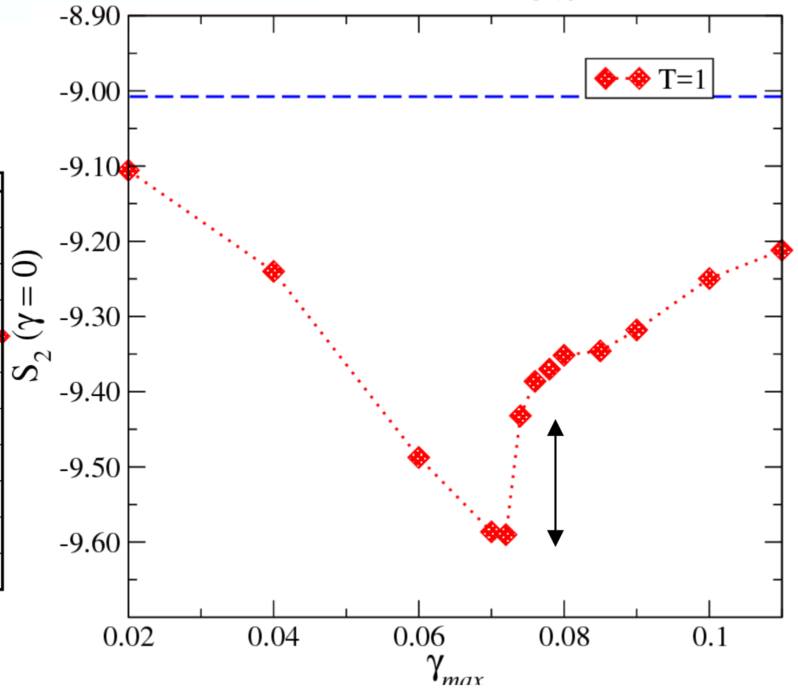
How about conventional structure based entropy? Pair excess entropy (S_2) for a binary system:

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

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

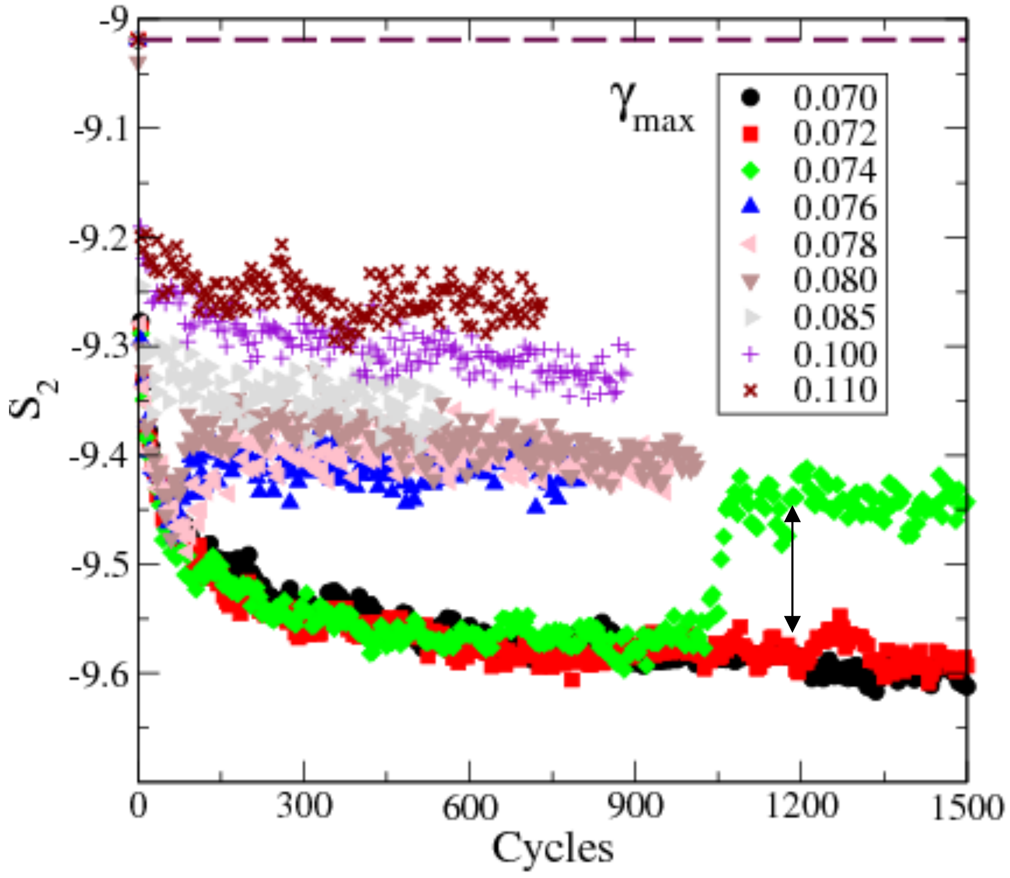
The S_2 and total energy jumps across the yielding amplitude.

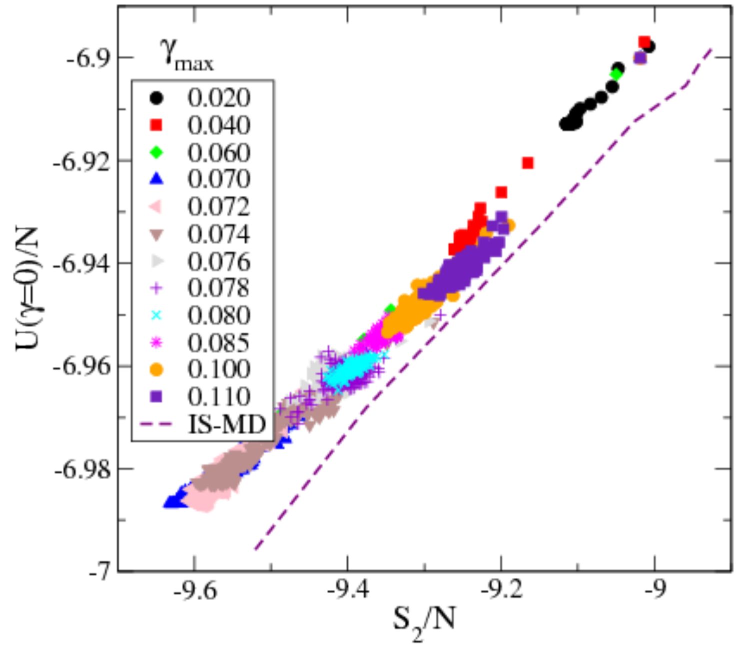


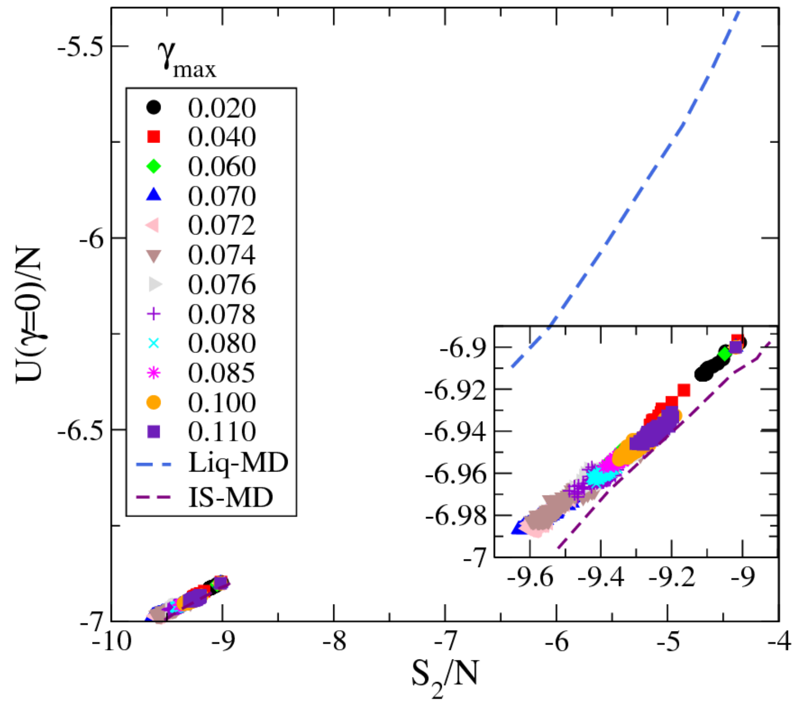


Entropic characterization of the yielding

- S_2 tracks the energy of the inherent structures.
- Close to relation found in T dependence for the liquid.







Summary

A non-equilibrium transition from a localized to a diffusive state (in configuration space) that resembles the glass to liquid transition and other non-ergodic to ergodic transitions.

Steady state energies in the diffusive state do not depend on initial conditions, whereas in the localized state they do.

Slow down of dynamics near the transition.

Critical strain a good way to characterize yield. Cyclic shear offers useful approach to studying the yielding transition.

The yielding transition appears to be a sharp, discontinuous, transition associated with the divergence of sizes of avalanches.

Behavior below yield at variance with some theoretical expectations. No critical-like signatures of approach to yielding.

The nature of the instability that leads to yielding to be fully worked out but the behavior is first order/spinodal-like.

Despite similarities, distinct differences from shear colloidal suspensions.

Observation of shear banding above the yielding point.