# Collective nonaffine rearrangements in binary glasses during large-amplitude oscillatory shear

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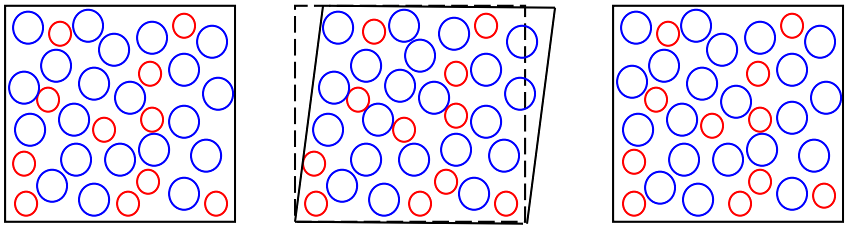
Movies, preprints @
http://www.wright.edu/~nikolai.priezjev/



N. V. Priezjev, "Collective nonaffine displacements in amorphous materials during large-amplitude oscillatory shear", *Phys. Rev. E* **95**, 023002 (2017).

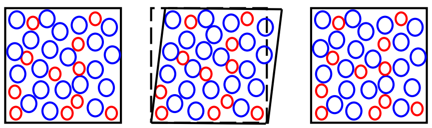
N. V. Priezjev, "Reversible plastic events during oscillatory deformation of amorphous solids", *Phys. Rev. E* **93**, 013001 (2016).

# Structural relaxation and dynamical heterogeneities in deformed glasses

Metallic glasses: mechanical properties include high strength and low ductility

Sun, Concustell, and Greer, Thermomechanical processing of metallic glasses: extending the range of the glassy state, *Nature Reviews Materials* **1**, 16039 (2016).

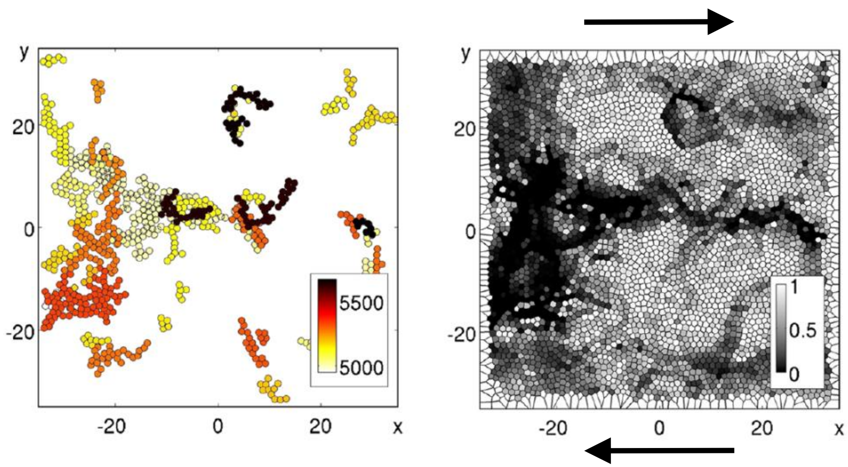
<u>Cyclic loading</u>: yielding transition, fatigue lifetime, failure mechanism, nonaffine motion (??)



Sha, Qu, Liu, Wang, Gao, Cyclic deformation in metallic glasses, *Nano Lett.* (2015).

Knowlton, Pine, and Cipelletti, A microscopic view of the yielding transition in concentrated emulsions, *Soft Matter* **10**, 6931 (2014).

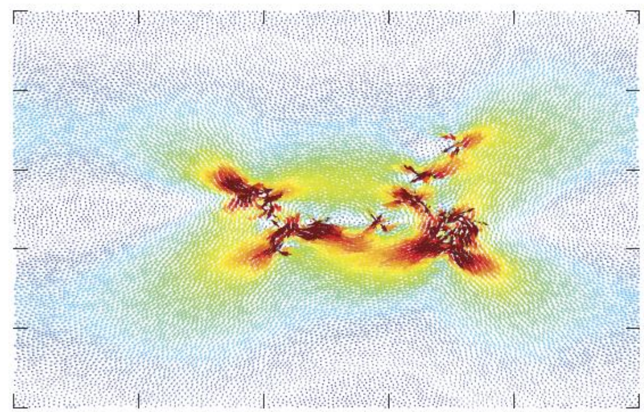
Cyclic shear experiment on dense 2D granular media:




Spatial location of successive clusters of cage jumps

Candelier, Dauchot, Biroli, *PRL* **102**, 088001 (2009)

Reversible avalanches in 2D amorphous solids:



Large particle displacements are completely reversed

Regev, Weber, Reichhardt, Dahmen, Lookman, *Nature* (2015)

# Details of molecular dynamics simulations and parameter values

Binary Lennard-Jones Kob-Andersen mixture:

$$V_{LJ}(r) = 4\varepsilon_{\alpha\beta}\left[\left(\frac{\sigma_{\alpha\beta}}{r}\right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r}\right)^{6}\right]$$

$Ni_{80}P_{20}$

Parameters for $\alpha\beta = A$ and $B$ particles:

$\varepsilon_{AA} = 1.0, \varepsilon_{AB} = 1.5, \ \varepsilon_{BB} = 0.5, m_A = m_B$

$\sigma_{AA} = 1.0, \sigma_{AB} = 0.8, \ \sigma_{BB} = 0.88$

Monomer density: $\rho = \rho_A + \rho_B = 1.20\,\sigma^{-3}$

Temperature: $T_{LJ} = 0.01\ \varepsilon/k_B << T_g = 0.435\ \varepsilon/k_B$

System size: $L = 36.84\,\sigma$, $N_p = 60000$

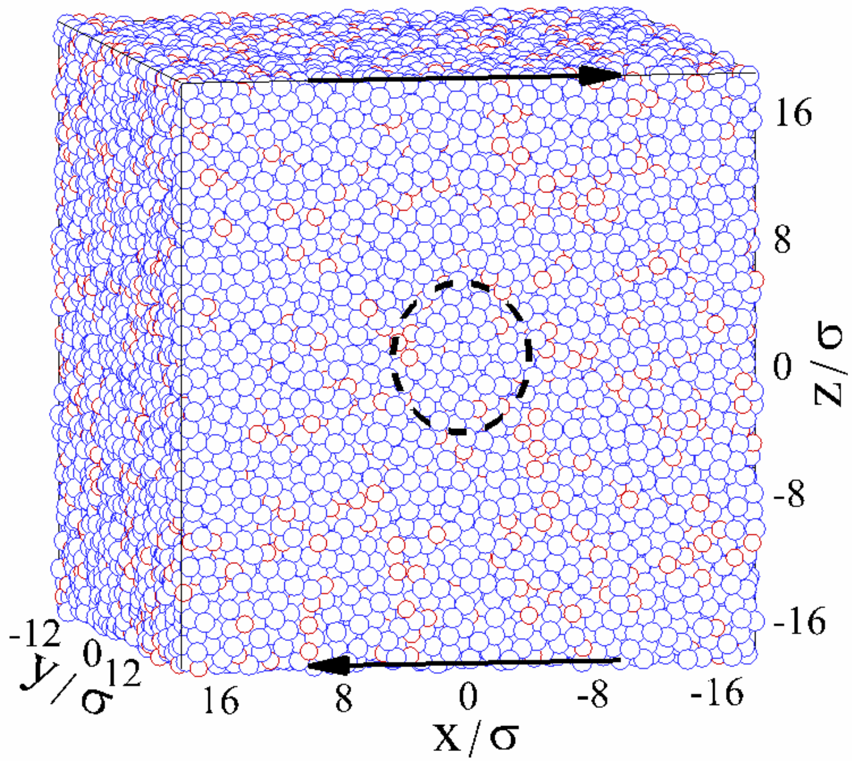
Lees-Edwards periodic boundary conditions

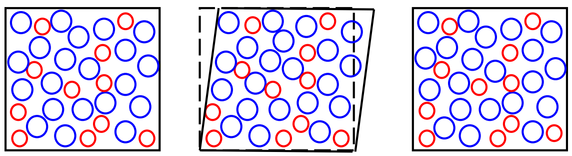
LAMMPS, DPD thermostat, $\Delta t_{MD} = 0.005\,\tau$

Slow annealing rate: $10^{-5}\ \varepsilon/k_B\tau$

Oscillatory shear strain: $\gamma(t) = \gamma_0 \sin(\omega t)$

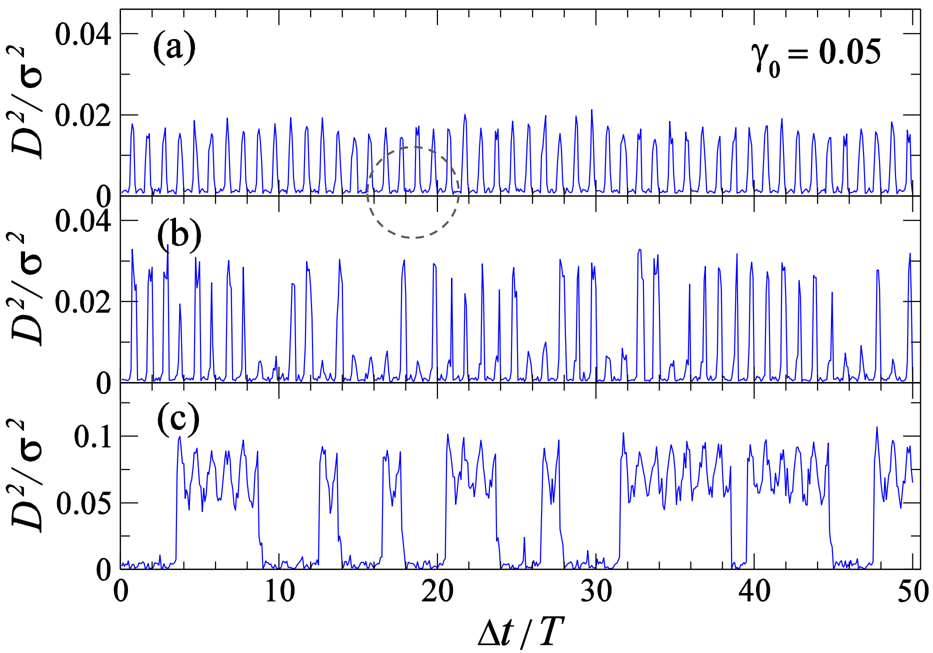
Oscillation period: $T = 2\pi/\omega = 5000\,\tau$

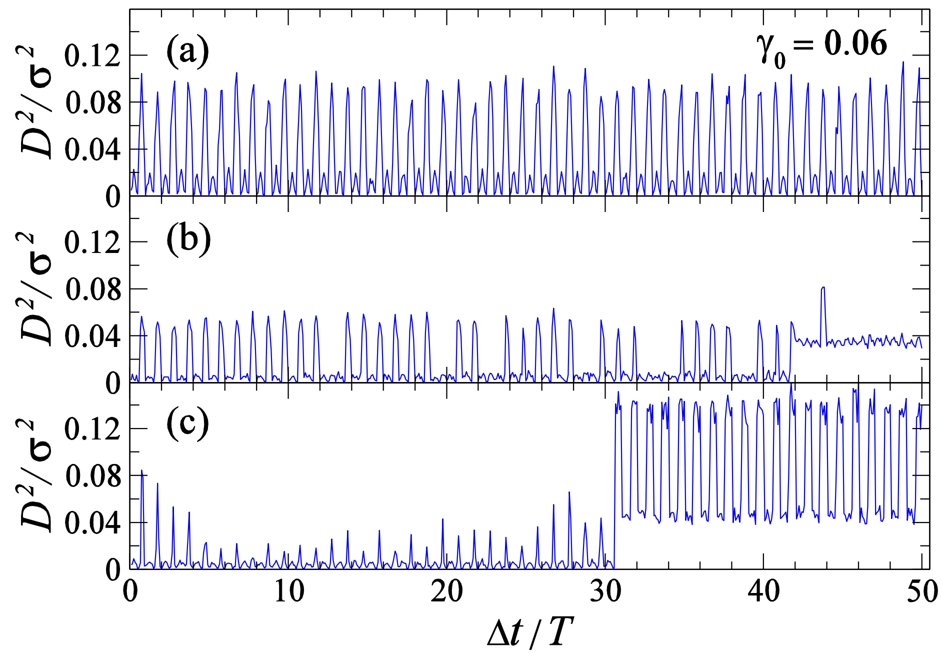


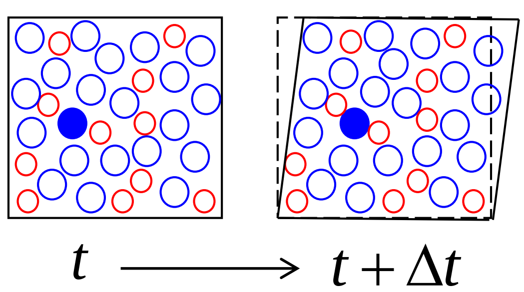



# Variation of nonaffine measure $D^2(0,\Delta t)$ for selected particles over 50 cycles

## Reversible / irreversible particle displacements



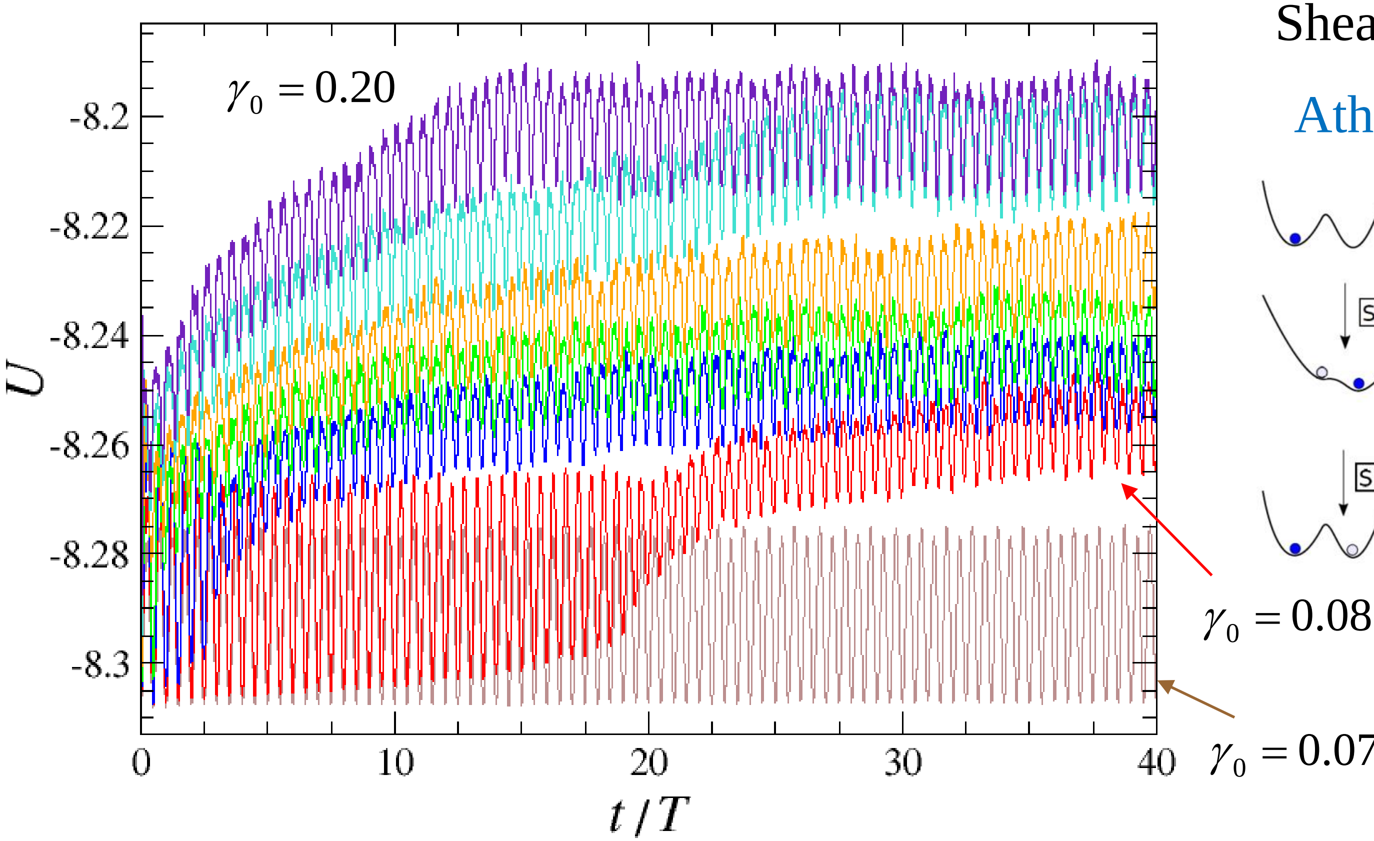

$$D^2(t,\Delta t) = \frac{1}{N_i}\sum_{j=1}^{N_i}\Big\{\mathbf{r}_j(t+\Delta t) - \mathbf{r}_i(t+\Delta t) - J_i[\mathbf{r}_j(t) - \mathbf{r}_i(t)]\Big\}^2$$

Excellent diagnostic for identifying particle rearrangements

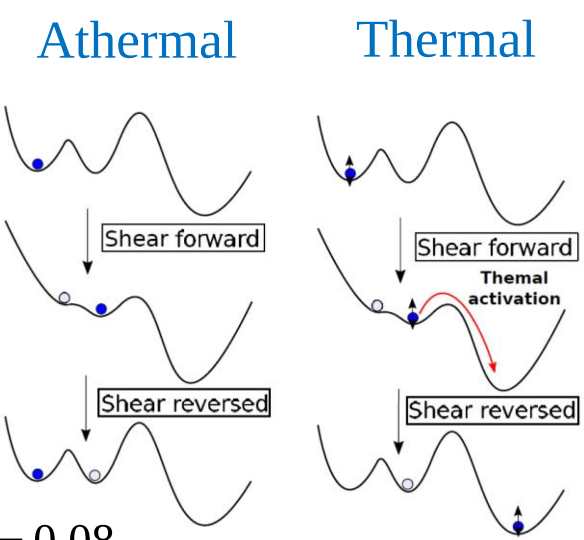
Falk and Langer, *Phys. Rev. E* **57**, 7192 (1998).

N. V. Priezjev, *Phys. Rev. E* **93**, 013001 (2016).

# Potential energy per particle $U$ during 40 oscillation cycles for different $\gamma_0$




Shear-induced activation:



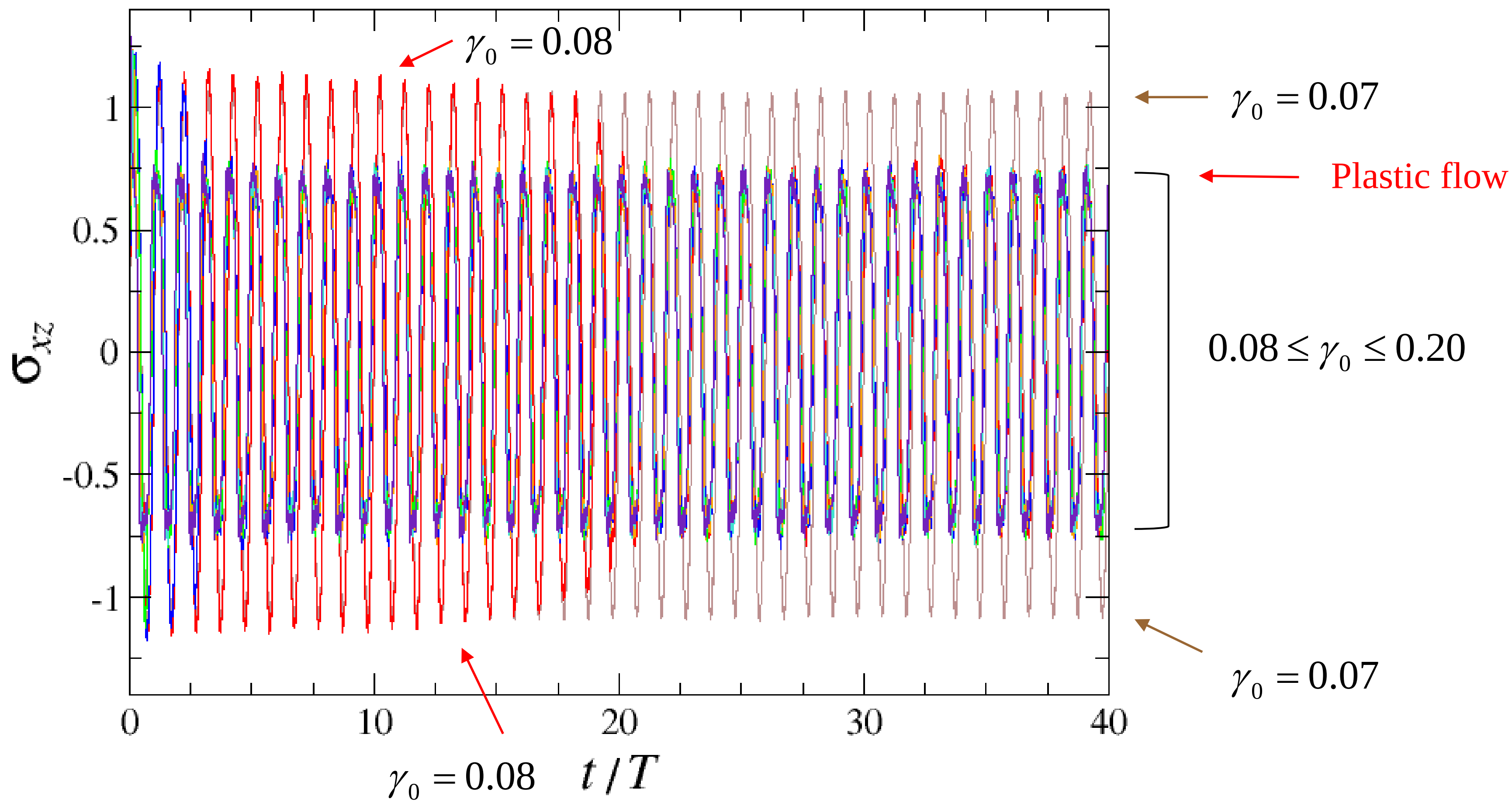

Farhadi & Arratia
arXiv:1608.07266

At the strain amplitude $\gamma_0 = 0.07$ the system dynamics is reversible after each cycle.

In contrast, at $\gamma_0 \geq 0.08$, some atoms undergo irreversible displacements leading to progressive increase of the potential energy $U/\varepsilon$

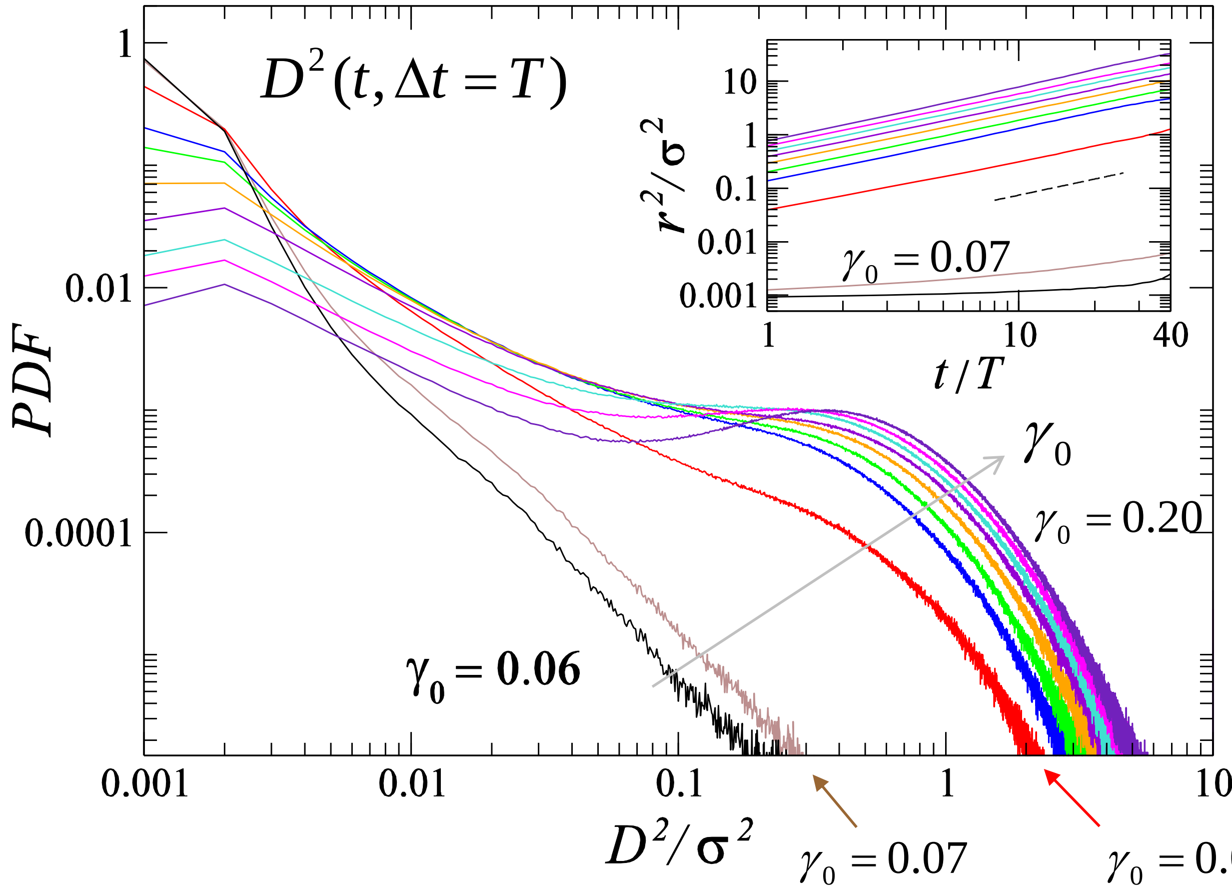
N. V. Priezjev, *Phys. Rev. E* **95**, 023002 (2017).

# Shear stress during 40 oscillation cycles for different strain amplitudes $\gamma_0$



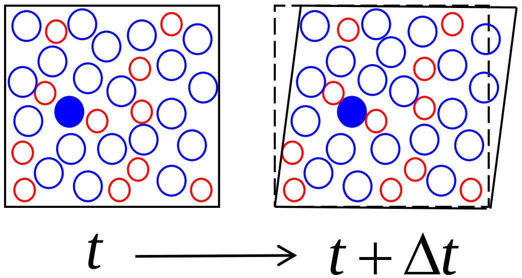

At the strain amplitude $\gamma_0$ = 0.07, the system dynamics is reversible, large stress amplitude. At $\gamma_0$ = 0.08, the shear stress amplitude is reduced after about 20 cycles: plastic flow and shear band formation. At $\gamma_0$ > 0.10, stress overshoot and large hysteresis loops.

# Probability distribution function of nonaffine measure $D^2(0,T)$ after one cycle




At the strain amplitude $\gamma_0 = 0.06$ and 0.07, the system dynamics is reversible and most atoms return to their cages after one cycle.

At large strain amplitudes $\gamma_0 \geq 0.08$, PDF with large nonaffine displacements (more cage breaking events).




$$D^2(t, \Delta t) = \frac{1}{N_i} \sum_{j=1}^{N_i} \left\{ \mathbf{r}_j(t+\Delta t) - \mathbf{r}_i(t+\Delta t) - J_i[\mathbf{r}_j(t) - \mathbf{r}_i(t)] \right\}^2$$

N. V. Priezjev, *Phys. Rev. E* **95**, 023002 (2017).

# Spatial configurations of atoms with large nonaffine displacements at $\gamma_0$=0.07

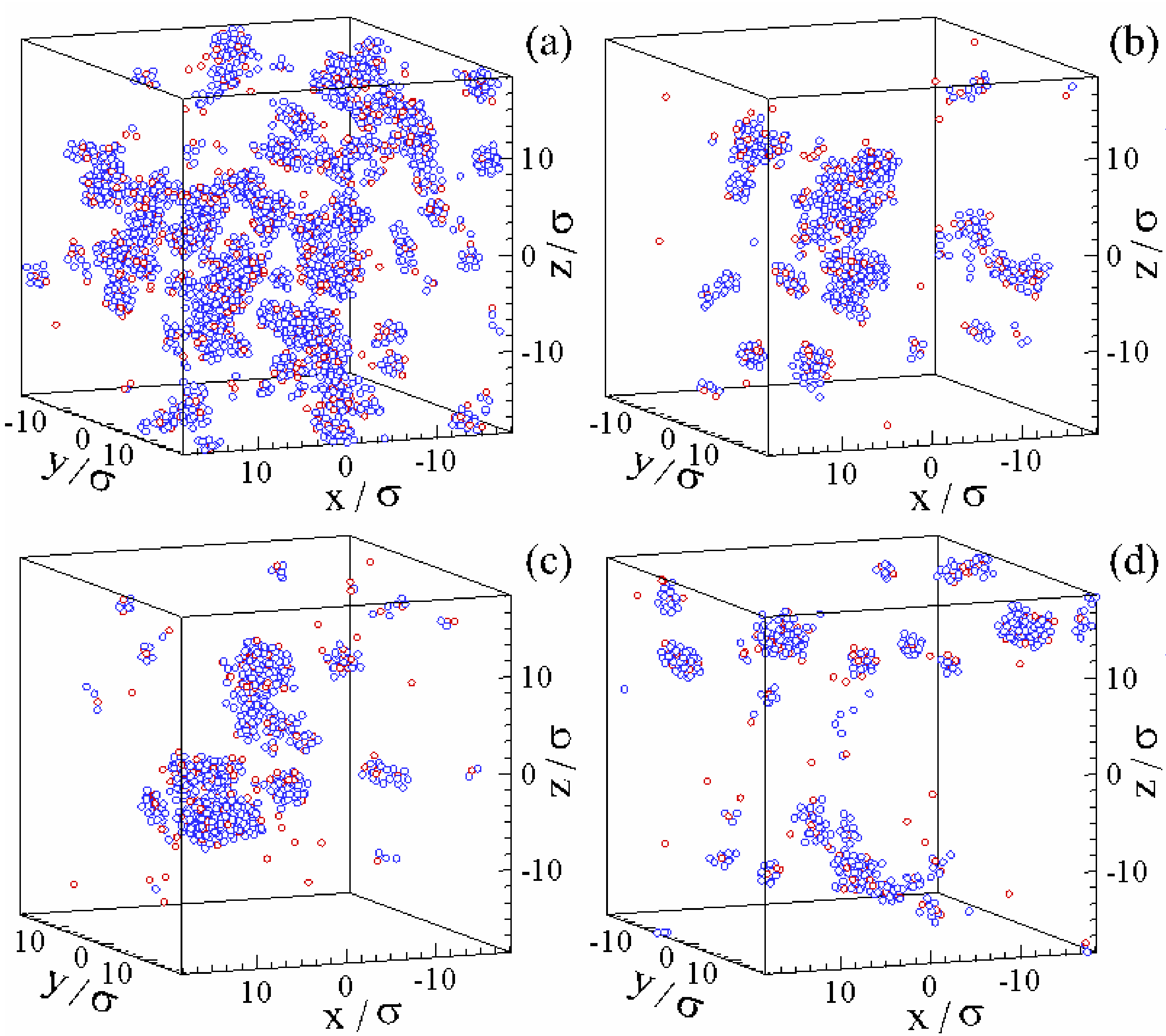
$$D^2(t,T) > 0.01\sigma^2 \approx r_{cage}^2$$

After 1st cycle

After 10th cycle

After 20th cycle

After 40th cycle



# Spatial configurations of atoms with large nonaffine displacements at $\gamma_0$=0.08

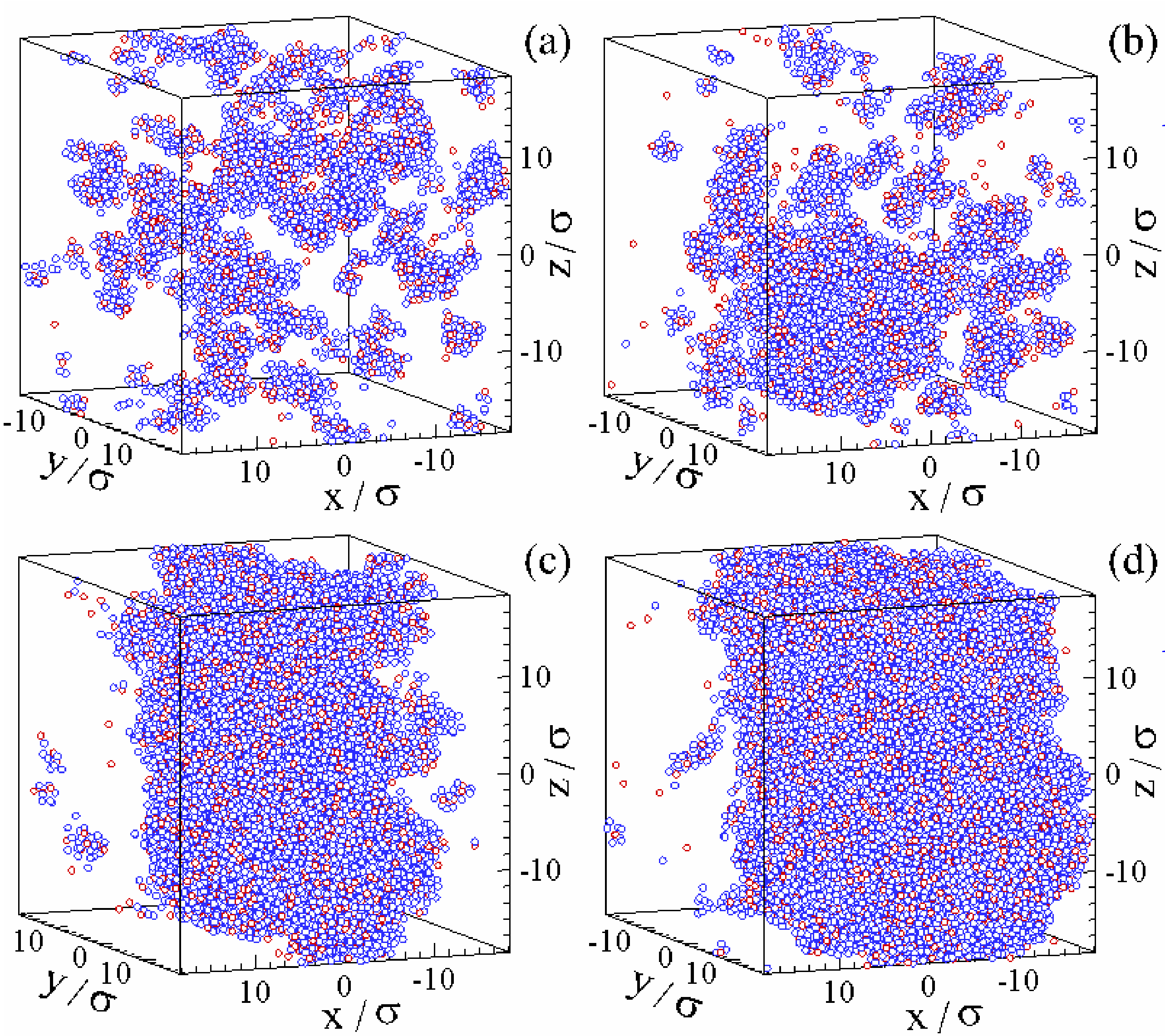
$$D^2(t,T) > 0.01\sigma^2 \approx r_{cage}^2$$

After 1st cycle

Large shear stress amplitude

Disconnected clusters

After 10th cycle




After 20th cycle

Small shear stress amplitude

Shear band formation

After 40th cycle

Finite width of shear band

# Spatial configurations of atoms with large nonaffine displacements at $\gamma_0$=0.10

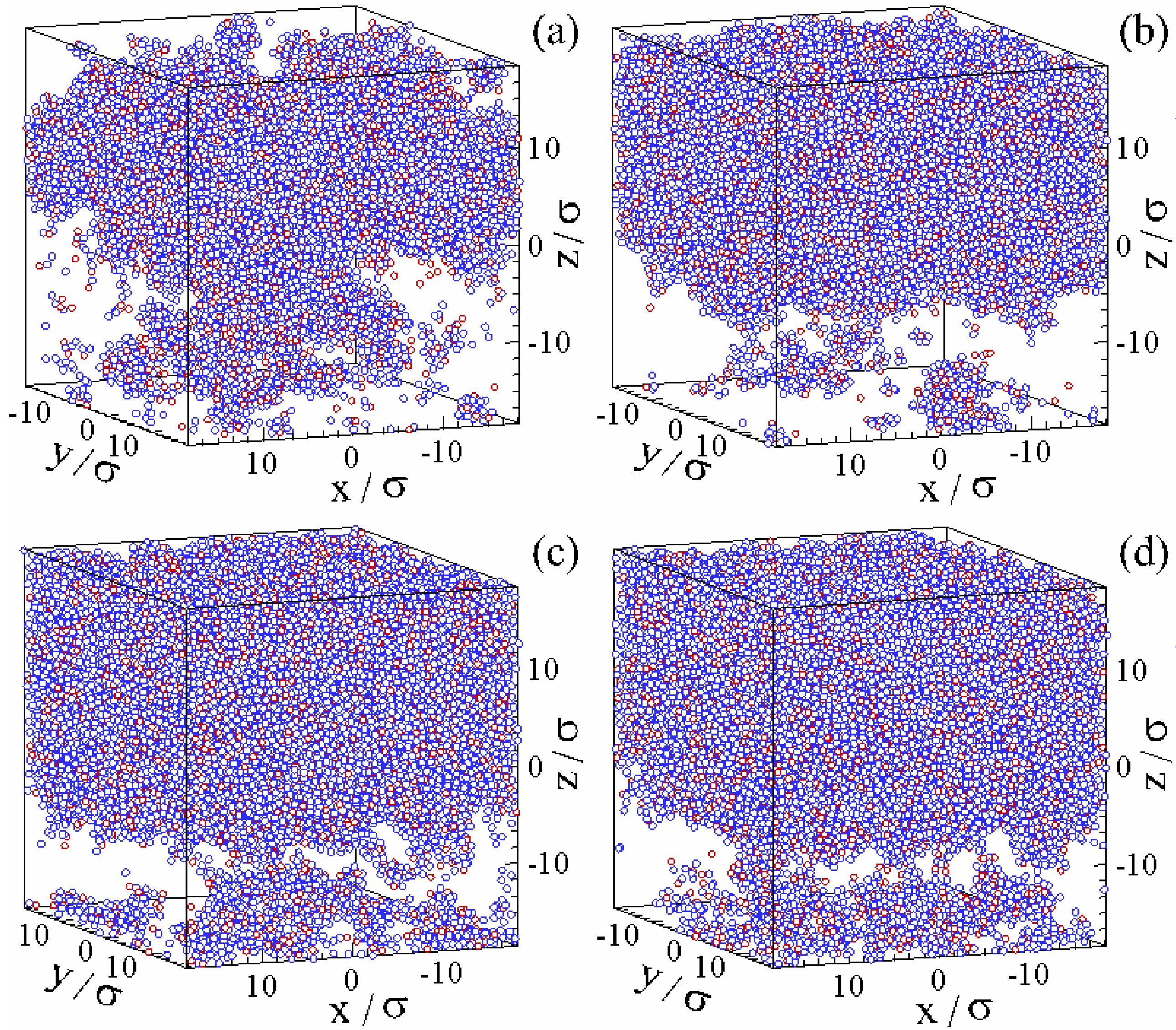
$$D^2(t,T) > 0.01\sigma^2 \approx r_{cage}^2$$

After 1st cycle

After 10th cycle

After 20th cycle

After 40th cycle




Finite width of shear band

# Spatial configurations of atoms with large nonaffine displacements at $\gamma_0$=0.16

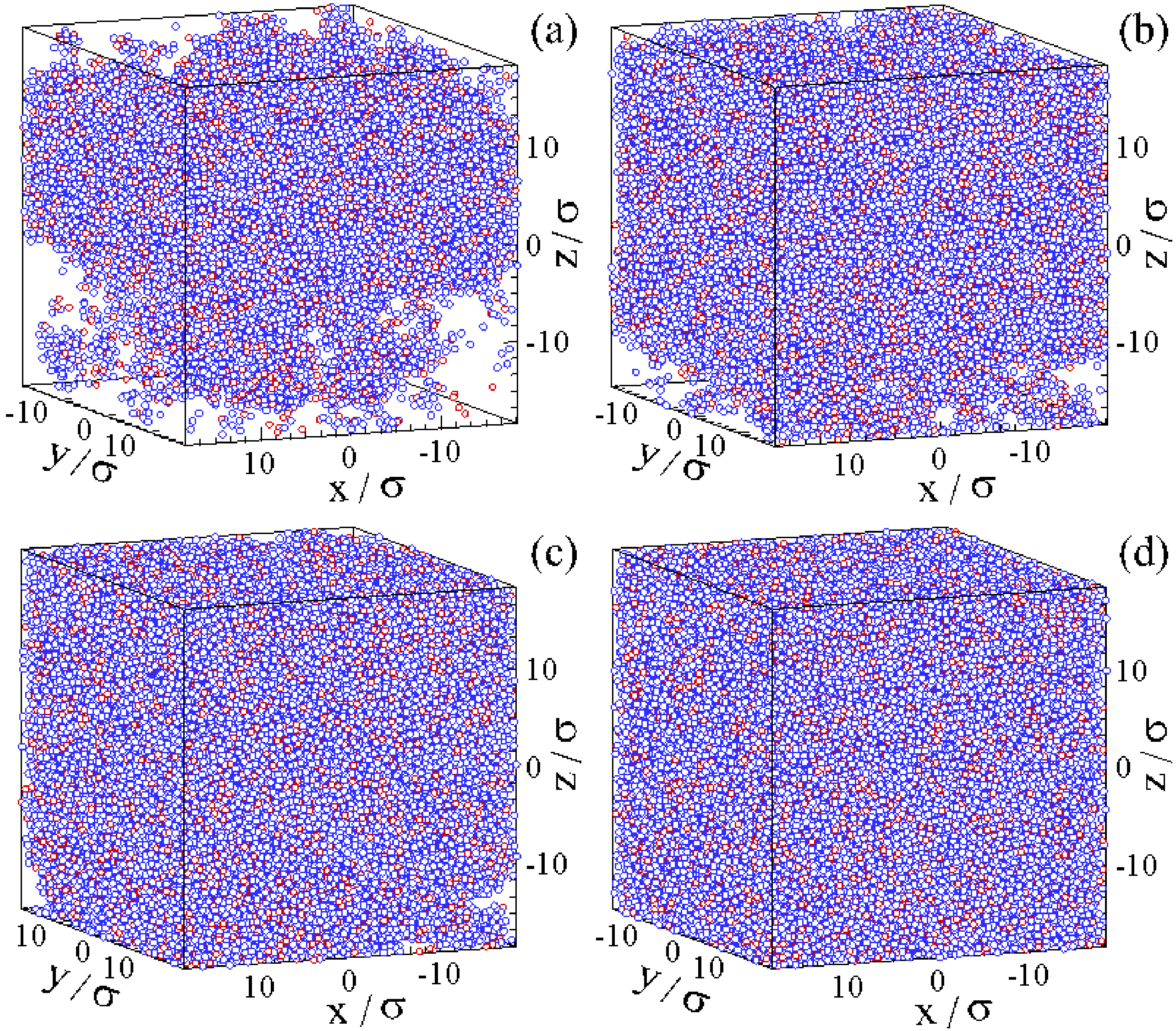
$$D^2(t,T) > 0.01\sigma^2 \approx r_{cage}^2$$

After 1st cycle

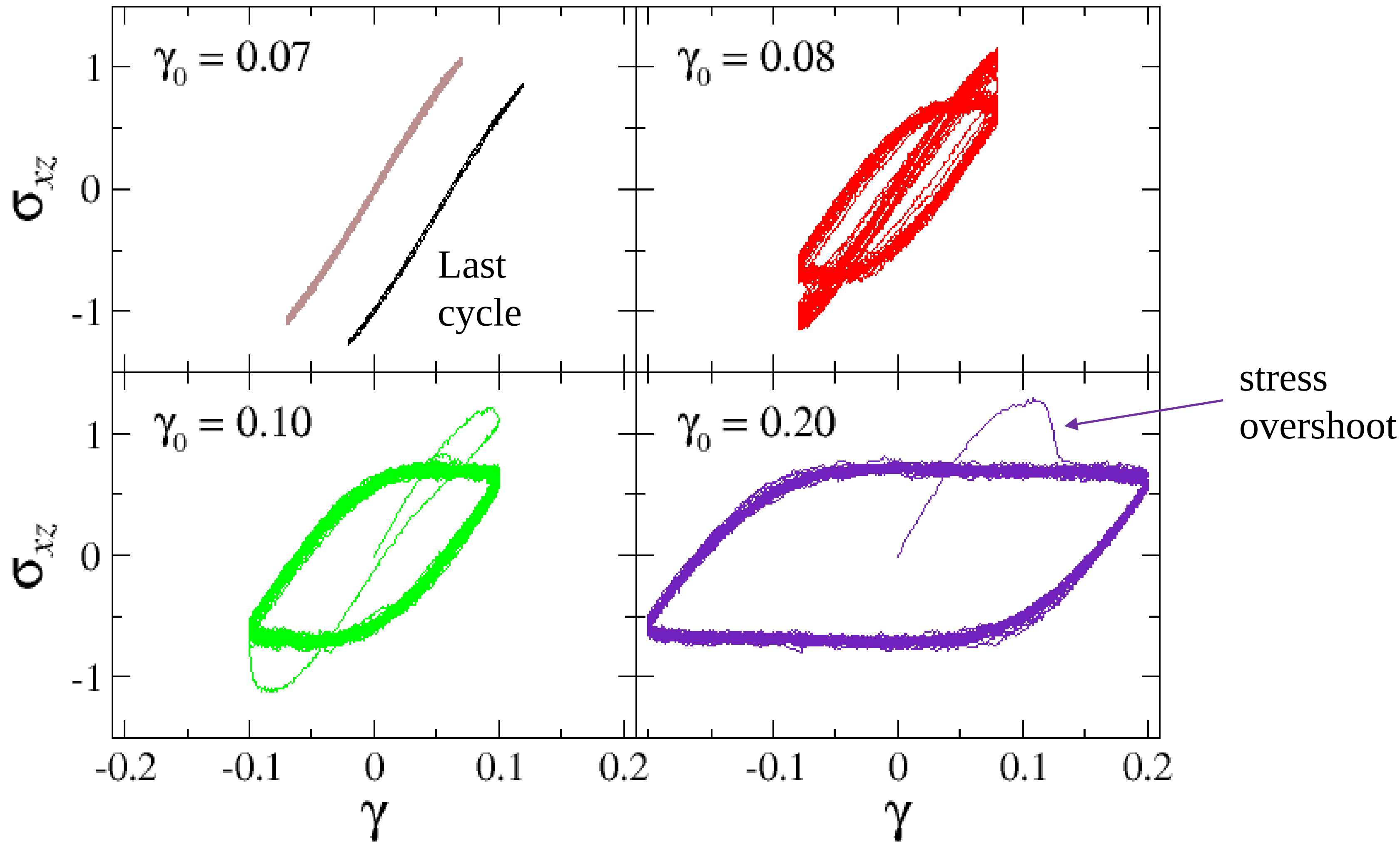
After 10th cycle

After 20th cycle

After 30th cycle



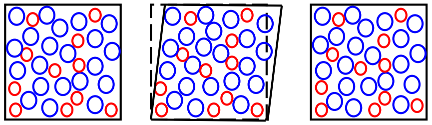
# Shear stress vs shear strain during 40 cycles for selected strain amplitudes $\gamma_0$




At the strain amplitude $\gamma_0$ = 0.07 the system dynamics is reversible but finite loop area.

At $\gamma_0$ = 0.08, the shear stress amplitude is reduced after about 20 cycles: plastic flow and shear band formation. At $\gamma_0$ = 0.10 and 0.20, stress overshoot and large loop area.

# Conclusions:



- MD simulations of binary 3D Lennard-Jones glasses under periodic shear strain at finite T.

- At small strain amplitudes, the mean square displacement exhibits a broad sub-diffusive plateau and the system undergoes nearly reversible deformation but finite hysteresis loop. Large clusters of particles undergo repetitive nonaffine displacements.

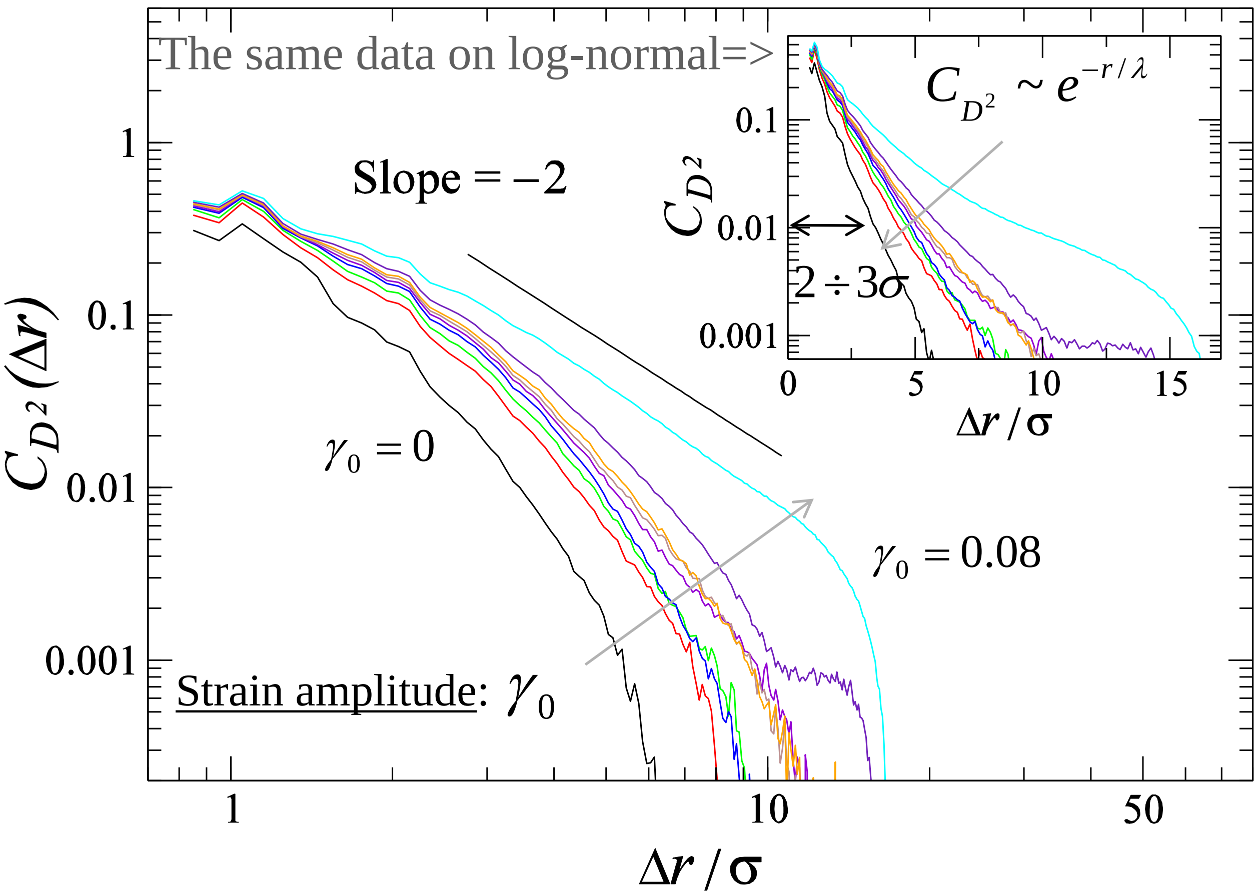
- Near the critical strain amplitude, the dynamic transition from disconnected clusters to a shear band of large nonaffine displacements: leads to drop in shear stress amplitude. The relaxation process involves intermittent bursts of large particle displacements.

- At large strain amplitudes: diffusive dynamics, quick formation & growth of shear bands, irreversible particle displacements lead to hysteresis & increase in the potential energy.

N. V. Priezjev, "Collective nonaffine displacements in amorphous materials during large-amplitude oscillatory shear", *Phys. Rev. E* **95**, 023002 (2017).

N. V. Priezjev, "Reversible plastic events during oscillatory deformation of amorphous solids", *Phys. Rev. E* **93**, 013001 (2016).

# Equal-time, spatial correlation function $C_{D^2}$ computed at max strain $\gamma(T/4) = \gamma_0$

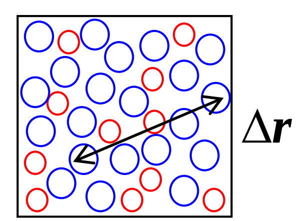



$$C_{D^2}(\Delta \mathbf{r}) = \frac{\langle D^2(\mathbf{r}+\Delta\mathbf{r}) D^2(\mathbf{r}) \rangle - \langle D^2(\mathbf{r}) \rangle^2}{\langle D^2(\mathbf{r})^2 \rangle - \langle D^2(\mathbf{r}) \rangle^2}$$

Quiescent glasses $\gamma_0 = 0$ or small $\gamma_0$, correlations of nonaffine displacements extend up to nearest-neighbor distances.

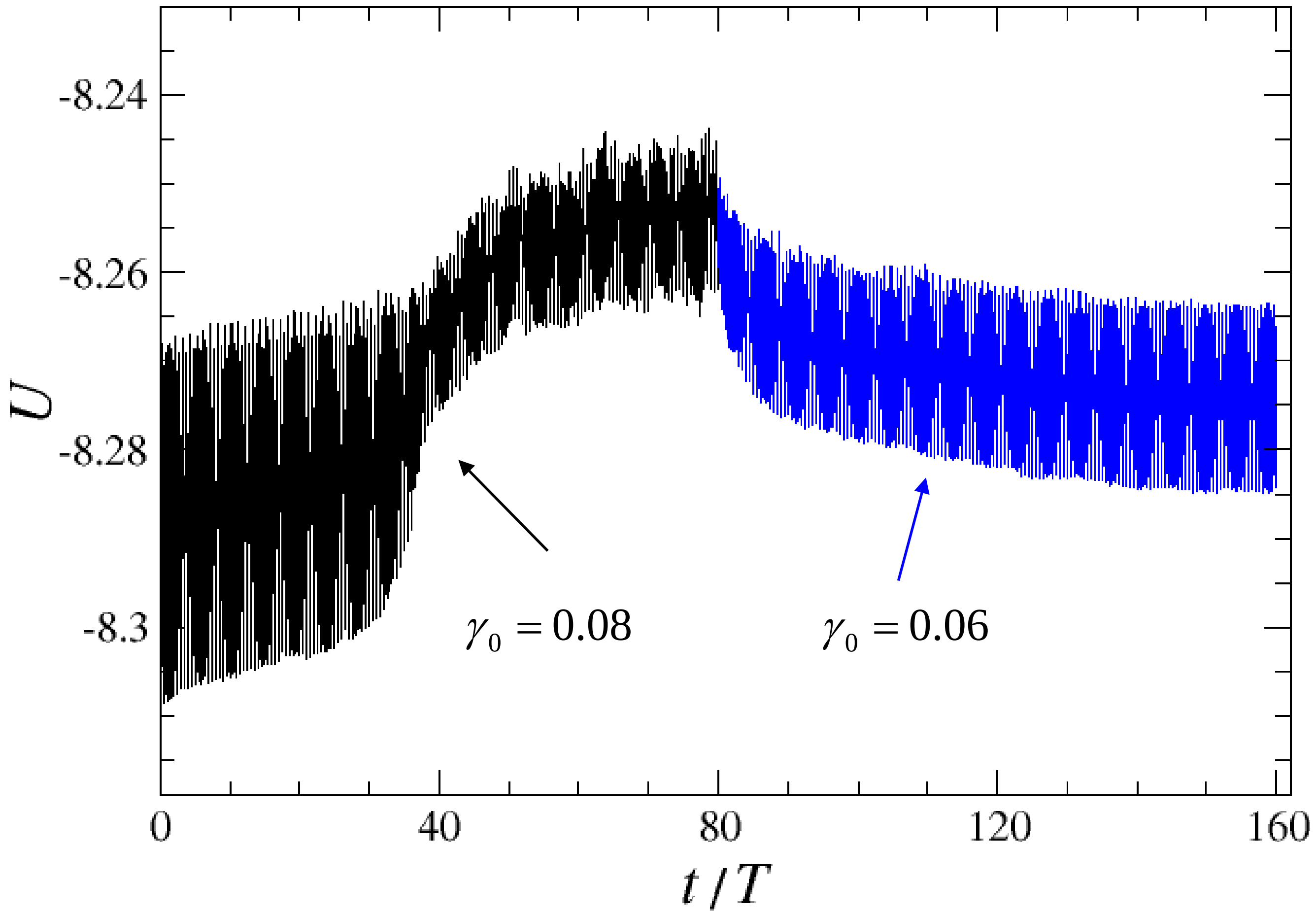
Large strain amplitude = power-law decay of $C_{D^2}$

In agreement with steadily sheared glasses Varnik *et al.* *Phys. Rev. E* **89**, 040301 (2014).




N. V. Priezjev, *Phys. Rev. E* **94**, 023004 (2016).

# Potential energy per particle $U$ during 160 oscillation cycles for different $\gamma_0$




At $\gamma_0 = 0.08$, shear band is formed during first 80 cycles leading to progressive increase of the potential energy $U$. Next, mechanical annealing for 80 cycles at $\gamma_0 = 0.06$, low $U$.