The yielding transition in periodically sheared binary glasses at finite temperature

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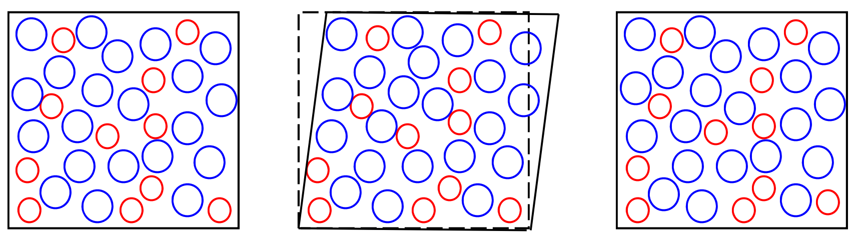
Movies, preprints @
http://www.wright.edu/~nikolai.priezjev/



N. V. Priezjev, The yielding transition in periodically sheared binary glasses at finite temperature, *Comput. Mater. Sci.* **150**, 162 (2018).

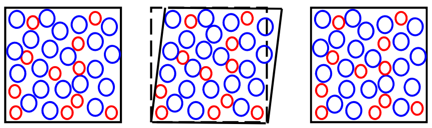
N. V. Priezjev, Molecular dynamics simulations of the mechanical annealing process in metallic glasses: Effects of strain amplitude and temperature, *J. Non-Cryst. Solids* **479**, 42 (2018).

Structural relaxation and dynamical heterogeneities in deformed glasses

<u>Metallic glasses</u>: 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).

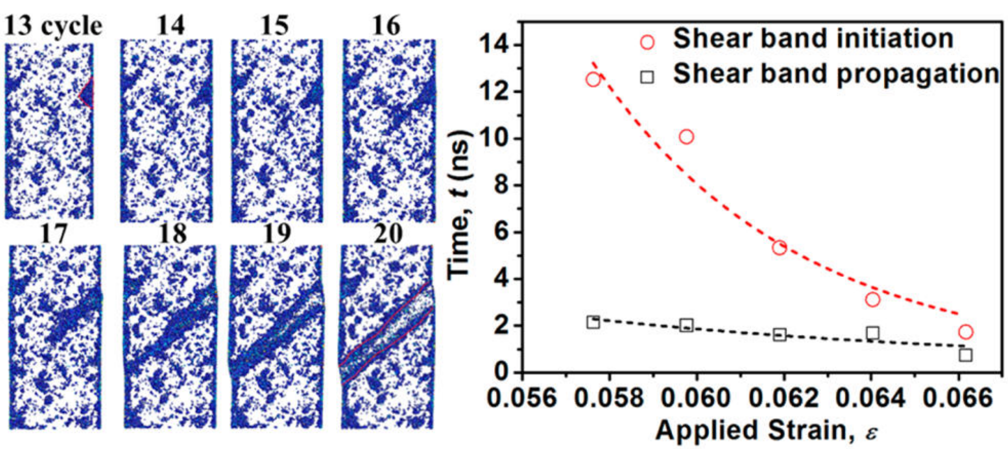
<u>Cyclic loading</u>: yielding transition, fatigue lifetime, failure mechanism, nonaffine motion (??)



Candelier, Dauchot, and Biroli, Dynamical heterogeneity in the cyclic shear experiment on dense 2D <u>granular media</u>, *Phys. Rev. Lett.* **102**, 088001 (2009).

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

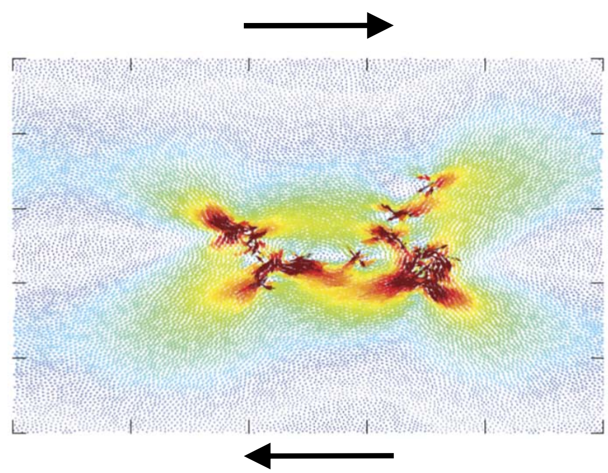
<u>Tension-compression cyclic loading of metallic glasses</u>:



Shear band due to accumulation of STZs at boundary

Sha, Qu, Liu, Wang, and Gao, *Nano Lett.* (2015)

<u>Reversible avalanches in 2D amorphous solids</u>:



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:

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

$Ni_{80}P_{20}$

<u>Parameters</u> 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: $T_{LJ} = 0.1\ \varepsilon / k_B < T_g = 0.435\ \varepsilon / k_B$

System size: $L = 36.84\,\sigma$, $N_p = 60{,}000$

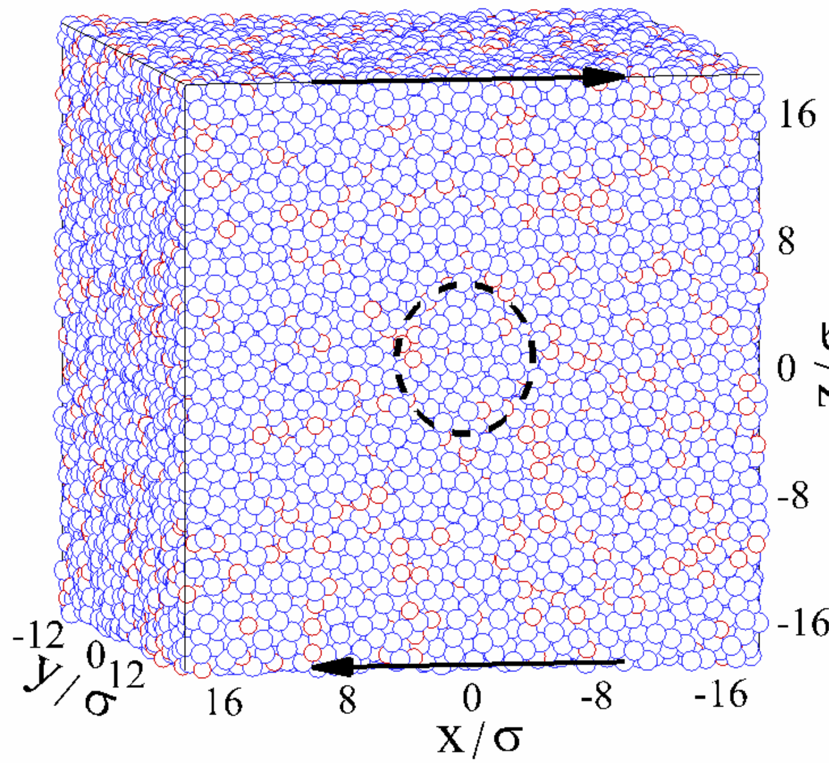
Lees-Edwards periodic boundary conditions

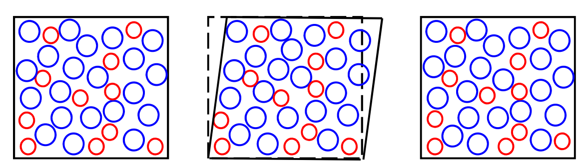
LAMMPS, <u>DPD thermostat</u>, $\Delta t_{MD} = 0.005\,\tau$

Instantaneous quenching to $T_{LJ} = 0.1\ \varepsilon / k_B$

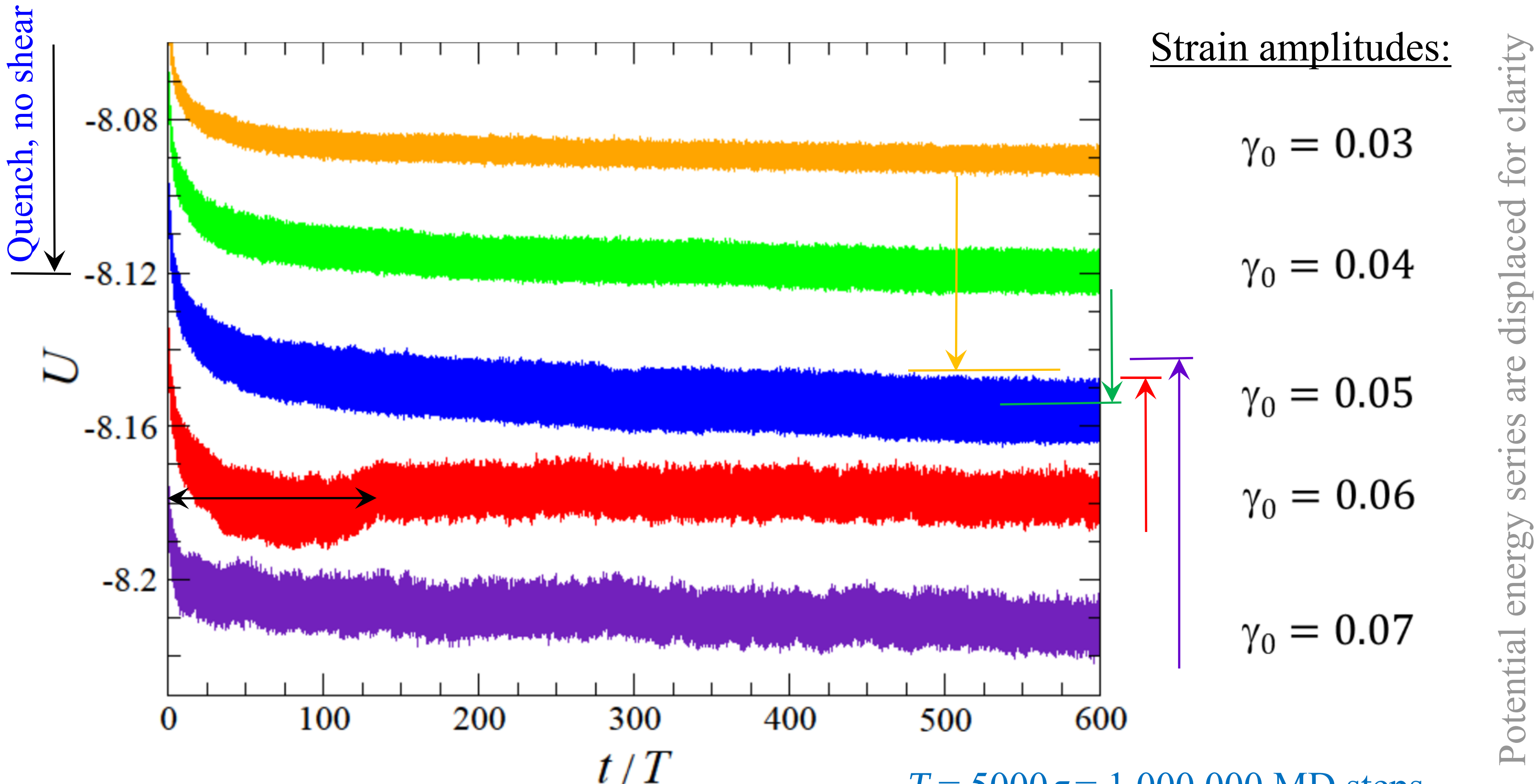
Oscillatory shear strain: $\gamma(t) = \gamma_0 \sin(\omega t)$

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





Potential energy per particle U/ε during 600 oscillation cycles for different γ_0

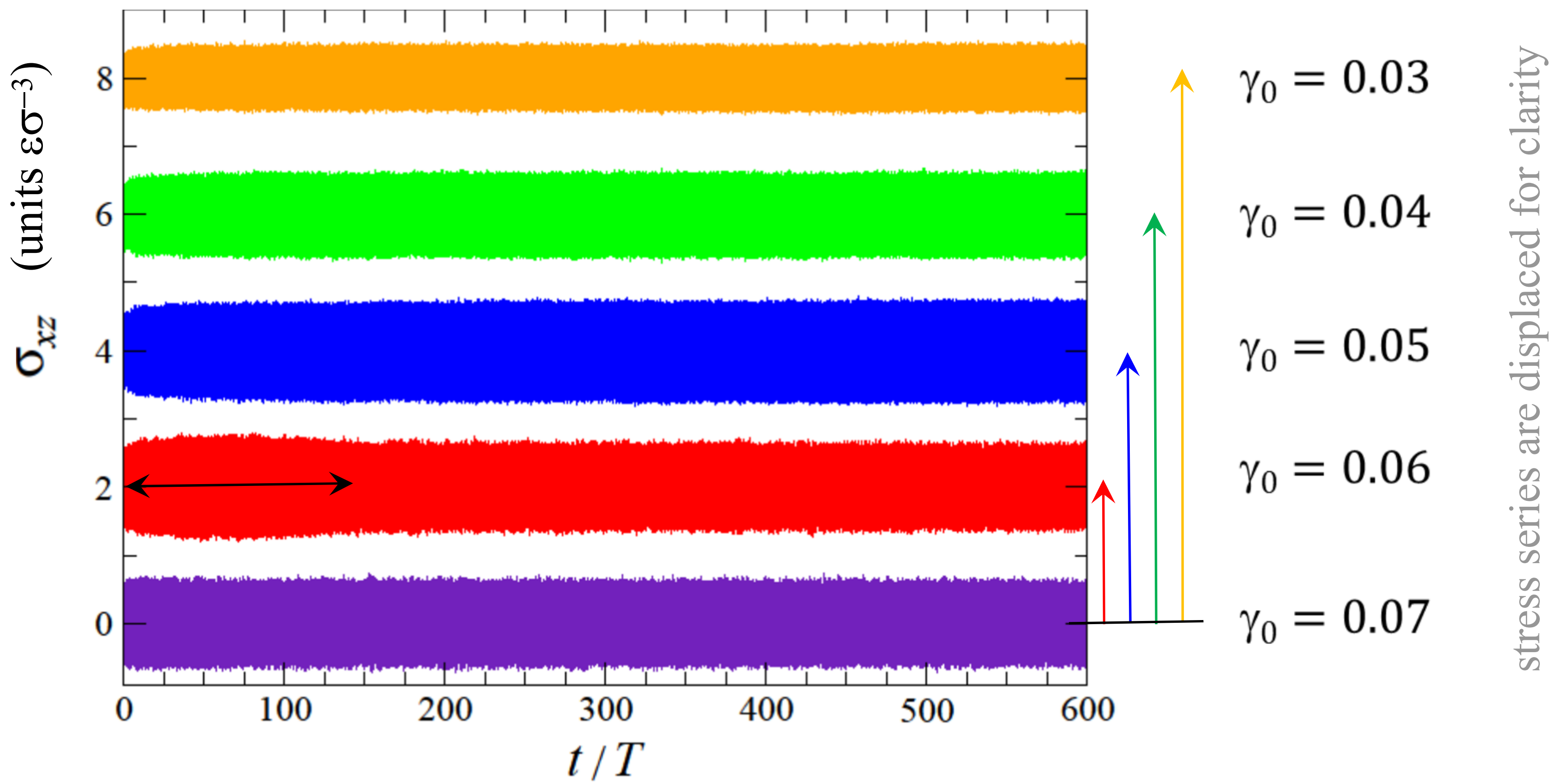


$T = 5000\,\tau = 1{,}000{,}000$ MD steps

At small strain amplitudes, $\gamma_0 \leq 0.05$, the potential energy acquires progressively lower minima with increasing strain amplitude. Minimum potential energy is at $\gamma_0 = 0.05$.

Near the yield transition, $\gamma_0 = 0.06$, shallow minimum in potential energy during first 150 cycles.

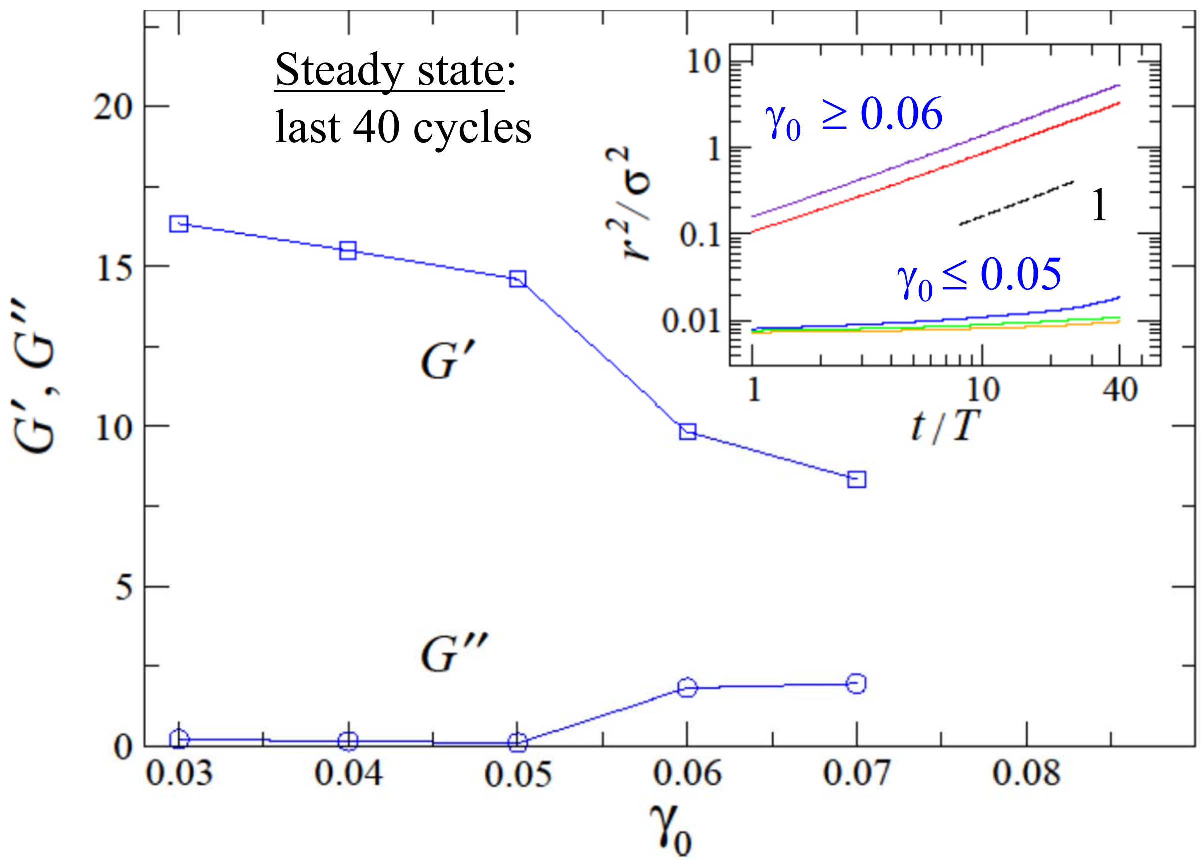
Shear stress during 600 oscillation cycles for different strain amplitudes γ_0



At <u>small strain amplitudes</u>, $\gamma_0 \le 0.05$: the amplitude of stress oscillations becomes larger with increasing strain amplitude; nearly reversible particle dynamics.

Near the <u>critical strain amplitude</u>, $\gamma_0 = 0.06$: shallow maximum in the amplitude of stress oscillations during first 150 cycles; then stress amplitude is reduced at $t > 150T$.

Storage and loss moduli and mean-square displacements for different γ_0



At small strain amplitudes, $\gamma_0 \leq 0.05$, the storage modulus *G'* dominates the response; nearly reversible particle dynamics.

At large strain amplitudes, $\gamma_0 \geq 0.06$, the loss modulus *G"* increases; irreversible particle diffusion; formation of shear band.

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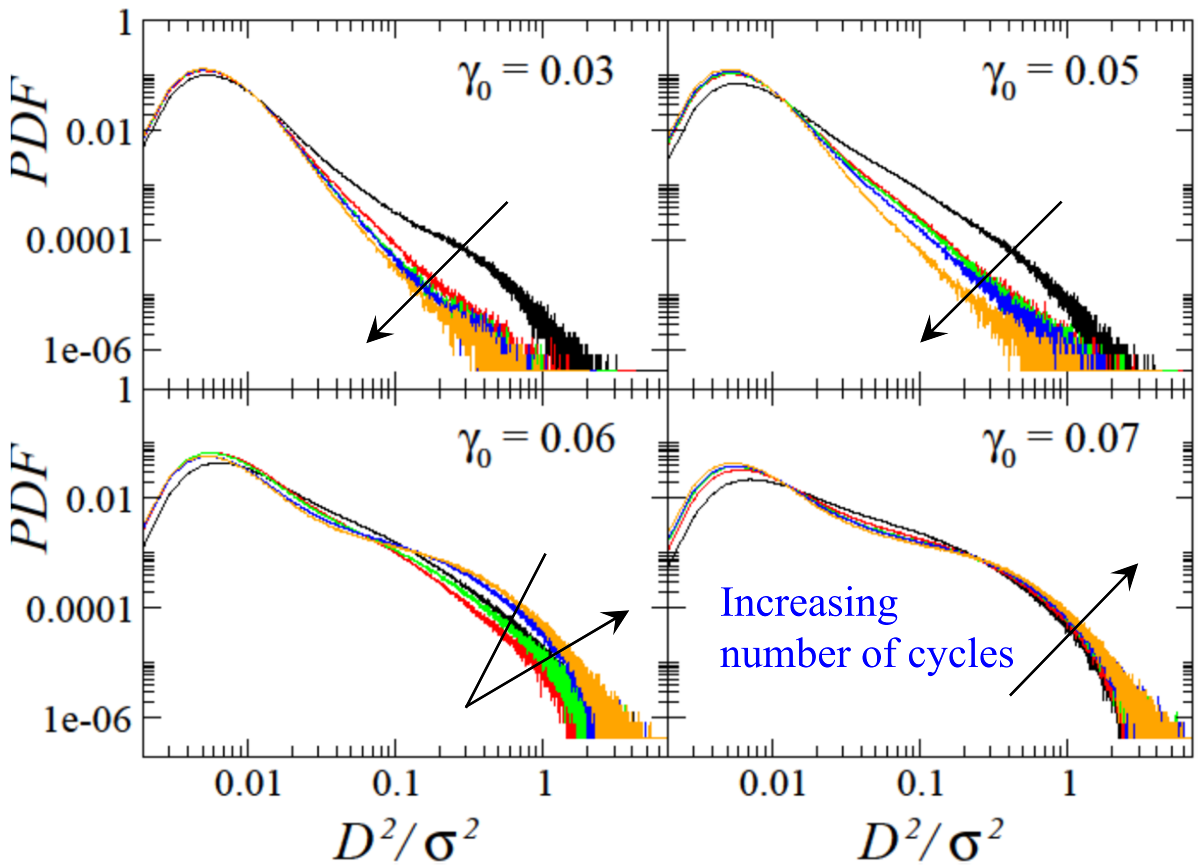
The critical strain amplitude, *G'=G"*, $\gamma_{\times} > \gamma_c$, onset of diffusion. Kawasaki & Berthier, *PRE* (2016).

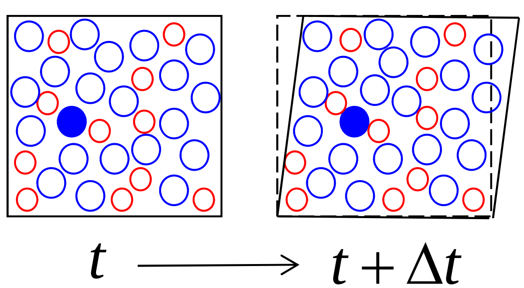
Probability distribution function of the nonaffine measure $D^2(t,T)$ after one cycle



At <u>small strain amplitudes</u>, $\gamma_0 \leq 0.05$, width of PDF is more narrow as the number of cycles increases; the system dynamics is nearly reversible after 600 cycles.

At <u>large strain amplitudes</u>, $\gamma_0 \geq 0.06$, PDFs become wider as the number of cycles increases; formation of shear band; enhanced particle diffusion.

$$D^2(t, \Delta t = T)$$



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

Excellent diagnostic for identifying particle rearrangements

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

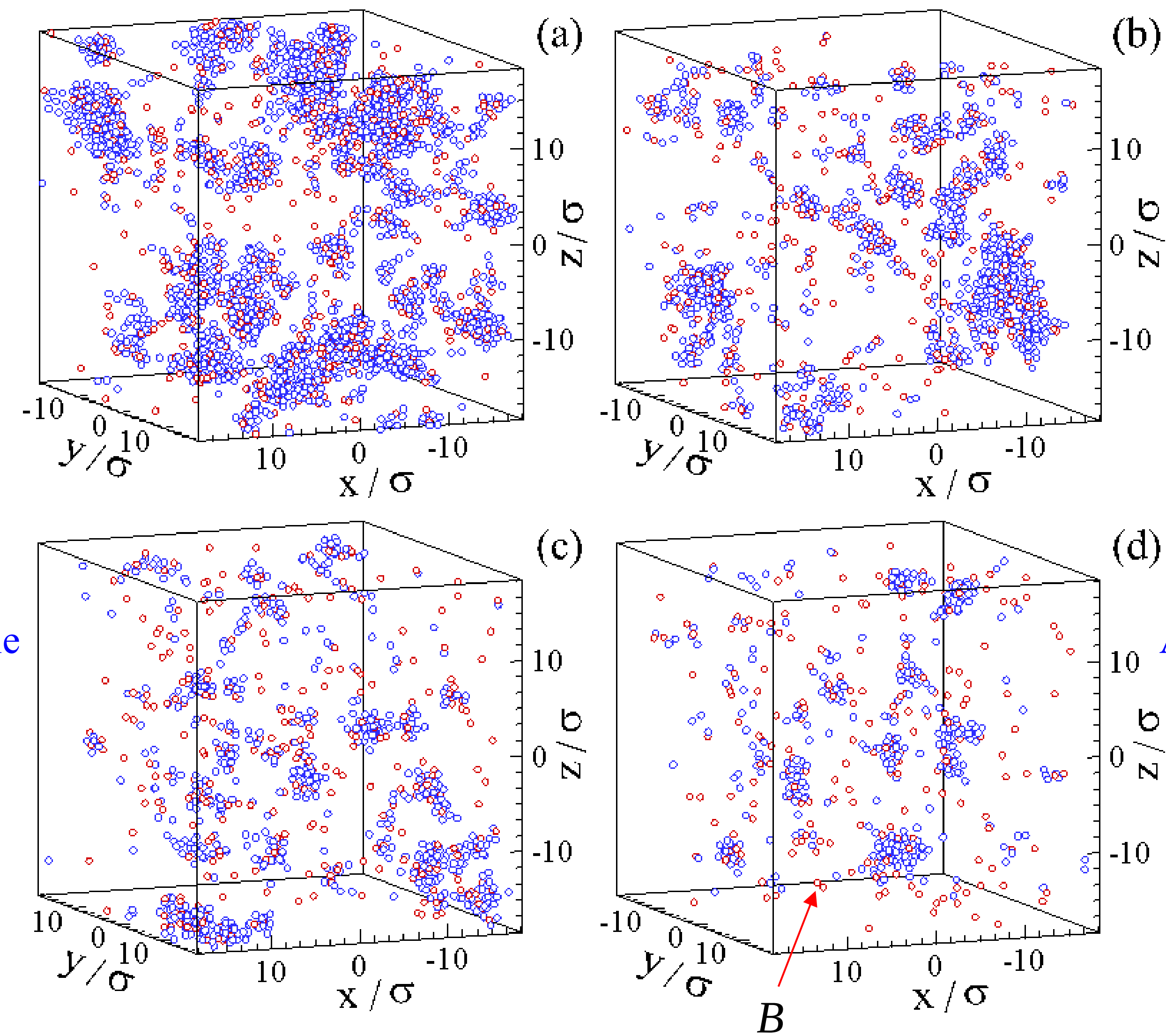
Spatial configurations of atoms with large nonaffine displacements at γ_0=0.03

$$D^2(t,T) > 0.04\,\sigma^2$$

After 20-th cycle

Disconnected sparse clusters

After 80-th cycle



After 200-th cycle

After 600-th cycle

Nearly reversible particle dynamics

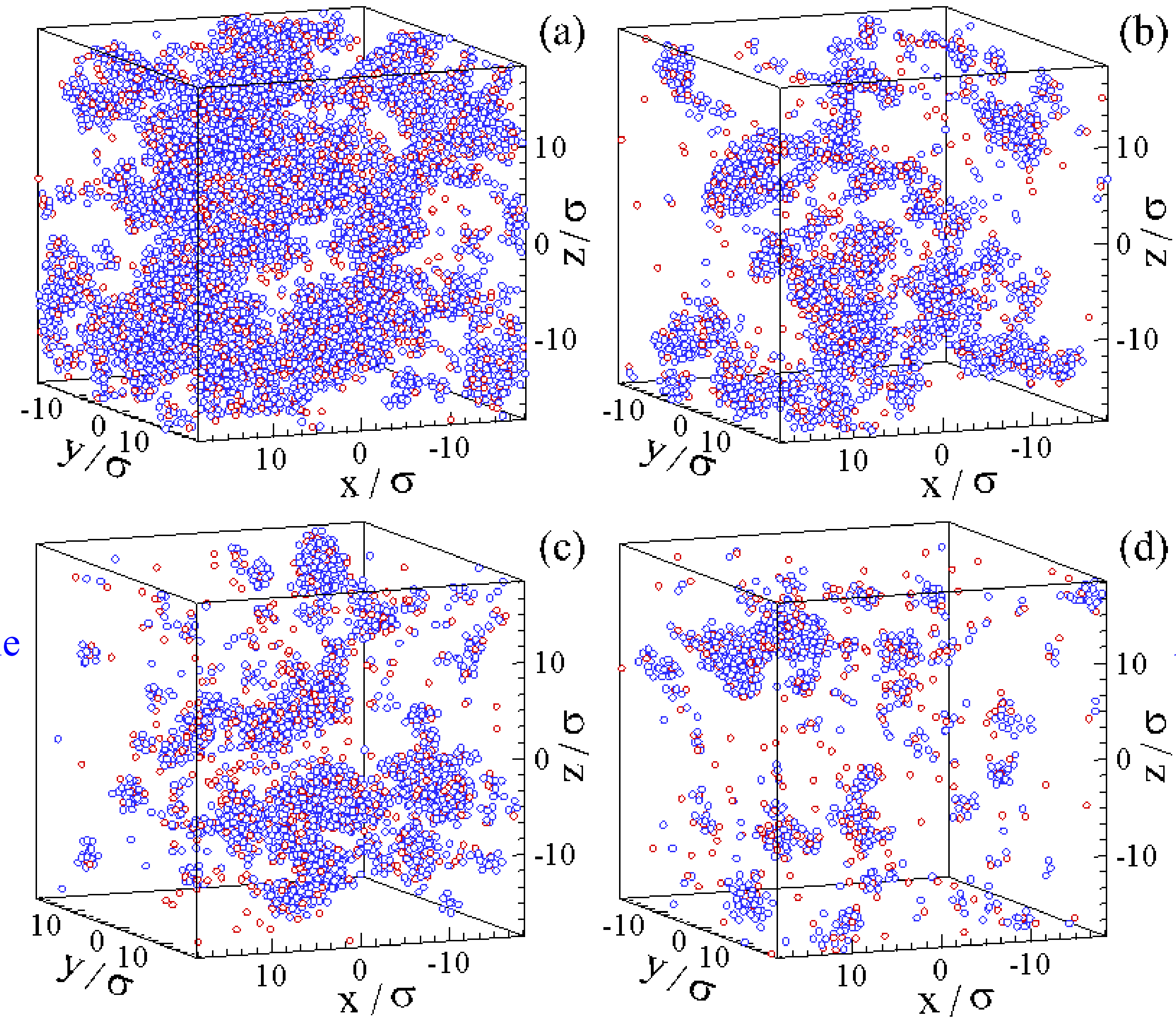
Spatial configurations of atoms with large nonaffine displacements at γ_0=0.05

$$D^2(t,T) > 0.04\,\sigma^2$$

After 20-th cycle

Large clusters of nonaffine displacements

After 80-th cycle



After 200-th cycle

Small clusters of nonaffine displacements

After 600-th cycle

Nearly reversible particle dynamics

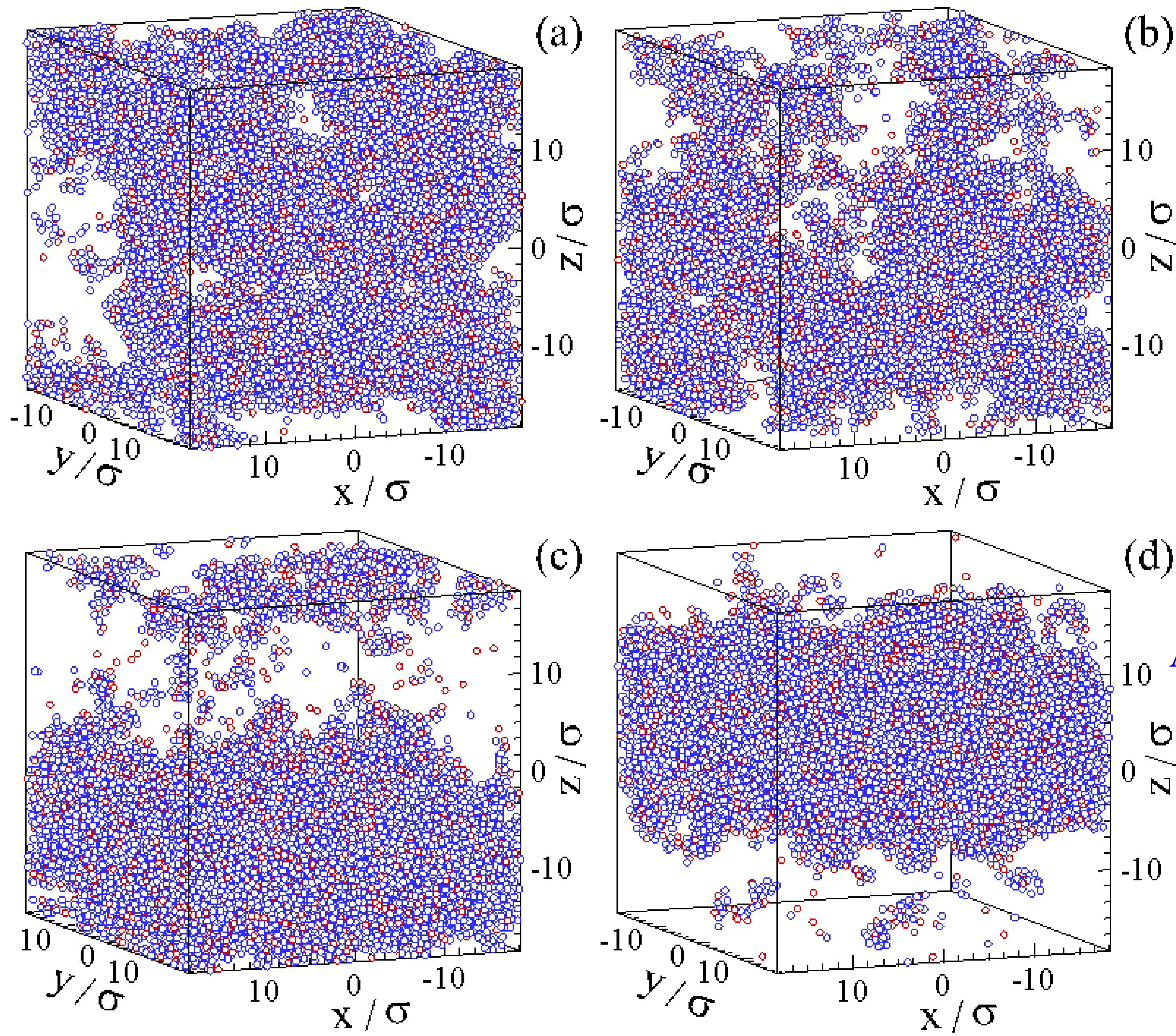
Spatial configurations of atoms with large nonaffine displacements at γ_0=0.06

$$D^2(t,T) > 0.04\,\sigma^2$$

After 20-th cycle

After 80-th cycle

Large shear stress amplitude



After 200-th cycle

Reduced shear stress amplitude

Shear band formation

After 600-th cycle

Finite width of shear band

Enhanced diffusion

Spatial configurations of atoms with large nonaffine displacements at γ_0=0.07

$$D^2(t,T) > 0.04\,\sigma^2$$

After 20-th cycle

After 80-th cycle

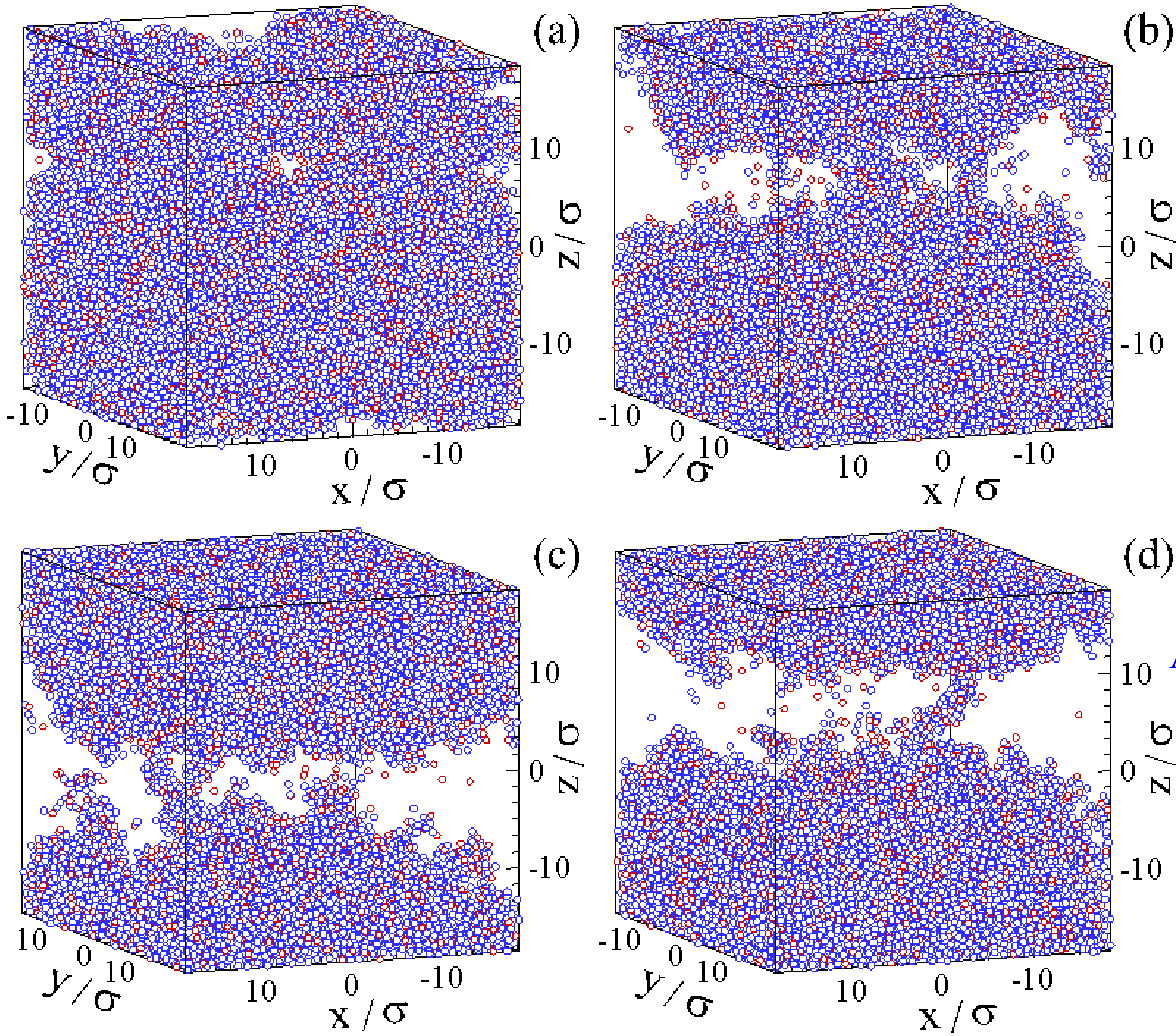
Reduced shear stress amplitude

Shear band formation

After 200-th cycle

After 600-th cycle

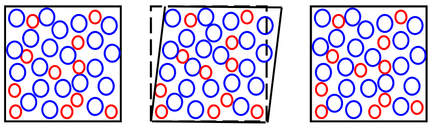
Finite width of shear band



The width of shear band increases with γ_0

LAMMPS, DPD thermostat

Conclusions:



600 cycles

- MD simulations of binary 3D Lennard-Jones glasses under periodic shear at finite T_{LJ}.

- At small strain amplitudes, $\gamma_0 \leq 0.05$: the potential energy acquires progressively lower minima; stress amplitude increases with γ_0; sparse transient clusters of atoms with large nonaffine displacements; nearly reversible particle dynamics.

- Near the critical strain amplitude, $\gamma_0 = 0.06$: the dynamic transition from disconnected clusters to a shear band of large nonaffine displacements: leads to drop in shear stress amplitude.

- At large strain amplitudes, $\gamma_0 \geq 0.07$: diffusive particle dynamics; quick formation and growth of shear bands; irreversible particle displacements lead to hysteresis & increase in the potential energy. The width of shear band increases with γ_0

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