Heterogeneous Relaxation Dynamics in Amorphous Materials under Cyclic Loading

March 22, 2013

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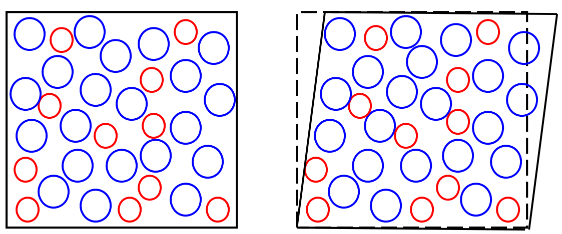
`Movies, preprints @ http://www.egr.msu.edu/~priezjev`

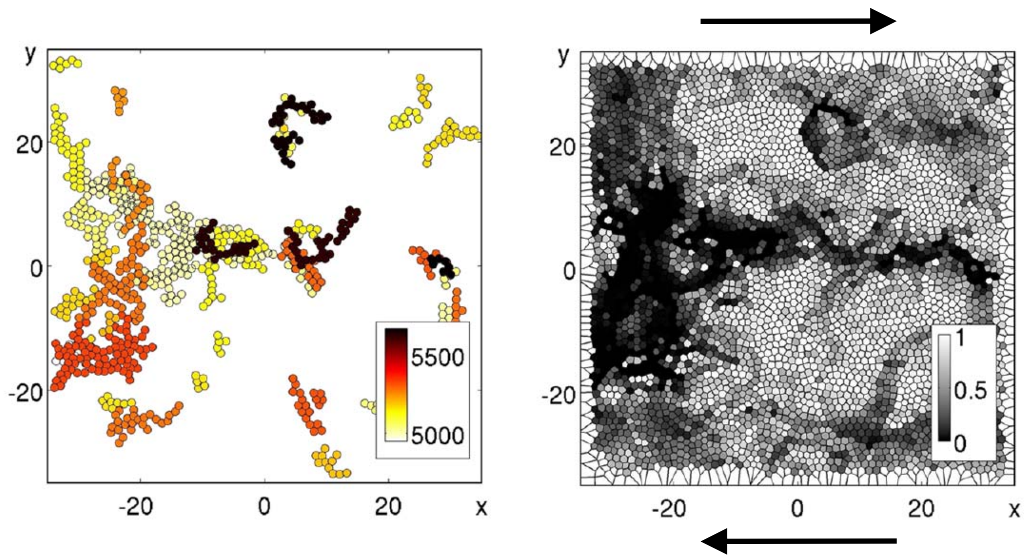


Acknowledgement:
NSF (CBET-1033662)

N. V. Priezjev, “Heterogeneous relaxation dynamics in amorphous materials under cyclic loading”, *Phys. Rev. E* **87**, 052302 (2013). Preprint: http://xxx.lanl.gov/abs/1301.1666

Dynamical Heterogeneities in Granular Media and Supercooled Liquids

• Cyclic Shear Experiment on Dense 2D Granular Media



Spatial location of successive clusters of cage jumps

Power-law distribution of clusters sizes

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

• Fluidized Bed Experiment: Monolayer of Bidisperse Beads

Candelier, Dauchot, and Biroli, *EPL* **92**, 24003 (2010).

• 2D Softly Repulsing Particle Molecular Dynamics Simulation (Supercooled Liquids at Eqm)

Candelier, Widmer-Cooper, Kummerfeld, Dauchot, Biroli, Harrowell, Reichman, *PRL* (2010).

Present study:

• 3D metallic glass under periodic strain?

• Particle diffusion depends on the strain amplitude

• Structural relaxation and dynamical heterogeneities

• Particle hopping dynamics clusters of mobile particles

• Dynamical facilitation of mobile particles

Details of molecular dynamics simulations and parameter values

Binary 3D Lennard-Jones Kob-Andersen mixture:

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

Interaction parameters for $\alpha\beta = A$ and B particles:

$$\varepsilon_{AA} = 1.0, \varepsilon_{AB} = 1.5, \ \varepsilon_{BB} = 0.5, m_A = m_B, N_p = 2940$$

$$\sigma_{AA} = 1.0, \sigma_{AB} = 0.8, \ \sigma_{BB} = 0.88, \ \tau = \sigma_{AA}\sqrt{m_A/\varepsilon_{AA}}$$

W. Kob and H. C. Andersen, *Phys. Rev. E* **51**, 4626 (1995).

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

Temperature: $T = 0.1\ \varepsilon/k_B < T_g = 0.45\ \varepsilon/k_B$

System dimensions: $12.81\,\sigma \times 14.79\,\sigma \times 12.94\,\sigma$

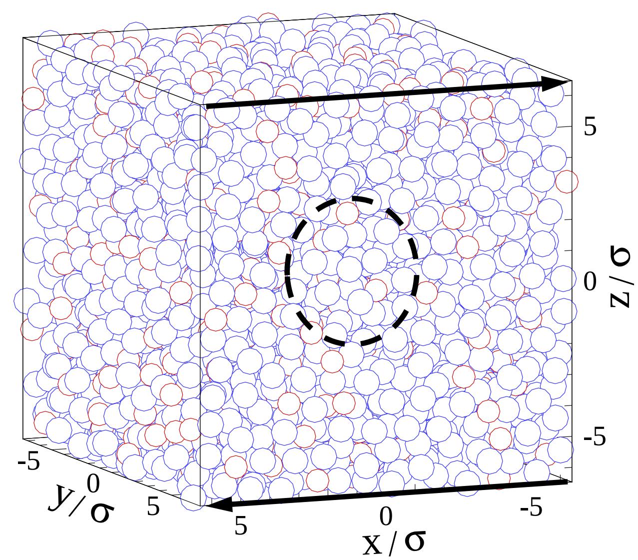
Lees-Edwards periodic boundary conditions

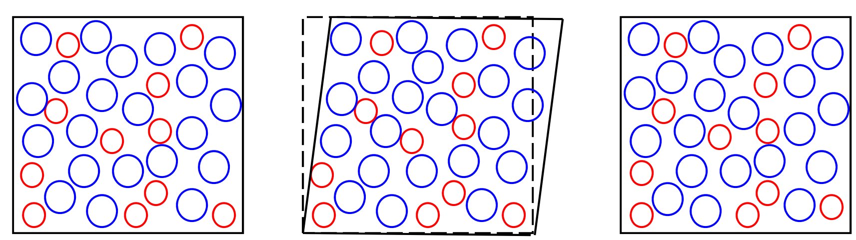
The SLLOD equations of motion: $\Delta t_{MD} = 0.005\,\tau$

Oscillatory shear strain: $\dot{\gamma}(t) = \dot{\gamma}_0 \cos(\omega t)$

Strain amplitude: $\gamma_0 = \dot{\gamma}_0 / \omega, \ \ \omega = 0.02\tau^{-1}$

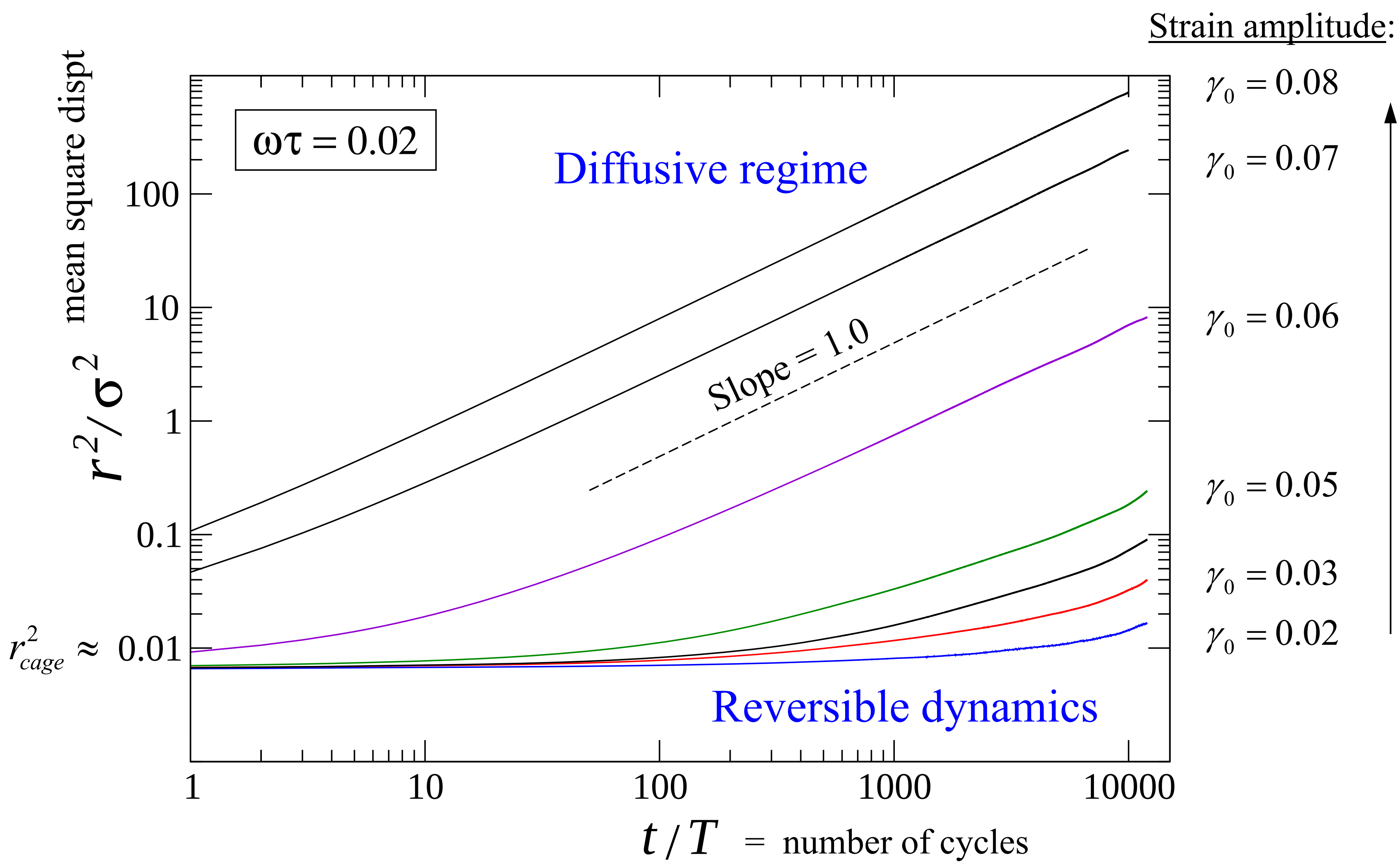
Oscillation period: $T = 2\pi / \omega = 314.16\,\tau$

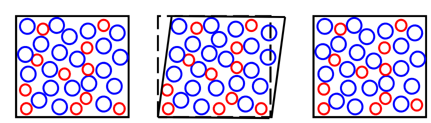




12,000 cycles ($\approx 7.5 \times 10^8$ MD steps)

Mean square displacement as a function of time for different strain amplitudes



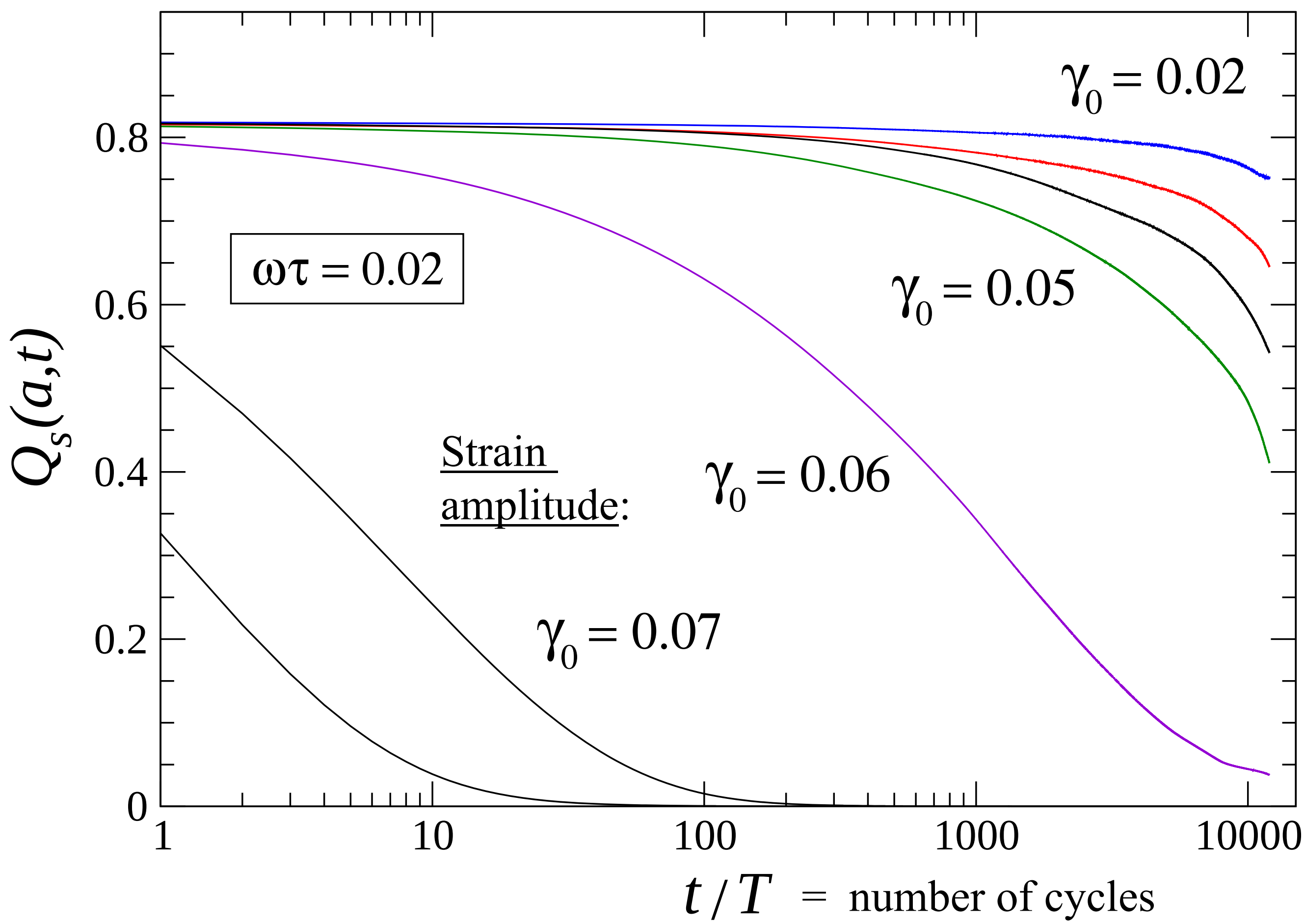


Oscillation period: $T = 2\pi / \omega = 314.16\,\tau$

Self-overlap order parameter $Q_s(a,t)$ for different strain amplitudes

$$Q_s(a,t) = \frac{1}{N_p}\sum_{i=1}^{N_p}\exp\left(-\frac{\Delta r_i(t)^2}{2a^2}\right)$$

$a = 0.12\sigma$ = probed length scale ~ max in $X_4(a,t)$



$Q_s(a,t)$ describes structural relaxation of the material.
Measure of the spatial overlap between particles positions.

Reversible dynamics:
$Q_s(t) \approx$ constant

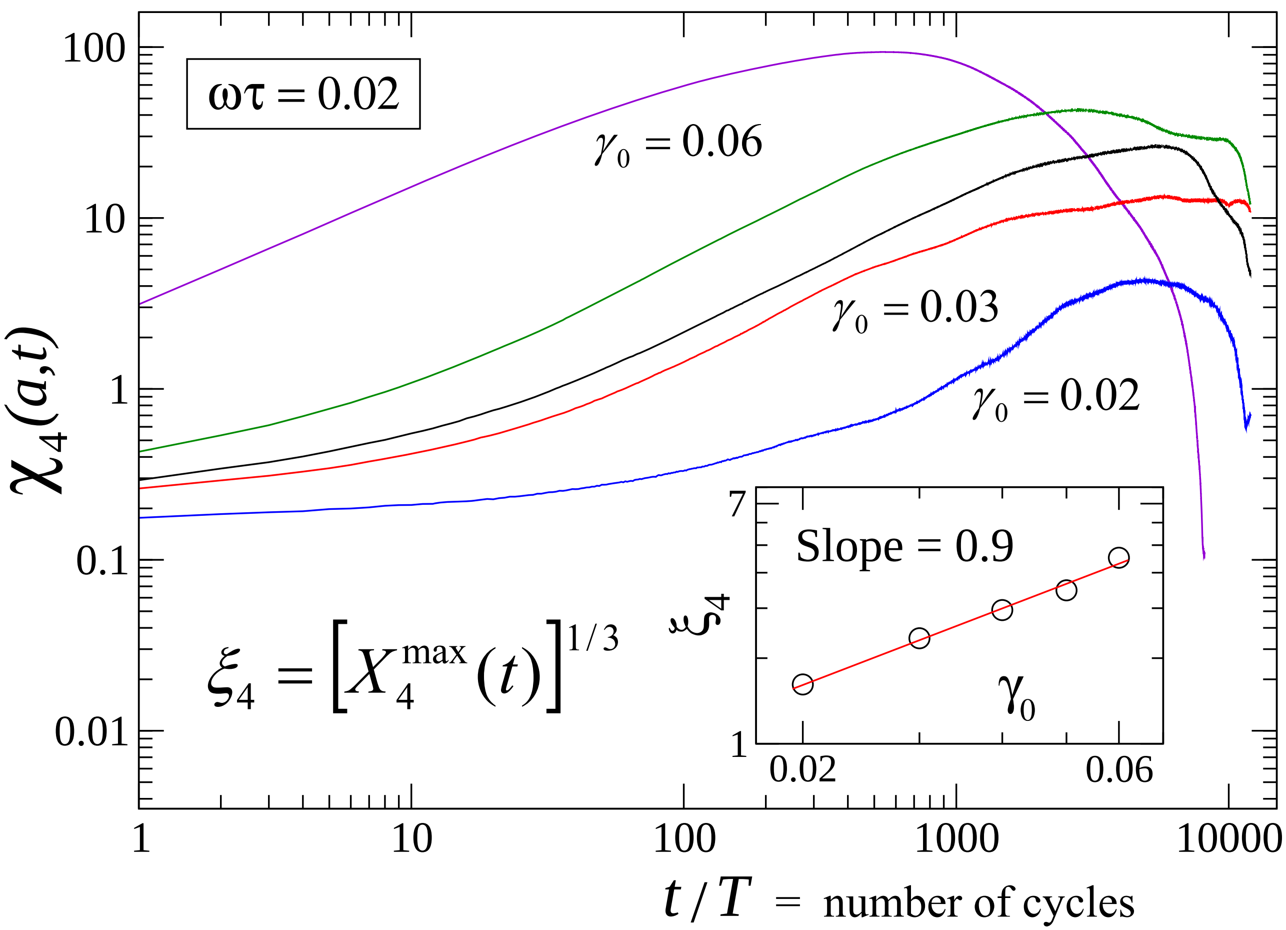
Diffusive regime:
$Q_s(t)$ vanishes at large t

Susceptibility
$X_4(a,t) = ?$

Dynamical susceptibility as a function of time for different strain amplitudes

$$X_4(a,t) = N_p\left(\left\langle Q_s(a,t)^2\right\rangle - \left\langle Q_s(a,t)\right\rangle^2\right)$$

$a = 0.12\sigma$ = probed length scale ~ max in $X_4(a,t)$



$X_4(a,t)$ is dynamical
sceptibility, which
the variance of Q_s.

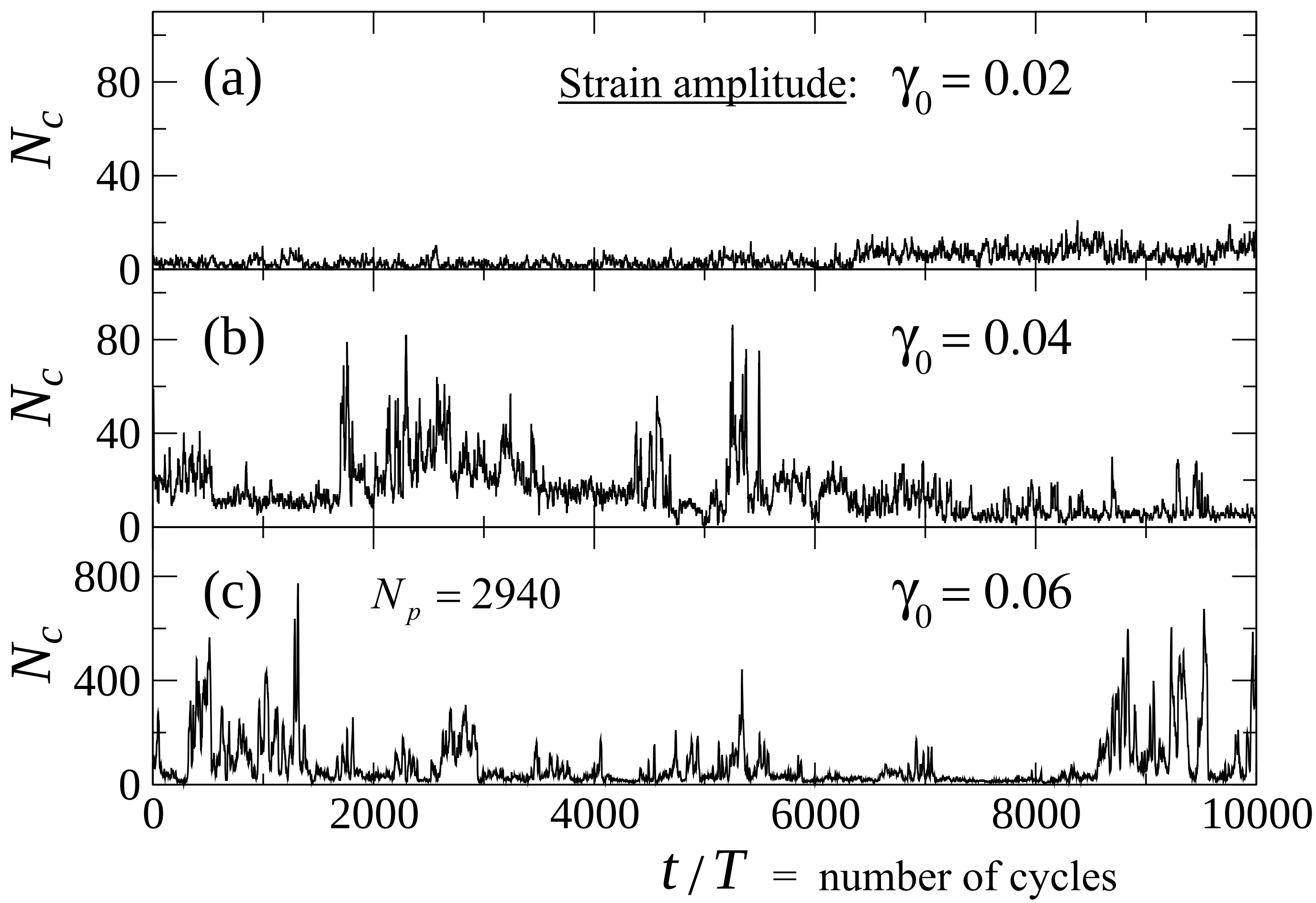
Maximum $X_4(a,t)$ indicates the largest spatial correlation between localized particles.

Berthier & Biroli (2011)

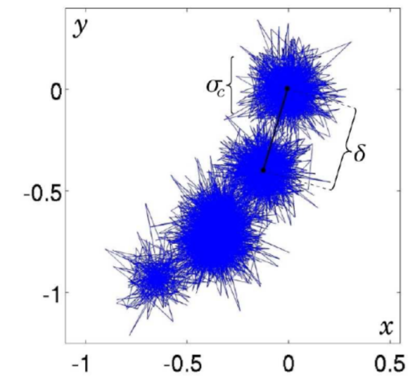
The dynamic correlation length increases with increasing strain amplitude (in contrast to steadily sheared supercooled liquids and glasses).

Mizuno & Yamamoto, *JCP* (2012); Tsamados, EPJE (2010)

Number of particles undergoing cage jumps N_c as a function of time t/T



Numerical algorithm for detection of cage jumps:



Candelier, Dauchot, Biroli, *PRL* (2009).

Periodic deformation = intermittent bursts of large particle displacements.

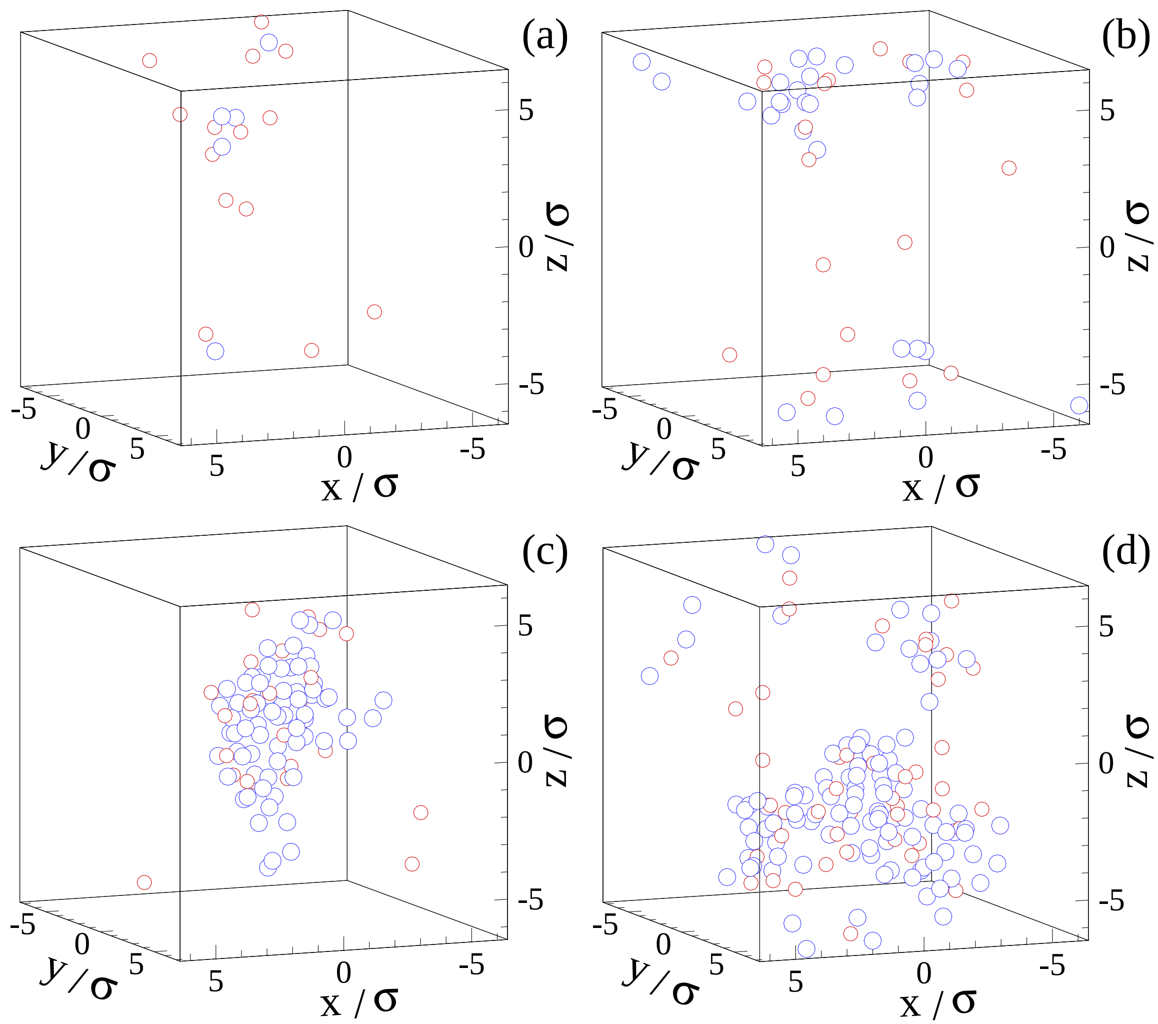
Power spectrum ~ frequency^{-2} = simple Brownian noise

Scale-invariant processes or Pink noise = "$1/f$ noise"

Typical clusters of mobile particles A (blue circles) and B (red circles)

$\gamma_0 = 0.02$

Single particle reversible jumps:



Strain amplitude:

$\gamma_0 = 0.03$

$\gamma_0 = 0.04$

Compact clusters; Irreversible jumps:

$$\xi_4 = \gamma_0^{0.9}$$

Strain amplitude:

$\gamma_0 = 0.05$

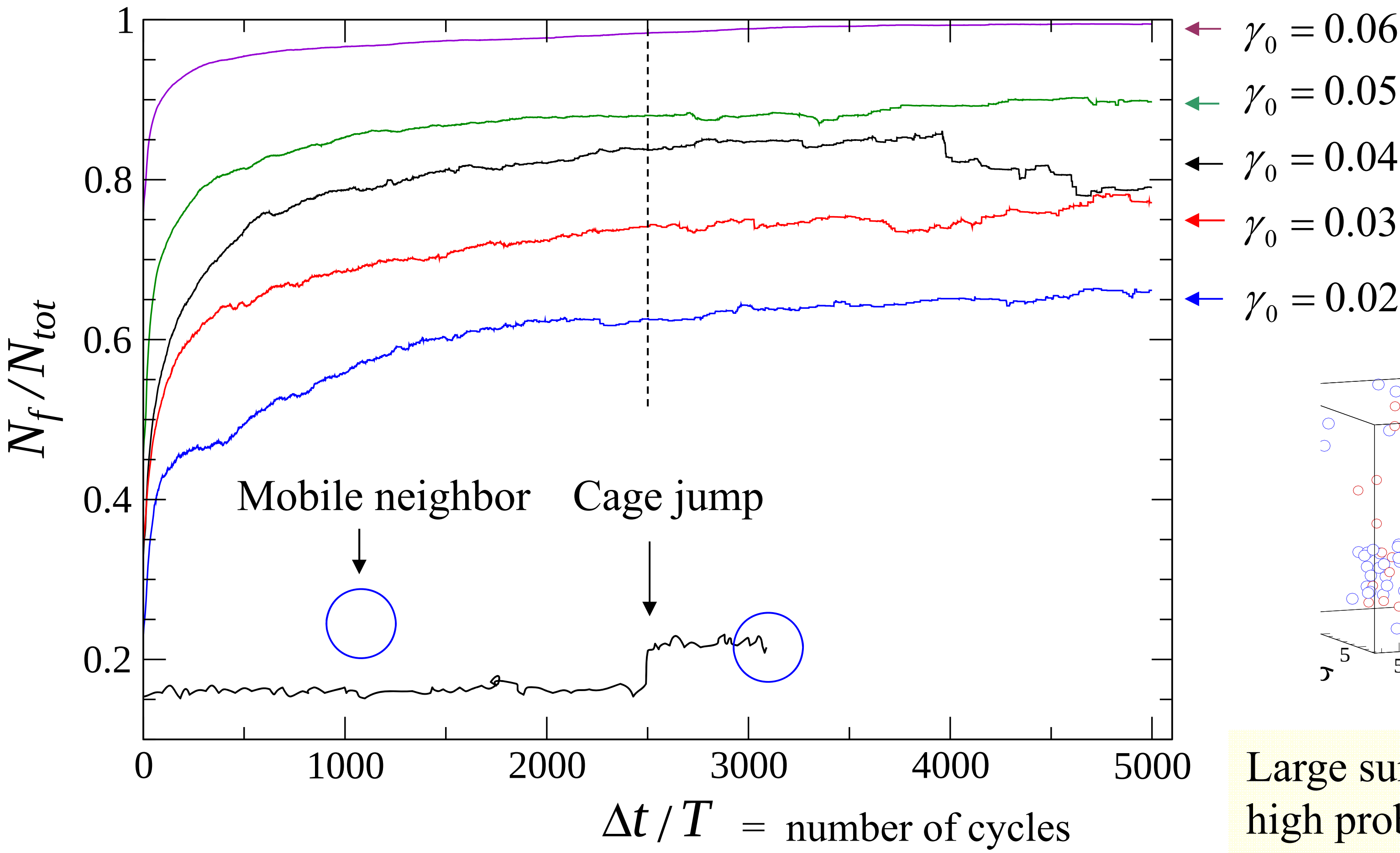
$\gamma_0 \geq 0.06$

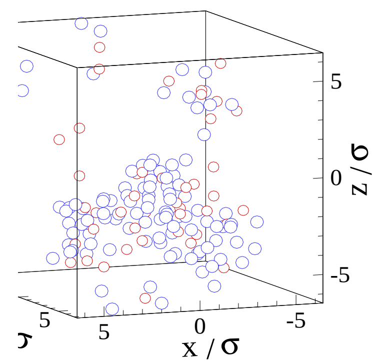
The system is fully relaxed over about 10^4 cycles

Fraction of dynamically facilitated particles increases with strain amplitude

Δt = time interval when a particles is immobile (inside the cage)

<u>Strain amplitude</u>:



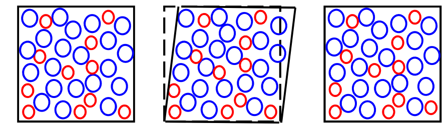


Large surface area = high probability to have mobile neighbors.

Oscillation period: $T = 2\pi / \omega = 314.16\,\tau$

Vogel and Glotzer, *Phys. Rev. Lett.* **92**, 255901 (2004).

Important conclusions:



- MD simulations of the binary 3D Lennard-Jones Kob-Andersen mixture at $T = 0.1\ \varepsilon / k_B$ under spatially homogeneous, time-periodic shear strain.

- At small strain amplitudes, the mean square displacement exhibits a broad sub-diffusive plateau and the system undergoes nearly reversible deformation over about 10^4 cycles.

- At larger strain amplitudes, the transition to the diffusive regime occurs at shorter time intervals and the relaxation process involves intermittent bursts of large particle displacements.

- The detailed analysis of particle hopping dynamics and the dynamic susceptibility $X_4(a,t)$ indicates that mobile particles aggregate into clusters whose sizes increase at larger strain amplitudes. (In contrast to sheared supercooled liquids and glasses). $\xi_4 = \gamma_0^{0.9}$

- Fraction of dynamically facilitated mobile particles increases at larger strain amplitudes.

N. V. Priezjev, "Heterogeneous relaxation dynamics in amorphous materials under cyclic loading", *Phys. Rev. E* **87**, 052302 (2013). Preprint: http://xxx.lanl.gov/abs/1301.1666