Heterogeneous Relaxation Dynamics in Amorphous Materials under Cyclic Loading

Nikolai V. Priezjev
Department of Mechanical Engineering
Michigan State University

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

Acknowledgement: NSF (CBET-1033662)

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  

- **Fluidized Bed Experiment: Monolayer of Bidisperse Beads**
  

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

**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:

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

\[ \sigma_{AA} = 1.0, \sigma_{AB} = 0.8, \sigma_{BB} = 0.88, \tau = \sigma_{AA} \sqrt{\frac{m_A}{\varepsilon_{AA}}} \]


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: \(\gamma_0 = \dot{\gamma}_0 / \omega, \quad \omega = 0.02\tau^{-1}\)

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

\[ \omega \tau = 0.02 \]

Diffusive regime

\[ \frac{r^2}{\sigma^2} \quad \text{mean square dispt} \]

\[ \frac{r^2}{\sigma^2} \approx 0.01 \]

Reversible dynamics

\[ r^2_{\text{cage}} \approx 0.01 \]

\( t / T \) = number of cycles

Oscillation period: \( T = \frac{2\pi}{\omega} = 314.16 \tau \)

Strain amplitude:

\( \gamma_0 = 0.08 \)
\( \gamma_0 = 0.07 \)
\( \gamma_0 = 0.06 \)
\( \gamma_0 = 0.05 \)
\( \gamma_0 = 0.03 \)
\( \gamma_0 = 0.02 \)
Self-overlap order parameter $Q_s(a,t)$ for different strain amplitudes

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

$t$ = number of cycles

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

Reversible dynamics:
$Q_s(t) \approx \text{constant}$

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

Susceptibility
$X_4(a,t) = ?$

$\gamma_0 = 0.02$

$\omega \tau = 0.02$

$\gamma_0 = 0.05$

$\gamma_0 = 0.06$

$\gamma_0 = 0.07$
Dynamical susceptibility as a function of time for different strain amplitudes

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

\[ a = 0.12\sigma = \text{probed length scale} \sim \text{max in } X_4(a,t) \]

\[ X_4(a,t) \text{ is dynamical susceptibility, which is the variance of } Q_s. \]

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 $t/T$

(a) Strain amplitude: $\gamma_0 = 0.02$

(b) $\gamma_0 = 0.04$

(c) $N_p = 2940$ $\gamma_0 = 0.06$

$t/T = \text{number of cycles}$

Power spectrum $\sim\text{frequency}^{-2} = \text{simple Brownian noise}$

Numerical algorithm for detection of cage jumps:


Periodic deformation = intermittent bursts of large particle displacements.

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:

\[ \gamma_0 = 0.04 \]

Compact clusters; Irreversible jumps:

\[ \xi_4 = \gamma_0^{0.9} \]

Strain amplitude:

- \( \gamma_0 = 0.03 \)
- \( \gamma_0 = 0.05 \)
- \( \gamma_0 \geq 0.06 \)

The system is fully relaxed over about \( 10^4 \) cycles.

Department of Mechanical Engineering
Michigan State University
Fraction of dynamically facilitated particles increases with strain amplitude

\[ \Delta t = \text{time interval when a particle is immobile (inside the cage)} \]

Strain amplitude:
- \( \gamma_0 = 0.06 \)
- \( \gamma_0 = 0.05 \)
- \( \gamma_0 = 0.04 \)
- \( \gamma_0 = 0.03 \)
- \( \gamma_0 = 0.02 \)

Large surface area = high probability to have mobile neighbors.

Oscillation period: \( T = 2\pi / \omega = 314.16 \tau \)

Important conclusions:

- MD simulations of the binary 3D Lennard-Jones Kob-Andersen mixture at \( T = 0.1 \frac{\varepsilon}{k_B} \) 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.