Atomistic modeling of cyclic loading and heat treatment processes for tuning the mechanical properties of amorphous alloys

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• Brief introduction (metallic glasses, amorphous structure, mechanical properties, etc)

• Part I: Cyclic loading with alternating shear orientation ("mechanical annealing")
  

• Part II: Cryogenic thermal cycling and mechanical properties of metallic glasses


• Part III: Aging and rejuvenation during elastostatic loading of amorphous alloys


• Conclusions
Thermomechanical processing: Structural relaxation and rejuvenation

Metallic glasses: mechanical properties include high strength and low ductility (brittle)


Rejuvenation: increase in stored energy

Relaxation: (1) cyclic loading or “mechanical annealing”, (2) ultrastable glasses by deposition
Part I: Cyclic loading with alternating shear orientation ("mechanical annealing")

Details of molecular dynamics simulations and parameter values

Binary Lennard-Jones Kob-Andersen mixture:

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

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, \( \Delta t_{MD} = 0.005\tau \)

Fast annealing rate: \( 10^{-2}\varepsilon/k_B\tau \) (poorly annealed glass)

\[ \gamma(t) = \gamma_0 \sin(\omega t) \]

Oscillation period: \( T = 2\pi/\omega = 5000\tau \)

higher energy sample
Potential energy per particle $U$ during 1400 oscillation cycles for different $\gamma_0$

With increasing strain amplitude $\gamma_0$ (below yield strain), the system relocates to deeper energy minima (via collective rearrangements of atoms).

Priezjev, JNCS (2019)
Potential energy minima during 4 different deformation protocols for $\gamma_0 = 0.06$.

For the strain amplitude $\gamma_0 = 0.06$ (just below yield strain), each additional alternation of the shear orientation in the deformation protocol results in lower energy states.
The potential energy $U$ during 3 deformation protocols for the indicated $\gamma_0$

For strain amplitudes $\gamma_0$ (below yield strain), each additional alternation of the shear orientation in the deformation protocol results in lower energy states.
The height of the yielding peak $\sigma_Y$ increases when an additional shear orientation is introduced in the cyclic loading protocol. The shear modulus $G$ is larger along the shear directions that were not used during cyclic deformation.

Snapshots of the strained glass after aging during 1400 T (no cyclic loading)

5% shear strain

10% shear strain

15% shear strain

20% shear strain

Nonaffine measure $D^2$
Snapshots of strained glass after 1400 alternating shear cycles ($xz$, $yz$, $xy$)

5% shear strain

10% shear strain

15% shear strain

20% shear strain

nonaffine measure $D^2$
Conclusions:

• Periodic shear deformation (in the “elastic” range) leads to relaxed, lower energy states ("mechanical annealing").

• For a fixed strain amplitude (below yield strain), each additional alternation of the shear orientation in the deformation protocol results in lower energy states.

• The yielding peak increases in glasses deformed at higher strain amplitudes.

• The shear modulus is larger along the shear directions that were not cyclically loaded.

Part II: The effect of cryogenic thermal cycling on potential energy states and mechanical properties of metallic glasses


Details of molecular dynamics simulations and parameter values

Binary Lennard-Jones Kob-Andersen mixture:

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

Parameters for \( \alpha, \beta = A \) and \( B \) particles:

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

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

Temperature: \( T_{LJ} = 0.01\varepsilon/k_B < T_g = 0.35\varepsilon/k_B \)

LAMMPS: \( N_p = 60000, \) MD step \( \Delta t_{MD} = 0.005\tau \)

Initial quench rates: \( 10^{-2}\varepsilon/k_B\tau \) to \( 10^{-5}\varepsilon/k_B\tau \)

Pressure \( P = 0 \) and thermal period \( T = 5000\tau = 10^6 \) MD steps
Potential energy per atom during 100 thermal cycles for different max $T_{LJ}$

Aging at constant temperature: $T_{LJ} = 0.01 \varepsilon / k_B$

Fast initial annealing rate: $10^{-2} \varepsilon / k_B \tau$, poorly-annealed glass

Potential energy per atom during 100 thermal cycles for different max $T_{LJ}$

Aging at constant temperature: $T_{LJ} = 0.01 \, \varepsilon/k_B$

Maximum $T_{LJ}$

- $T_{LJ} = 0.4 \, \varepsilon/k_B$
- $T_{LJ} = 0.3 \, \varepsilon/k_B$
- $T_{LJ} = 0.2 \, \varepsilon/k_B$
- $T_{LJ} = 0.1 \, \varepsilon/k_B$

Slow initial annealing rate: $10^{-5} \, \varepsilon/k_B \tau$, well-annealed glass

Tensile stress vs strain after 100 cycles: effects of quench rate and max $T_{LJ}$

Strain rate $= 10^{-5} \, 1/\tau$

Aged glasses (black curves): Higher yield peak at slower quench rates

Highest yield peak (blue curves) at maximum $T_{LJ} = 0.30 \, \varepsilon/k_B$

Maximum $T_{LJ}$

- $T_{LJ} = 0.4 \, \varepsilon/k_B$
- $T_{LJ} = 0.30 \, \varepsilon/k_B$
- $T_{LJ} = 0.2 \, \varepsilon/k_B$
- $T_{LJ} = 0.1 \, \varepsilon/k_B$
- $T_{LJ} = 0.01 \, \varepsilon/k_B$

Aged glasses
The yielding peak $\sigma_Y$, elastic modulus $E$, and $U_{min}$ versus maximum $T_{LJ}$

- Highest yield peak and elastic modulus after thermal loading with maximum $T_{LJ} = 0.30 \, \varepsilon / k_B$
- A correlation between minimum potential energy $U_{min}$ and maximum values of $\sigma_Y$ and $E$. 

Initial quench rates:
- (color code)
  - $10^{-2} \, \varepsilon / k_B \tau$
  - $10^{-3} \, \varepsilon / k_B \tau$
  - $10^{-4} \, \varepsilon / k_B \tau$
  - $10^{-5} \, \varepsilon / k_B \tau$

Pressure $P = 0$
- $T_g = 0.35 \, \varepsilon / k_B$
Conclusions:

• MD simulations of binary 3D Lennard-Jones glasses that are initially prepared with different cooling rates and then subjected to repeated cycles of heating and cooling.

• The potential energy in rapidly annealed glasses decreases during thermal cycling, while the energy in slowly annealed glasses increases at large cycling amplitudes ($T_g$).

• The elastic modulus and the yielding peak (after the thermal treatment) acquire maximum values at a particular $max T_{LJ}$ which coincides with the minimum of the potential energy.

Part III: Aging and rejuvenation during elastostatic loading of amorphous alloys

Constant applied stress $\sigma_{zz}$

At what stress, temperature to load, and for how long?

Setup: Temperature profiles, annealing time, glass transition temperature

Reference state: \( P = 0 \) and \( T_{LJ} = 0.01 \ \varepsilon/k_B \)

The stress \( \sigma_{zz} \) was ramped up to a certain value during the annealing time.

Elastostatic loading: constant stress \( \sigma_{zz} \)

Pressure \( P = 0 \)

\( T_g = 0.35 \ \varepsilon/k_B \)
Variation of the potential energy vs. annealing time at different temp $T_a$

Constant applied stress $\sigma_{zz}$ is up to ~70-80% of the yielding peak at a given temperature $T_a$

Aging: high $T_a < T_g = 0.35 \, \varepsilon/k_B$ and low stress $\sigma_{zz}$  Rejuvenation: low $T_a$ and high $\sigma_{zz}$
Collective nonaffine displacements vs. annealing time at $T_a = 0.1 \varepsilon/k_B$

Empty regions correspond to atoms that remained in their cages during the annealing time.

Elastostatic loading: constant applied stress: $\sigma_{zz} = 1.5 \varepsilon \sigma^{-3}$

$D^2(0, 10^5\tau) > 0.04\sigma^2$

$D^2(0, 2 \times 10^5\tau) > 0.04\sigma^2$

$D^2(0, 1.6 \times 10^6\tau) > 0.04\sigma^2$

$D^2(0, 2.4 \times 10^6\tau) > 0.04\sigma^2$
The elastic modulus $E$ vs. annealing time $t_a$ at different temperatures $T_a$.

- $T_a = 0.05 \, \epsilon / k_B$
- $T_a = 0.10 \, \epsilon / k_B$
- $T_a = 0.20 \, \epsilon / k_B$
- $T_a = 0.25 \, \epsilon / k_B$

Maximum effect of rejuvenation due to elastostatic loading: about 10% decrease in $E$.
Conclusions:

• Well-annealed binary glass at zero pressure is elastostatically loaded during extended time intervals (~$10^8$ MD steps) in a wide range of annealing temperatures.

• **Aging**: high $T_a < T_g = 0.35 \, \varepsilon / k_B$ and low stress $\sigma_{zz}$  
  **Rejuvenation**: low $T_a$ and high $\sigma_{zz}$

  \[ T_a < 0.6 \, T_g \quad \sigma_{zz} \approx 0.8 \, \sigma_Y \]

• Maximum effect of rejuvenation due to elastostatic loading: about 10% decrease in $E$