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


Thermal treatment and mechanical cycling of metallic glasses

**Metallic glasses**: mechanical properties include high strength and low ductility


Rejuvenated states offer improvements in plasticity, while relaxed states exhibit high yield stress and greater chemical stability.

**Periodic shear**: yielding transition, relaxation dynamics, failure mechanism, nonaffine motion


**“Mechanical annealing” during sub-yield cycling**

**Thermal loading**: aging or rejuvenation, structural relaxation, ductile vs brittle fracture (??)


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: \( T_{LJ} = 0.01 \varepsilon/k_B < T_g = 0.435 \varepsilon/k_B \)

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 $T_{LJ}$

Black horizontal line = 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 quench rate: $10^{-5} \, \varepsilon / k_B \tau$
Potential energy $U$ during 1000 thermal cycles for different maximum $T_{LJ}$

Transition to low $U$ states after few 100 thermal cycles.

- Higher max $T_{LJ}$ $\Rightarrow$ lower $U_{\text{min}}$

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

Slow initial quench rate: $10^{-5} \; \varepsilon/k_B \tau$
Potential energy minima during 1000 thermal cycles for different max $T_{LJ}$

Data in (a)-(d) for indicated initial quench rates

Quench rate: $10^{-3} \varepsilon/k_B \tau$

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

Lowest $U_{\text{min}}$ at max $T_{LJ} = 0.35 \varepsilon/k_B$
Configurations of atoms with large nonaffine displacements after 1 cycle

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

\[ \max T_{LJ} = 0.35 \frac{\varepsilon}{k_B} \]

- After 1-st cycle
  - Large clusters of atoms with large nonaffine displacements

- After 200-th cycle

- After 100-th cycle

- After 1000-th cycle
  - Nearly reversible particle dynamics

Slow initial quench rate: \(10^{-5} \frac{\varepsilon}{k_B \tau}\)

B small atom type
Tensile stress vs strain after 1000 cycles: effects of quench rate and max $T_{LJ}$

Quench rate = $10^{-2}$

- Quench rate = $10^{-3}$
- Quench rate = $10^{-4}$
- Quench rate = $10^{-5}$

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

Highest yield peak (blue curves) at maximum $T_{LJ} = 0.35 \, \varepsilon/k_B$

- $T_{LJ} = 0.4 \, \varepsilon/k_B$
- $T_{LJ} = 0.35 \, \varepsilon/k_B$
- $T_{LJ} = 0.2 \, \varepsilon/k_B$
- $T_{LJ} = 0.1 \, \varepsilon/k_B$
- $T_{LJ} = 0.01 \, \varepsilon/k_B$

Strain rate = $10^{-5} \, 1/\tau$
The yielding peak $\sigma_Y$, the elastic modulus $E$, and $U_{\text{min}}$ versus maximum $T_{\text{LJ}}$

Highest yield peak and elastic modulus after thermal loading with maximum $T_{\text{LJ}} = 0.35 \varepsilon/k_B$

A correlation between $U_{\text{min}}$ and maximum values of $\sigma_Y$ and $E$.

Initial quench rates:

$10^{-2} \varepsilon/k_B \tau$

$10^{-3} \varepsilon/k_B \tau$

$10^{-4} \varepsilon/k_B \tau$

$10^{-5} \varepsilon/k_B \tau$
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.

• With increasing cycle number, the potential energy minima saturate to a constant value that depends on the thermal amplitude ($max T_{LJ}$) and the initial cooling rate.

• 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.

• In the steady state, the glasses thermally expand and contract but most of the atoms return to their cages after each cycle, similar to limit cycles in periodically driven glasses.

