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

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Thermal treatment and mechanical cycling of metallic glasses

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

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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

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

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

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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:

\[ \varepsilon_{AA} = 1.0, \quad \varepsilon_{AB} = 1.5, \quad \varepsilon_{BB} = 0.5, \quad m_A = m_B \]
\[ \sigma_{AA} = 1.0, \quad \sigma_{AB} = 0.8, \quad \sigma_{BB} = 0.88 \]

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

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

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

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

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

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

**Slow initial annealing rate:** $10^{-5} \varepsilon / k_B \tau$

Potential energy $U$ during 1000 thermal cycles for different maximum $T_{LJ}$

$T_{LJ} = 0.10 \frac{\varepsilon}{k_B}$

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

$T_{LJ} = 0.35 \frac{\varepsilon}{k_B}$

Higher max $T_{LJ}$ => lower $U_{min}$

$T = 5000\tau = 10^6$ MD steps

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

Slow initial annealing rate: $10^{-5} \frac{\varepsilon}{k_B \tau}$

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Potential energy minima during 1000 thermal cycles for different max $T_{LJ}$

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

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

- Black curves = Aging at constant temperature: $T_{LJ} = 0.01 \varepsilon / k_B$
- Lowest $U_{min}$ at max $T_{LJ} = 0.35 \varepsilon / k_B$

- (a) $10^{-2}$
  - $T_{LJ} = 0.4 \varepsilon / k_B$
- (b) $10^{-3}$
  - $T_{LJ} = 0.35 \varepsilon / k_B$
- (c) $10^{-4}$
  - $T_{LJ} = 0.3 \varepsilon / k_B$
- (d) $10^{-5}$
  - $T_{LJ} = 0.25 \varepsilon / k_B$
  - $T_{LJ} = 0.2 \varepsilon / k_B$
  - $T_{LJ} = 0.1 \varepsilon / k_B$
Configurations of atoms with large nonaffine displacements after 1 cycle

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

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

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

After 100-th cycle
Nearly reversible particle dynamics

After 200-th cycle

After 1000-th cycle

B small atom type

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

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

$\sigma_{xx}$ (units $\varepsilon \sigma^{-3}$)

Quench rate = $10^{-3}$

$\varepsilon_{xx}$

(a) $10^{-2}$

(b) $10^{-4}$

(c) $10^{-5}$

(d)

$\varepsilon_{xx}$

Maximum $T_{LJ}$

$T_{LJ} = 0.4 \varepsilon/k_B$

$T_{LJ} = 0.35 \varepsilon/k_B$

$T_{LJ} = 0.2 \varepsilon/k_B$

$T_{LJ} = 0.1 \varepsilon/k_B$

$T_{LJ} = 0.01 \varepsilon/k_B$

Aged glasses

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

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

Highest yield peak (blue curves) at maximum $T_{LJ} = 0.35 \varepsilon/k_B$
The yielding peak $\sigma_Y$, the elastic modulus $E$, and $U_{min}$ versus maximum $T_{LJ}$

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

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

Initial quench rates:

- $10^{-2} \varepsilon/k_B \tau$
- $10^{-3} \varepsilon/k_B \tau$
- $10^{-4} \varepsilon/k_B \tau$
- $10^{-5} \varepsilon/k_B \tau$

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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.

