The influence of complex thermal treatment on mechanical properties of metallic glass

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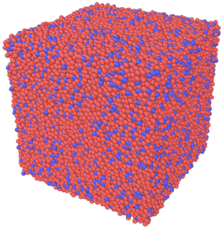
How thermal cycling treatment change the properties of metallic glasses?



1, Pros of metallic glass:
high strength and elastic limit, high resistance to corrosion, etc.

2, Cons of metallic glass:
low ductility, brittle fracture due to shear band formation, especially in aged samples.

3, Our purpose:
investigate the microscopic details of the thermal cycling processing on metallic glass, as well as the degree of relaxation, elastic, etc.

4, Our method:
MD simulation to heat the samples above T_g, quench with different cooling rates and apply thermal cycling treatments.

Details of the model

Lennard-Jones (LJ) potential for Kob-Andersen binary mixture model:

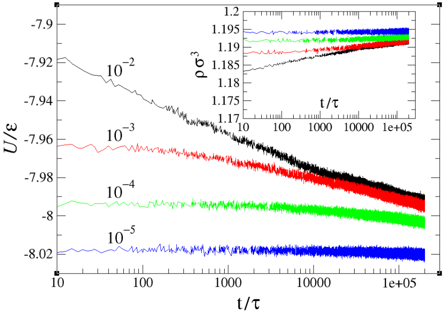
$$V_{\alpha\beta}(r) = 4\,\varepsilon_{\alpha\beta}\left[\left(\frac{\sigma_{\alpha\beta}}{r}\right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r}\right)^{6}\right]$$

1,Parameters for $\alpha, \beta = A, B$ particles:
$\varepsilon_{AA} = 1.0$, $\varepsilon_{AB} = 1.5$, $\varepsilon_{BB} = 0.5$,
$\sigma_{AA} = 1.0$,$\sigma_{AB} = 0.8$,$\sigma_{BB} = 0.88$, and
$m_A = m_B$
2, Number of A atoms: 48 000
3, Number of B atoms: 12 000
4, Glass transition temperature of the KA model, $T_g \approx 0.435, \varepsilon/k_B$ (reduced units)
5, 3D periodic boundary conditions
6, Nosé-Hoover thermostat, LAMMPS package

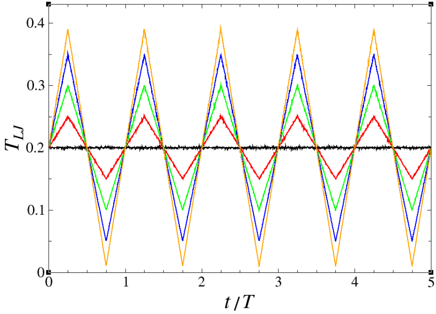
Steps:

1. Equilibrate the sample at $T = 0.7\,\varepsilon/k_B$, higher than T_g.
2. Anneal the sample to $T_{LJ} = 0.2\,\varepsilon/k_B$ with **four** different cooling rates $10^{-2}\varepsilon/k_B\tau$, $10^{-3}\varepsilon/k_B\tau$, $10^{-4}\varepsilon/k_B\tau$, and $10^{-5}\varepsilon/k_B\tau$.
3. Repeatedly heat and cool the samples at $P = 0$, with the thermal amplitude ΔT_{LJ} from 0.0 to $0.19\,\varepsilon/k_B$ during 100 cycles with the period $T = 2000\,\tau$.
4. Samples were strained along the $\hat{x}$ direction at $P = 0$ with the strain rate $\dot{\varepsilon}_{xx} = 10^{-5}\,\tau^{-1}$.

Aging, density and thermal amplitudes

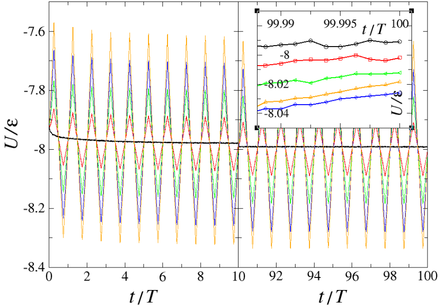


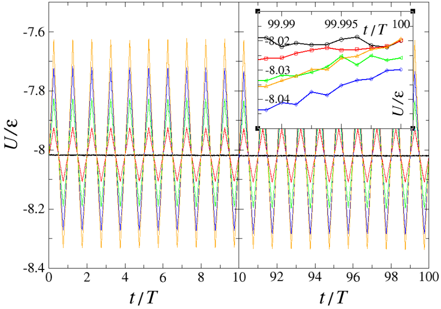
The variation of the potential energy per atom for binary glasses prepared with different cooling rates (in units of $\varepsilon/k_B\tau$). The inset shows the glass density as a function of time for the same samples.



The variation of temperature T_{LJ} (in units of ε/k_B) during first 5 periods, for the thermal amplitudes $\Delta T_{LJ} = 0.05\,\varepsilon/k_B$, $0.10\,\varepsilon/k_B$, $0.15\,\varepsilon/k_B$, and $0.19\,\varepsilon/k_B$. The black line denotes the data at the constant temperature $T_{LJ} = 0.2\,\varepsilon/k_B$.

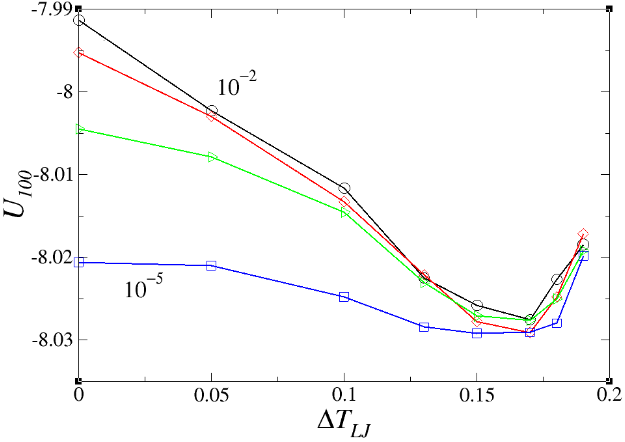
Potential energy vs period





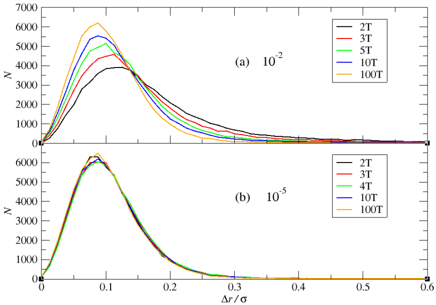
The potential energy series during the first and last ten cycles with the thermal amplitudes $\Delta T_{LJ} = 0.0$, $0.05\,\varepsilon/k_B$, $0.1\,\varepsilon/k_B$, $0.15\,\varepsilon/k_B$, and $0.19\,\varepsilon/k_B$. The sample was initially annealed with the cooling rate of 10^{-2} *(left)*, $10^{-5}\varepsilon/k_B\tau$ *(right)* , respectively. The enlarged view of the same data at the end of the last cycle is displayed in the inset.

Potential energy vs ΔT_{LJ}

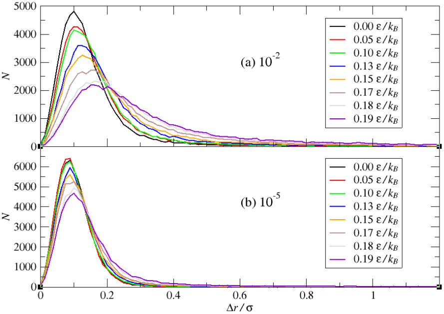


The dependence of the potential energy after 100 cycles, U_{100}/ε, as a function of the thermal amplitude ΔT_{LJ} (in units of ε/k_B) for glasses initially annealed with the cooling rates of $10^{-2}\varepsilon/k_B\tau$, $10^{-3}\varepsilon/k_B\tau$, $10^{-4}\varepsilon/k_B\tau$, and $10^{-5}\varepsilon/k_B\tau$.

Distribution of atomic displacements

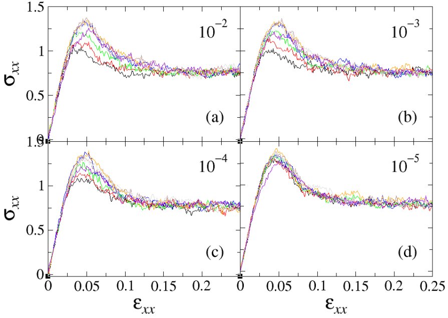


The distribution of atomic displacements during one cycle for the thermal amplitude $\Delta T_{LJ} = 0.10\,\varepsilon/k_B$.

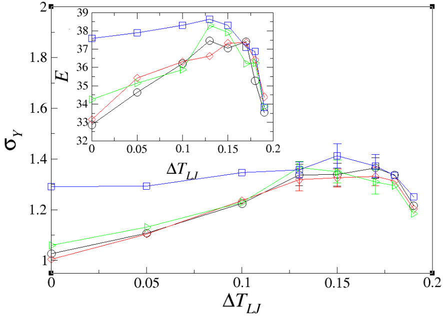


The probability distribution of atomic displacements during the second cycle for the indicated values of the thermal amplitude ΔT_{LJ}.

Stress-strain curves and elastic modulus



The variation of tensile stress, σ_{xx} (in units of $\varepsilon\sigma^{-3}$), as a function of strain, ε_{xx}, for samples annealed with four different cooling rates. The strain rate is $\dot{\varepsilon}_{xx} = 10^{-5}\,\tau^{-1}$. The tensile tests were performed after the thermal treatment with amplitudes $\Delta T_{LJ} = 0.0$, $0.05\ \varepsilon/k_B$, $0.10\ \varepsilon/k_B$, $0.13\ \varepsilon/k_B$, $0.15\ \varepsilon/k_B$, $0.17\ \varepsilon/k_B$, and $0.19\ \varepsilon/k_B$.



The dependence of the stress overshoot σ_Y (in units of $\varepsilon\sigma^{-3}$) as a function of samples annealed with cooling rates $10^{-2}\varepsilon/k_B\tau$, $10^{-3}\varepsilon/k_B\tau$, $10^{-4}\varepsilon/k_B\tau$, and $10^{-5}\varepsilon/k_B\tau$. The variation of the elastic modulus E (in units of $\varepsilon\sigma^{-3}$) versus thermal amplitude is shown in the inset.

Conclusions

1. MD simulations of binary Lennard-Jones glasses under periodic thermal treatment ($\Delta T_{LJ} < T_g$).
2. Thermal cycling leads to relaxed states, potential energy levels lower than those in the aged samples.
3. Potential energy first decreases and acquires a local minimum as ΔT_{LJ} increasing, then go up.
4. Stress overshoot and the elastic modulus weakly depend on the cooling rate except for the lowest rate.
5. Inverse correlation between the potential energy levels and mechanical properties.

Thanks for your attention!
Any suggestions?