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

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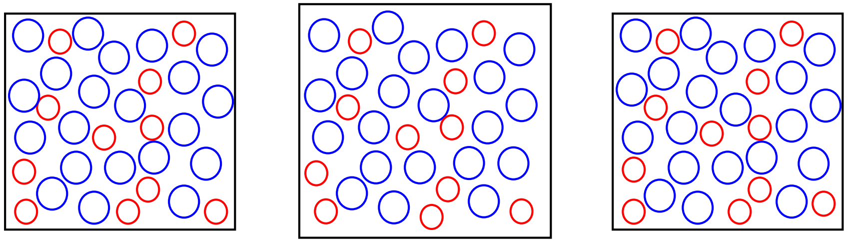
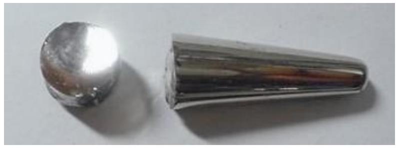


N. V. Priezjev, The potential energy states and mechanical properties of thermally cycled binary glasses (2019). Preprint: cond-mat/1810.10877

N. V. Priezjev, The effect of cryogenic thermal cycling on aging, rejuvenation, and mechanical properties of metallic glasses, *J. Non-Cryst. Solids* **503-504**, 131-138 (2019).

Thermal treatment and mechanical cycling of metallic glasses

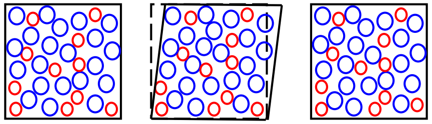
Metallic glasses: mechanical properties include high strength and low ductility



Sun, Concustell, and Greer, Thermomechanical processing of metallic glasses: extending the range of the glassy state, *Nature Reviews Materials* **1**, 16039 (2016).

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



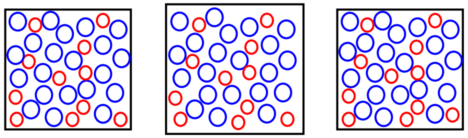
"Mechanical annealing" during sub-yield cycling

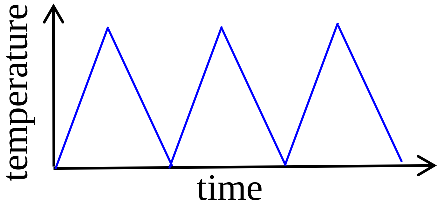
Candelier, Dauchot, and Biroli, Dynamical heterogeneity in the cyclic shear experiment on dense 2D granular media, *Phys. Rev. Lett.* **102**, 088001 (2009).

Knowlton, Pine, and Cipelletti, A microscopic view of the yielding transition in concentrated emulsions, *Soft Matter* **10**, 6931 (2014).

Priezjev, The yielding transition in periodically sheared binary glasses at finite temperature, *Comput. Mater. Sci.* **150**, 162 (2018).

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





Ketov, Sun, Nachum, Lu, Checchi, Beraldin, Bai, Wang, Louzguine-Luzgin, Carpenter, and Greer, Rejuvenation of metallic glasses by non-affine thermal strain, *Nature* **524**, 200 (2015).

Shang, Guan, and Barrat, Role of thermal expansion heterogeneity in the cryogenic rejuvenation of metallic glasses, *J. Phys.: Mater.* **1**, 015001 (2018).

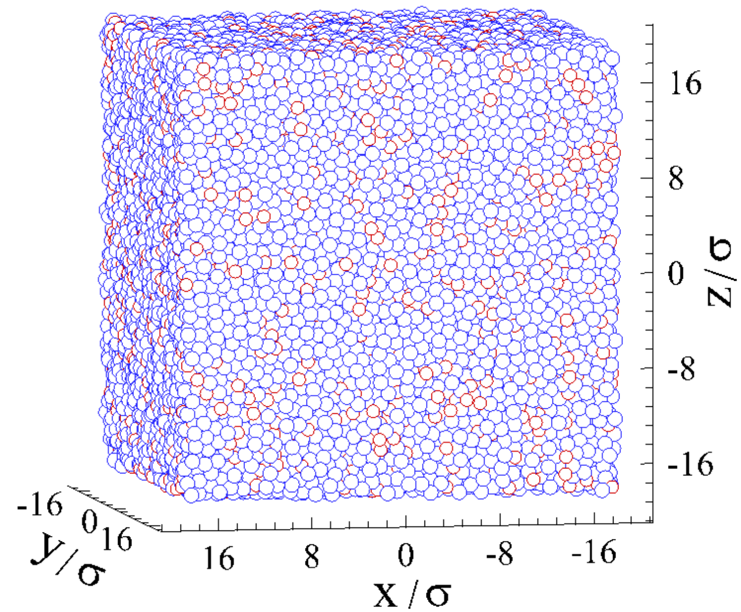
Priezjev, The effect of cryogenic thermal cycling on aging, rejuvenation, and mechanical properties of metallic glasses, *J. Non-Cryst. Solids* **503-504**, 131 (2019).

Details of molecular dynamics simulations and parameter values

Binary Lennard-Jones Kob-Andersen mixture:

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

$Ni_{80}P_{20}$



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

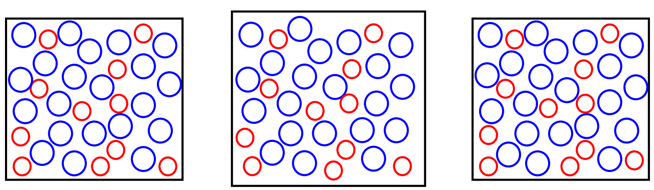
$\varepsilon_{AA} = 1.0, \varepsilon_{AB} = 1.5, \ \varepsilon_{BB} = 0.5, m_A = m_B$

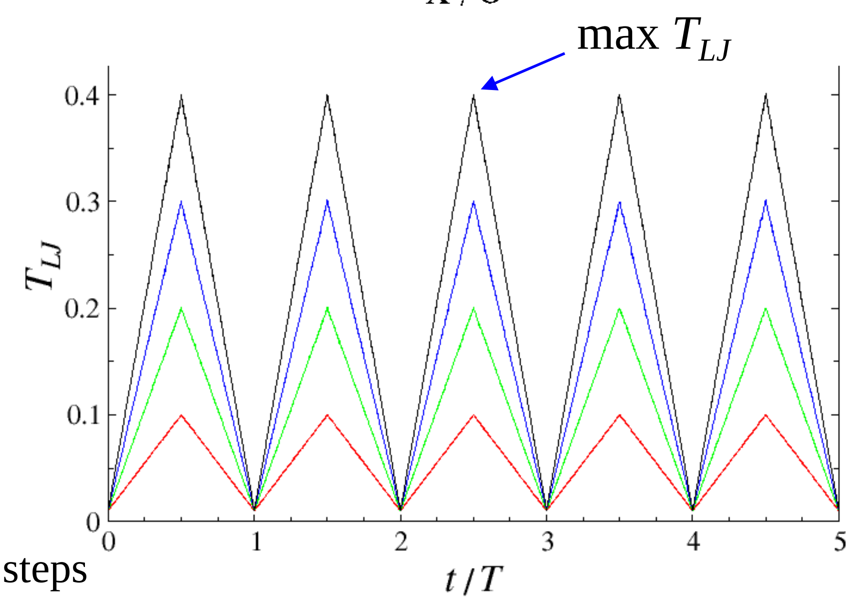
$\sigma_{AA} = 1.0, \sigma_{AB} = 0.8, \ \sigma_{BB} = 0.88$

Temperature: T_{LJ} = 0.01 ε / k_B < T_g = 0.435 ε / k_B

LAMMPS: N_p = 60000, MD step Δt_{MD}= 0.005τ

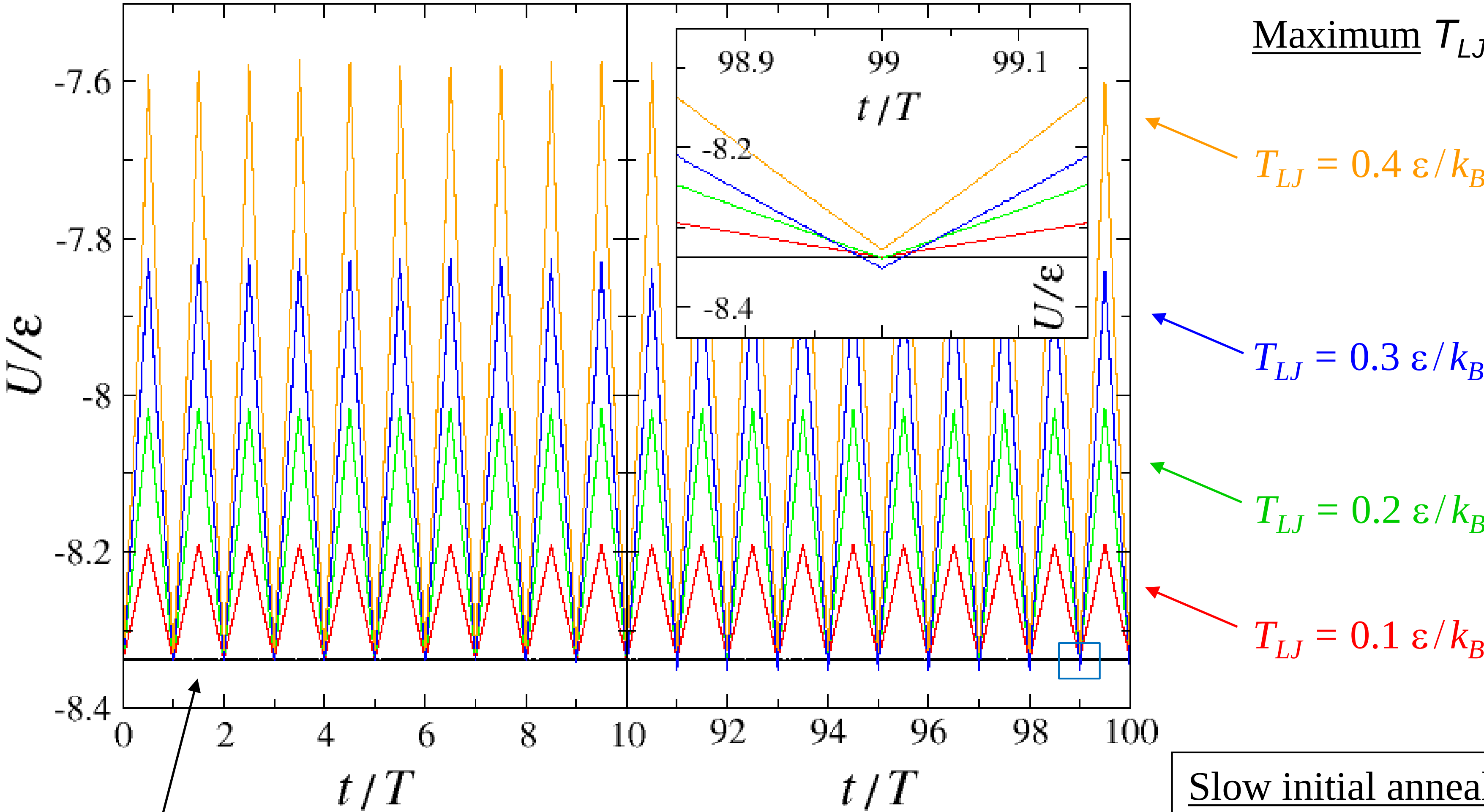
Initial quench rates: 10^{-2} $\varepsilon / k_B\tau$ to 10^{-5} $\varepsilon / k_B\tau$





Pressure P = 0 and thermal period T = 5000τ = 10^6 MD steps

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



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

Aging at constant temperature: T_{LJ} = 0.01 ε/k_B

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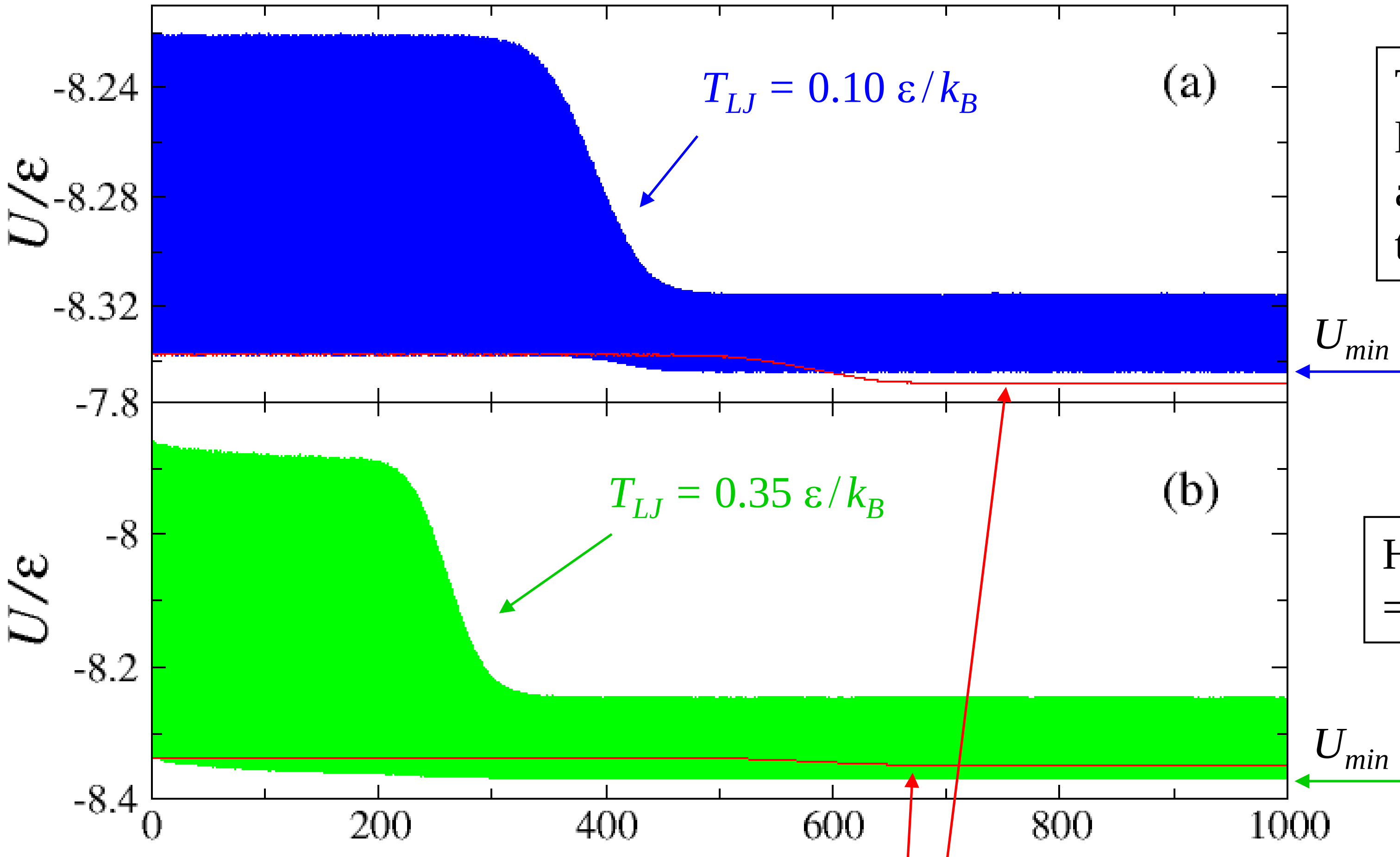
Potential energy U during 1000 thermal cycles for different maximum T_{LJ}



Transition to low U states after few 100 thermal cycles

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

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

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

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

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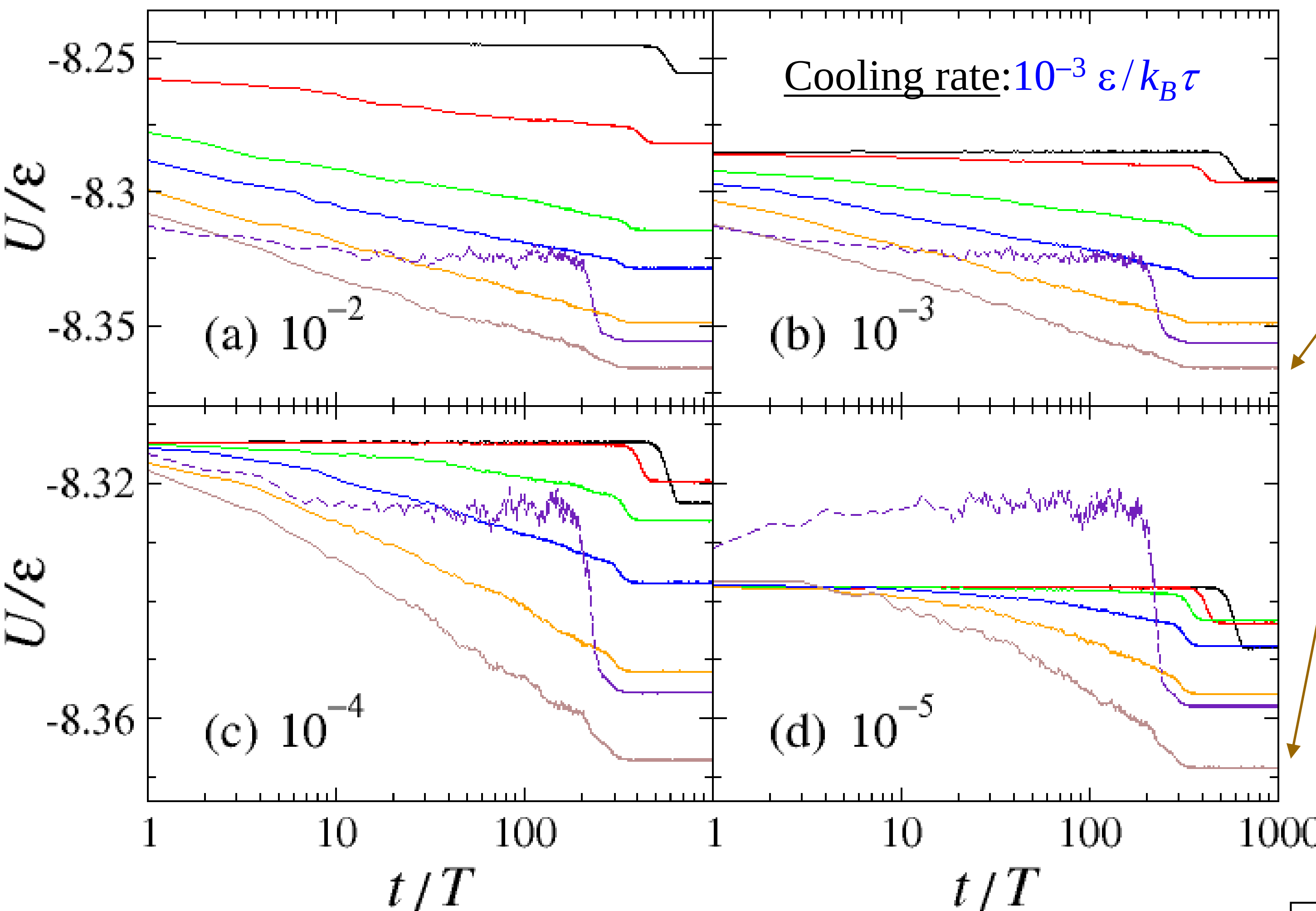
Potential energy minima during 1000 thermal cycles for different max T_{LJ}

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



maximum T_{LJ}

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

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

$T_{LJ} = 0.3\ \varepsilon/k_B$

$T_{LJ} = 0.25\ \varepsilon/k_B$

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

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

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

Lowest U_{min} at max $T_{LJ} = 0.35\ \varepsilon/k_B$

Configurations of atoms with large nonaffine displacements after 1 cycle

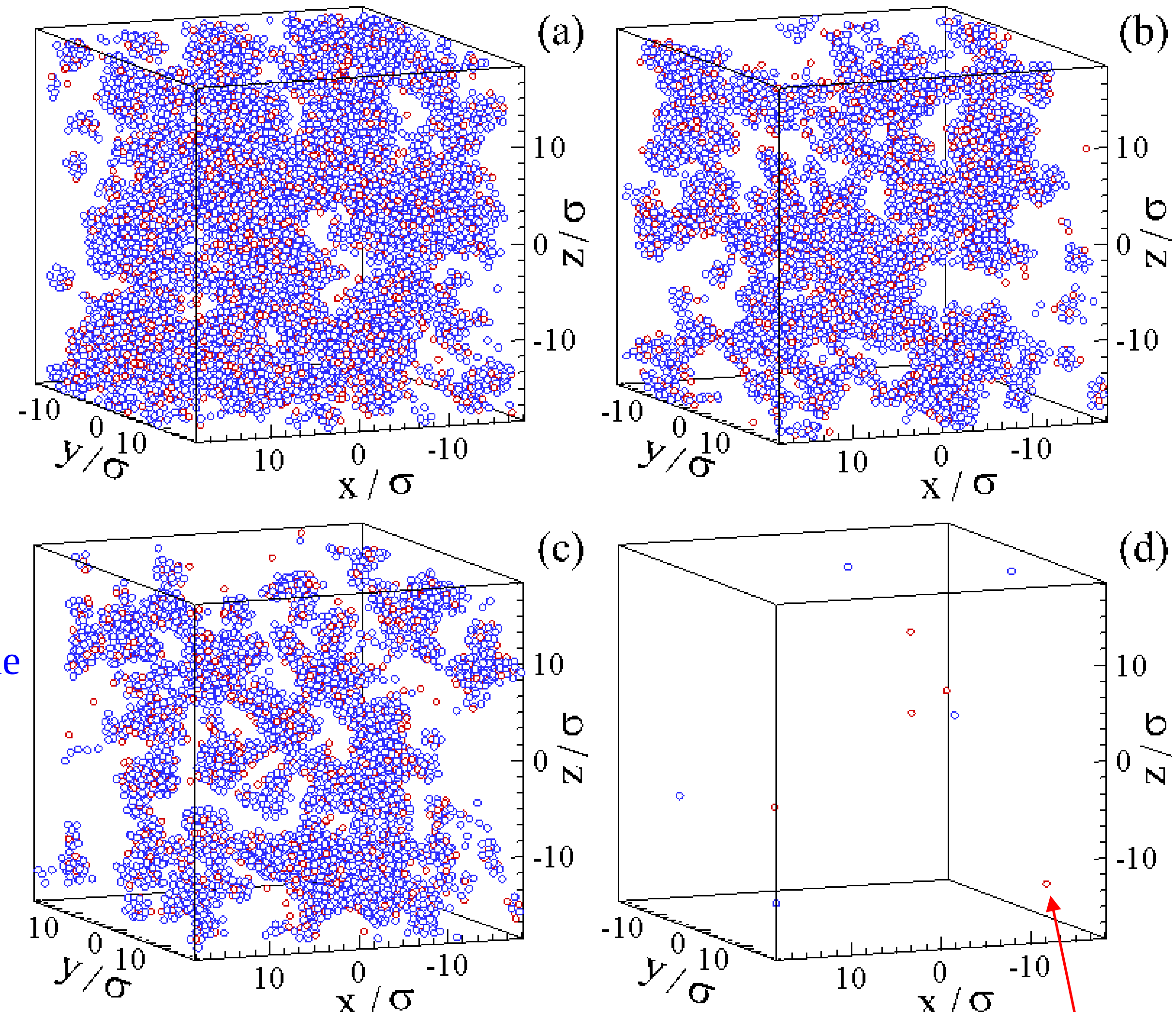
$$D^2(t,T) > 0.04\,\sigma^2$$

max T_{LJ} **= 0.35** ε/k_B

After 1-st cycle

After 100-th cycle

Large clusters of atoms with large nonaffine displacements



After 200-th cycle

After 1000-th cycle

Nearly reversible particle dynamics

B small atom type

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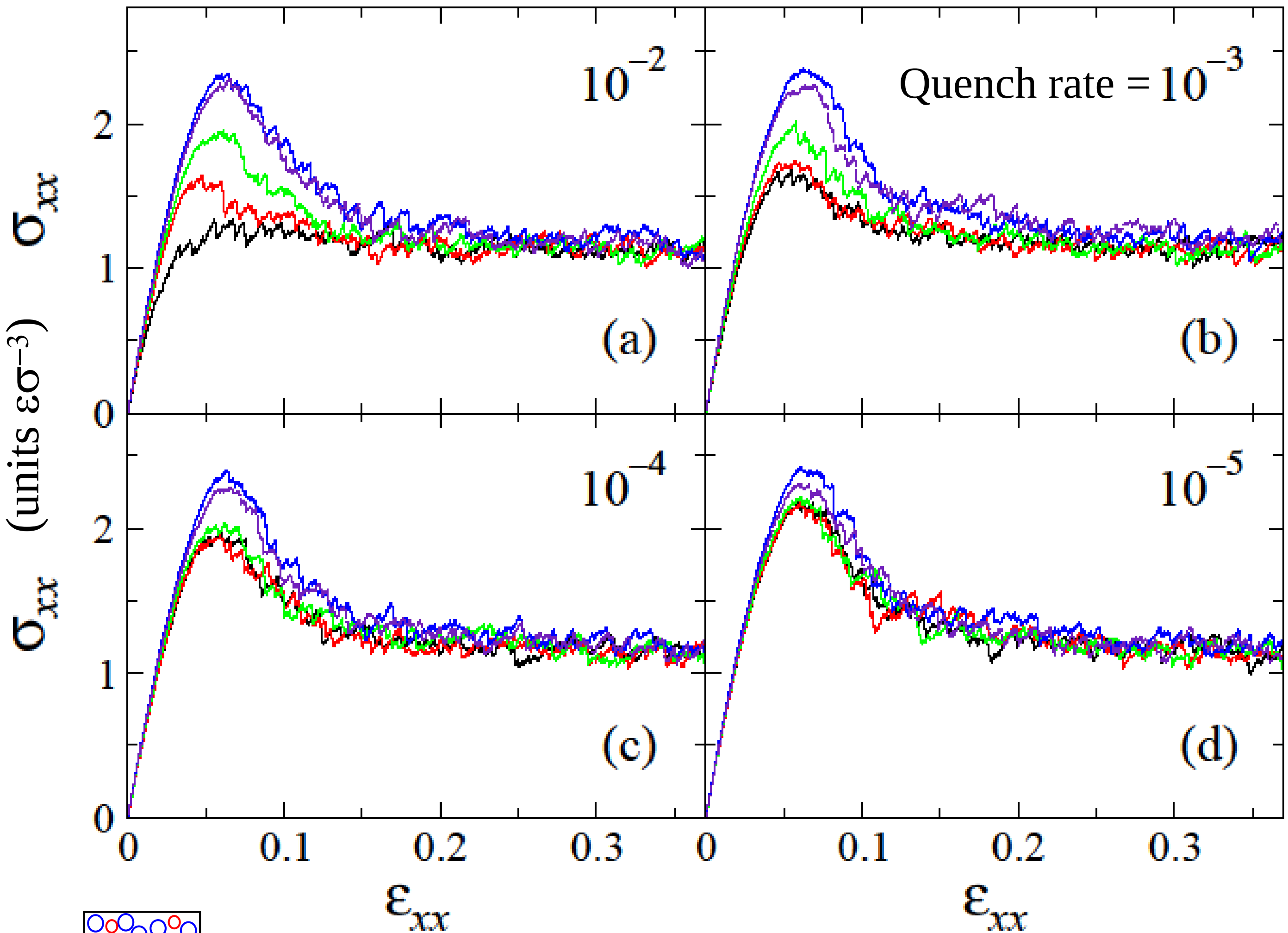
Slow initial quench rate: $10^{-5}\ \varepsilon/k_B\tau$

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



maximum T_{LJ}

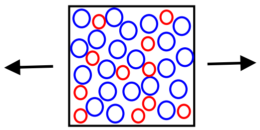
$T_{LJ} = 0.4\ \varepsilon/k_B$

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

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

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

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

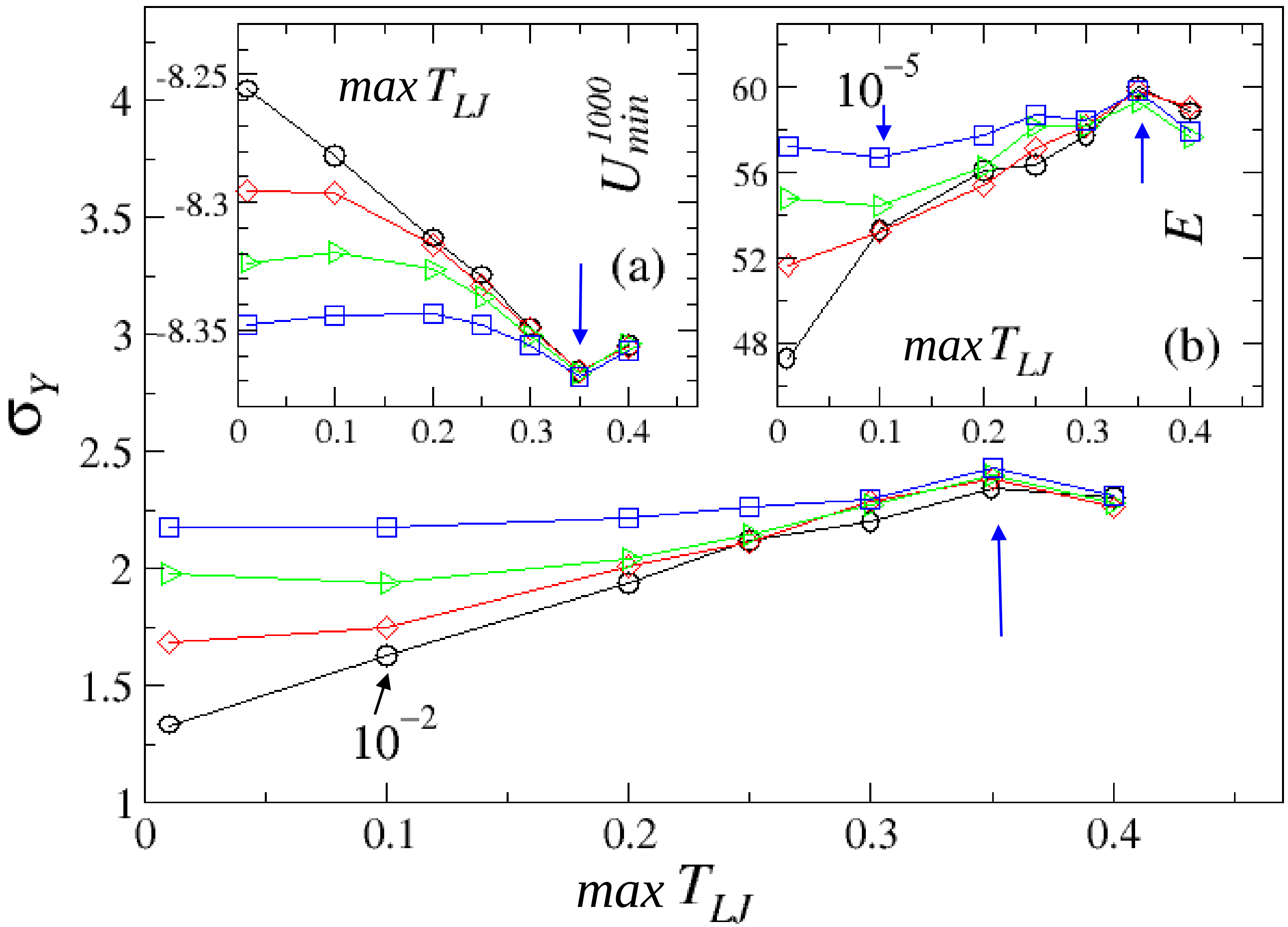


Strain rate = $10^{-5}\ 1/\tau$

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 σ_Y, the elastic modulus E, and U_{min} versus maximum T_{LJ}



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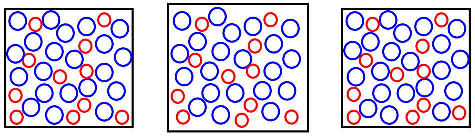
Highest yield peak and elastic modulus after thermal loading with maximum $T_{LJ} = 0.35\ \varepsilon/k_B$

A correlation between U_{min} and maximum values of σ_Y and E.

Conclusions:



1000 cycles

- 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.

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Q.-L. Liu and N. V. Priezjev, "The influence of complex thermal treatment on mechanical properties of amorphous materials", *Computational Materials Science* **161**, 93-98 (2019).

N. V. Priezjev, The effect of cryogenic thermal cycling on aging, rejuvenation, and mechanical properties of metallic glasses, *Journal of Non-Crystalline Solids* **503-504**, 131-138 (2019).