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

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Movies, preprints @
http://www.wright.edu/~nikolai.priezjev/
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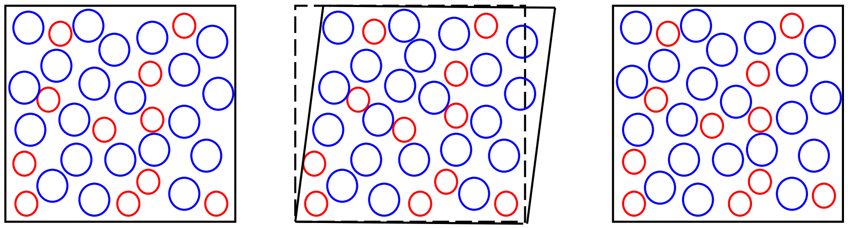


N. V. Priezjev, Accelerated relaxation in disordered solids under cyclic loading with alternating shear orientation, *J. Non-Cryst. Solids* **525**, 119683 (2019).

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

Outline

- Brief introduction (metallic glasses, amorphous structure, mechanical properties, etc)
- Part I: Cyclic loading with alternating shear orientation ("*mechanical annealing*")

  N. V. Priezjev, Accelerated relaxation in disordered solids under cyclic loading with alternating shear orientation, *J. Non-Cryst. Solids* **525**, 119683 (2019).

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

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

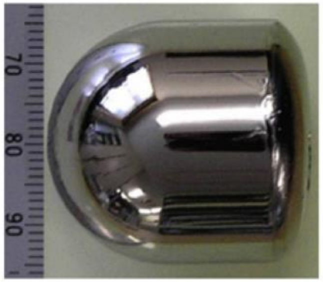
- Part III: Aging and rejuvenation during elastostatic loading of amorphous alloys

  N. V. Priezjev, Aging and rejuvenation during elastostatic loading of amorphous alloys: A molecular dynamics simulation study, *Comput. Mater. Sci.* **168**, 125 (2019).

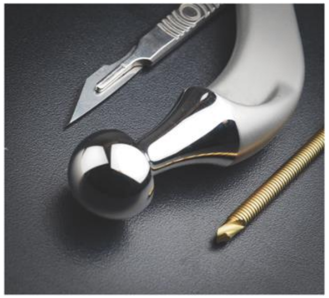
- Conclusions

Amorphous structure, dynamical heterogeneity, and shear transformations

Metallic glasses: multicomponent alloys; high strength and elastic limit but low ductility



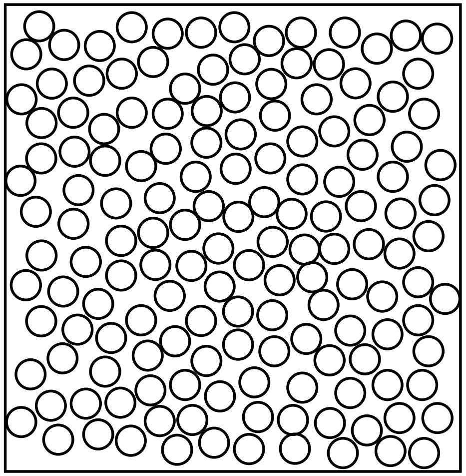
Cu-Zr-Al-Ag; ~30mm
Inoue & Takeuchi (2011)



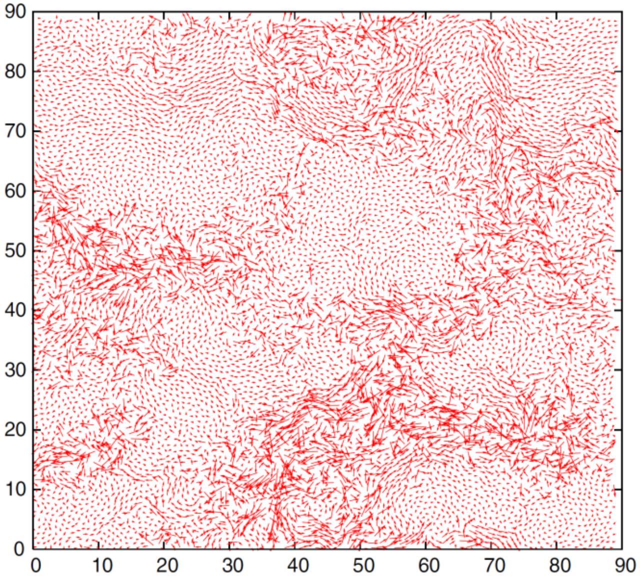
Biocompatible: Implantable medical devices and surgical tools (Mg-based)

Wear, corrosion resistant

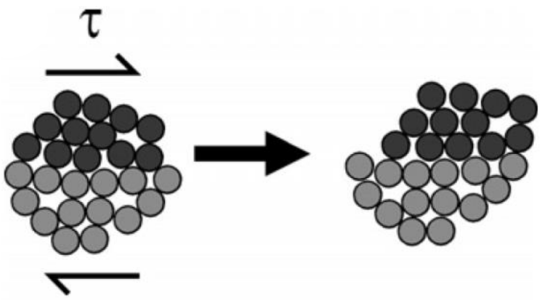
Sporting goods: *e.g.*, golf clubs



Disordered structure; no long-range order



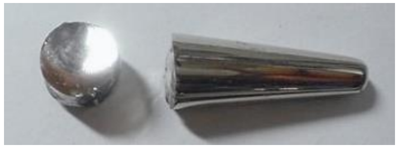
Spatial map of single-particle displacements, Berthier & Biroli (2011)



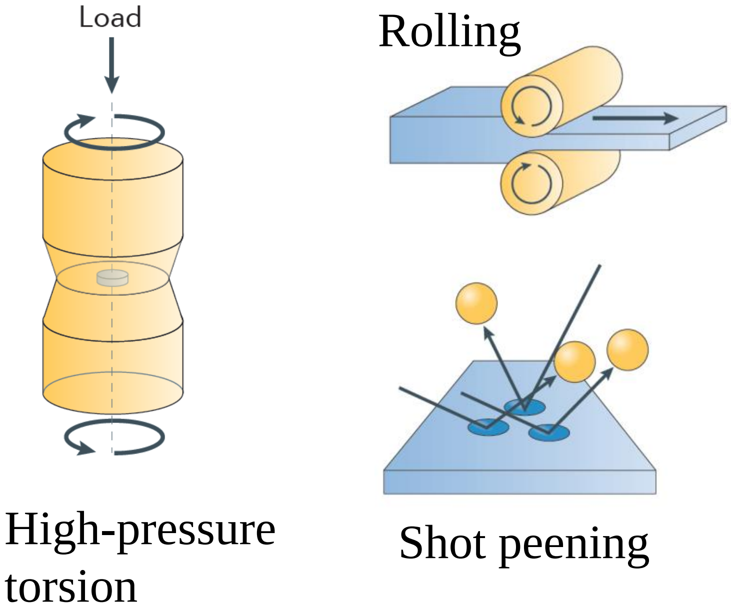
Localized shear transformations Spaepen (1977) & Argon (1979)

Thermomechanical processing: Structural relaxation and rejuvenation

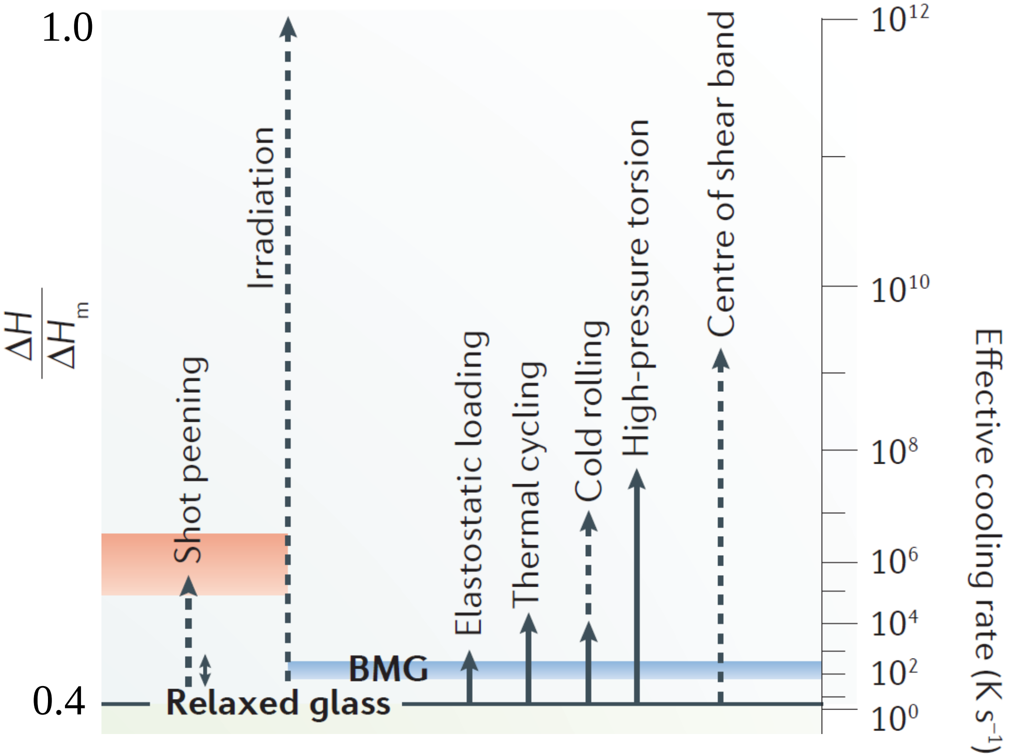
Metallic glasses: mechanical properties include high strength and low ductility (brittle)

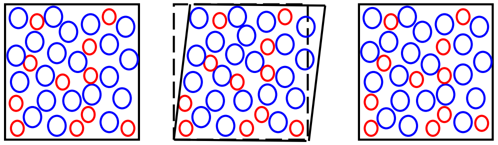


Sun, Concustell, and Greer, Thermomechanical processing of metallic glasses: extending the range of the glassy state, *Nature Reviews Materials* **1**, 16039 (2016).



Rejuvenation: increase in stored energy

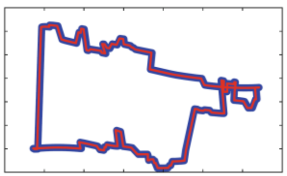




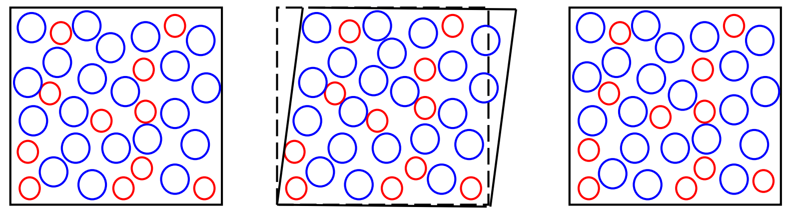
Relaxation: (1) cyclic loading or *"mechanical annealing"*, (2) ultrastable glasses by deposition

Part I: Cyclic loading with alternating shear orientation
(*“mechanical annealing”*)

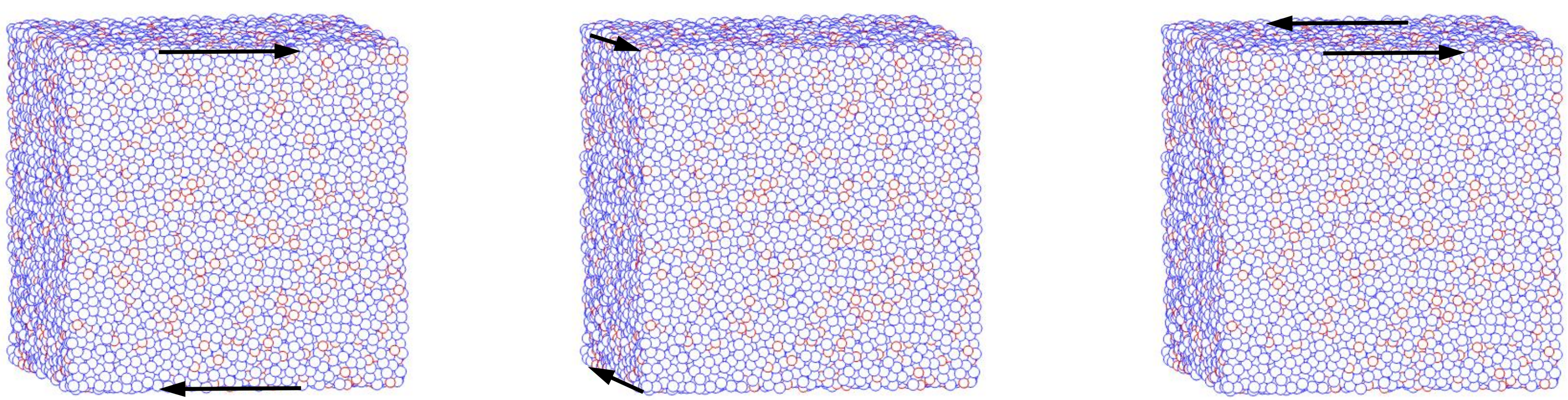
2 cycles at T=0



Regev *et al.* 2015



Periodic shear; one plane
Priezjev *JNCS* (2018)
Sastry *et al.* (2017)



N. V. Priezjev, Accelerated relaxation in disordered solids under cyclic loading with alternating shear orientation, *J. Non-Cryst. Solids* **525**, 119683 (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:

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

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

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

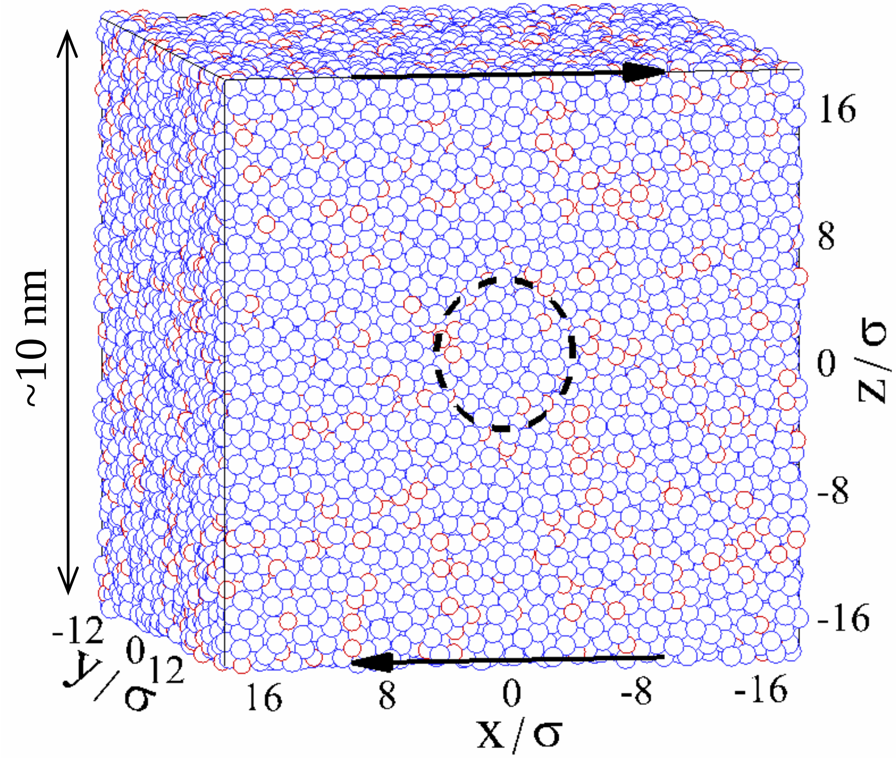
LAMMPS, Nose-Hoover thermostat, $\Delta t_{MD} = 0.005\,\tau$

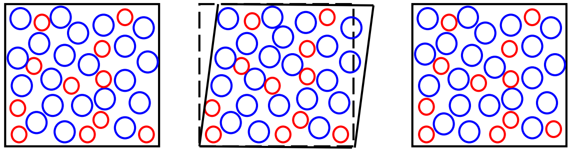
Fast annealing rate: $10^{-2}\ \varepsilon/k_B\tau$ (**poorly annealed glass**)

higher energy sample

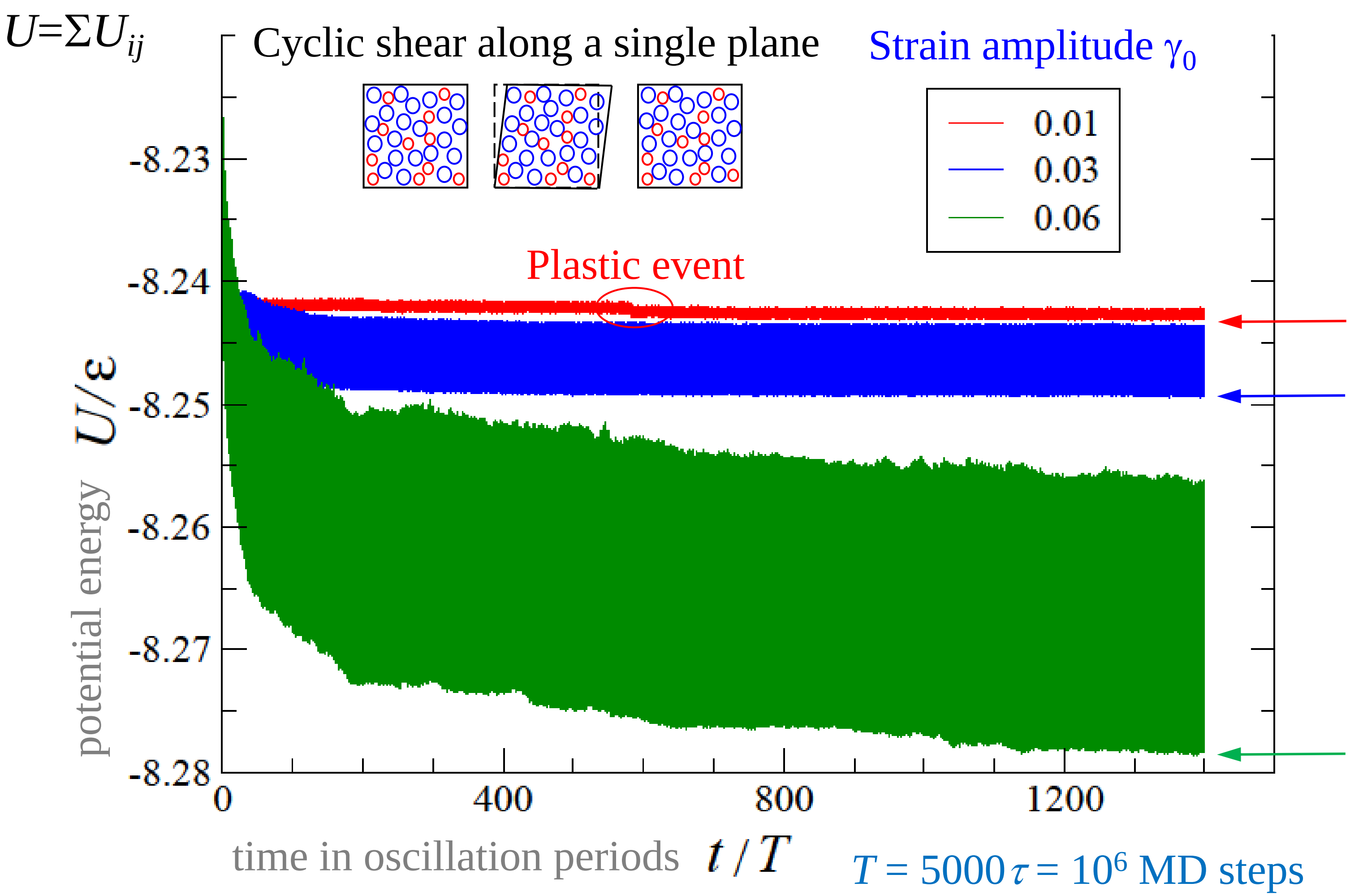
Oscillatory shear strain: $\gamma(t) = \gamma_0 \sin(\omega t)$

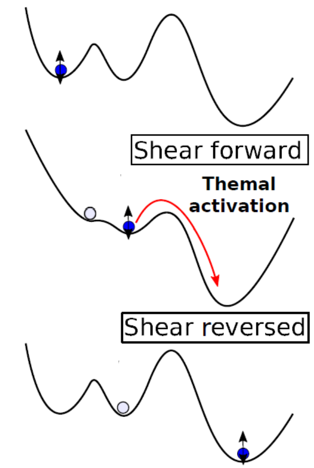
Oscillation period: $T = 2\pi/\omega = 5000\,\tau$





Potential energy per particle U during 1400 oscillation cycles for different γ_0





Energy minima (at zero strain)

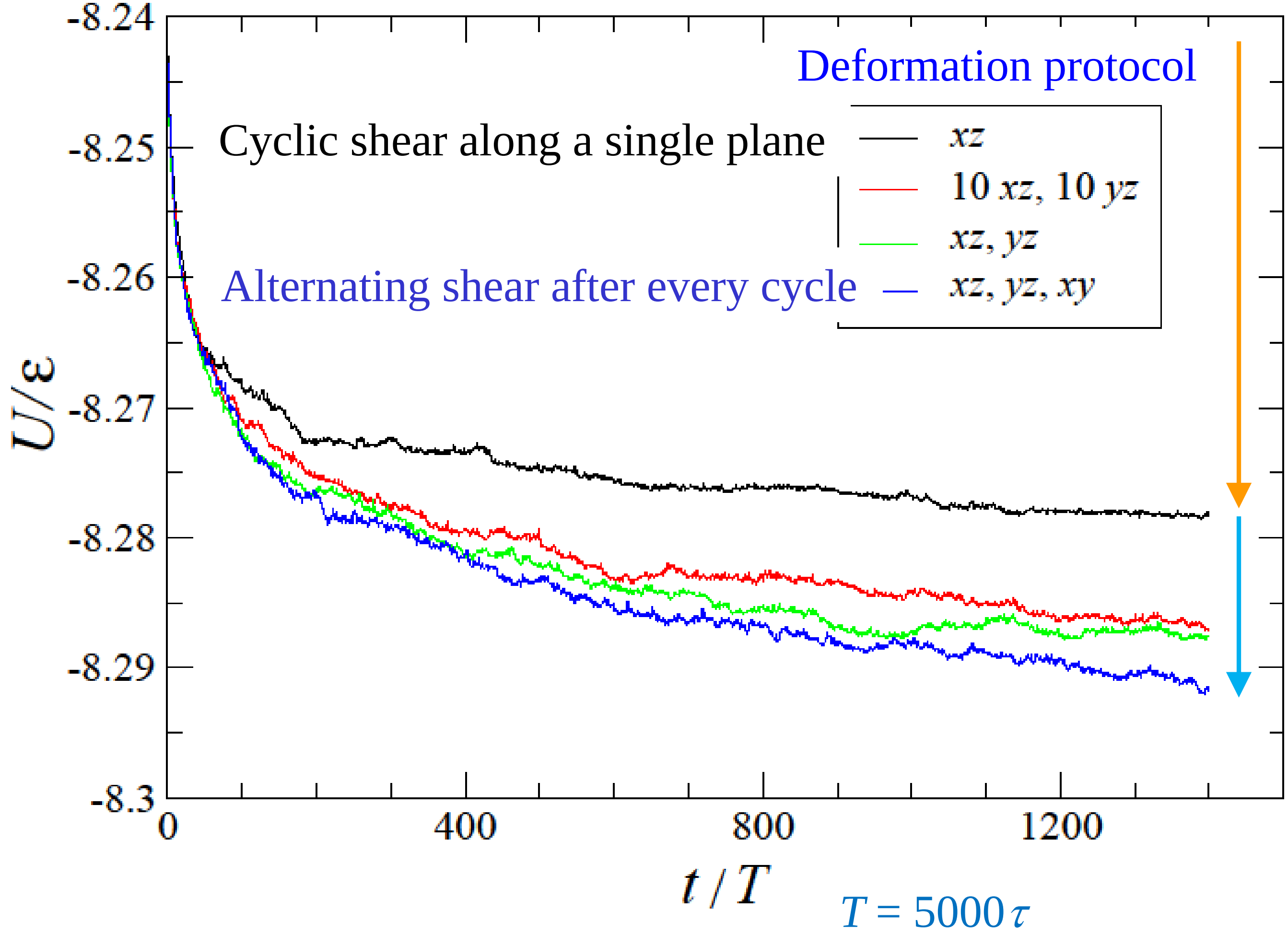
$T = 5000\,\tau = 10^6$ MD steps

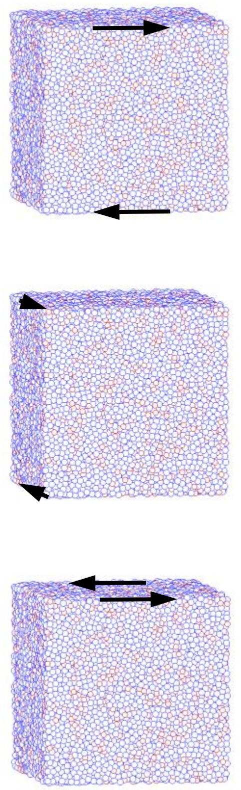
~ 900h 40prcs

With increasing strain amplitude γ_0 (below yield strain), the system relocates to deeper energy minima (via collective rearrangements of atoms).

Priezjev, *J. Non-Cryst. Solids* (2019)

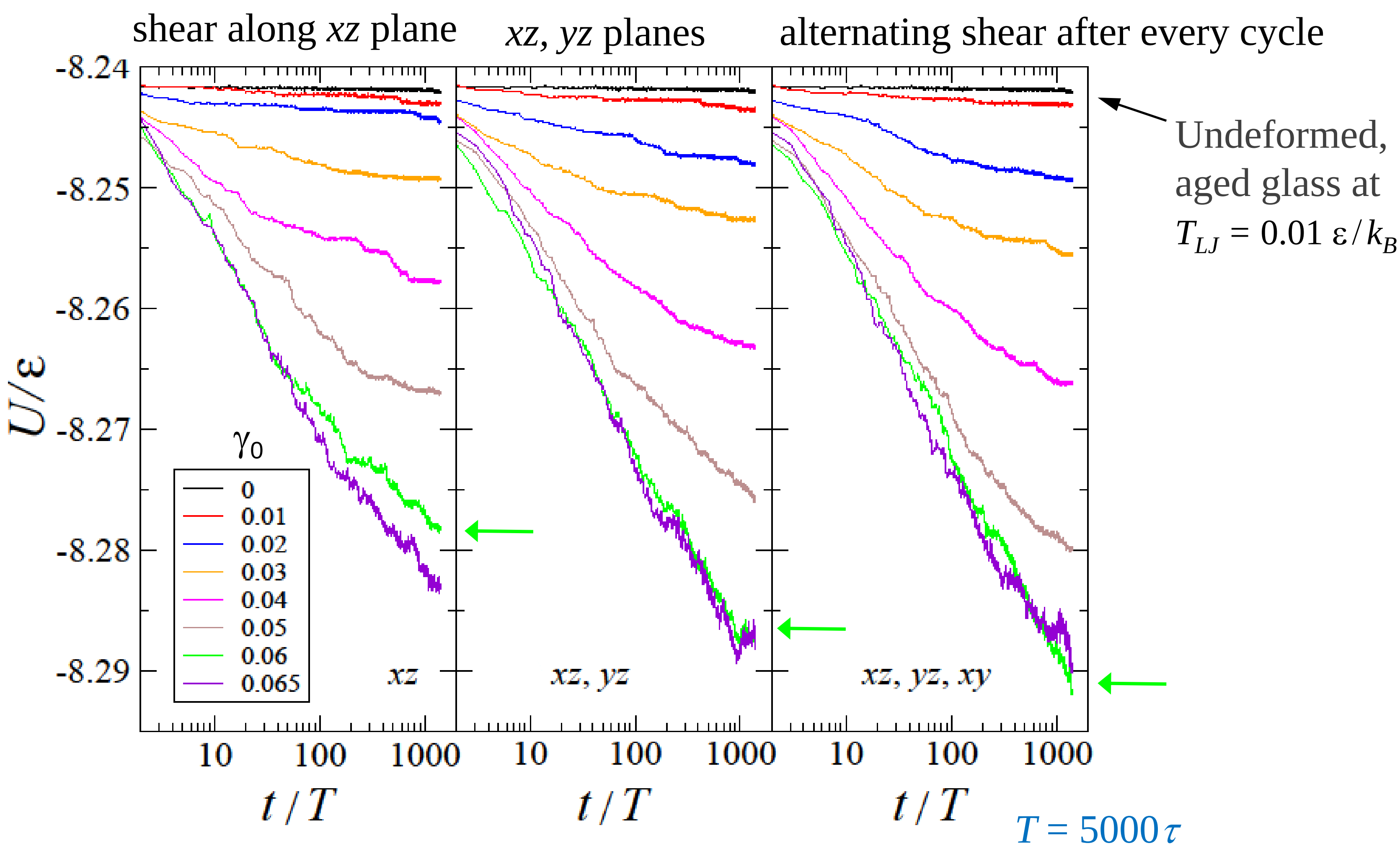
Potential energy minima during 4 different deformation protocols for $\gamma_0 = 0.06$





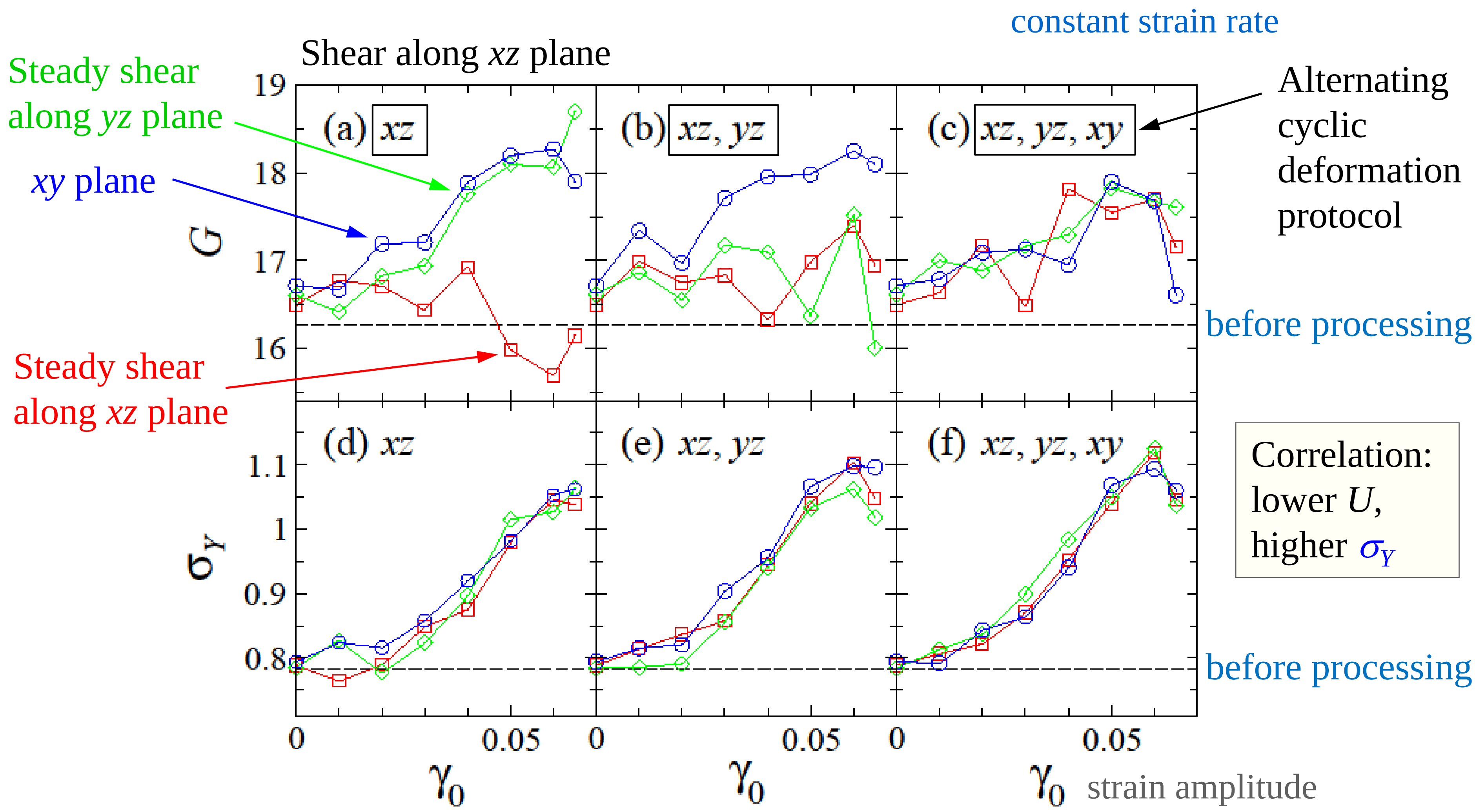
For the strain amplitude $\gamma_0 = 0.06$ (just below yield strain), each additional alternation of the shear orientation in the deformation protocol results in lower energy states.

The potential energy U during 3 deformation protocols for the indicated γ_0



For strain amplitudes γ_0 (below yield strain), each additional alternation of the shear orientation in the deformation protocol results in lower energy states.

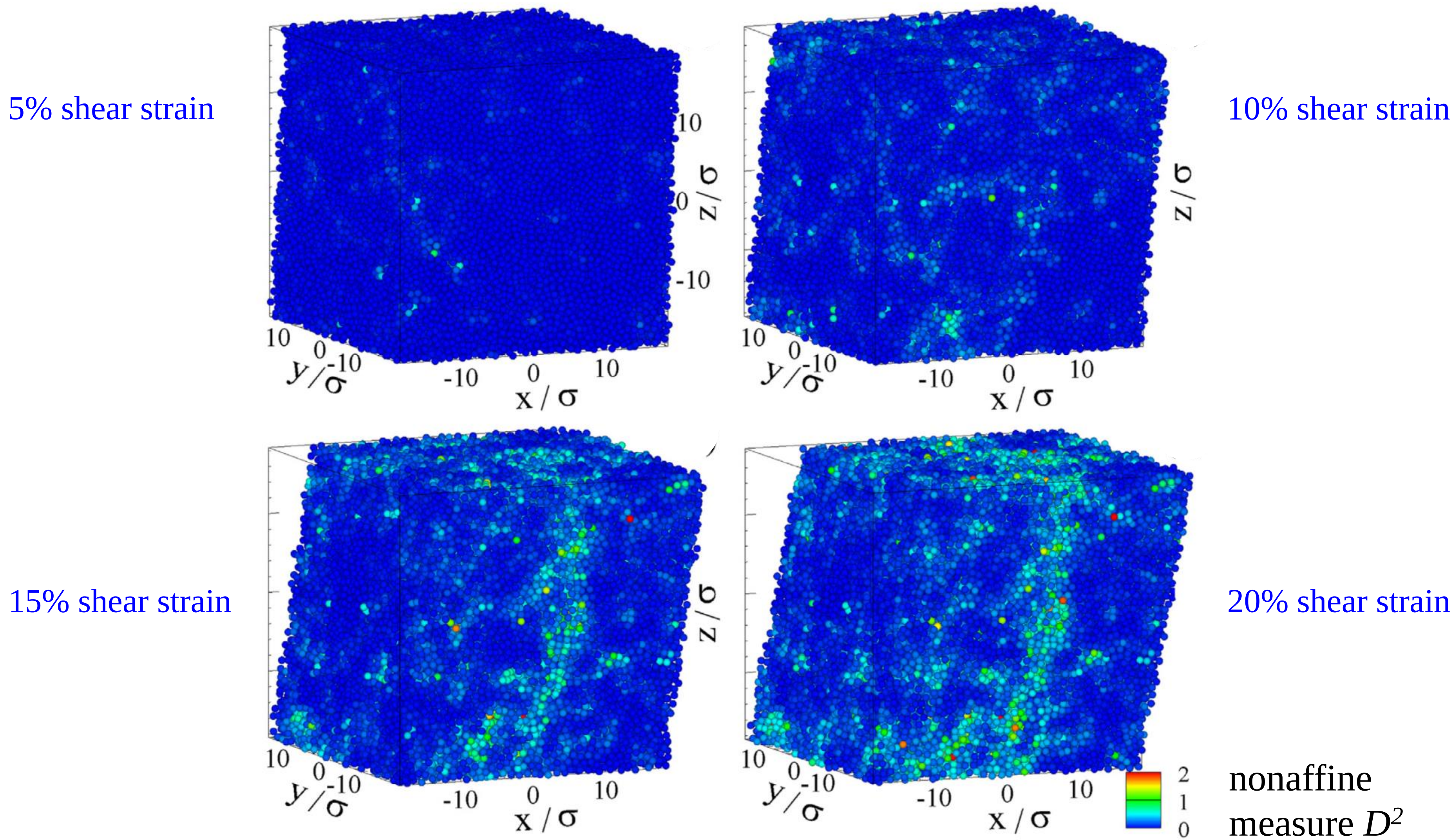
Shear modulus G and yielding peak σ_Y during startup shear deformation



The height of the yielding peak σ_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.

Priezjev, *J. Non-Cryst. Solids* (2019)

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



N. V. Priezjev, *J. Non-Cryst. Solids* **525**, 119683 (2019).

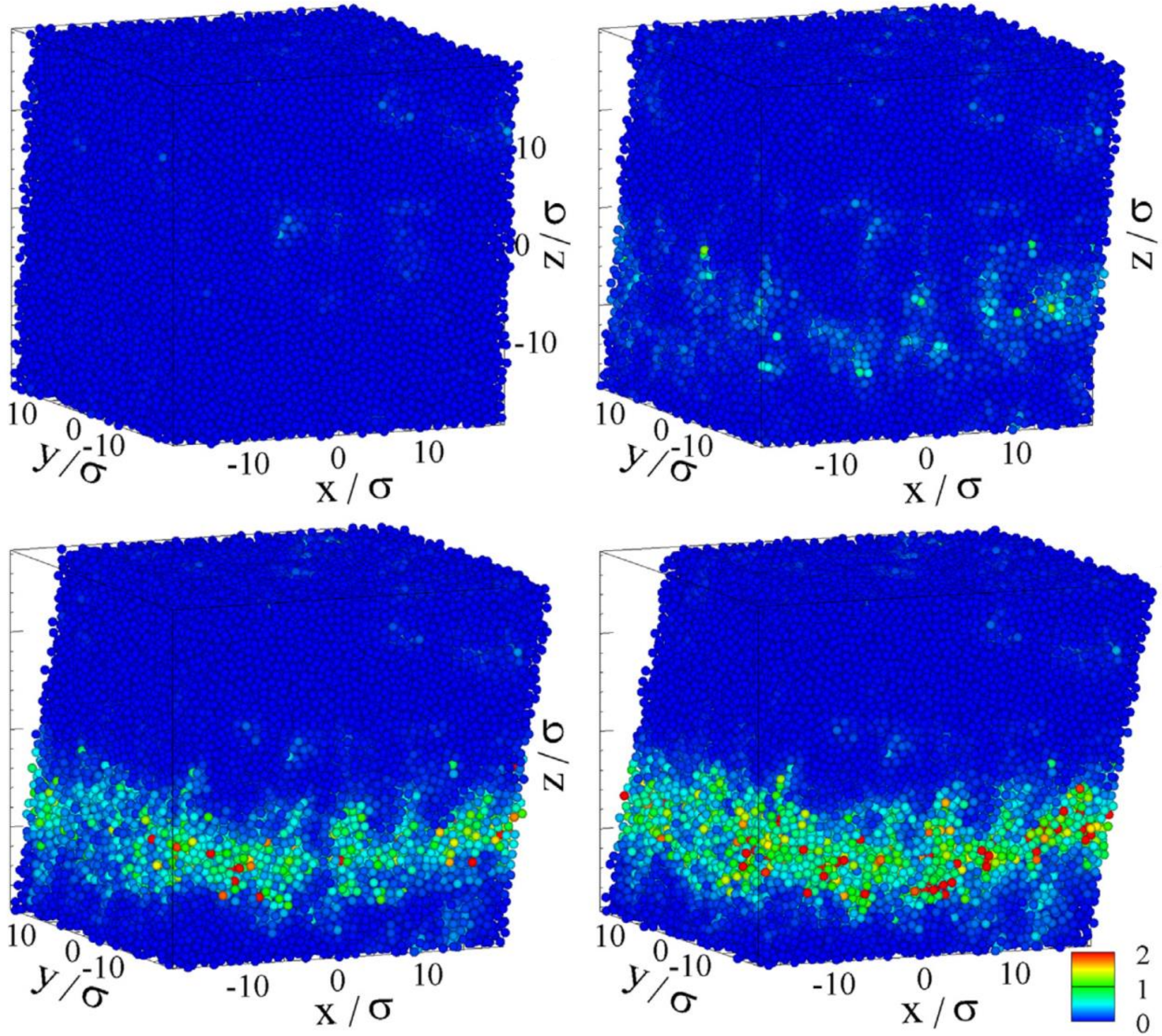
Snapshots of strained glass after 1400 alternating shear cycles (*xz, yz, xy*)

5% shear strain

10% shear strain

15% shear strain

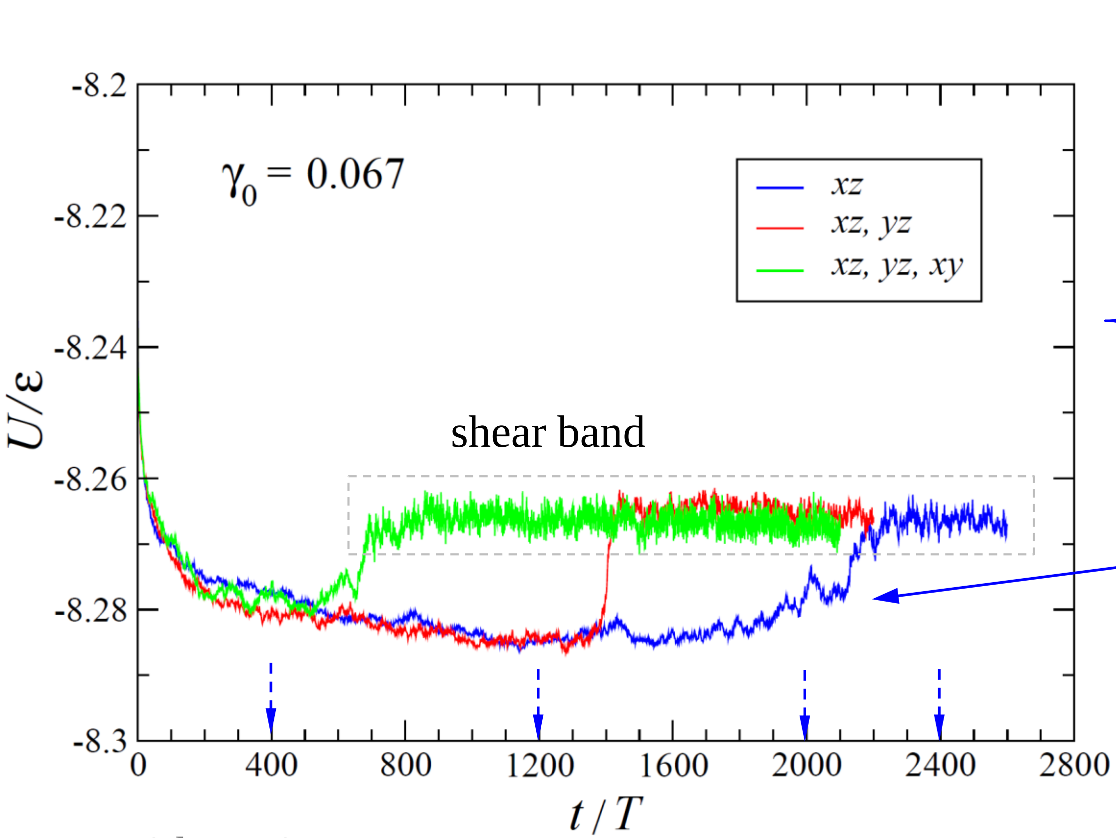
20% shear strain

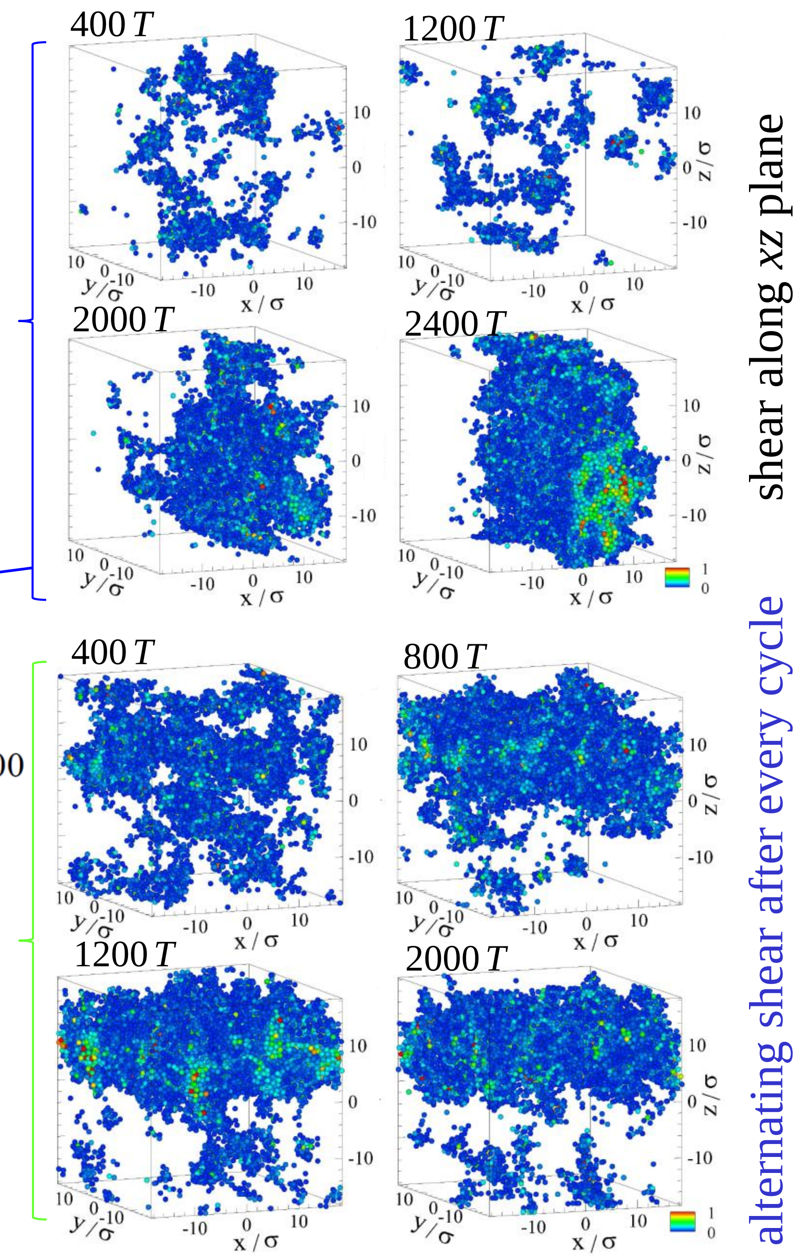


nonaffine measure D^2

N. V. Priezjev, *J. Non-Cryst. Solids* **525**, 119683 (2019).

Yielding transition and shear band at the critical strain amplitude γ_0=0.067



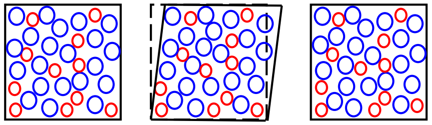


~ 70days 40prcs

Alternating shear orientation facilitates yielding but the critical strain amplitude remains unchanged for different deformation protocols.

N.V. Priezjev, arXiv:2001.06853 (2020)

Conclusions:



2400 shear cycles

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

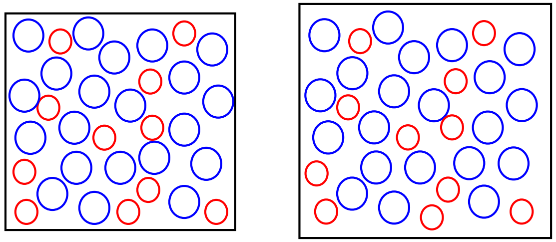
- For a fixed strain amplitude (below yield strain), each additional alternation of the shear orientation in the deformation protocol results in lower energy states.

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

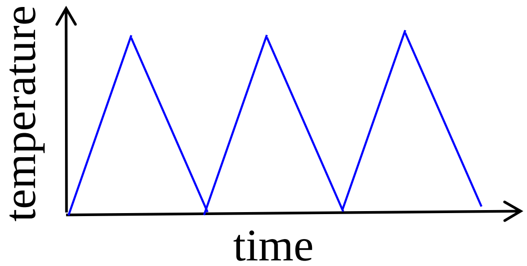
- The shear modulus is larger along the shear directions that were not cyclically loaded.

N. V. Priezjev, Accelerated relaxation in disordered solids under cyclic loading with alternating shear orientation, *J. Non-Cryst. Solids* **525**, 119683 (2019).

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



100 thermal cycles



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).

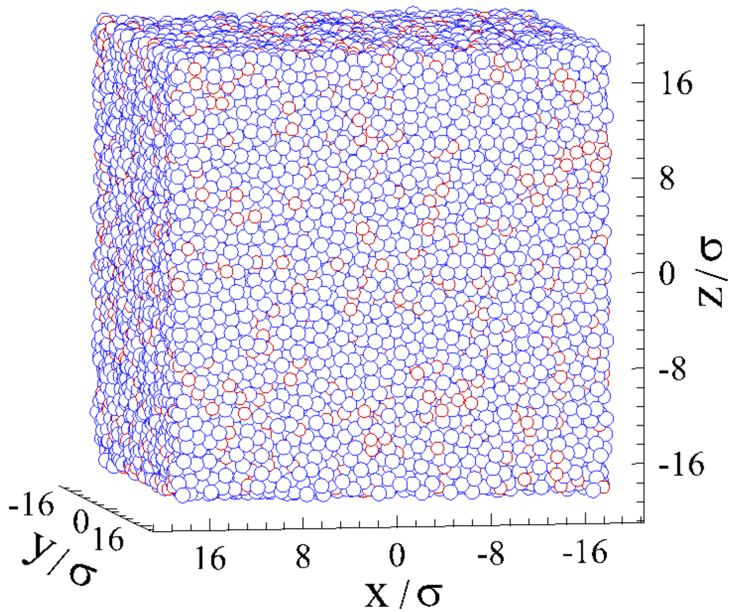
Priezjev, The effect of cryogenic thermal cycling on aging, rejuvenation, and mechanical properties of metallic glasses, *J. Non-Cryst. Solids* **503**, 131 (2019).

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:

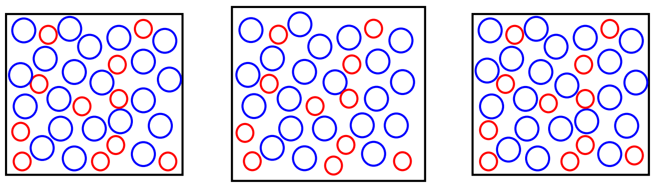
$\varepsilon_{AA} = 1.0, \varepsilon_{AB} = 1.5, \ \varepsilon_{BB} = 0.5, m_A = m_B$

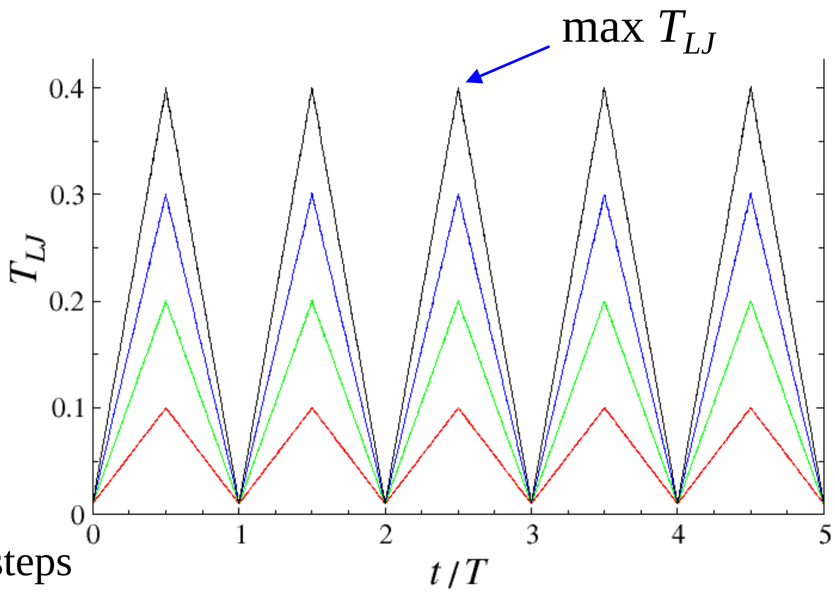
$\sigma_{AA} = 1.0, \sigma_{AB} = 0.8, \ \sigma_{BB} = 0.88$

Temperature: $T_{LJ} = 0.01\ \varepsilon/k_B < T_g \approx 0.35\ \varepsilon/k_B$

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

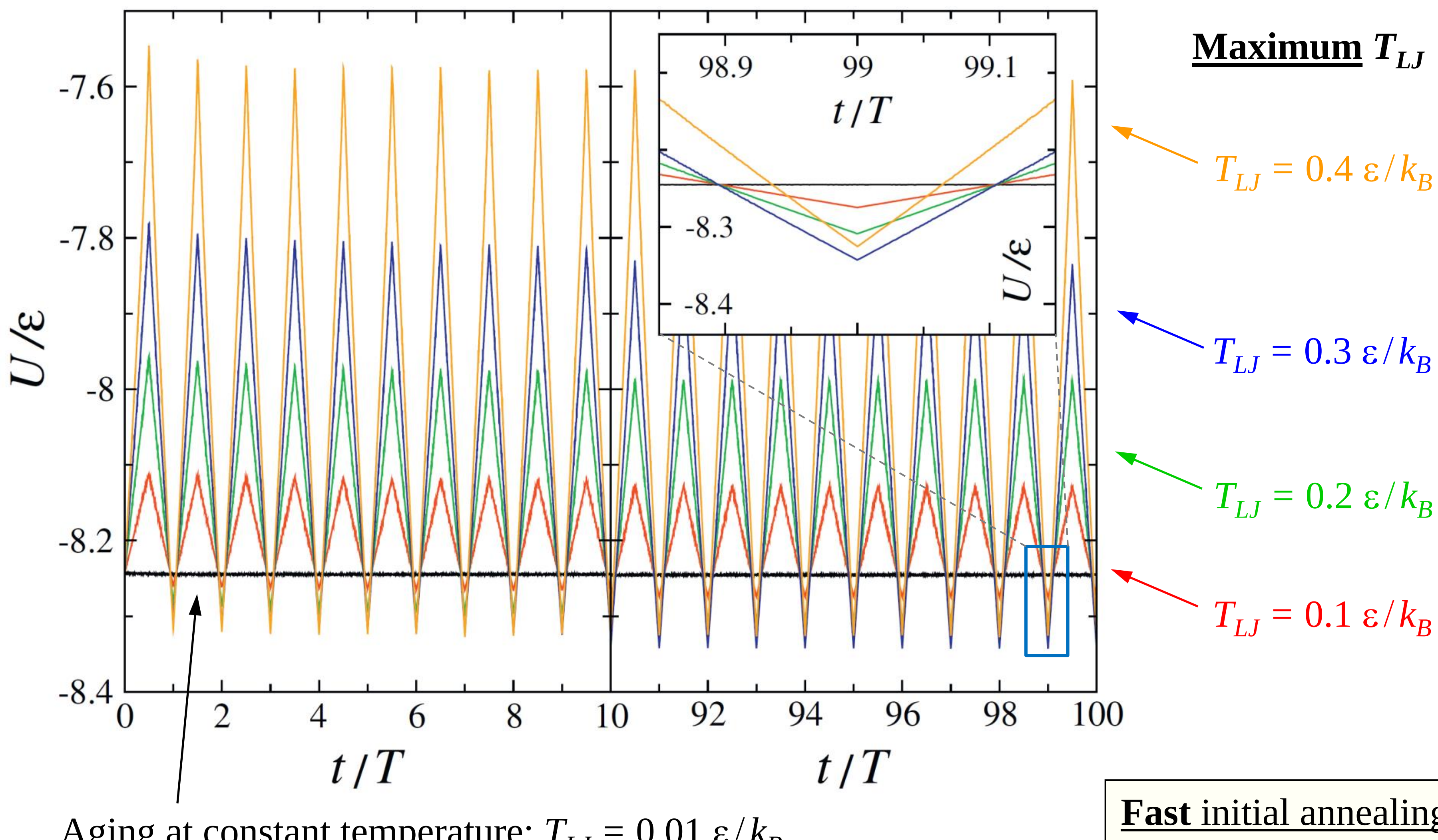
Initial quench rates: $10^{-2}\ \varepsilon/k_B\tau$ to $10^{-5}\ \varepsilon/k_B\tau$





Pressure $P = 0$ and thermal period $T = 5000\tau = 10^6$ MD steps

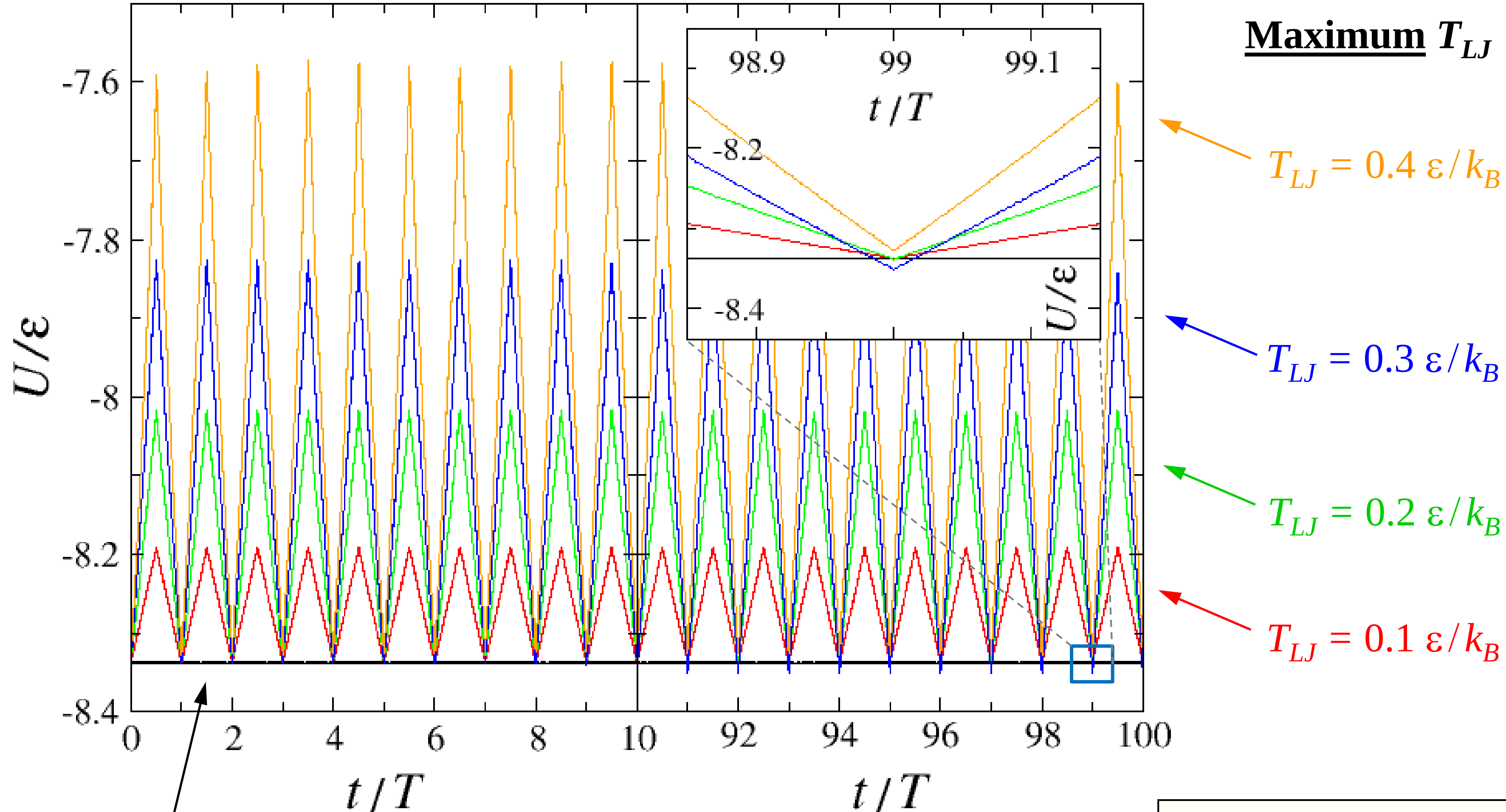
Potential energy per atom during 100 thermal cycles for different max T_{LJ}



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

N. V. Priezjev, *J. Non-Cryst. Solids* **503**, 131 (2019).

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

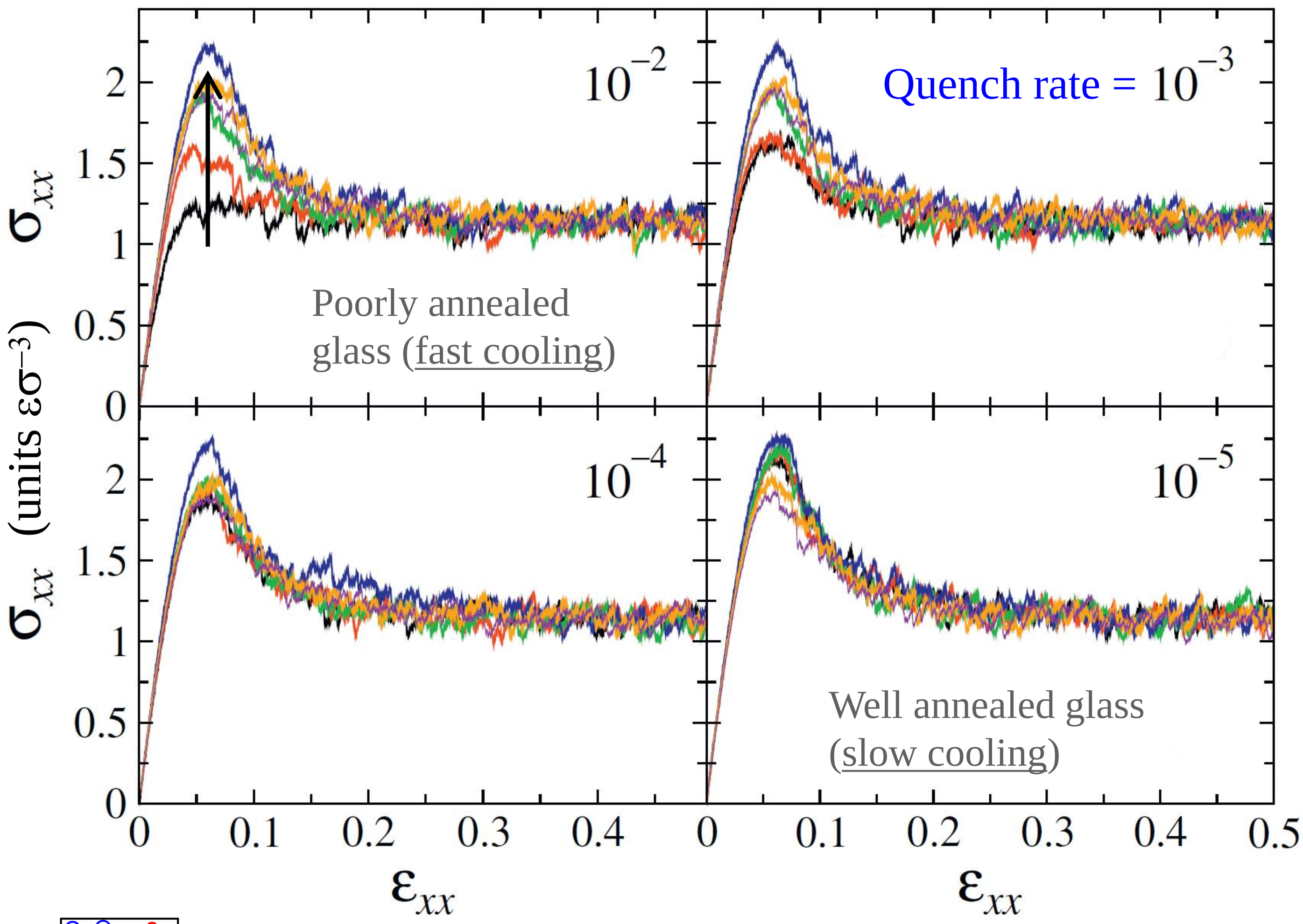


Aging at constant temperature: $T_{LJ} = 0.01\ \varepsilon/k_B$

N. V. Priezjev, *J. Non-Cryst. Solids* **503**, 131 (2019).

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}



Maximum T_{LJ}

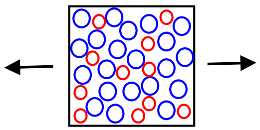
$T_{LJ} = 0.4\ \varepsilon/k_B$

$T_{LJ} = 0.30\ \varepsilon/k_B$

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

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

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

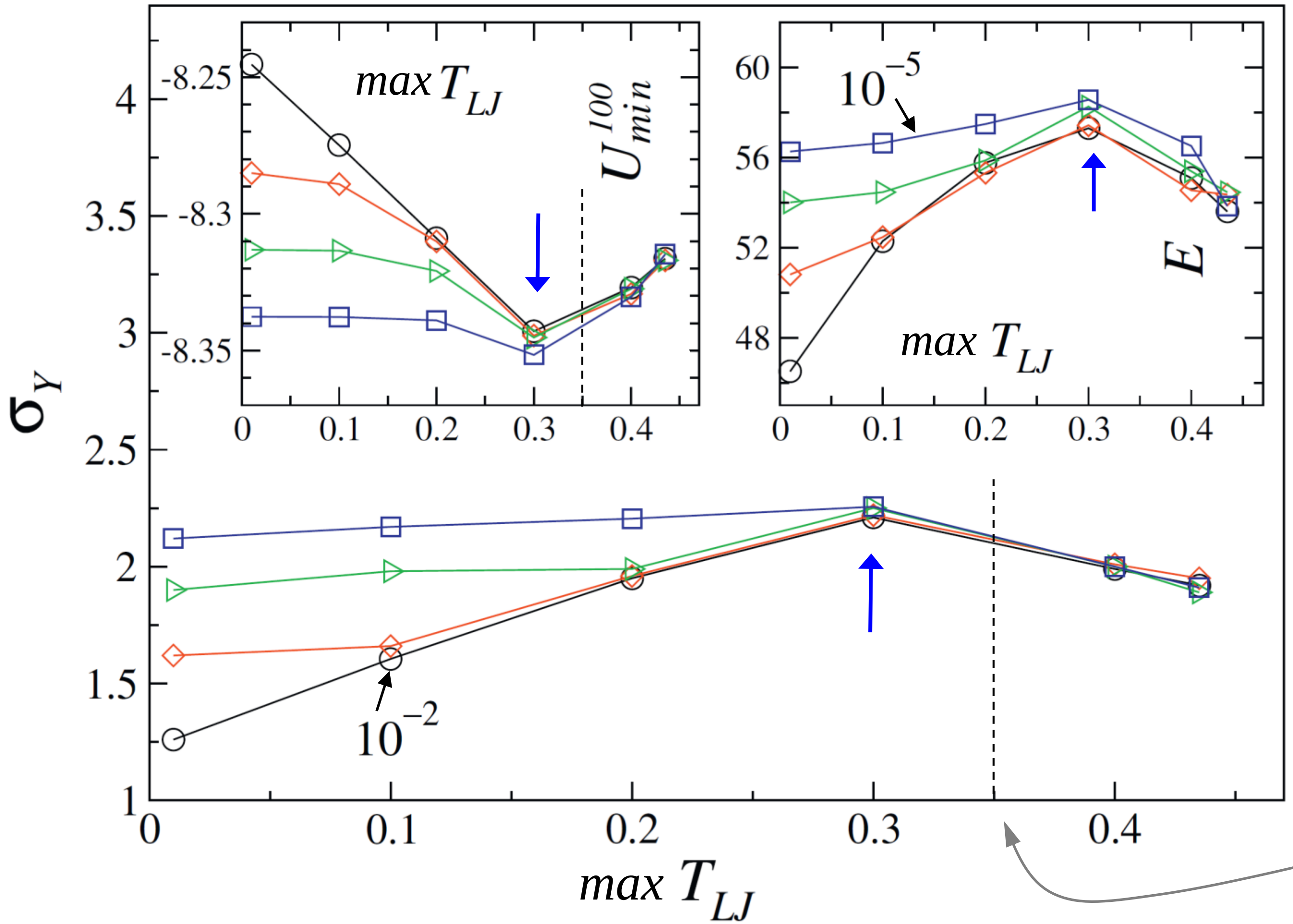


Strain rate = $10^{-5}\ 1/\tau$

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

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

The yielding peak σ_Y, elastic modulus E, and U_{min} versus maximum T_{LJ}



Initial quench rates:
(color code)

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

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

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

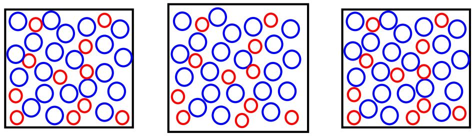
$10^{-5}\ \varepsilon/k_B\tau$

Pressure $P = 0$

$T_g \approx 0.35\ \varepsilon/k_B$

- 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 σ_Y and E.

Conclusions:



100 thermal 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.

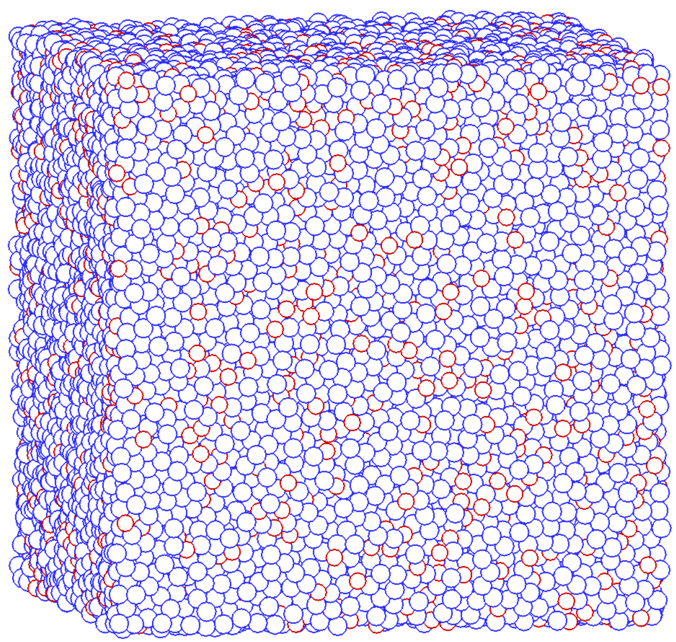
- The potential energy in rapidly annealed glasses decreases during thermal cycling, while the energy in slowly annealed glasses increases at large cycling amplitudes ($>T_g$).

- 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.

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).

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

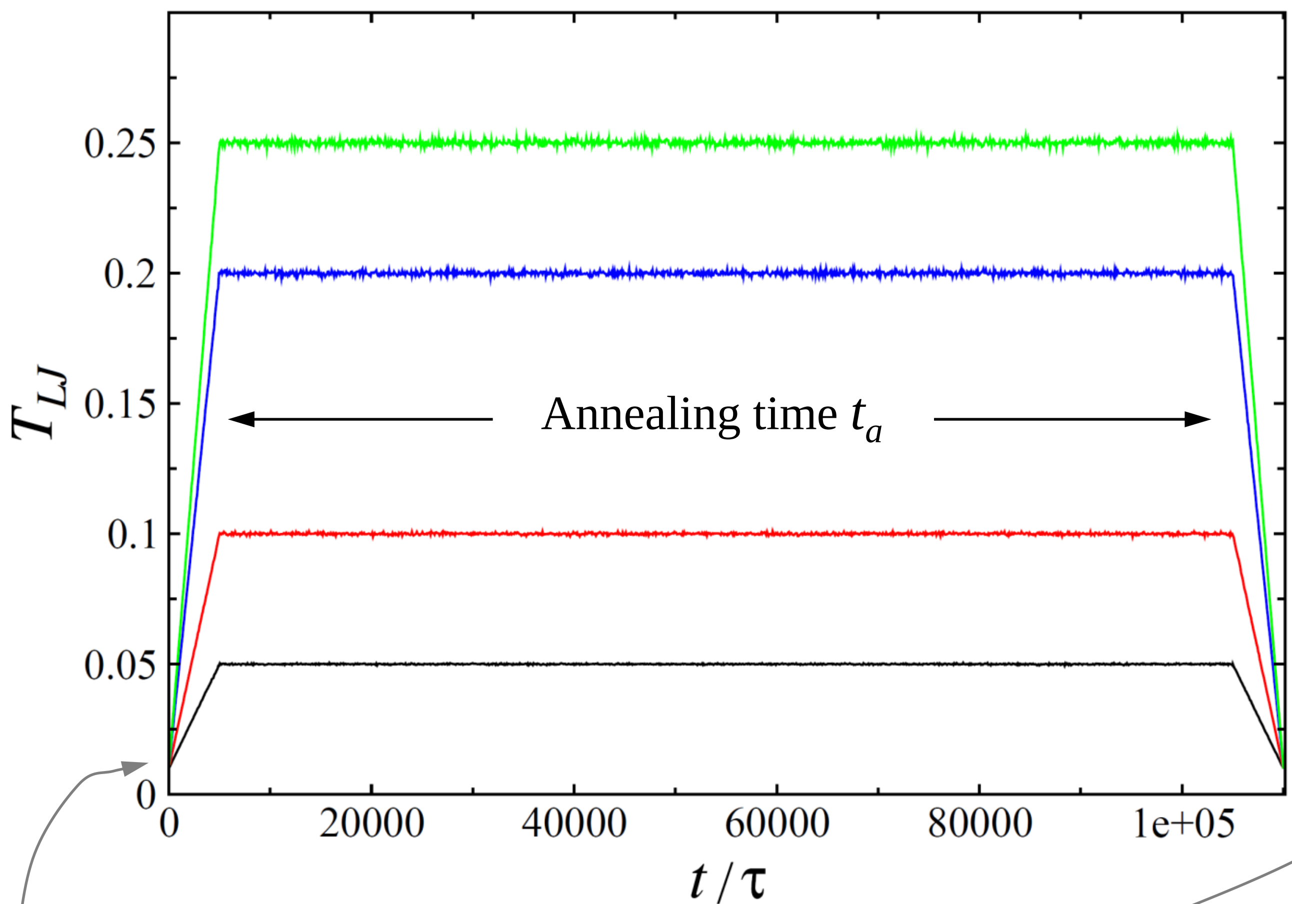
Constant applied stress σ_{zz}

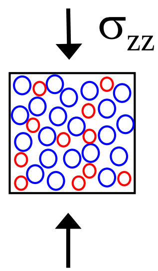


At what stress, temperature to load, and for how long?

N. V. Priezjev, Aging and rejuvenation during elastostatic loading of amorphous alloys: A molecular dynamics simulation study, *Comput. Mater. Sci.* **168**, 125 (2019).

Setup: Temperature profiles, annealing time, glass transition temperature





Elastostatic loading: constant stress σ_{zz}

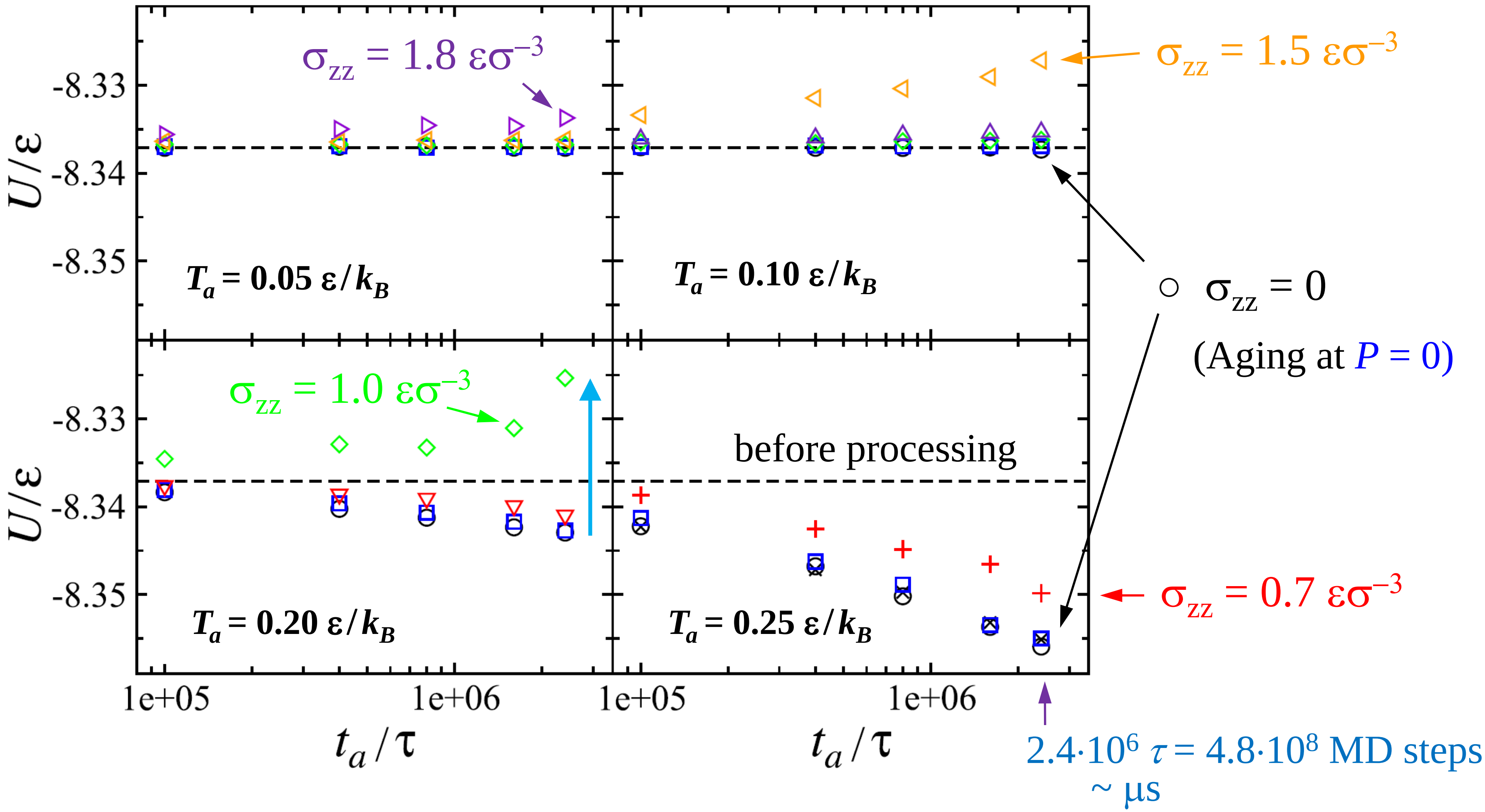
The stress σ_{zz} was ramped up to a certain value during the annealing time

Pressure $P = 0$

$T_g = 0.35\ \varepsilon / k_B$

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

Variation of the potential energy vs. annealing time at different temp T_a



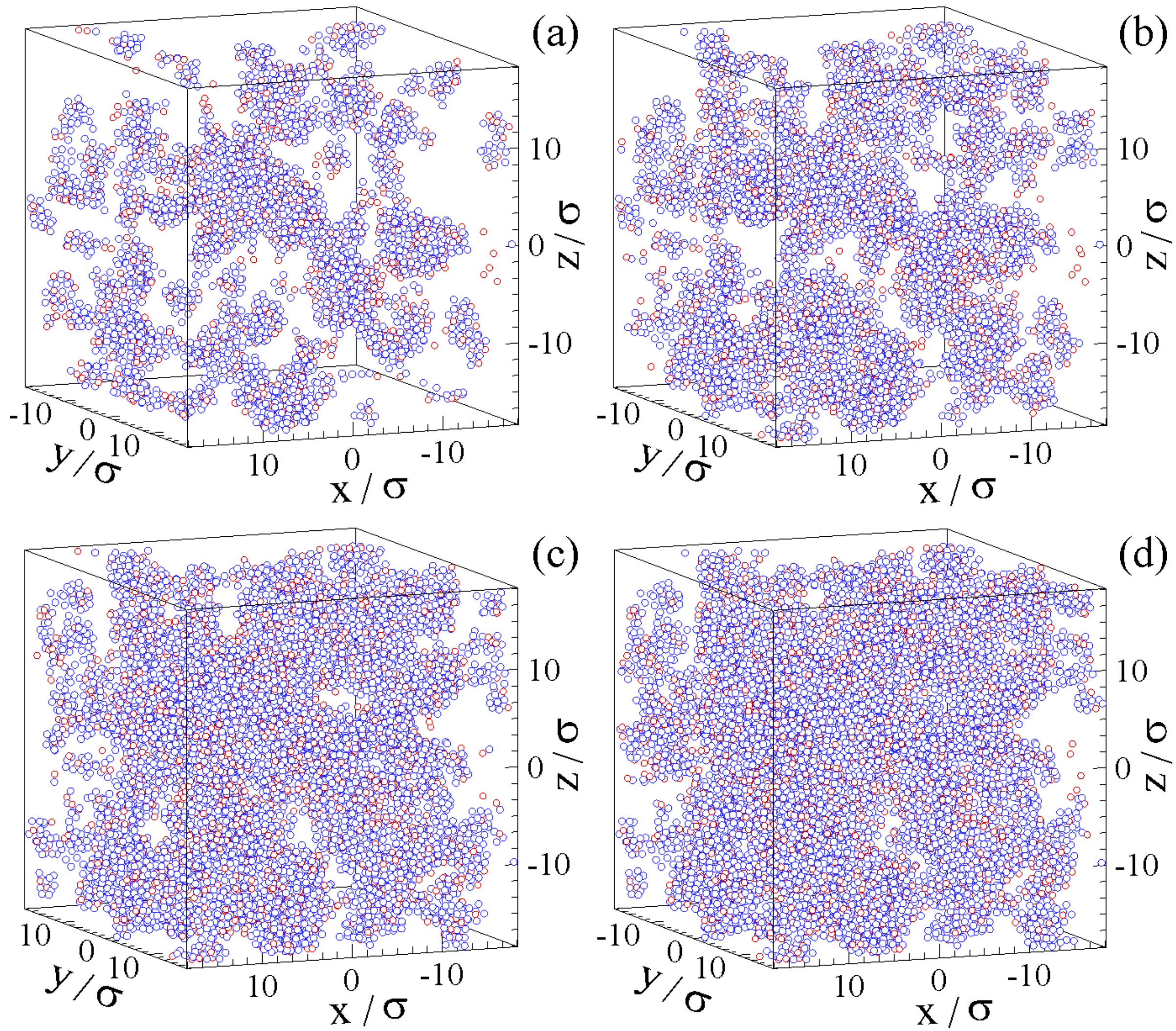
Constant applied stress σ_{zz} is up to ~70-80% of the yielding peak at a given temperature T_a

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

Collective nonaffine displacements vs. annealing time at T_a = 0.1 ε/k_B

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

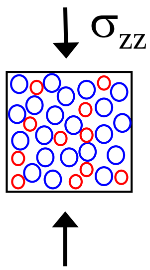
$D^2(0,\ \underline{10^5\tau}) > 0.04\sigma^2$ $D^2(0,\ \underline{4\times10^5\tau}) > 0.04\sigma^2$



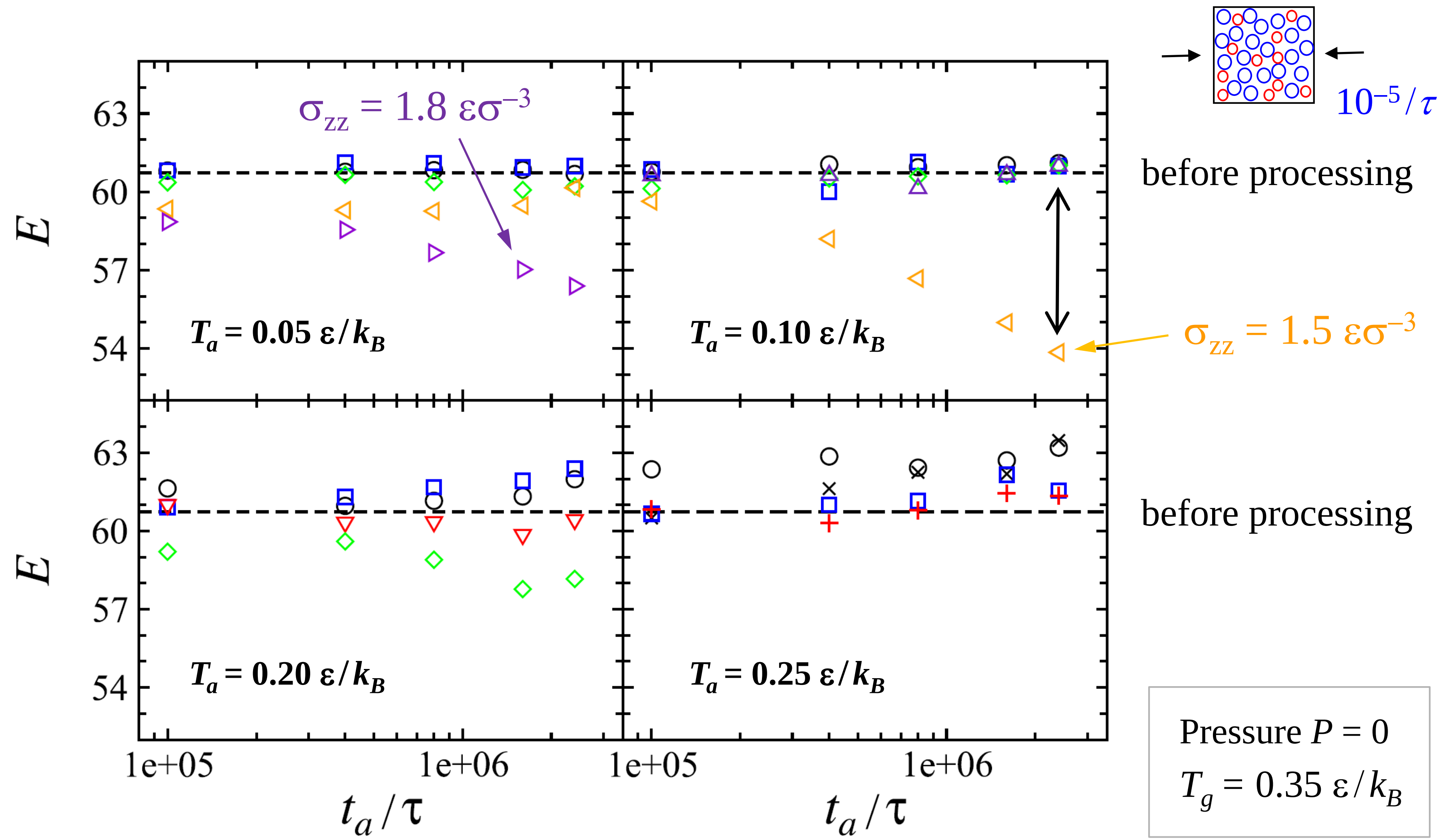
$D^2(0,\ \underline{1.6\times10^6\tau}) > 0.04\sigma^2$ $D^2(0,\ \underline{2.4\times10^6\tau}) > 0.04\sigma^2$

Elastostatic loading: constant applied stress:

$\sigma_{zz} = 1.5\ \varepsilon\sigma^{-3}$



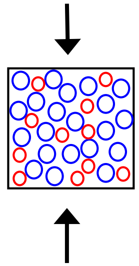
The elastic modulus E vs. annealing time t_a at different temperatures T_a



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

Conclusions:

Elastostatic loading: constant stress σ_{zz}



- 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.

- Annealing: high $T_a < T_g = 0.35\ \varepsilon / k_B$ and low stress σ_{zz} Rejuvenation: low T_a and high σ_{zz}

  $T_a < 0.6\ T_g$ $\sigma_{zz} \approx 0.8\ \sigma_Y$

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

N. V. Priezjev, Aging and rejuvenation during elastostatic loading of amorphous alloys: A molecular dynamics simulation study, *Comput. Mater. Sci.* **168**, 125 (2019).