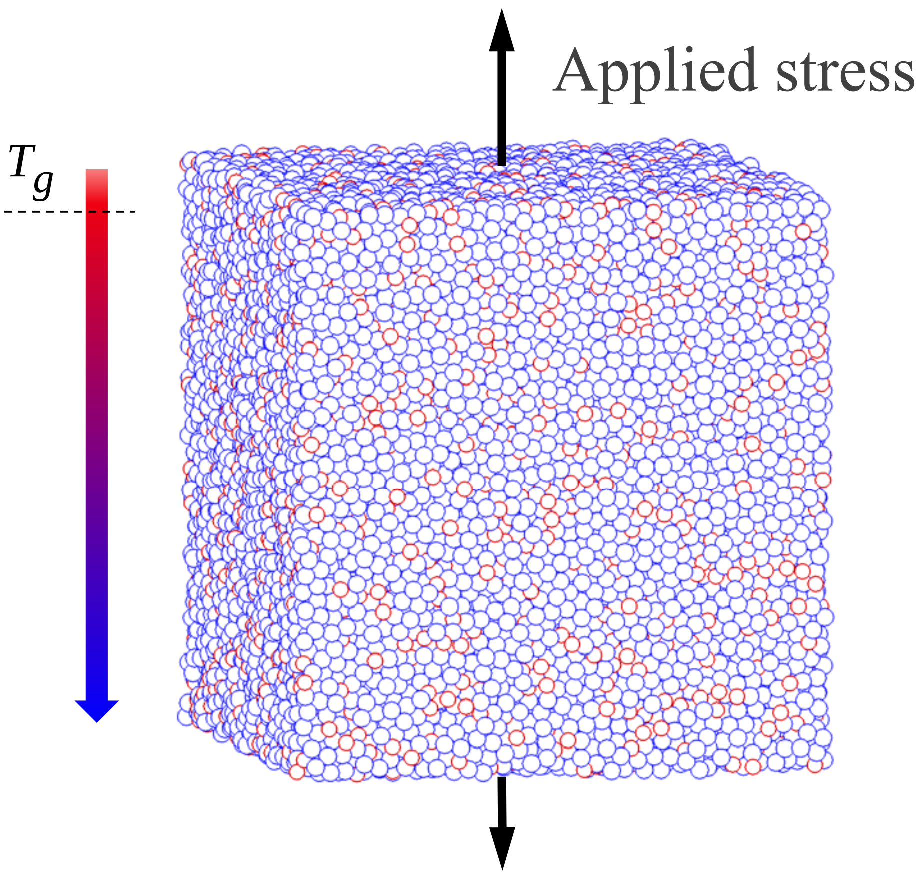
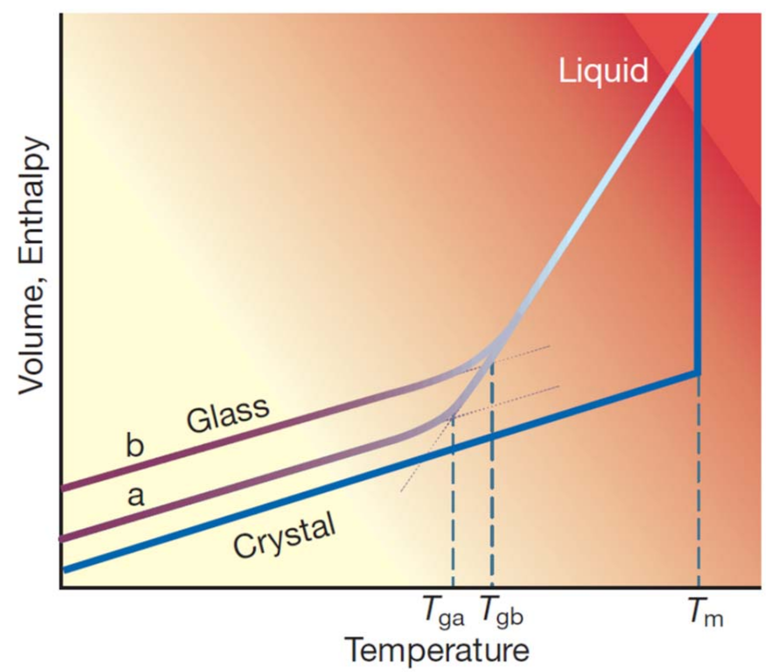
Rapidly cooling metallic glasses across the glass transition temperature under applied stress



Debenedetti & Stillinger, Nature (2001)



N. V. Priezjev, Cooling under applied stress rejuvenates amorphous alloys and enhances their ductility, *Metals* **11**, 67 (2021). J. Schroers et al., Enhancing ductility in bulk metallic glasses by straining during cooling, *Commun. Mater.* **2**, 23 (2021).

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:

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

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

Glass transition temperature: $T_g \approx 0.35\ \varepsilon / k_B$

Periodic boundary conditions: 60,000 atoms

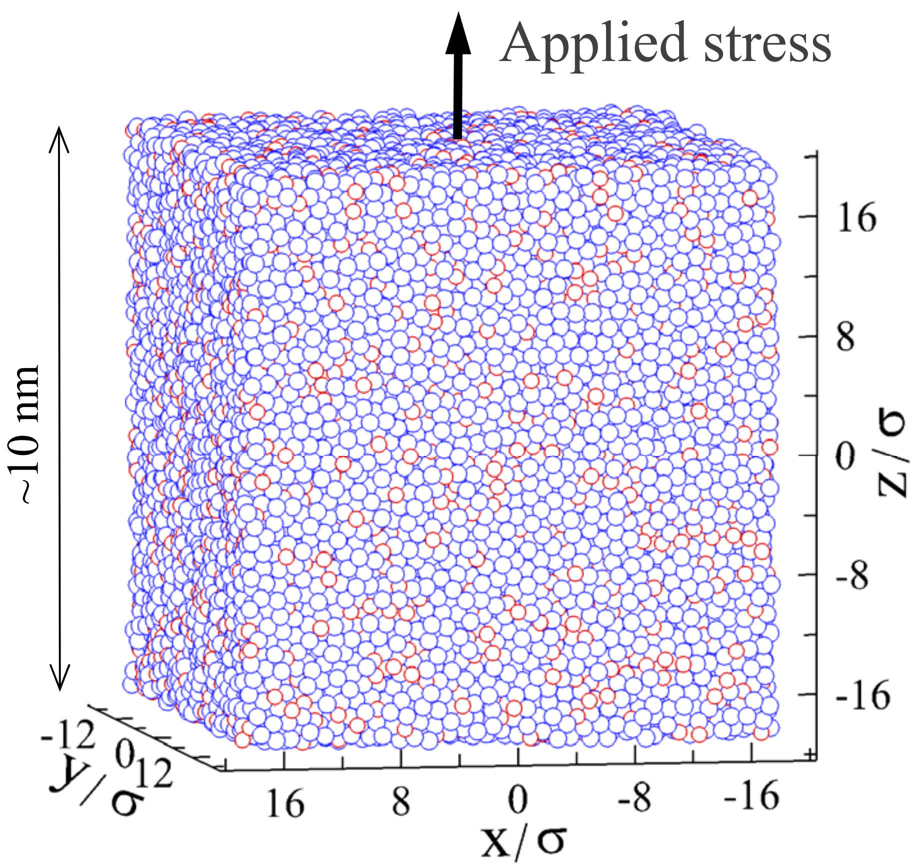
LAMMPS, Nose-Hoover thermostat

Integration time step: $\Delta t_{MD} = 0.005\ \tau$

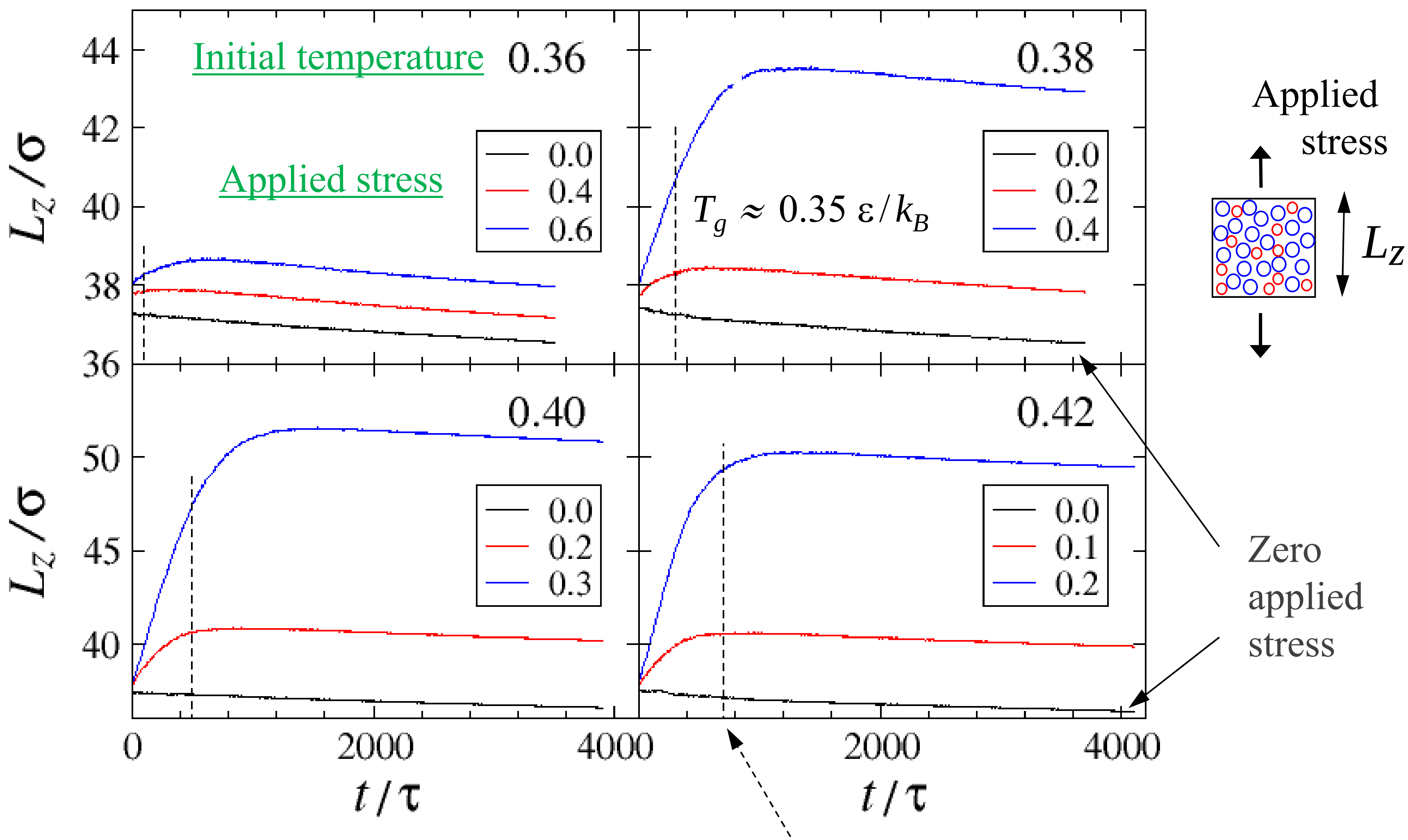
Fixed cooling rate: $10^{-4}\ \varepsilon / k_B \tau$

Variable parameters:

- Initial temperature (just above T_g)
- Applied normal stress (along z axis)

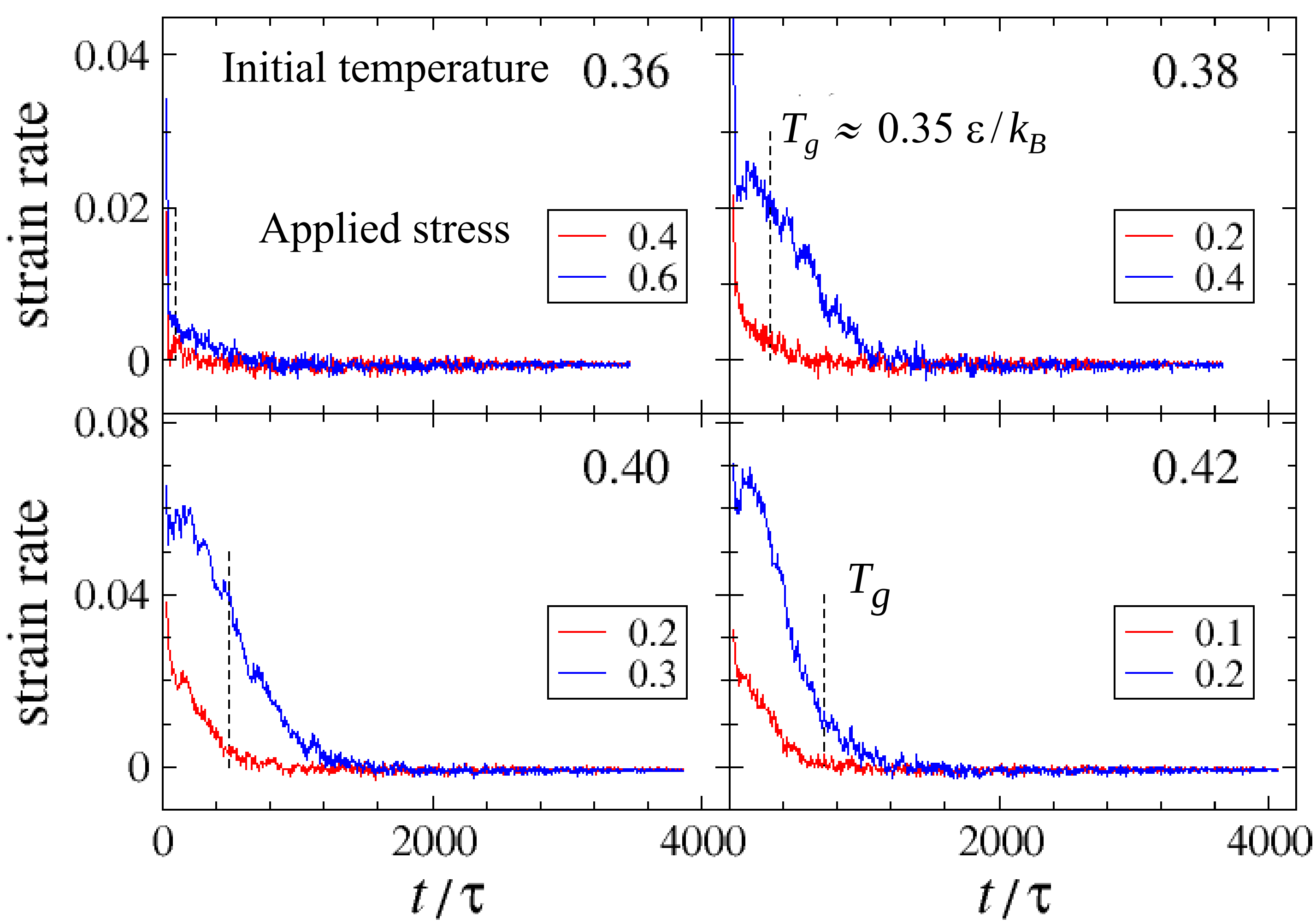


The time dependence of the system size L_Z upon cooling under applied stress



At higher applied stress, pronounced deformation near T_g (marked by vertical dashed lines)

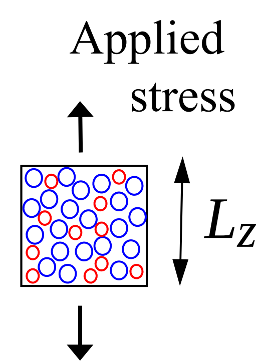
The time dependence of the strain rate upon cooling under applied stress



Fixed cooling rate: $10^{-4}\ \varepsilon/k_B\tau$

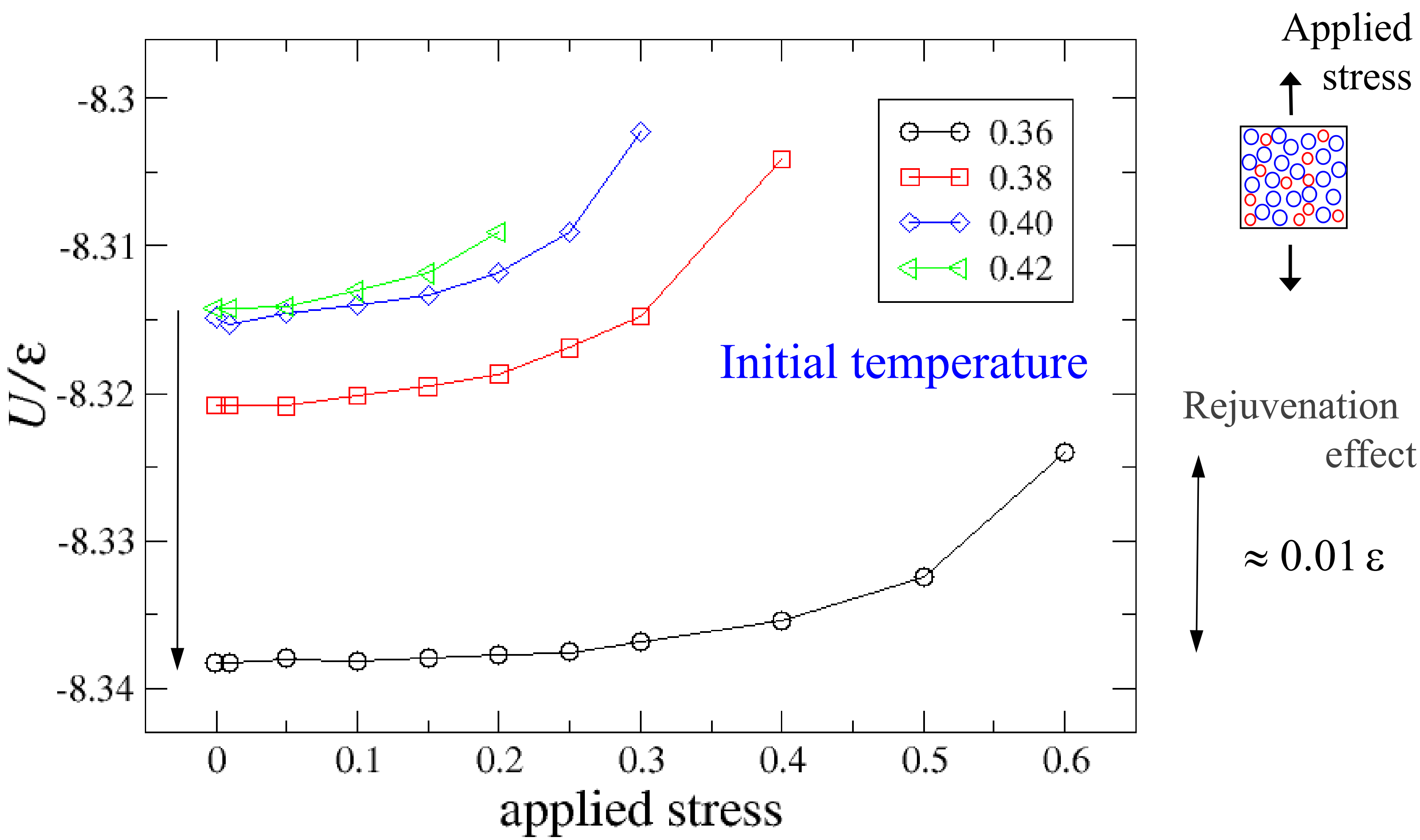
Inverse cooling rate: $10{,}000\,\tau$

Time scale set by strain rate: $0.05/0.01 \approx 5\,\tau$



At larger applied stress, higher strain rate near T_g (marked by vertical dashed lines).

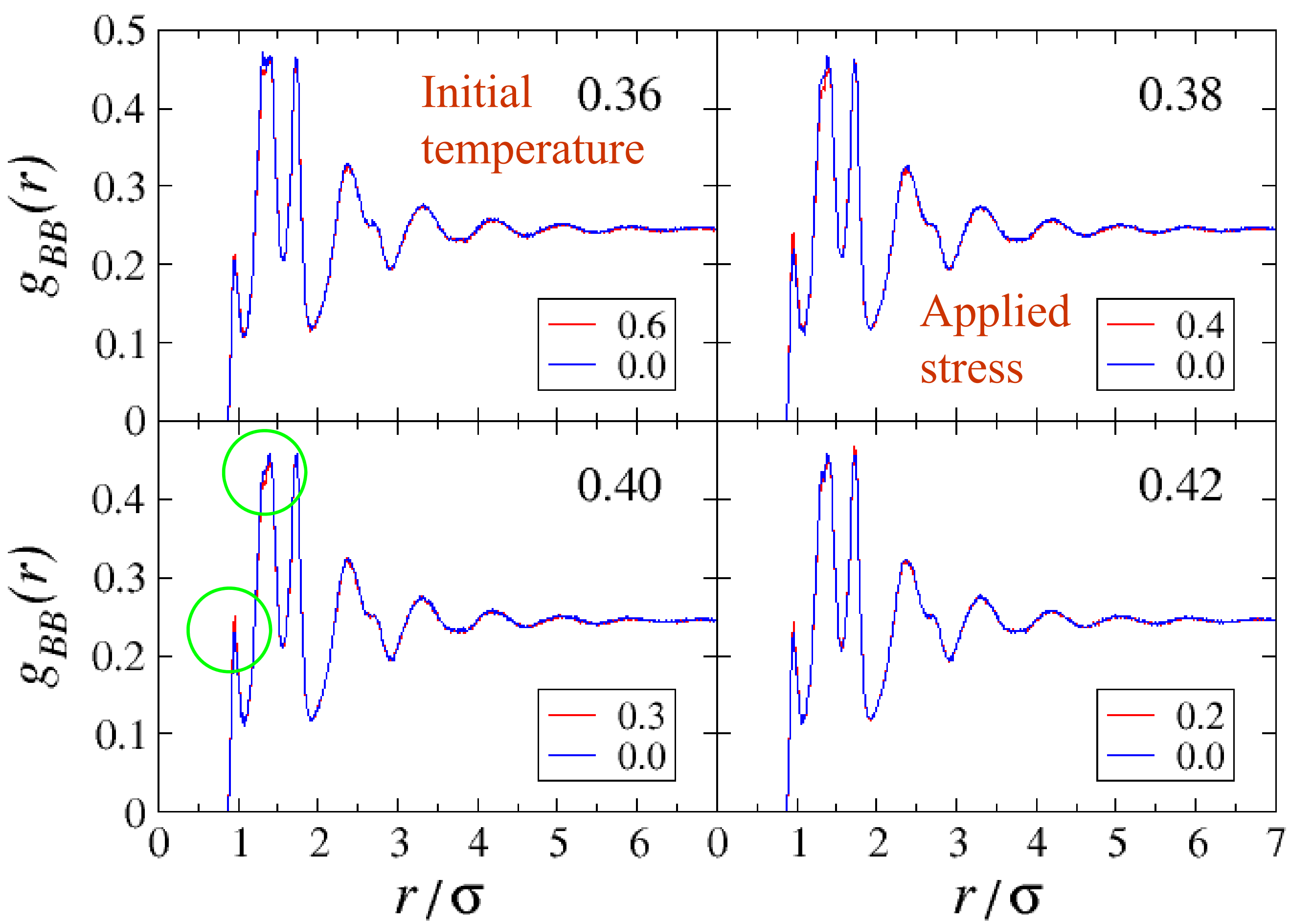
The potential energy *U* versus applied stress for 4 initial temperatures



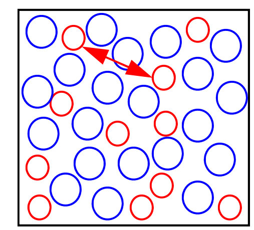
With increasing applied stress, the binary glass is relocated to progressively higher energy states as it freezes at higher strain.

N. V. Priezjev, *Metals* **11**, 67 (2021).

The radial distribution function after cooling at applied stress to low T



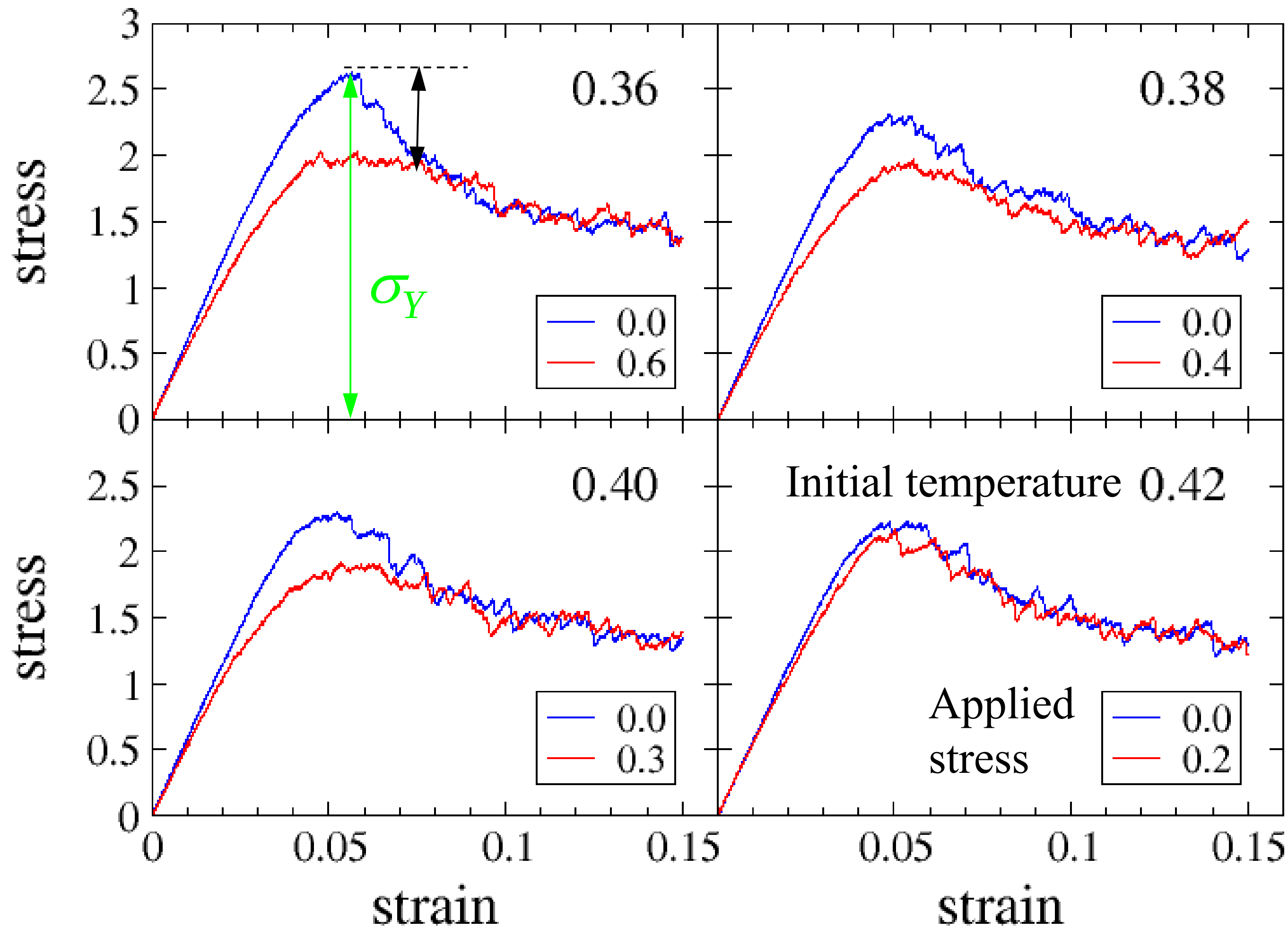
In *well-annealed* glasses, smaller type neighbors *B* effectively repel each other.



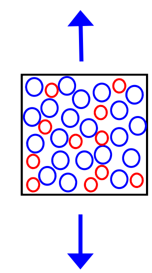
In *rejuvenated* glasses, structure is more 'random', thus more contacts between *B*–*B* type atoms.

Upon cooling under applied stress, the glass former freezes into a more 'random' configuration, which is reflected in larger number of contacts between *B*–*B* atoms.

The tensile stress vs. strain during loading at low T and *constant* strain rate



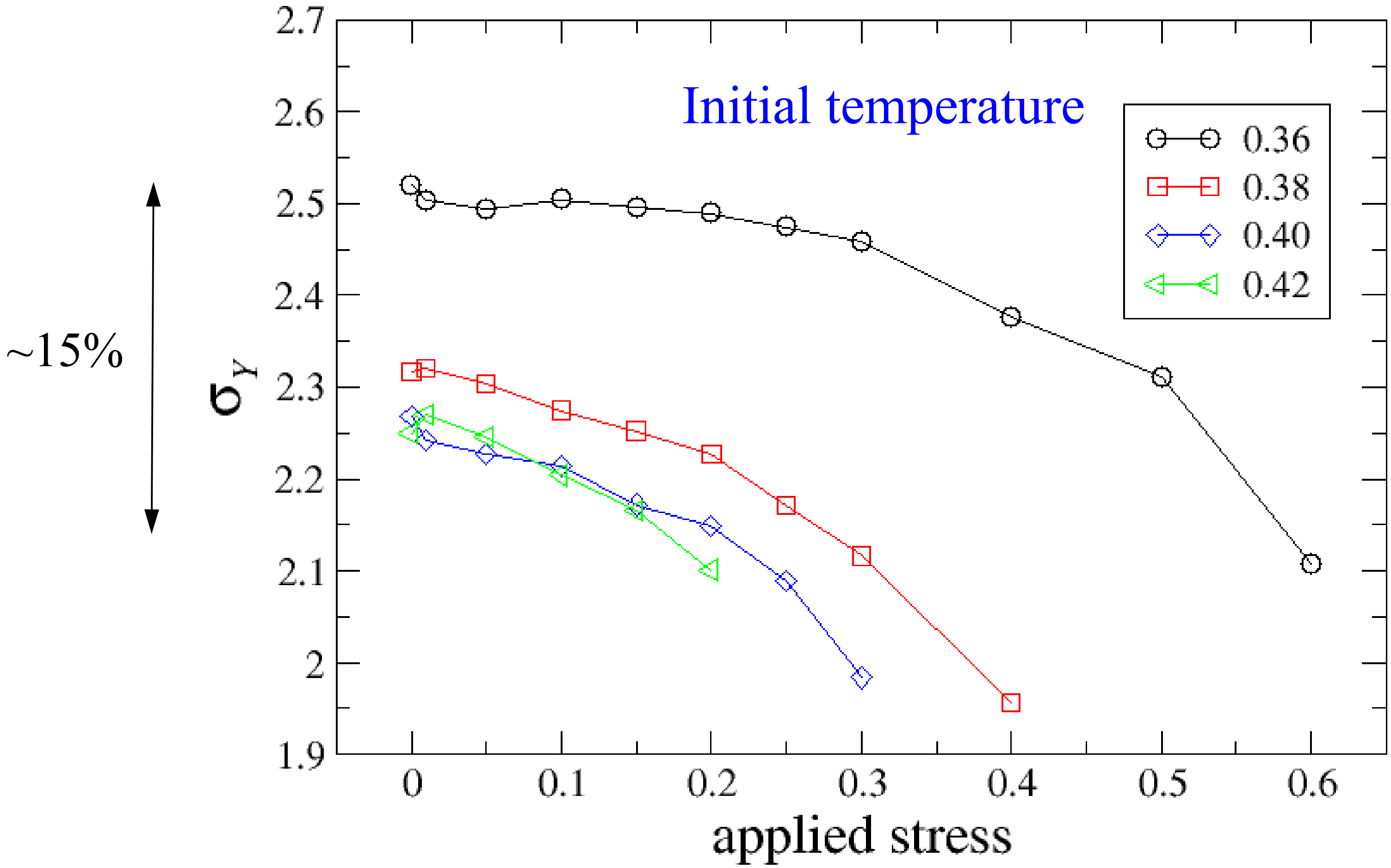
Tensile tests to probe mechanical properties



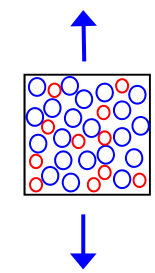
Strain rate $= 10^{-5}\ 1/\tau$

The yielding peak, σ_Y, is reduced in highly rejuvenated samples initially cooled at the maximum applied stress. The maximum difference in the yield stress becomes more pronounced for binary glasses prepared at lower initial temperatures.

The yielding peak as a function of the applied stress for 4 initial temperatures



Tensile tests to probe mechanical properties



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

The ductility is enhanced as the elastic modulus and the yielding peak are reduced in glasses that were cooled at larger tensile stresses and higher initial temperatures.

Conclusions:

- Rapid cooling across the glass transition temperature under applied stress leads to rejuvenation of metallic glasses (*i.e.*, higher energy and modified atomic structure).

- The yielding peak and elastic modulus are reduced in rejuvenated samples, indicating enhanced ductility (*i.e.*, improved mechanical properties).

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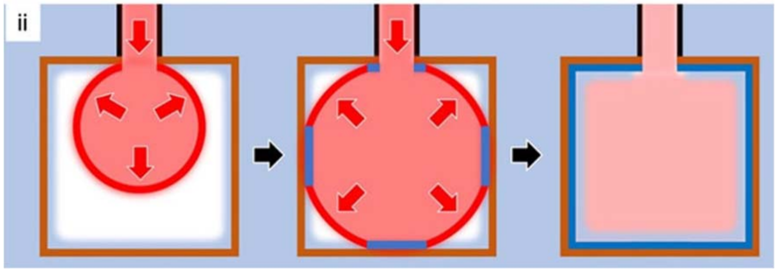

Blow molding against a cold mold results into excited liquid cooling and hence enables to net-shape BMG articles into their ductile state.

Mota, Lund, Sohn, Browne, Hofmann, Curtarolo, Van Walle & Schroers, Enhancing ductility in bulk metallic glasses by straining during cooling, *Commun. Mater.* **2**, 23 (2021).