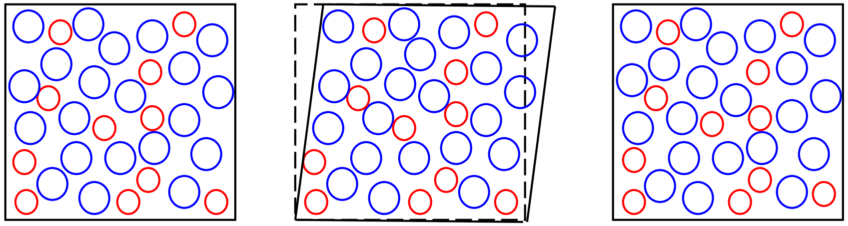
Fatigue failure of metallic glasses under cyclic shear deformation

Nikolai V. Priezjev

Department of Civil and Environmental Engineering

Howard University

`Movies, preprints: youtube.com/@nikolaipriezjev9047`

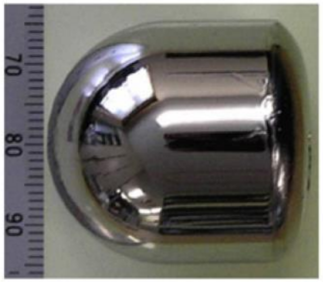


N. V. Priezjev, Fatigue failure of amorphous alloys under cyclic shear deformation, *Computational Materials Science* **226**, 112230 (2023).

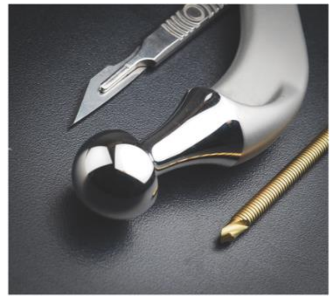
N. V. Priezjev, Shear band formation in amorphous materials under oscillatory shear deformation, *Metals* **10**, 300 (2020).

Amorphous structure, dynamical heterogeneity, and shear transformations

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



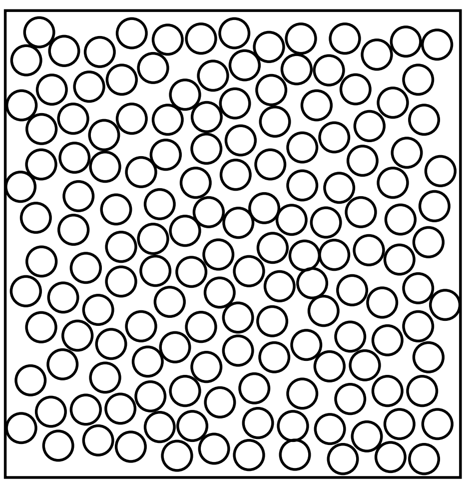
Cu-Zr-Al-Ag; ~30mm
Inoue & Takeuchi (2011)



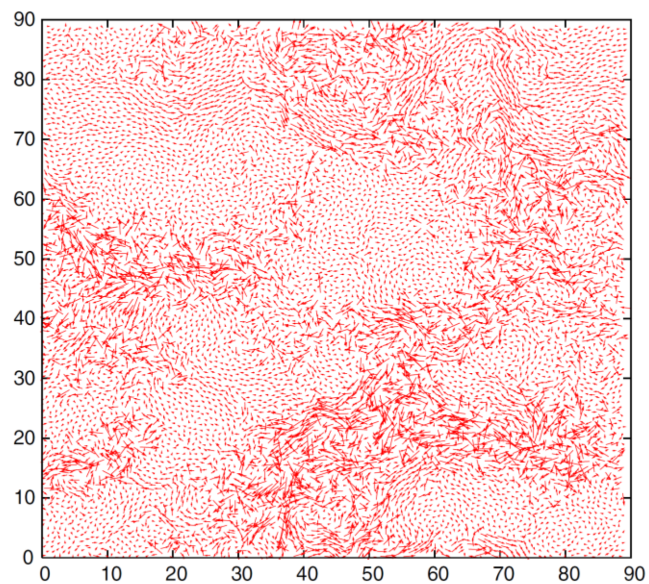
Biocompatible: Implantable medical devices and surgical tools (Mg-based)

Wear, corrosion resistant

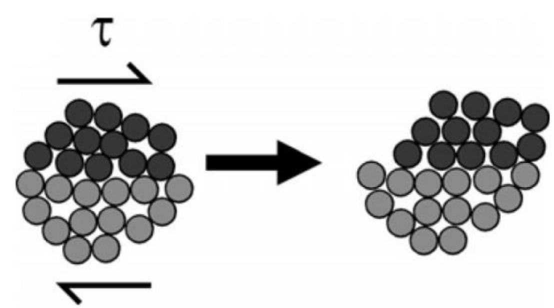
Sporting goods: *e.g.*, golf clubs



Disordered structure; no long-range order

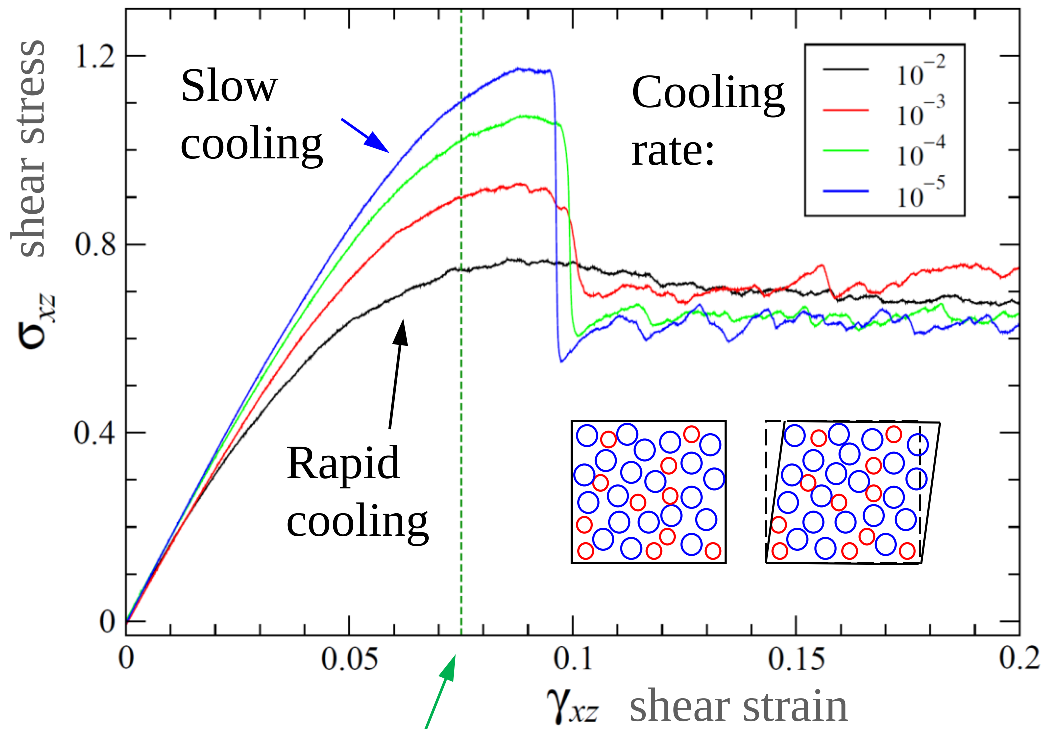


Spatial map of single-particle dis-placements, Berthier & Biroli (2011)



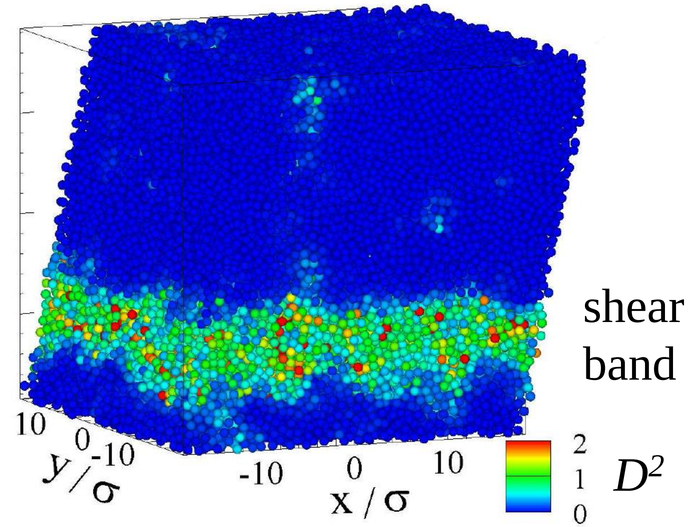
Localized shear transformations
Spaepen (1977) & Argon (1979)

Thermal history and stress response to mechanical deformation

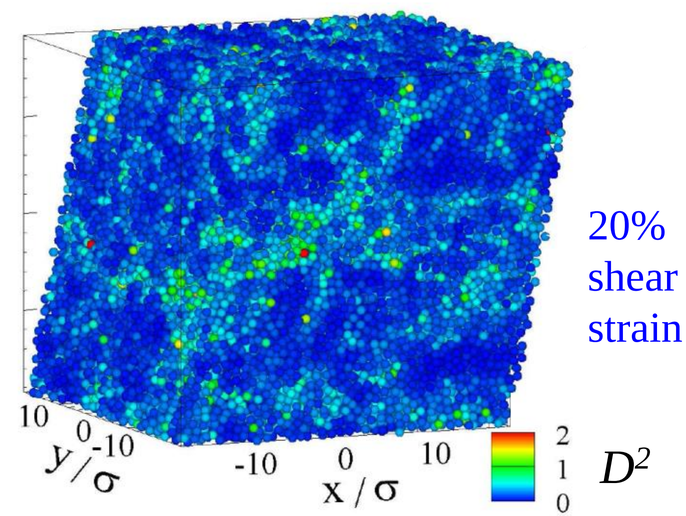


Critical strain amplitude during oscillatory shear

Well annealed glass (slow cooling)



Poorly annealed glass (fast cooling)



Upon slow cooling, glasses become more relaxed and exhibit a yielding peak; while rapidly cooled glasses show smooth crossover when strained.

N.V. Priezjev, *Metals* **10**, 300 (2020).

N.V. Priezjev, *Comp. Mat. Sci.* (2020).

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: $L = 94.10\,\sigma$, $N_p = 1{,}000{,}000$

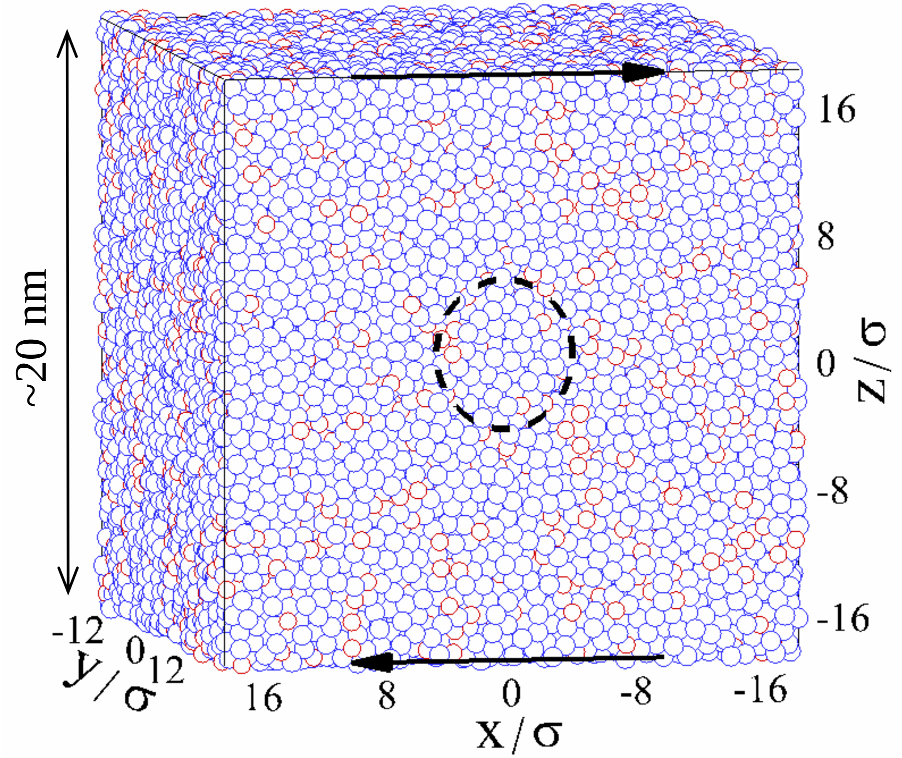
Lees-Edwards periodic boundary conditions

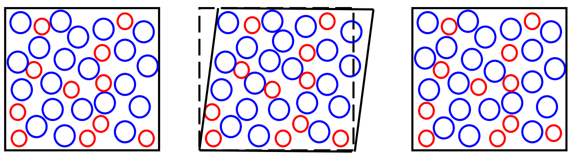
LAMMPS, Nose-Hoover thermostat, $\Delta t_{MD} = 0.005\,\tau$

Slow annealing rate: $10^{-5}\ \varepsilon / k_B \tau$ (**well-annealed glass**)

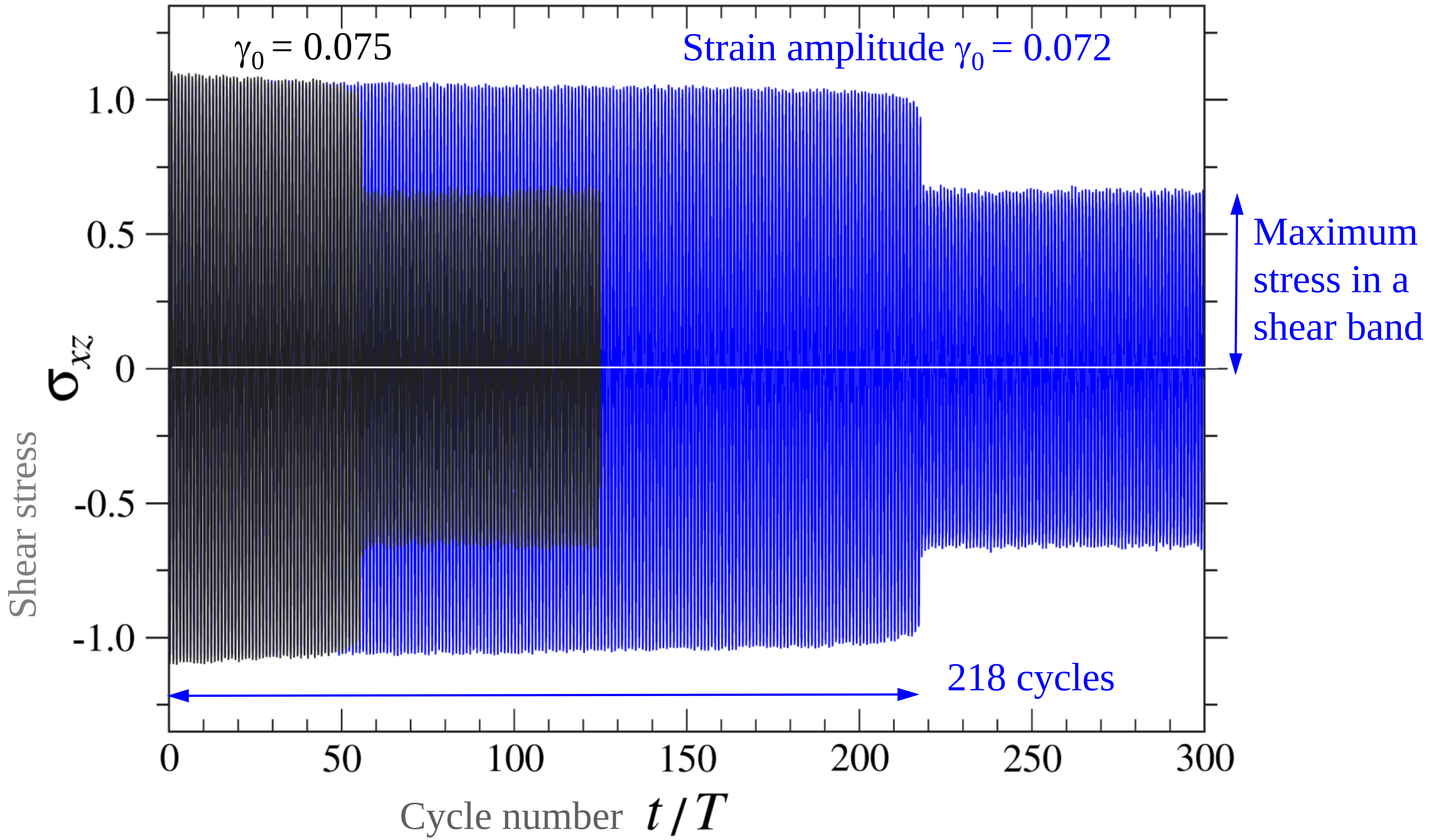
Oscillatory shear strain: $\gamma(t) = \gamma_0 \sin(\omega t)$

Strain amplitude: $0.069 \le \gamma_0 \le 0.075$



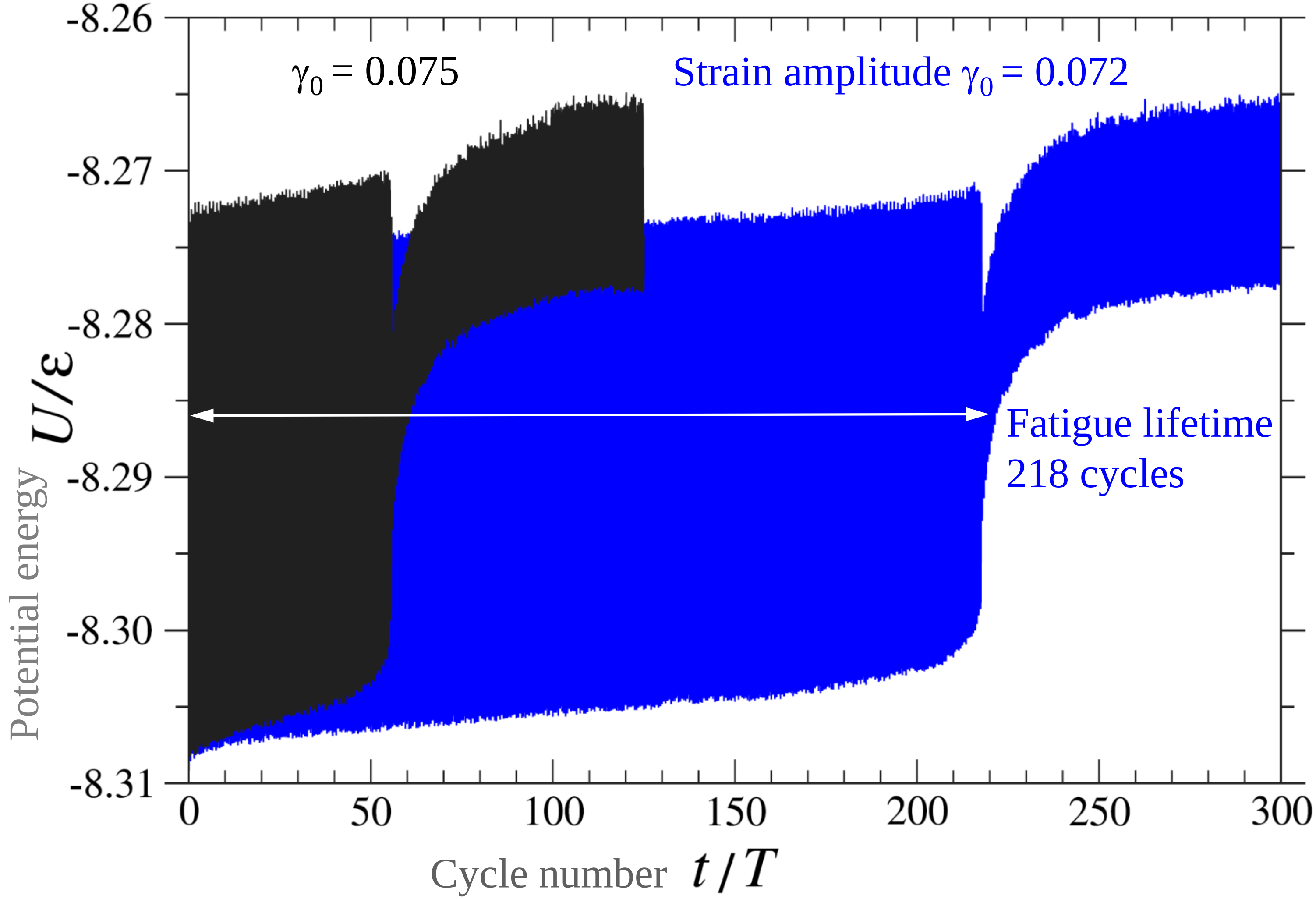


Shear stress during 300 cycles for strain amplitudes γ_0 = 0.072 and 0.075



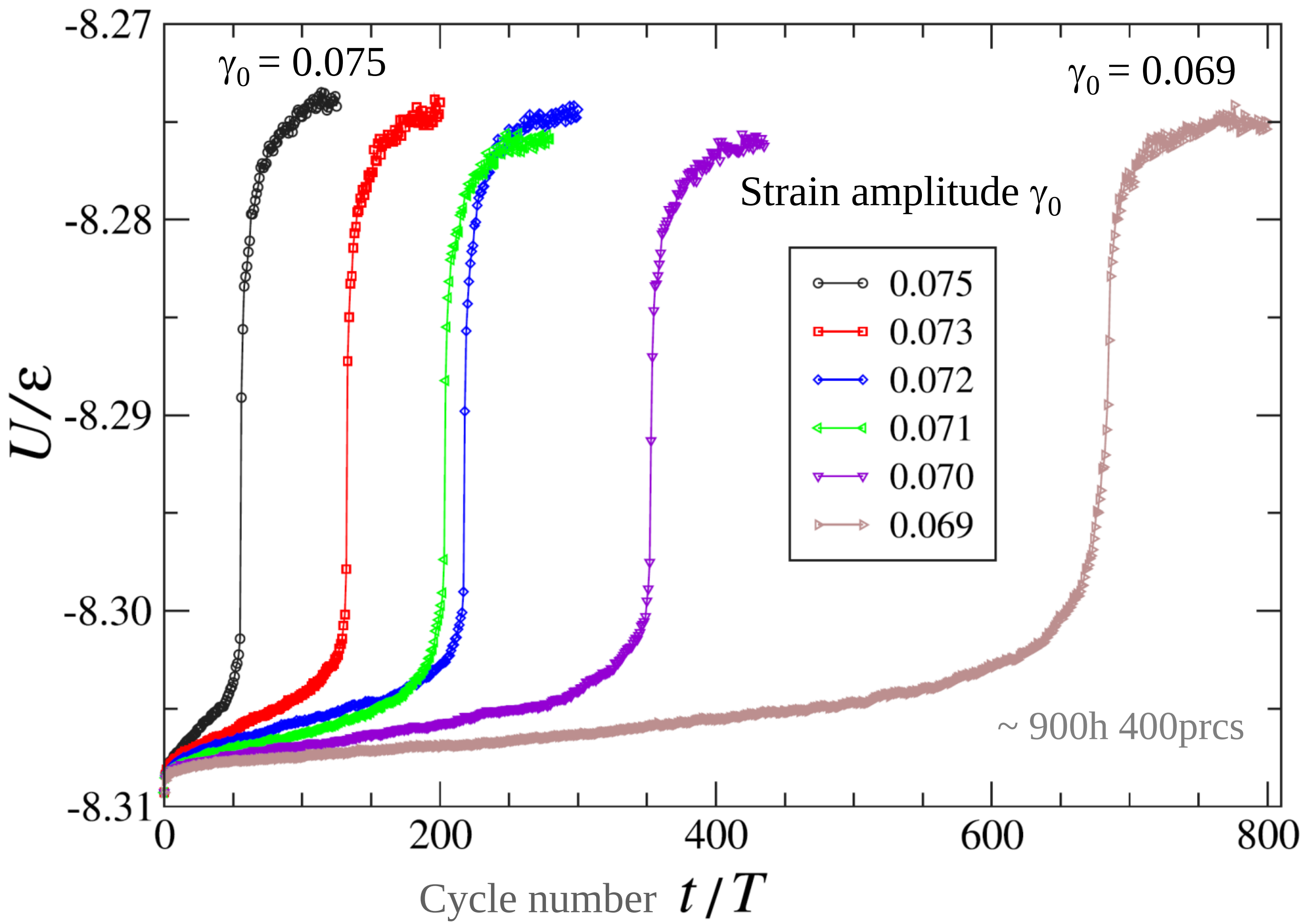
The amplitude of shear stress oscillations slightly decreases upon continued loading until a sudden drop during one shear cycle. Fatigue lifetime is longer at smaller γ_0

Potential energy per particle U for strain amplitudes $\gamma_0 = 0.072$ and 0.075



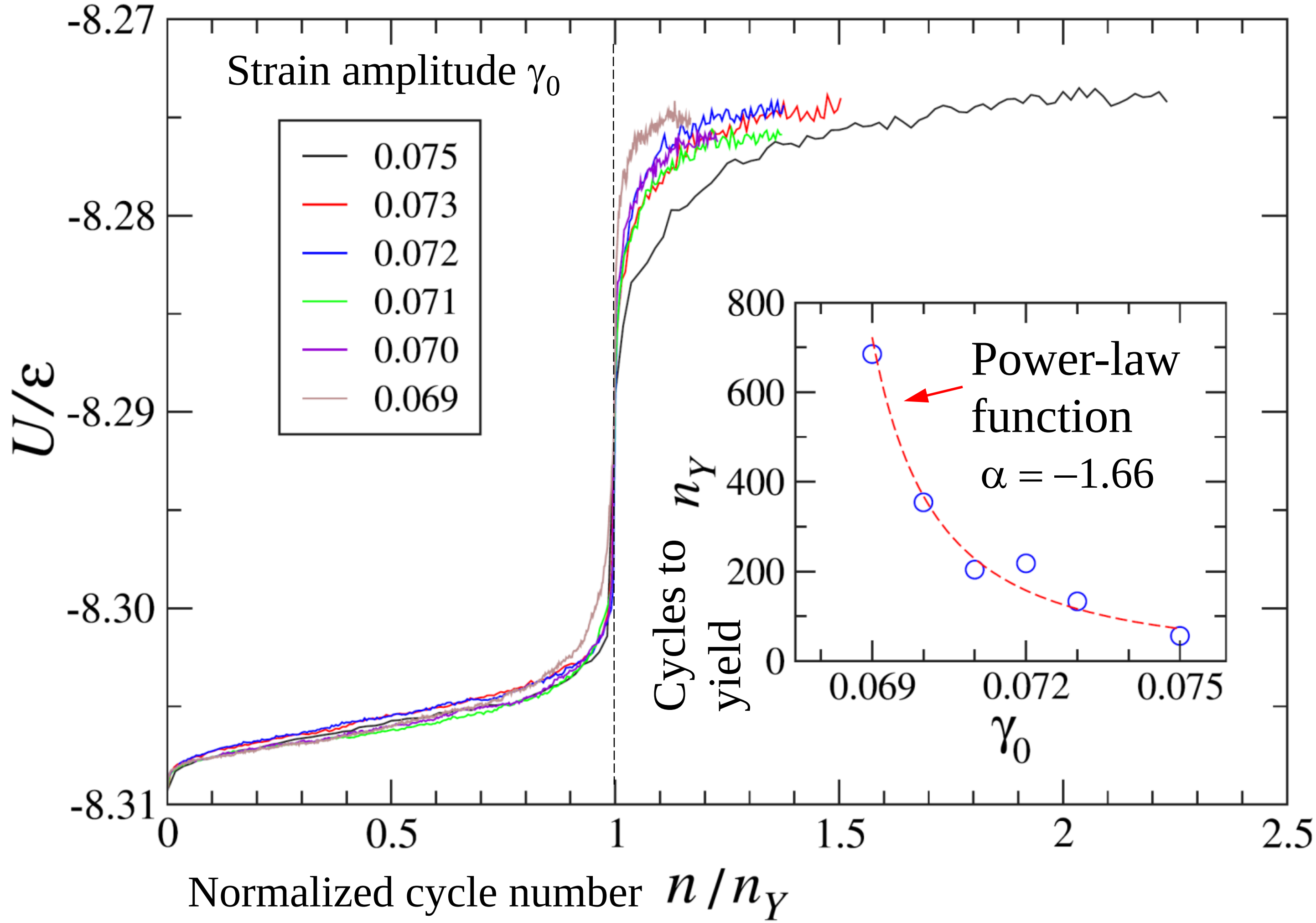
The potential energy gradually increases via collective rearrangements of atoms. A sharp increase at the yielding transition is associated with formation of a shear band.

Potential energy minima vs cycle number for selected strain amplitudes γ_0



Upon reducing strain amplitude γ_0 towards a critical value, the yielding transition becomes significantly delayed.

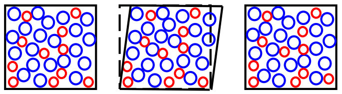
The potential energy minima U vs normalized cycle number for selected γ_0

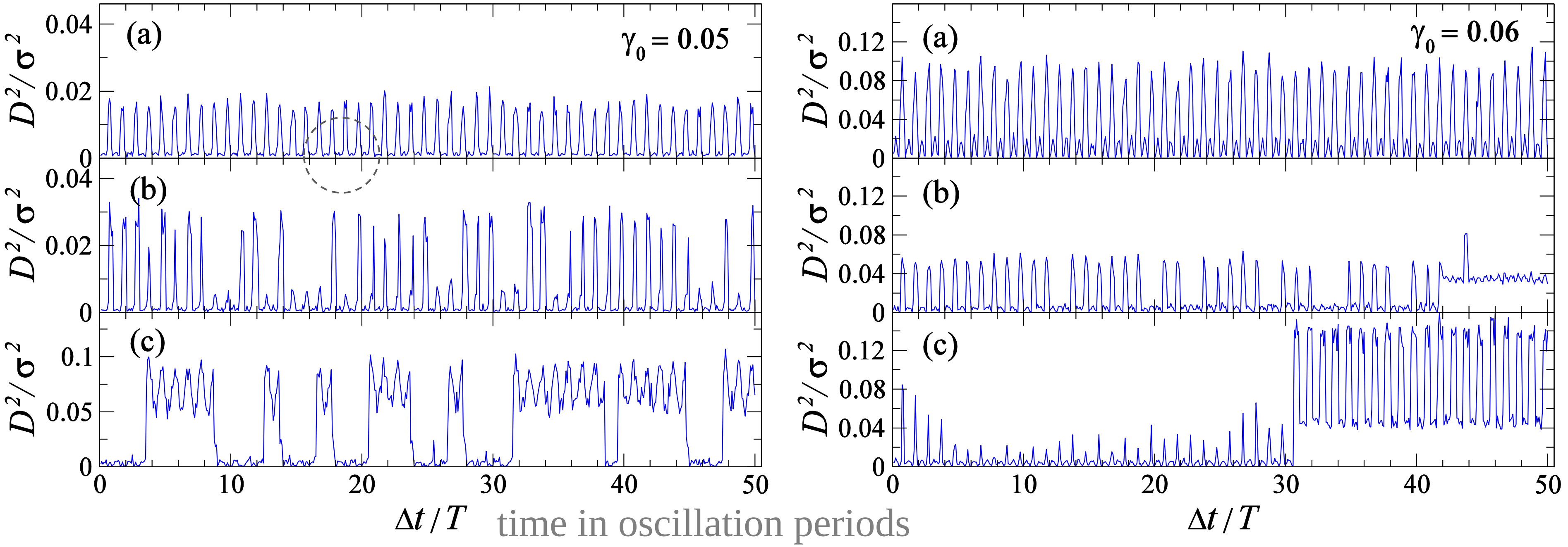


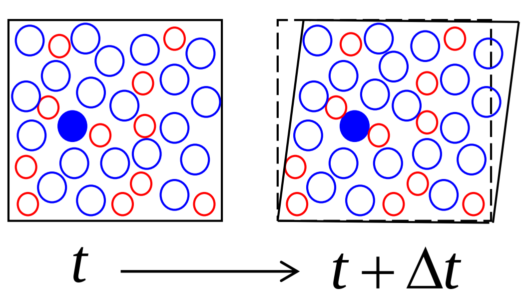
The potential energy minima for different γ_0 closely follow a master curve. The number of cycles until the yielding transition, n_Y, is well described by a power-law function.

Variation of nonaffine measure $D^2(0,\Delta t)$ for selected particles over 50 cycles

Reversible / irreversible particle displacements







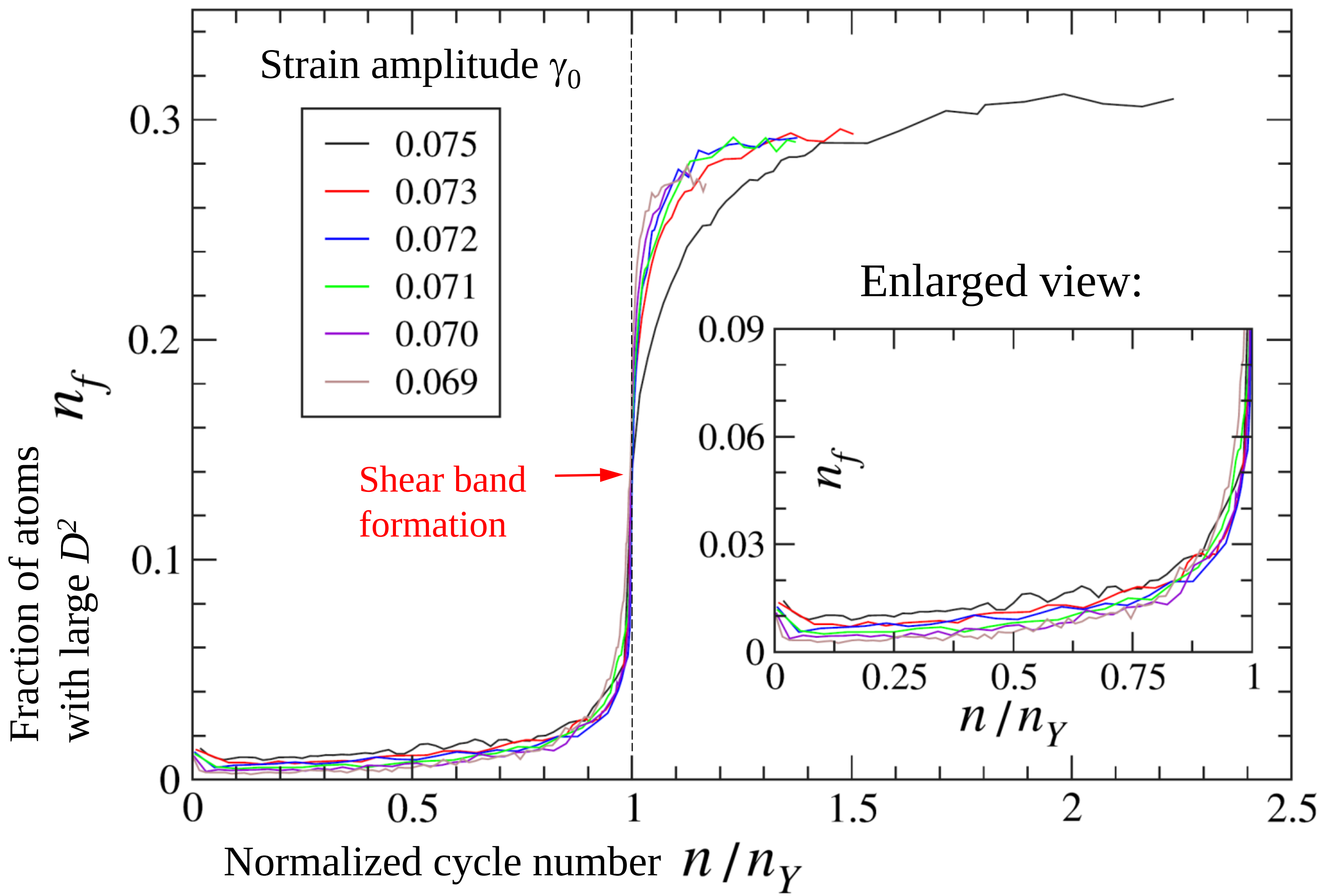
$$D^2(t,\Delta t) = \frac{1}{N_i}\sum_{j=1}^{N_i}\Big\{\mathbf{r}_j(t+\Delta t) - \mathbf{r}_i(t+\Delta t) - J_i[\mathbf{r}_j(t) - \mathbf{r}_i(t)]\Big\}^2$$

Excellent diagnostic for identifying particle rearrangements

Falk and Langer, *Phys. Rev. E* **57**, 7192 (1998).

N. V. Priezjev, *Phys. Rev. E* **93**, 013001 (2016).

Number of plastic events vs normalized number of cycles for selected γ_0

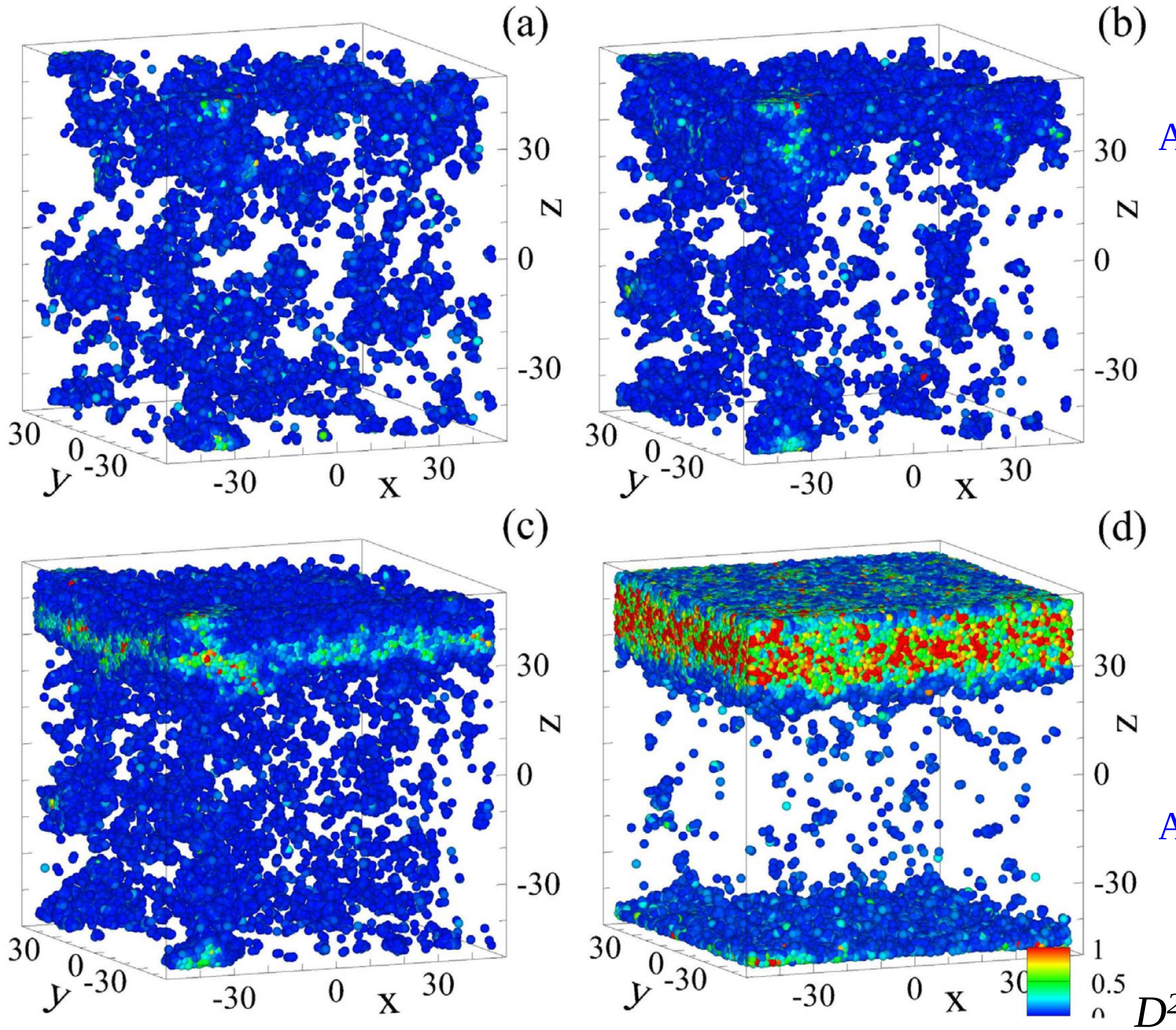


Plastic rearrangements of only about 1% of atoms during the first $n_Y/2$ cycles result in the increase of the potential energy U (rejuvenation).

Spatial configurations of atoms with large nonaffine displacements at γ_0=0.072

After 201st cycle

After 217th cycle



Shear band formation

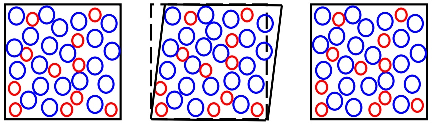
After 218th cycle

Finite width of shear band

After 225th cycle

youtube.com/@nikolaipriezjev9047

Conclusions:



Cyclic shear deformation

• The fatigue process proceeds via a sequence of irreversible rearrangements of small clusters of atoms until a sudden formation of a shear band at the yielding transition.

• The potential energy at the end of each cycle as a function of the normalized number of cycles is nearly independent of the strain amplitude, which allows for estimation of the fatigue lifetime at a given strain amplitude.

• Upon approaching a critical strain amplitude from above, the number of shear cycles until the yielding transition is well described by a power-law function.

N. V. Priezjev, Fatigue failure of amorphous alloys under cyclic shear deformation, *Computational Materials Science* **226**, 112230 (2023).