Plastic deformation of a model glass induced by a local shear transformation

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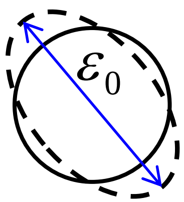
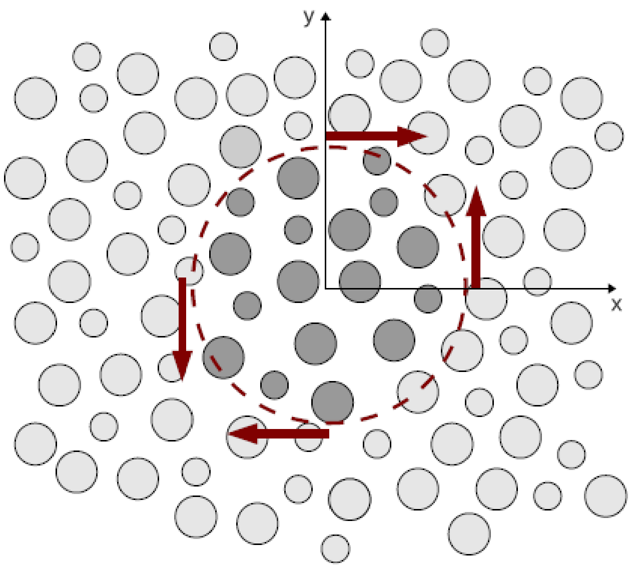
APS March 3, 2015

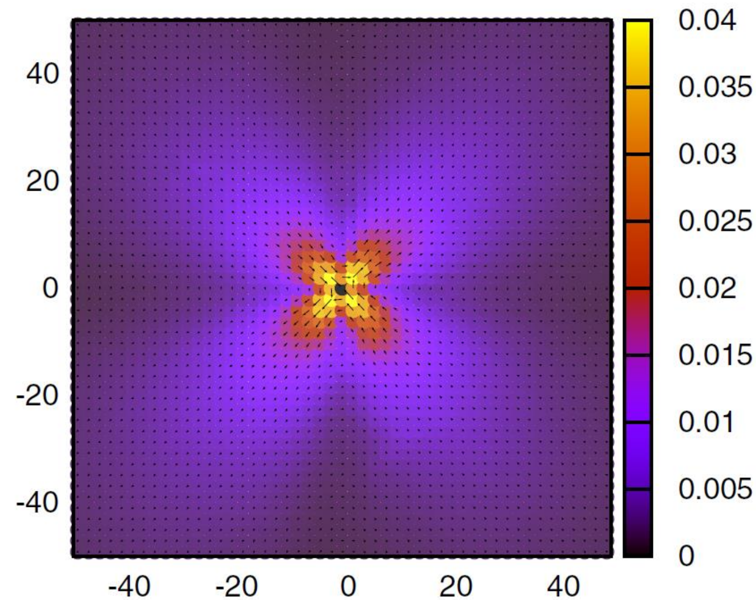


N. V. Priezjev, "Plastic deformation of a model glass induced by a local shear transformation", *Physical Review E* **91**, 032412 (2015); "The effect of a reversible shear transformation on plastic deformation of an amorphous solid", *J. Phys.: Condens. Matter* **27**, 435002 (2015).

Time-dependent elastic response to a local shear transformation in 2D glass



Instantaneously strain circular inclusion into an ellipse (elementary plastic event in deformed glasses)



Long-time mean displacement field with quadrupolar symmetry

1. Long-time response averages out to continuum solution despite large fluctuations
2. A crossover from a propagative transmission in the case of weakly damped dynamics to a diffusive transmission for strong damping (large friction)

Eshelby inclusion problem (1957)

Puosi, Rottler, Barrat, *Phys. Rev. E* **89**, 042302 (2014).

Details of molecular dynamics simulations and parameter values

Binary 3D Lennard-Jones Kob-Andersen mixture:

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

Interaction parameters for $\alpha\beta = A$ and B particles:

$$\varepsilon_{AA} = 1.0, \varepsilon_{AB} = 1.5, \ \varepsilon_{BB} = 0.5, m_A = m_B, N_p = 10000$$

$$\sigma_{AA} = 1.0, \sigma_{AB} = 0.8, \ \sigma_{BB} = 0.88, \ \ \tau = \sigma_{AA}\sqrt{m_A/\varepsilon_{AA}}$$

Kob & Andersen, *Phys. Rev. E* **51**, 4626 (1995).

Monomer density: $\rho = \rho_A + \rho_B = 1.20\,\sigma^{-3}$

Temperature: $T = 0.01\ \varepsilon/k_B \ll T_g = 0.45\ \varepsilon/k_B$

System dimensions: $20.27\sigma \times 20.27\sigma \times 20.27\sigma$

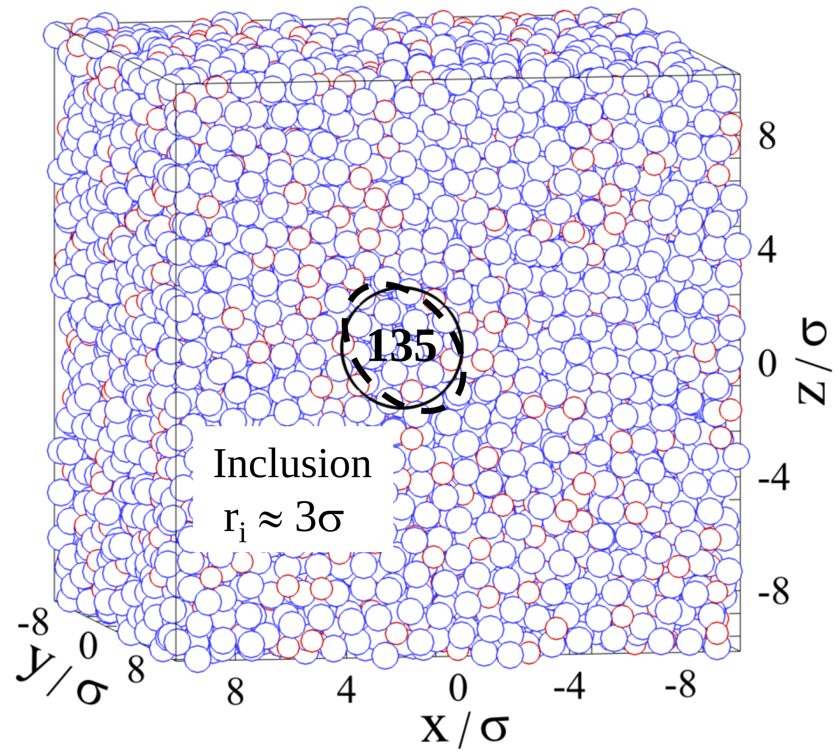
Periodic boundary conditions $\quad \Delta t_{MD} = 0.005\,\tau$

Langevin dynamics

$$m\ddot{x}_i + m\Gamma\dot{x}_i = -\sum_{i \neq j}\frac{\partial V_{ij}}{\partial x_i} + f_i$$

Oscillatory shear strain: $\varepsilon(t) = \varepsilon_0 \sin(\pi\, t/\tau_i)$

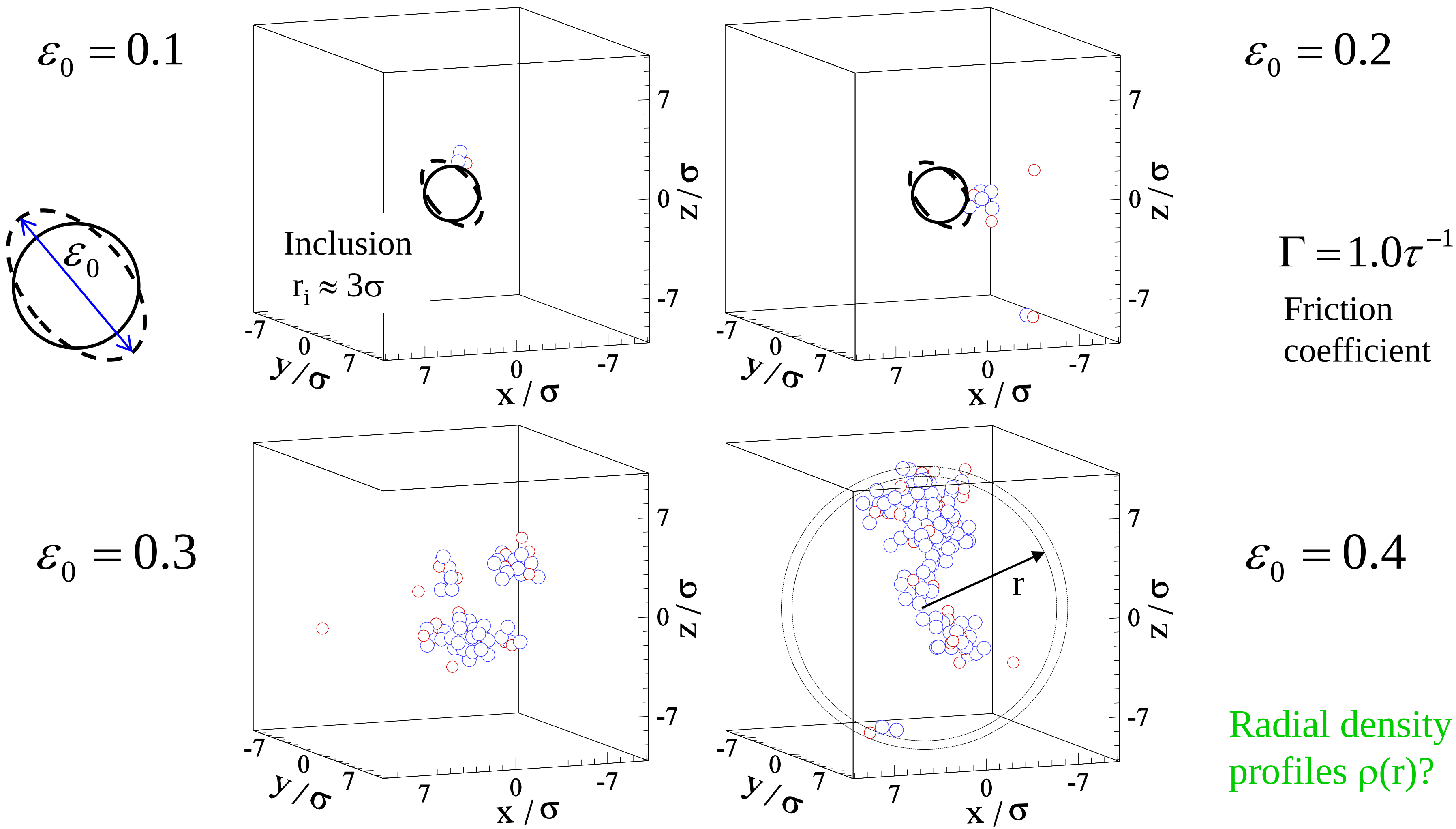
Time scale of shear event: $\boxed{0 < t < \tau_i}$



Plastic deformation after reversible shear event (averaged over 504 independent samples)

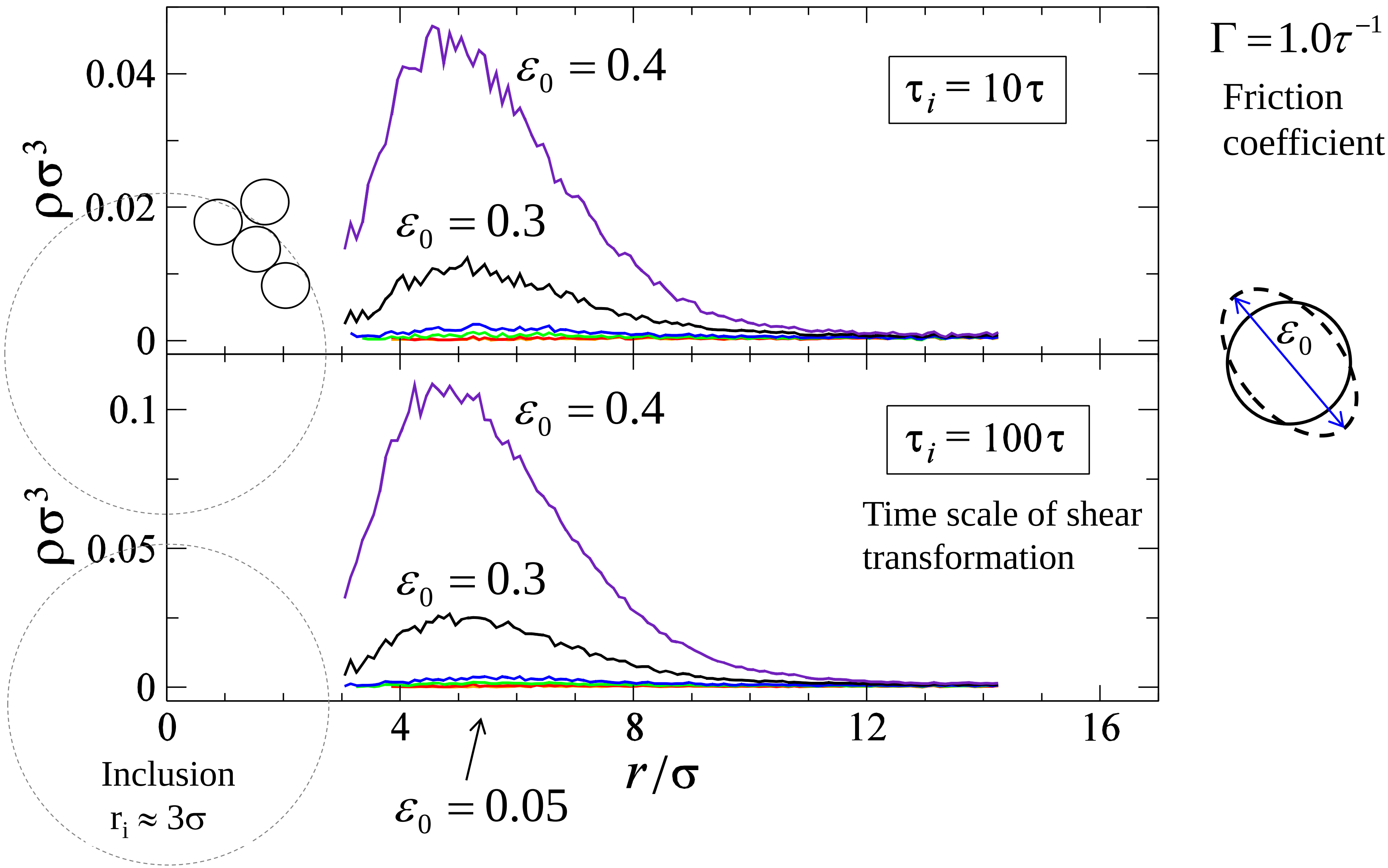
Friction coefficient Γ, duration of shear event τ_i

Snapshots of cage jump configurations for different strain amplitudes ε_o



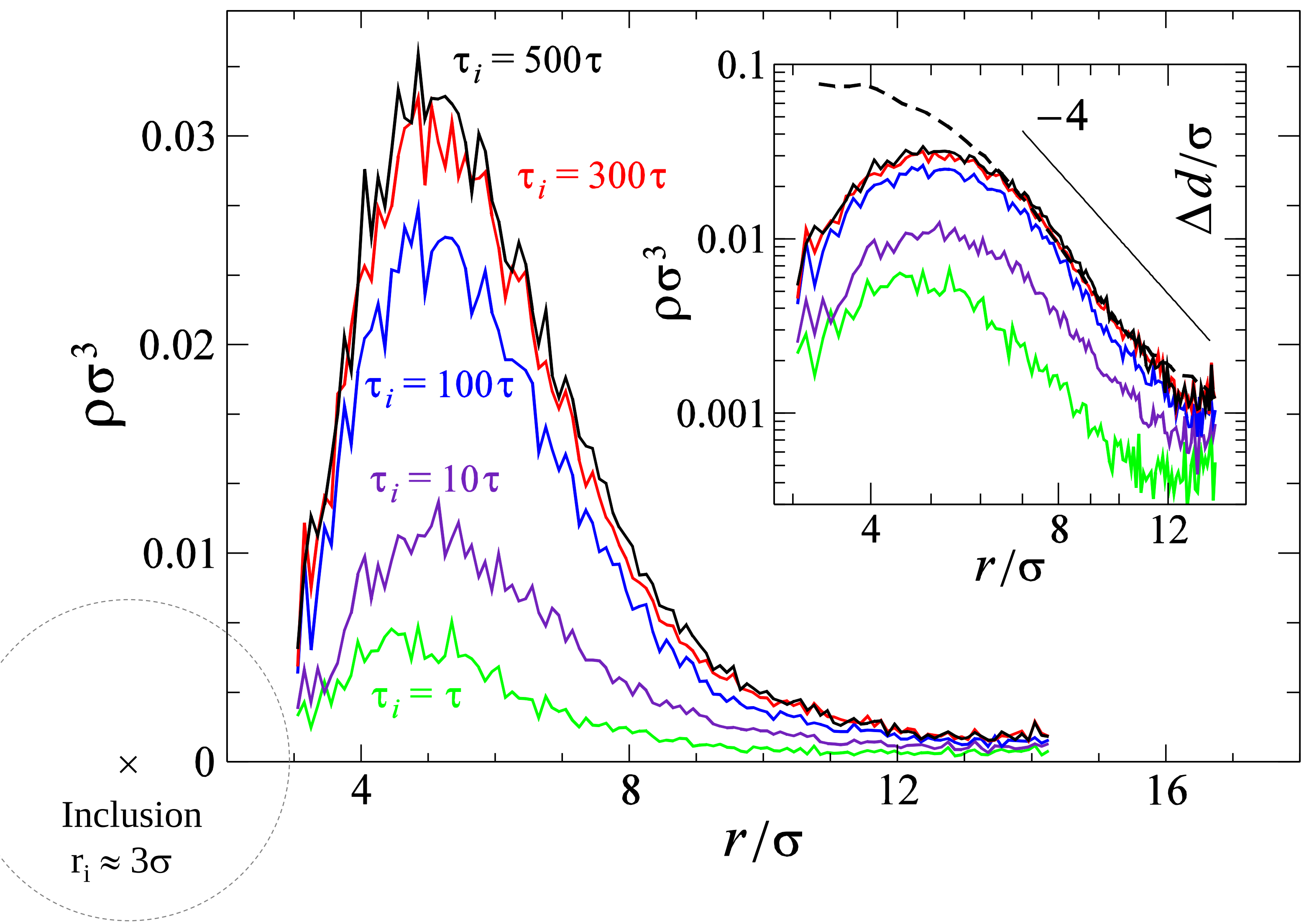
With increasing strain amplitude ε_o, the number of cage jumps increases and they tend to aggregate into compact clusters.

Radial density profiles of cage jumps ρ(r) for different strain amplitudes ε_o



The average density of cage jumps ρ(r) becomes larger as the strain amplitude increases.

Radial density profiles of cage jumps $\rho(r)$ for different times of shear event τ_i

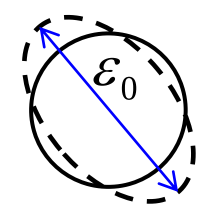


$\Gamma = 1.0\tau^{-1}$

Friction coefficient

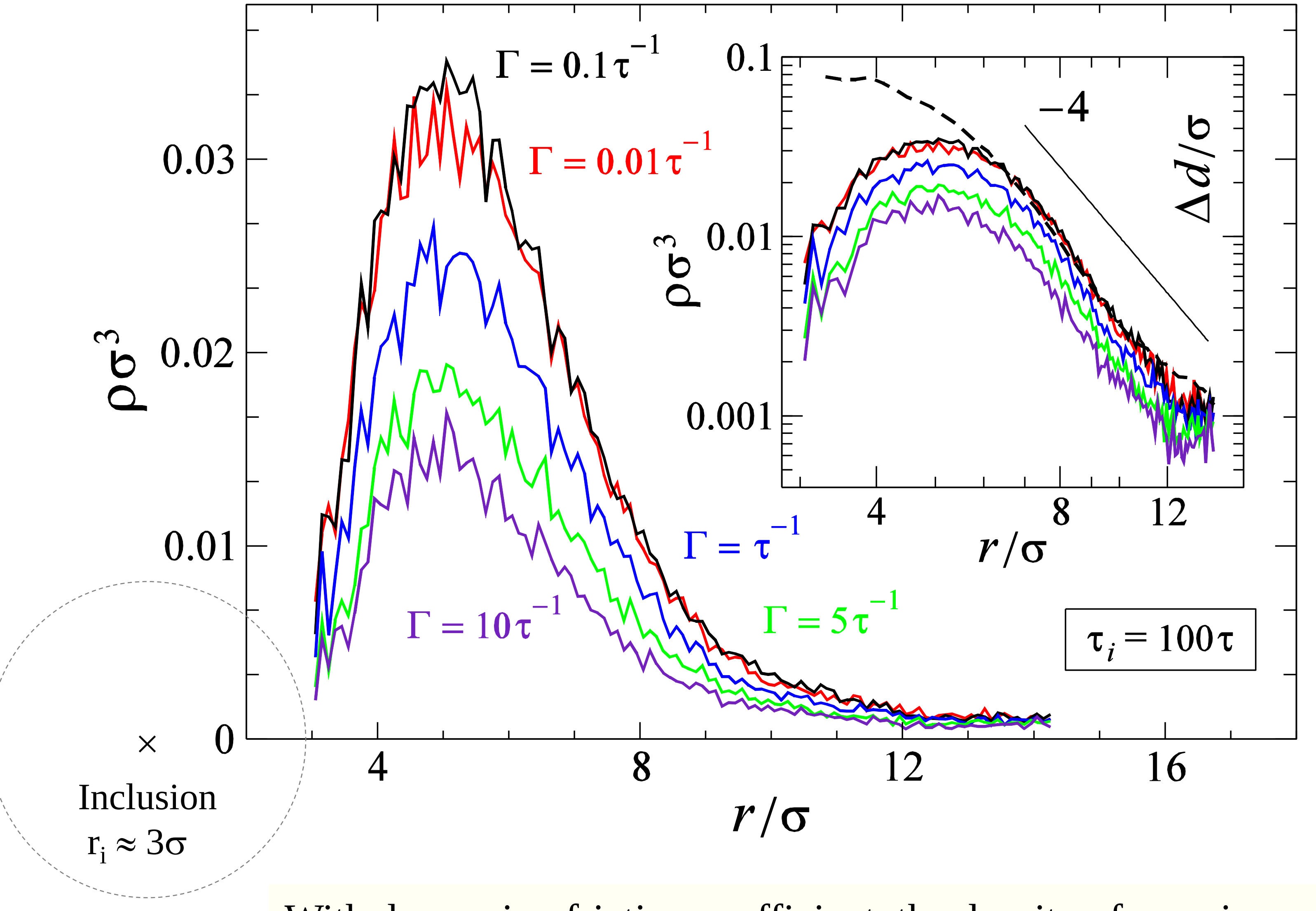
$\varepsilon_0 = 0.3$

Strain amplitude



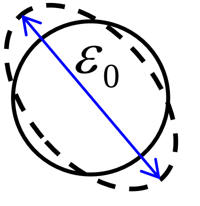
The density of cage jumps increases with increasing shear transformation time scale τ_i.

Radial density profiles of cage jumps ρ(r) for different friction coefficients Γ



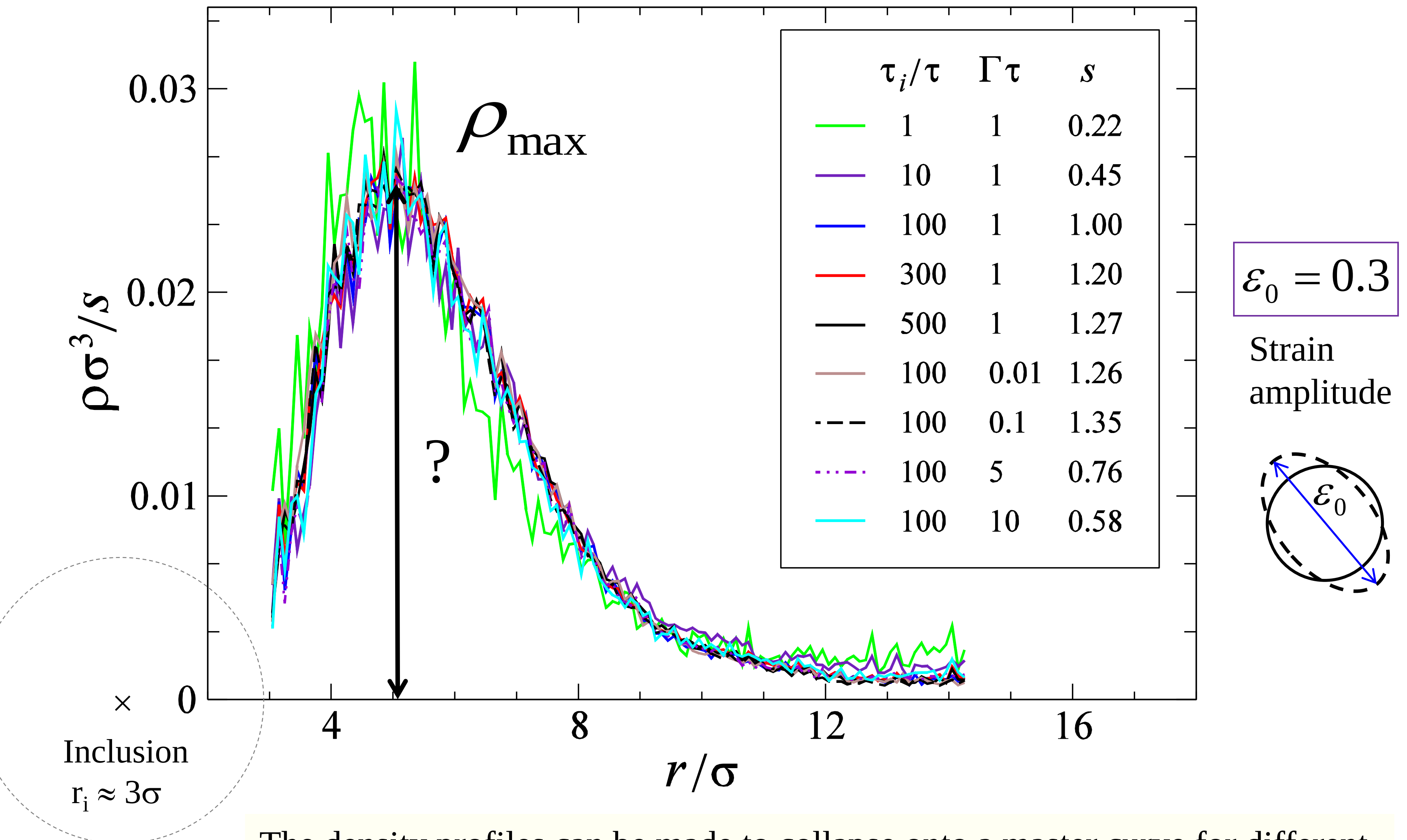
$\varepsilon_0 = 0.3$

Strain amplitude



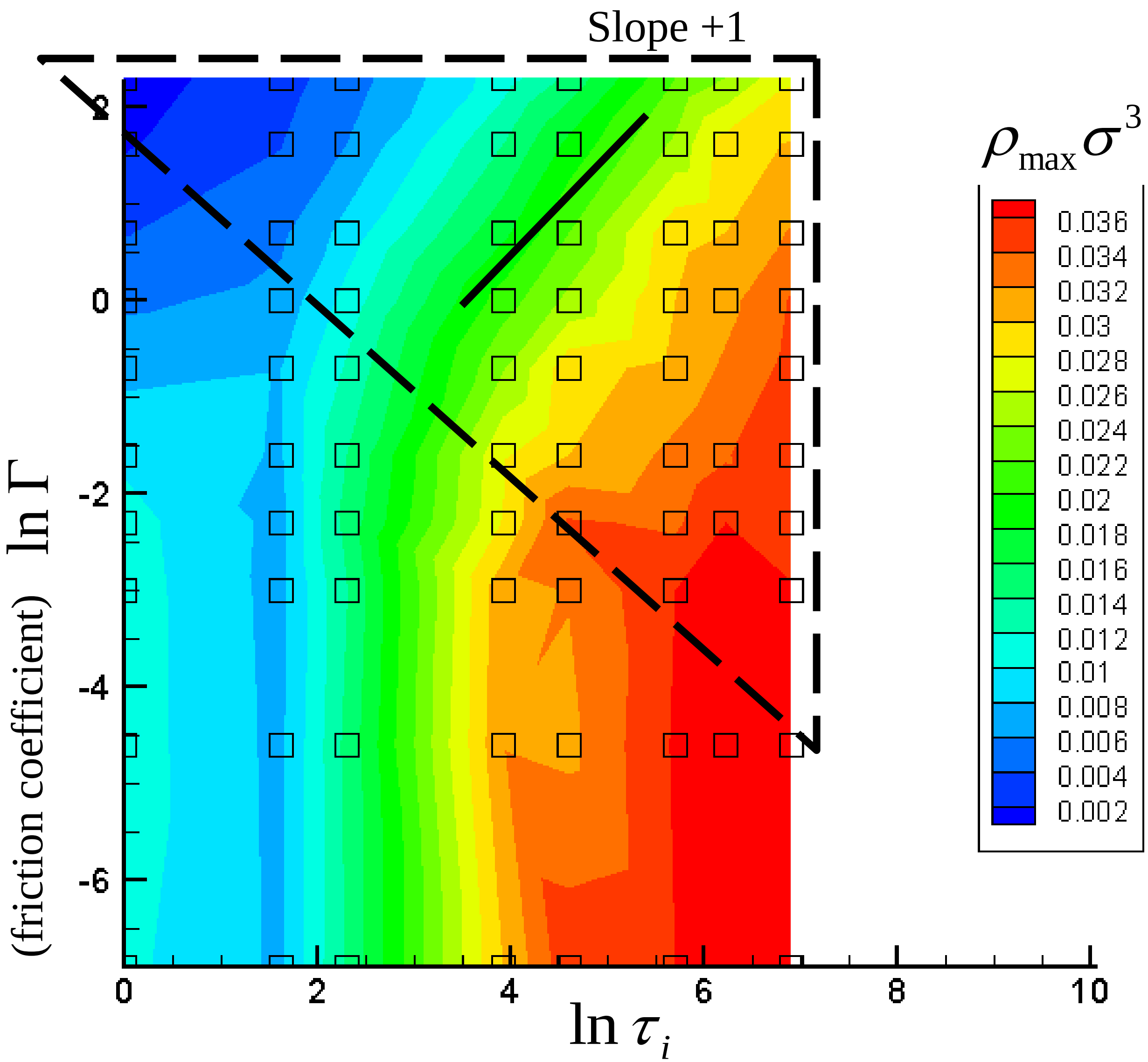
With decreasing friction coefficient, the density of cage jumps increases and it appears to saturate at small values of Γ.

Rescaled radial density profiles of cage jumps ρ for different τ_i and Γ



The density profiles can be made to collapse onto a master curve for different values of the friction coefficient Γ and the time scale of shear event τ_i.

Peak value of density profiles of cage jumps as a function of τ_i and Γ

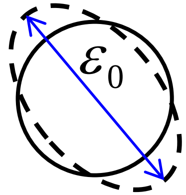


$\Gamma \sim \tau_i^{+1}$

$\rho_{\max}(\Gamma / \tau_i) = \text{const}$

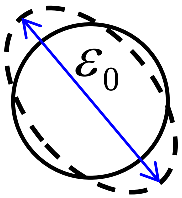
$\varepsilon_0 = 0.3$

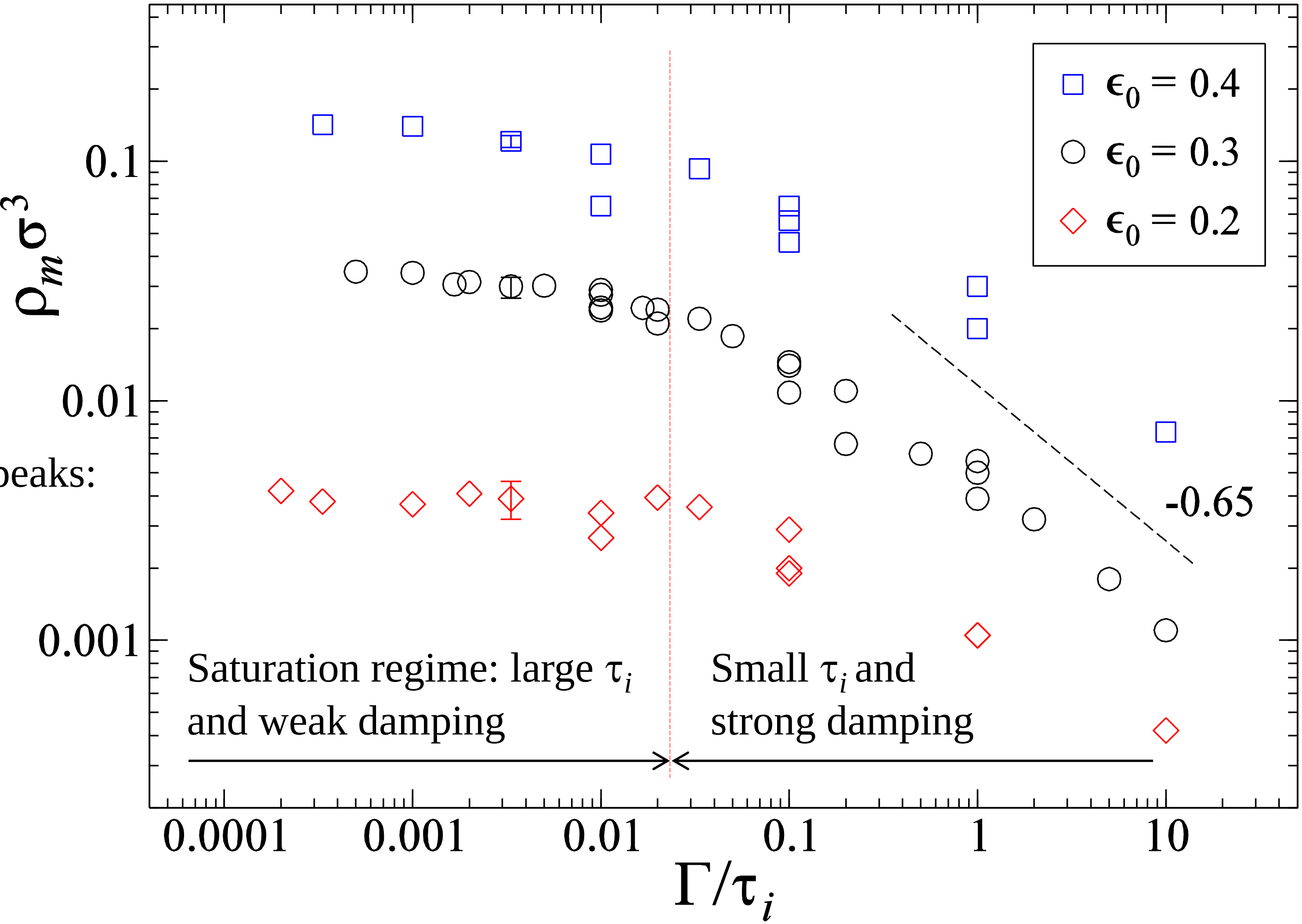
Strain amplitude



Log-log contour plot of the maximum of density profiles of cage jumps.

Maximum of density profiles of cage jumps as a function of Γ/τ_i



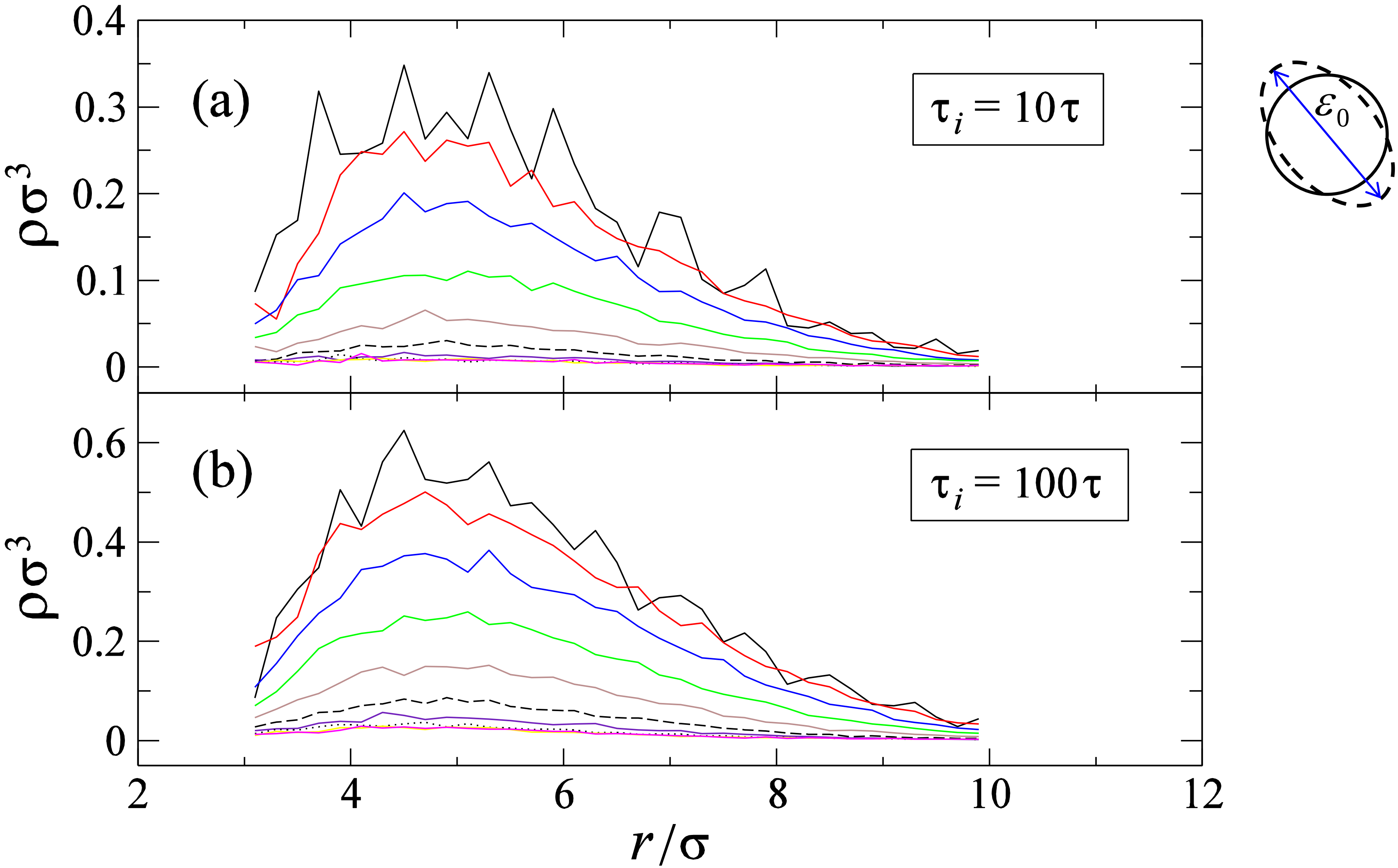


Rescale density peaks:

$$\rho_m \rightarrow \frac{\rho_m}{\varepsilon_o^5}$$

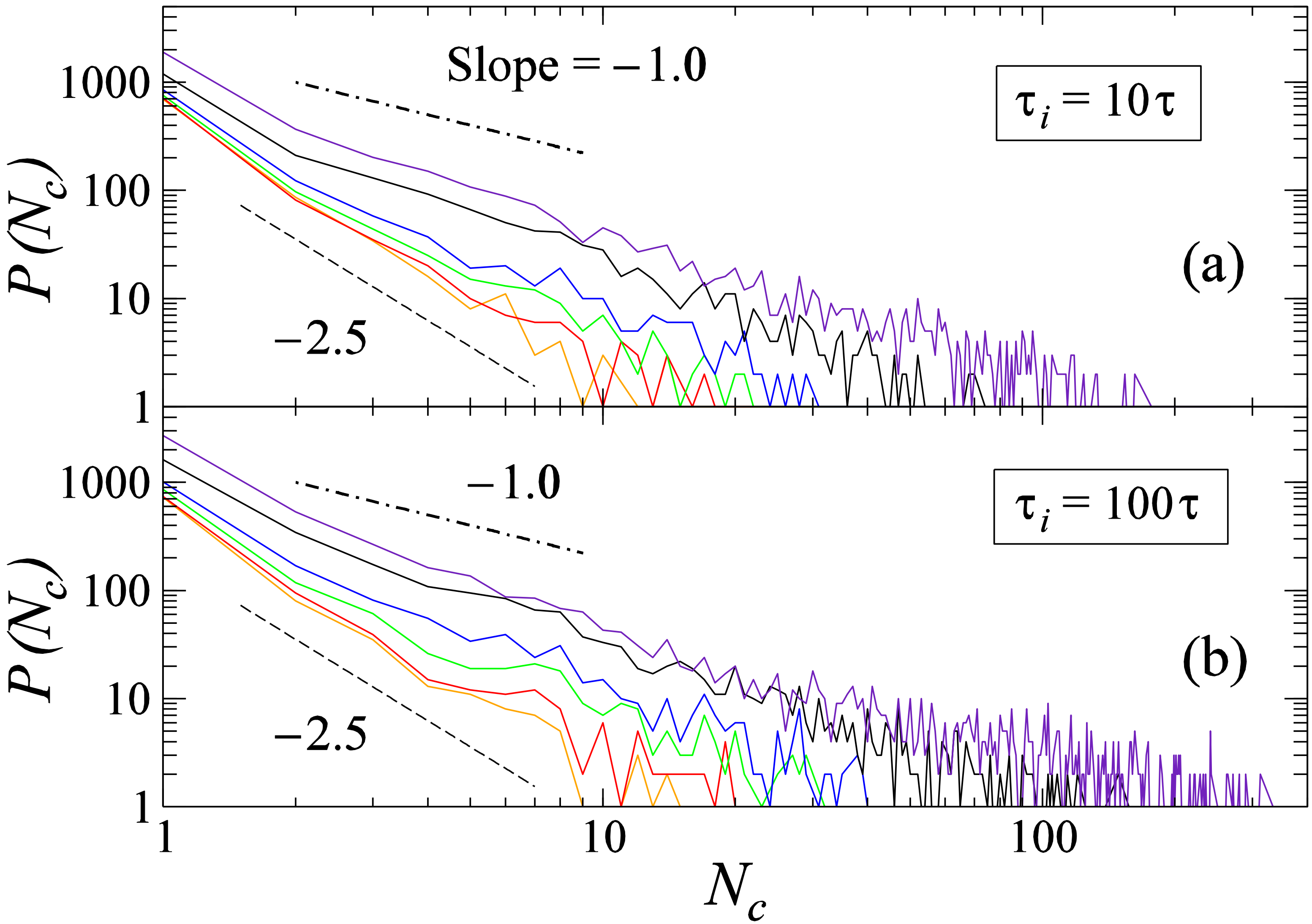
For a given strain amplitude, the peak values of the cage density profiles collapse onto a master curve as a function of the ratio Γ/τ_i : constant to power-law decay with the slope −0.65.

Angular dependence of the density profiles of cage jumps



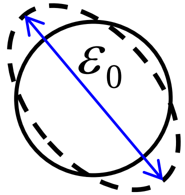
The angle is $\theta = 0^\circ, 10^\circ, 20^\circ, 30^\circ, 40^\circ, 50^\circ, 60^\circ, 70^\circ, 80^\circ, 90^\circ$ from top to bottom.

The probability distribution of cluster sizes of cage jumps



The strain amplitude is ε_0 = 0.05, 0.1, 0.15, 0.2, 0.3, and 0.4 from bottom to top.

Conclusions:



- Plastic deformation after <u>reversible local shear transformation</u> is studied using MD simulations of the binary 3D Lennard-Jones Kob-Andersen mixture.

- It was found that, in general, the density of irreversible cage jumps increases with increasing strain amplitude of the shear transformation.

- For a given strain amplitude ε_o, the density of cage jumps increases upon either increasing time scale of the shear event or decreasing friction coefficient.

- The peak values of the density profiles of cage jumps collapse onto master curves as a function of Γ/τ_i : crossover from constant to power-law decay $\rho_m \sim (\Gamma/\tau_i)^{-0.65}$.

$$\boxed{\rho_m \rightarrow \frac{\rho_m}{\varepsilon_o^5}}$$

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Numerical algorithm for detection of cage jumps

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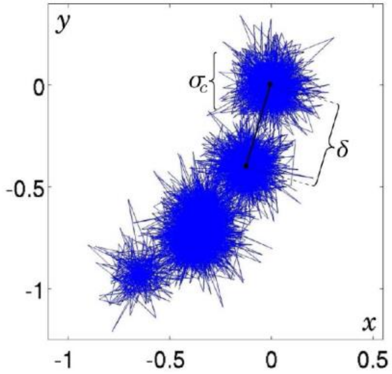

Candelier, Dauchot, Biroli, *PRL* (2009).