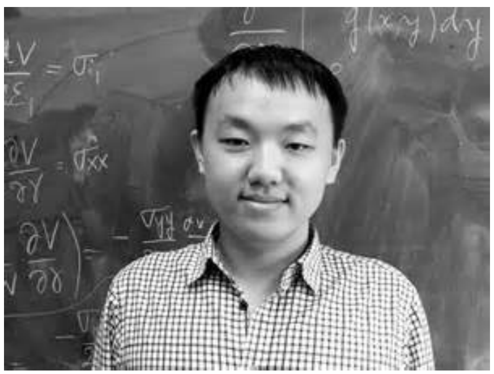
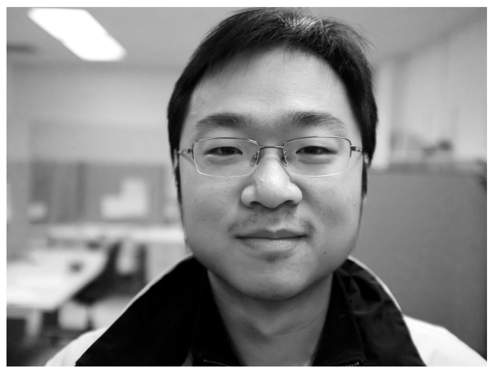
Mechanical properties of glasses: Rearrangements, reversibility, and ductility

Corey S. O'Hern
Department of Mechanical Engineering & Materials Science
Department of Physics
Department of Applied Physics
Yale University





Meng Fan, Yale

Minglei Wang, Yale

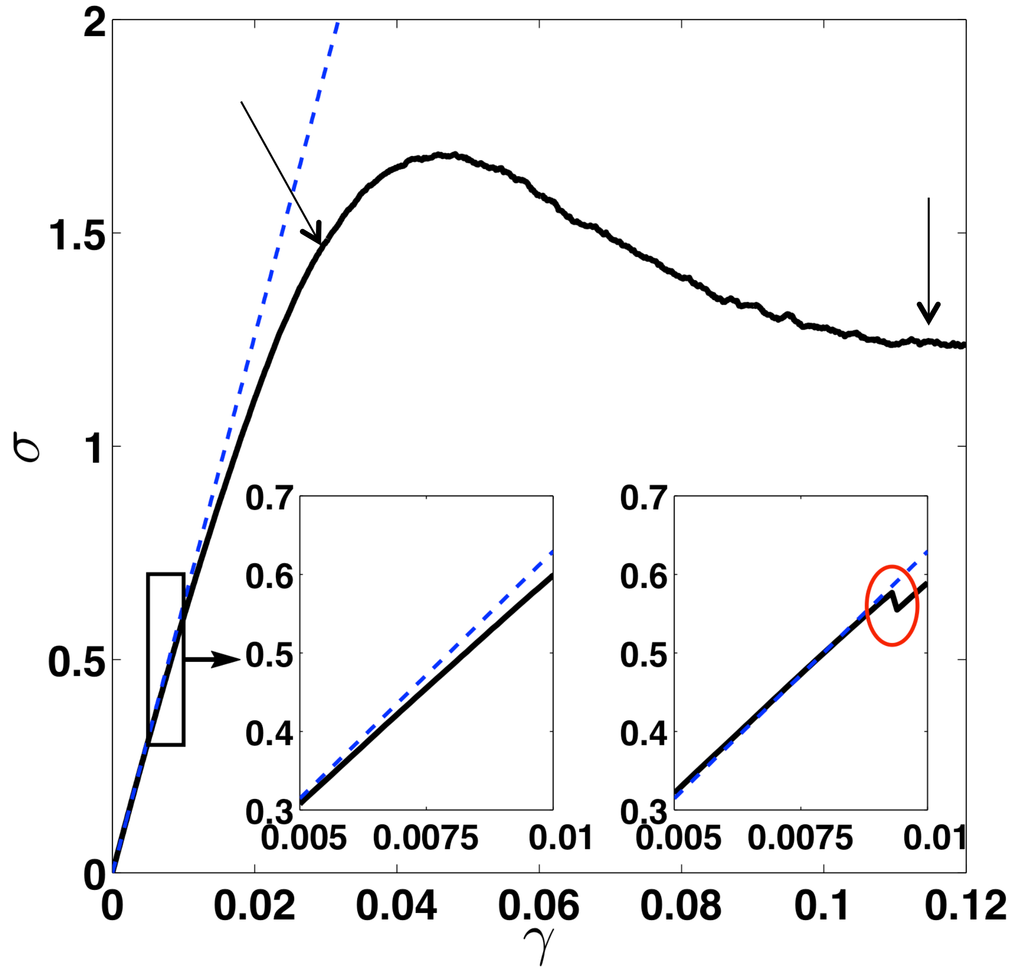
Jan Schroers, Yale

Mark D. Shattuck CCNY

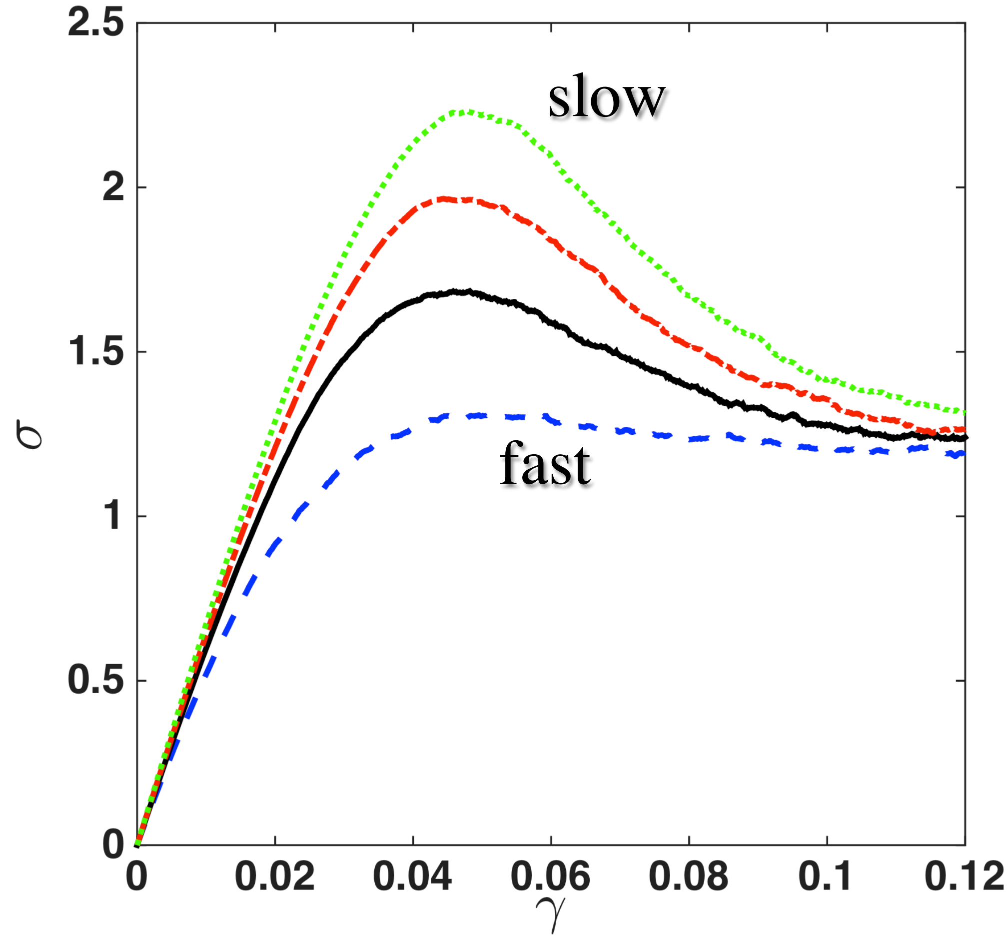
NSF MRSEC DMR-1119826 and CMMI-1462439

CRISP Center for Research on Interface Structures & Phenomena

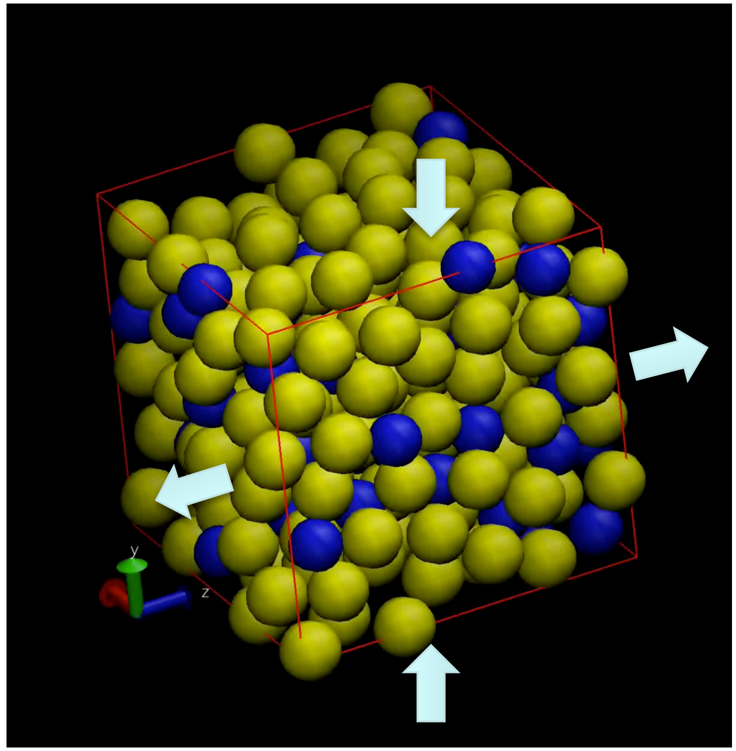
Nonlinear mechanical response (ensemble averages)



Cooling rate-dependent mechanical response



Mechanical Response to Pure Shear



γ=0.2

Athermal, quasistatic “pure shear” at constant pressure

Kob-Andersen binary Lennard-Jones mixtures

$$U(r_{ij}) = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]$$

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

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

$T(t) = T_0 - Rt$ $T_f=0$ $10^{-6} < R < 1$

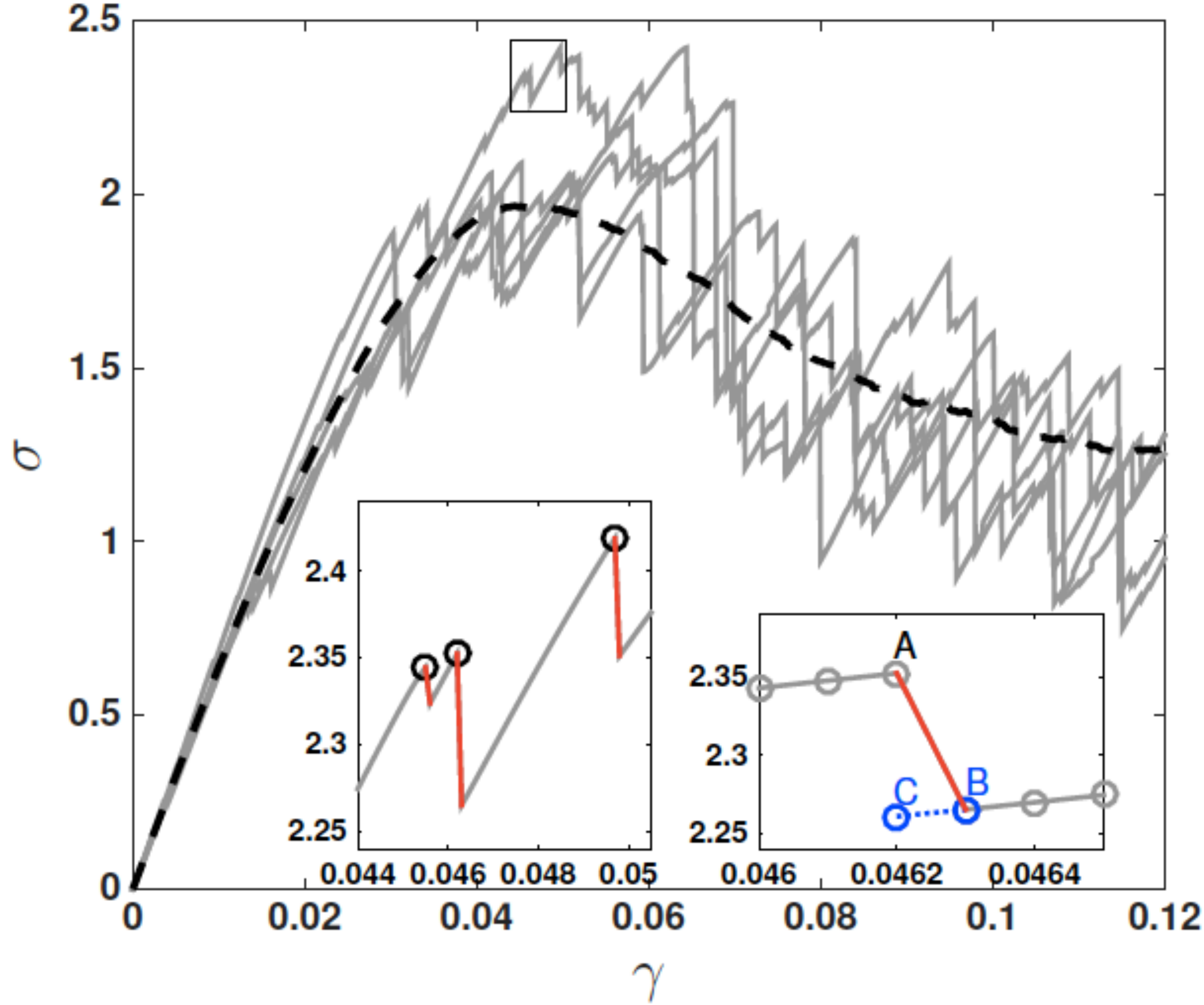
Stress Tensor

$$\hat{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{pmatrix}$$

$$U = \frac{1}{N}\sum_{i<j} U\left(r_{ij}\right)$$

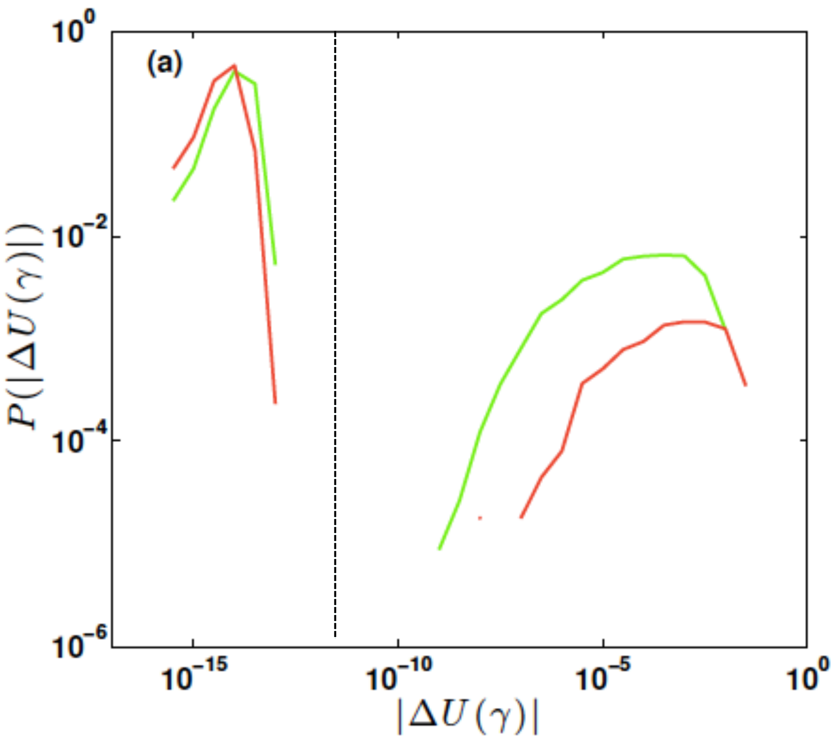
$$\vec{F}_i = \vec{\nabla}_i U\left(r_{ij}\right)$$

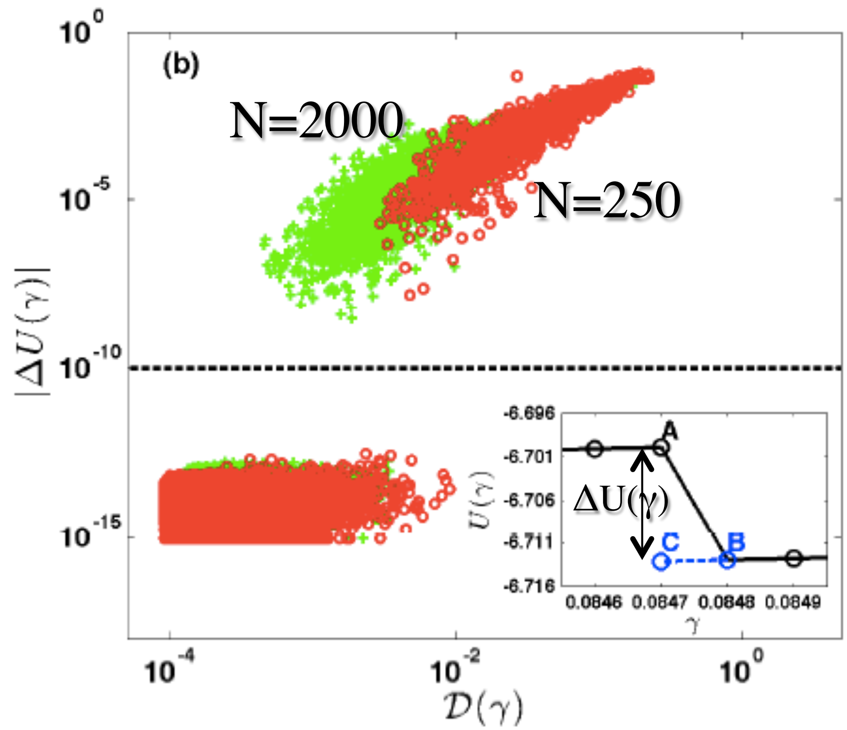
$$\sigma_{\alpha\beta} = V^{-1}\sum_{i<j} r_{ij\alpha} F_{ij\beta}$$



2.5
2
1.5
1
0.5
0
0.02
0.04
0.06
0.08
0.1
0.12
σ
γ
2.4
2.35
2.3
2.25
0.044
0.046
0.048
0.05
A
B
C
0.0462
0.0464

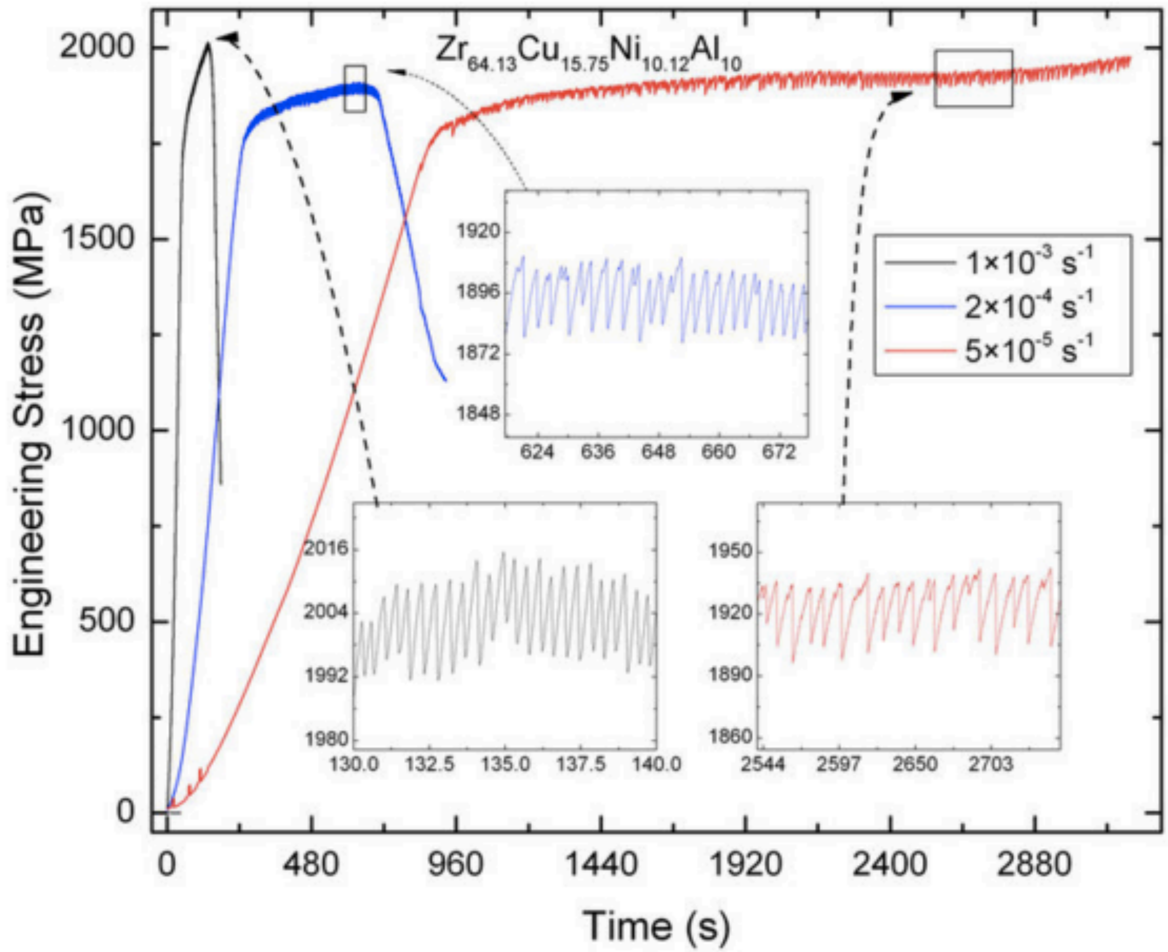
Particle Rearrangement Events





$$D(\gamma) = \frac{\left|\vec{R}(\gamma + d\gamma) - \vec{R}(\gamma) J(d\gamma)\right|}{N}$$

Figure 2: Compression stress-time profiles of $Zr_{64.13}Cu_{15.75}Ni_{10.12}Al_{10}$ ingots (by atomic percent)[13,14].



Cylindrical samples, 2 mm in diameter and 4 mm in length, have been compressed along their 4-mm axis at fixed strain rates and at room temperature, 298 K. Insets show sudden drops in the applied stress, as the ingots are compressed at various constant strain rates. These stress drops indicate the occurrence of slip avalanches in the material.

"Tuned critical avalanche scaling in bulk metallic glasses," J. Antonaglia, X. Xie, G. Schwarz, M. Wraith, J. Qiao, Y. Zhang, P. K. Liaw, J. T. Uhl, and K. A. Dahmen, Scientific Reports 4 (2014) 4382.

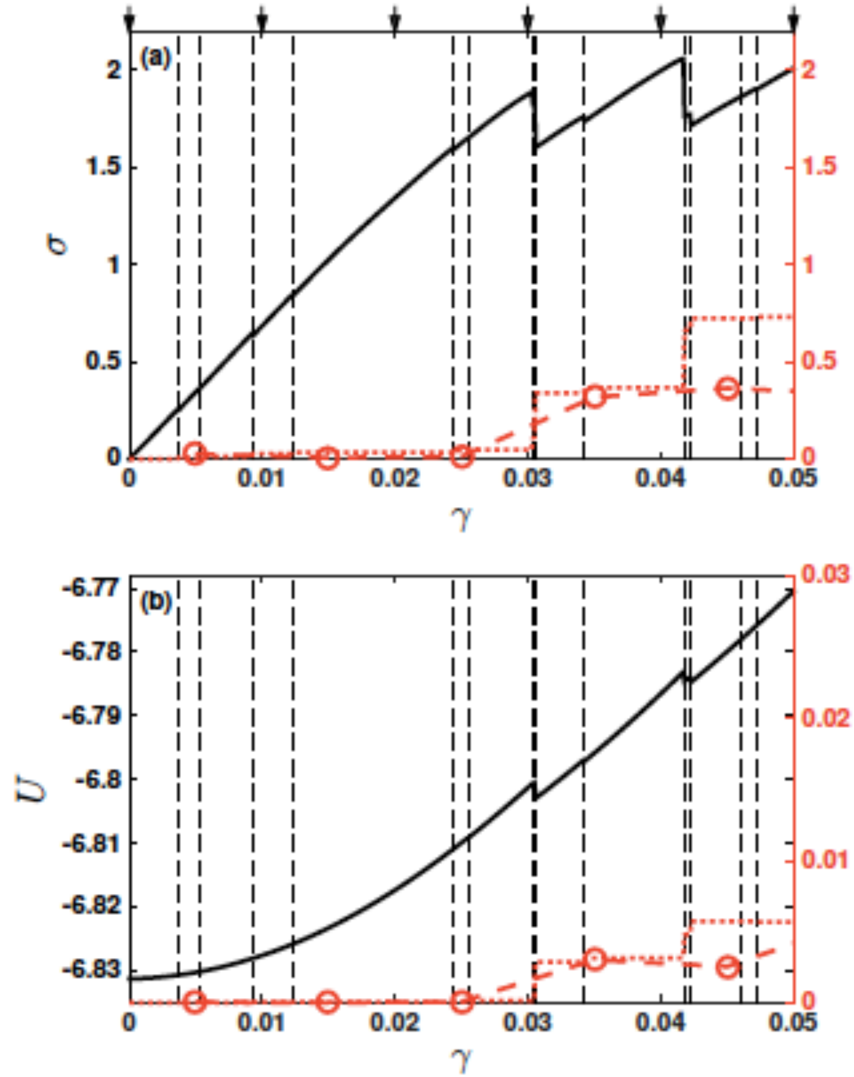
$$\sigma(\gamma) = \sigma_{\text{elastic}}(\gamma) - \overbrace{\sigma_{\text{loss}}(\gamma)}^{\text{rearrangements}} - \overbrace{\sigma'_{\text{loss}}(\gamma)}^{\text{softening}}$$

$$U(\gamma) = U_{\text{elastic}}(\gamma) - U_{\text{loss}}(\gamma) - U'_{\text{loss}}(\gamma)$$

Rearrangements

$$\sigma_{\mathrm{loss}}(\gamma) = \sum_{i=1}^{N_r(\gamma)} |\Delta\sigma(\gamma_i)|$$

$$U_{\mathrm{loss}}(\gamma) = \sum_{i=1}^{N_r(\gamma)} |\Delta U(\gamma_i)|,$$



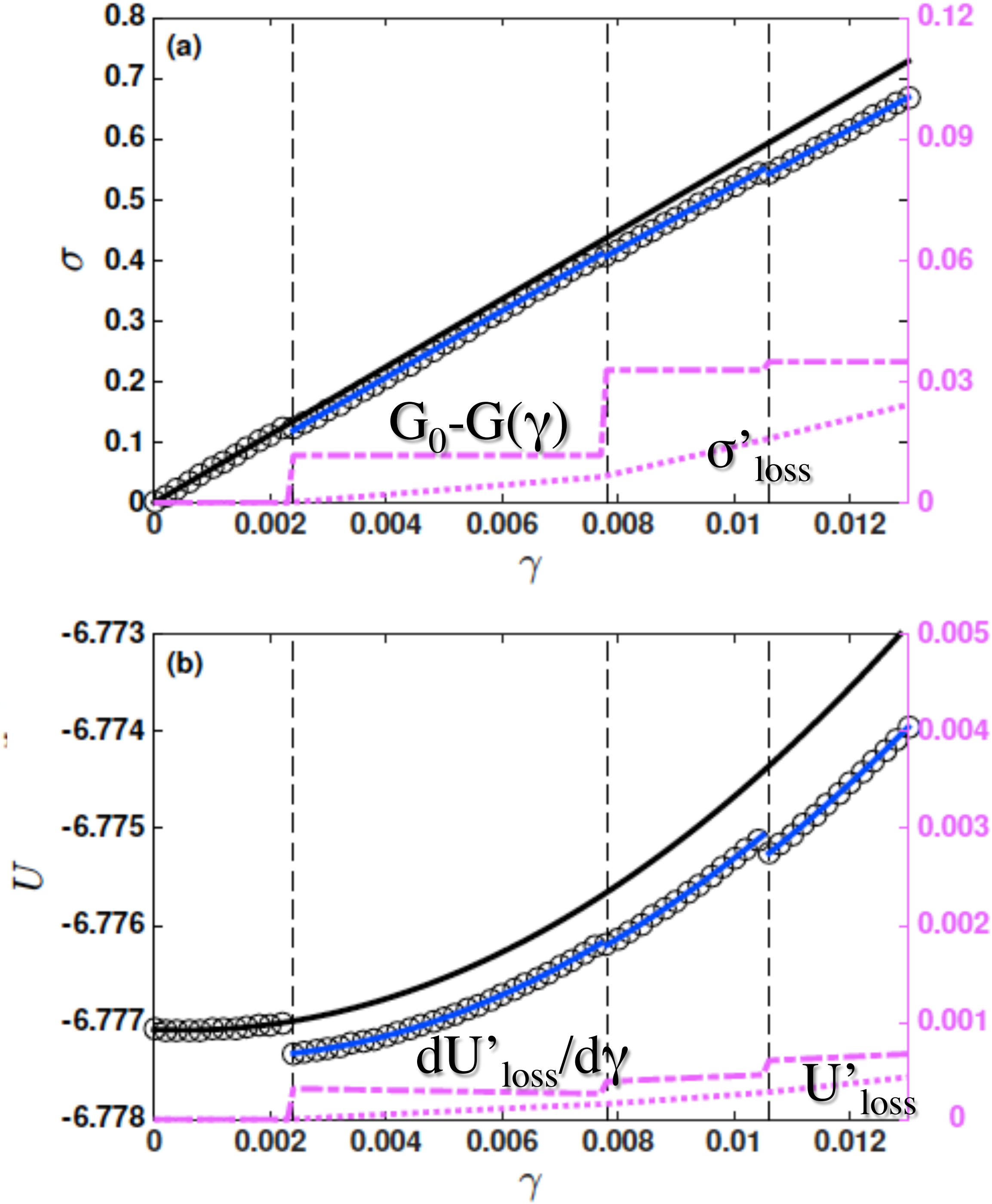
σ_{loss}

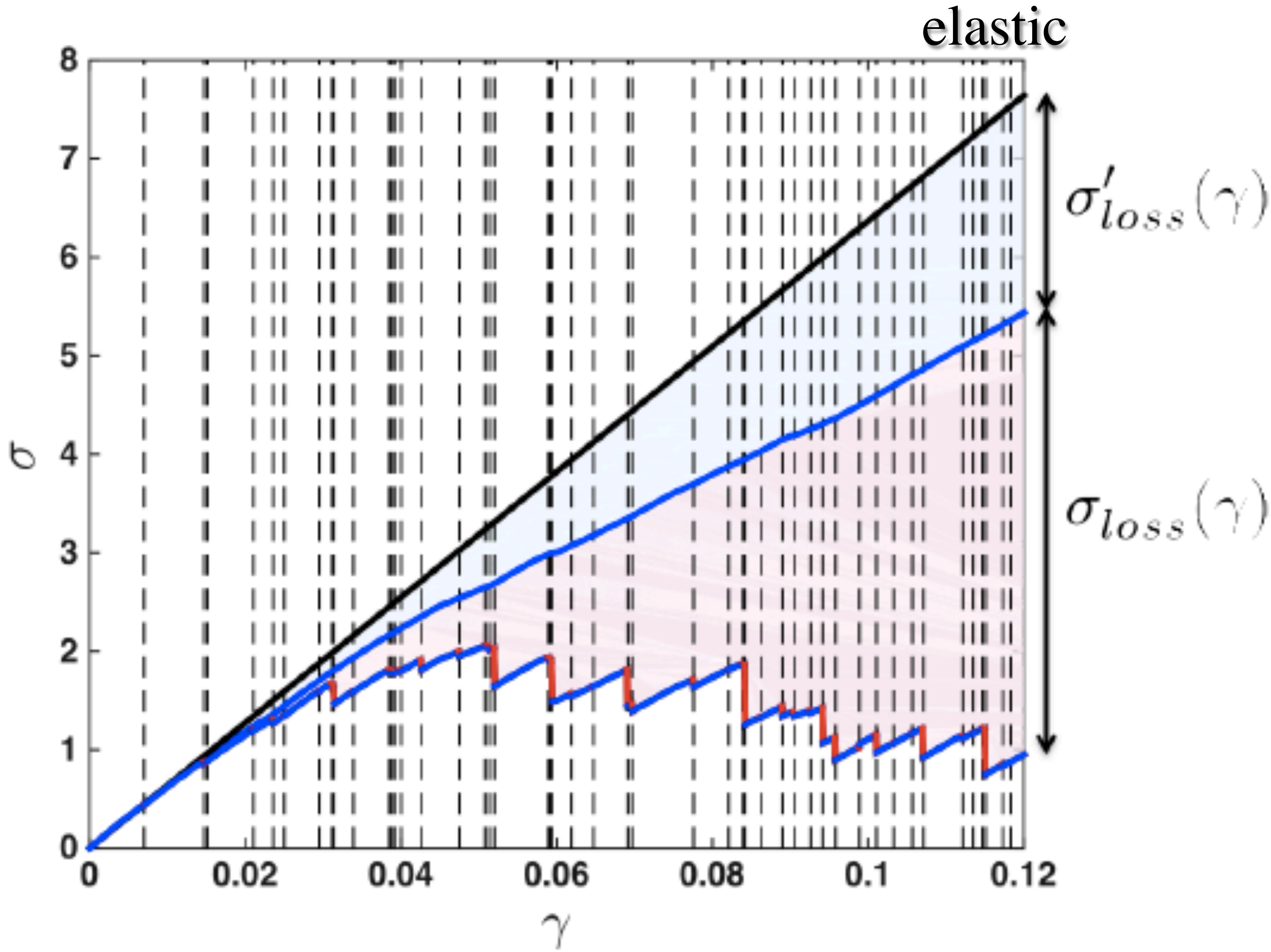
U_{loss}

Softening

$$\left[\frac{d\sigma'_{\rm loss}}{d\gamma}\right](\gamma) = G_0 - G(\gamma)$$

$$\sigma'_{\rm loss}(\gamma) = \int_0^{\gamma} (d\sigma'_{\rm loss}/d\gamma')d\gamma'$$





elastic
$\sigma'_{loss}(\gamma)$
$\sigma_{loss}(\gamma)$
σ
γ
0
0.02
0.04
0.06
0.08
0.1
0.12
1
2
3
4
5
6
7
8

Rearrangements

$$\frac{d\sigma_{loss}}{d\gamma} = \frac{d\sigma_{loss}}{dN_r}\frac{dN_r}{d\gamma}$$

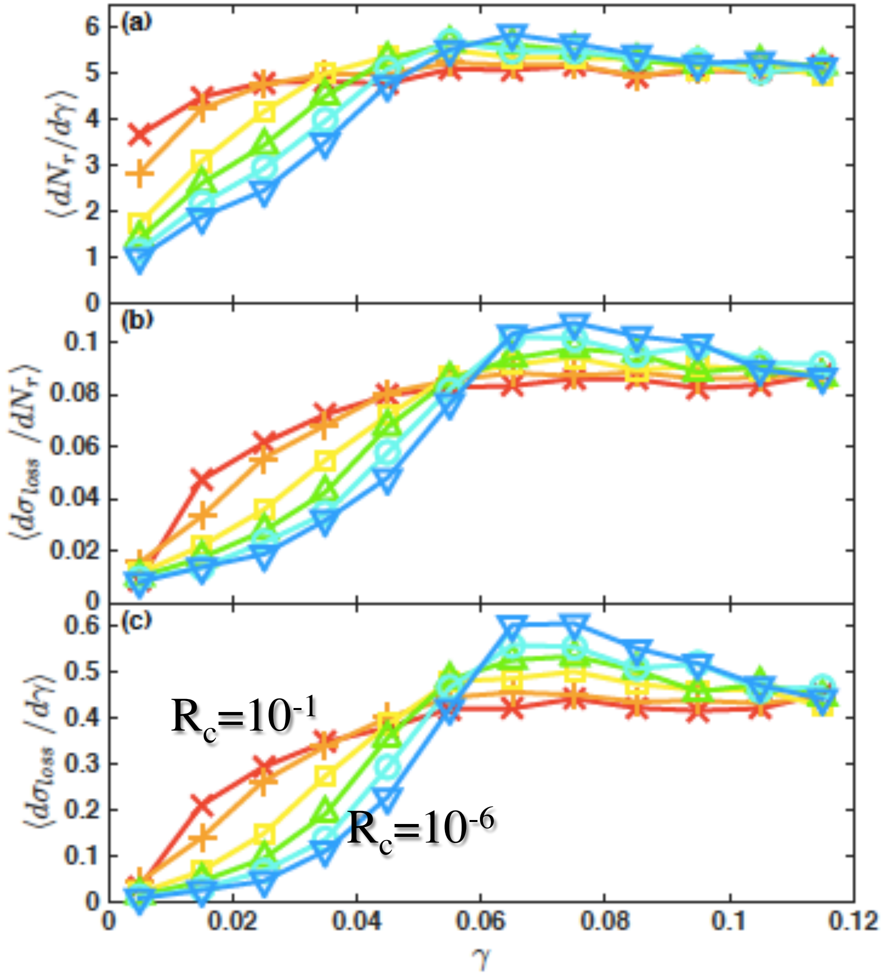
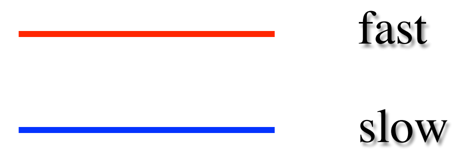


Figure 5: Ensemble-averaged (a) rearrangement frequency $\langle dN_r/d\gamma \rangle$, (b) stress loss per rearrangement $\langle d\sigma_{\text{loss}}/dN_r \rangle$, and (c) rearrangement-induced stress loss per (1%) strain $\langle d\sigma_{\text{loss}}/d\gamma \rangle$ plotted versus strain γ for glasses undergoing AQS pure shear. The glasses were prepared using cooling rates $R = 10^{-1}$ (crosses), 10^{-2} (plus signs), 10^{-3} (squares), 10^{-4} (upward triangles), 10^{-5} (circles), and 10^{-6} (downward triangles). All data is obtained by averaging over 500 independent samples with $N = 2000$.



Softening

fast

slow

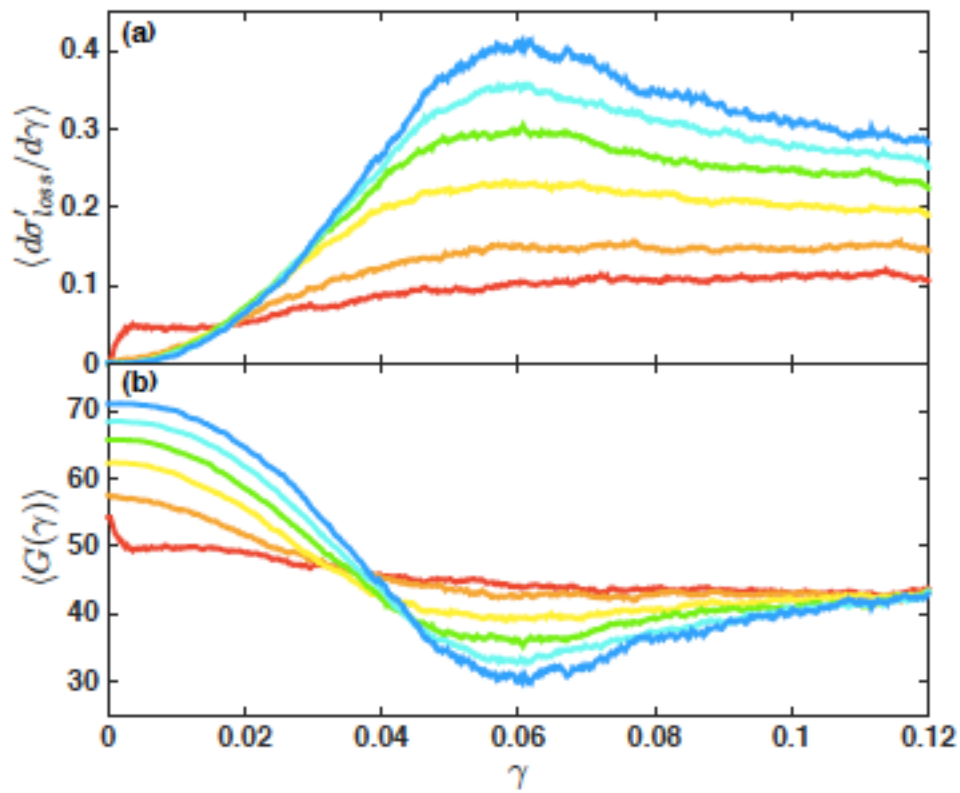


Figure 6: Ensemble-averaged (a) softening-induced stress loss per (1%) strain $\langle d\sigma'_{\rm loss}/d\gamma \rangle$ and (b) local slope of the continuous stress versus strain segments $\langle G(\gamma) \rangle$ plotted versus strain γ for cooling rates $R = 10^{-1}$ (red), 10^{-2} (orange), 10^{-3} (yellow), 10^{-4} (green), 10^{-5} (cyan), and 10^{-6} (blue). All data is obtained by averaging over 500 configurations with $N = 2000$.

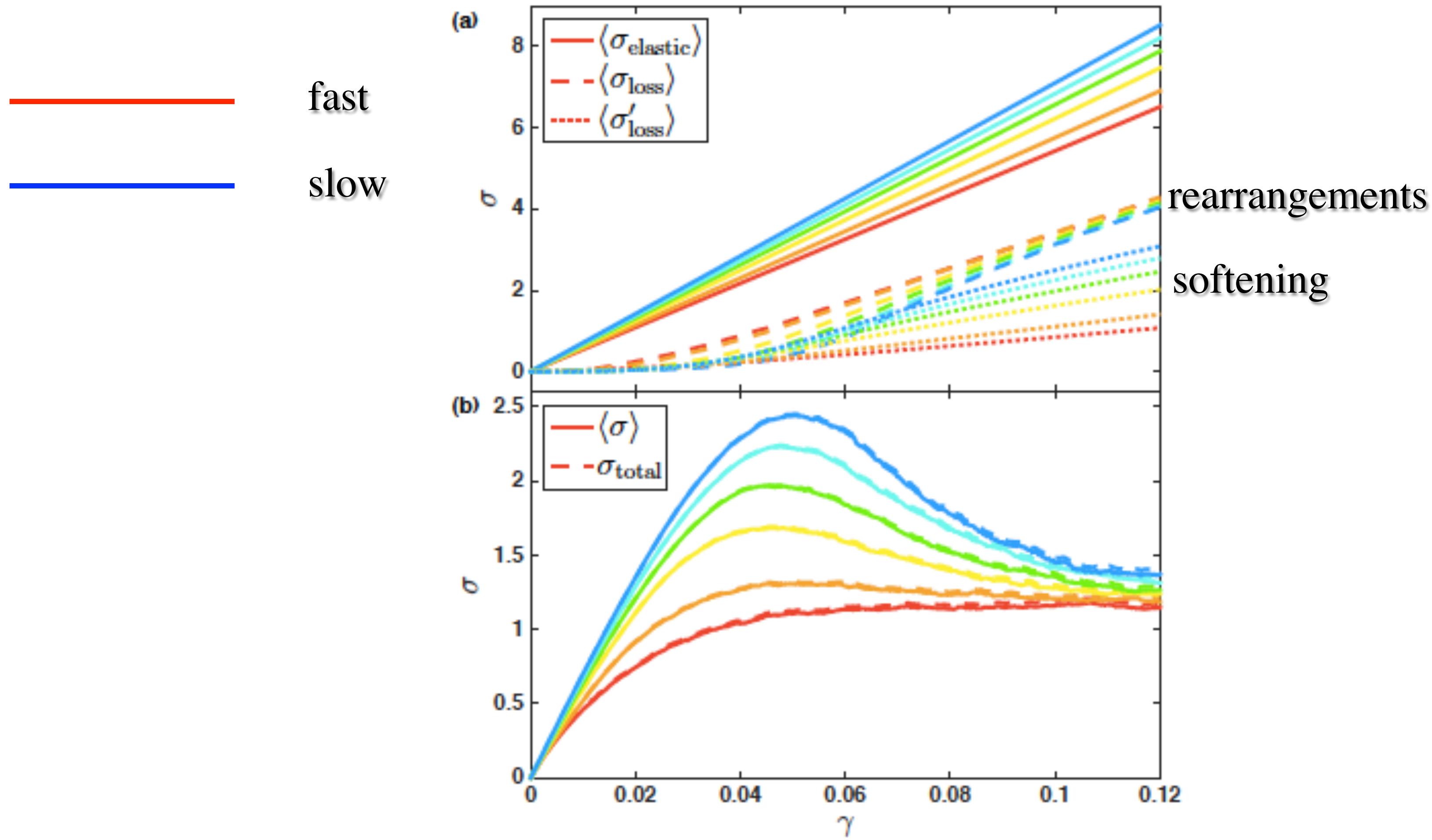
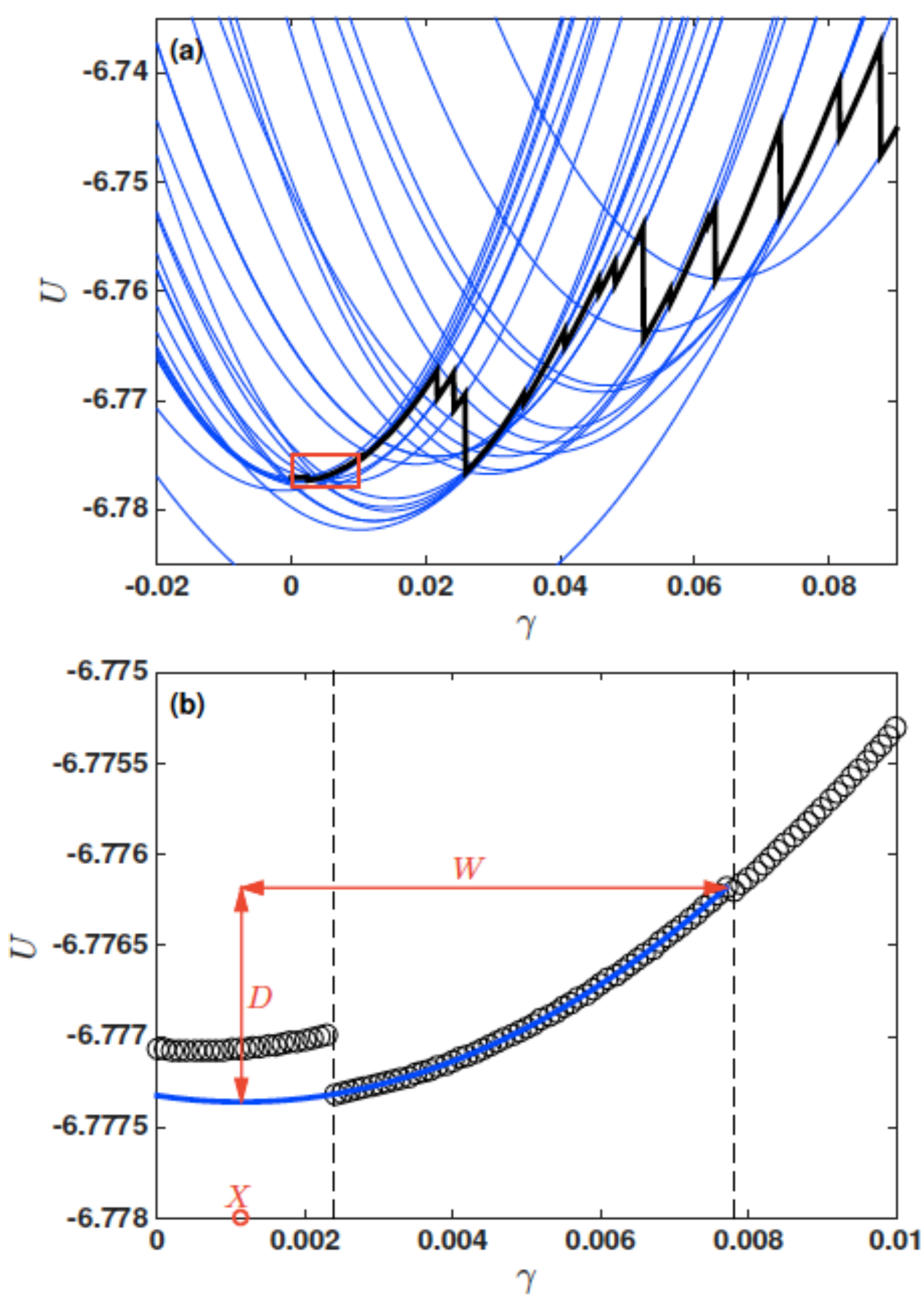
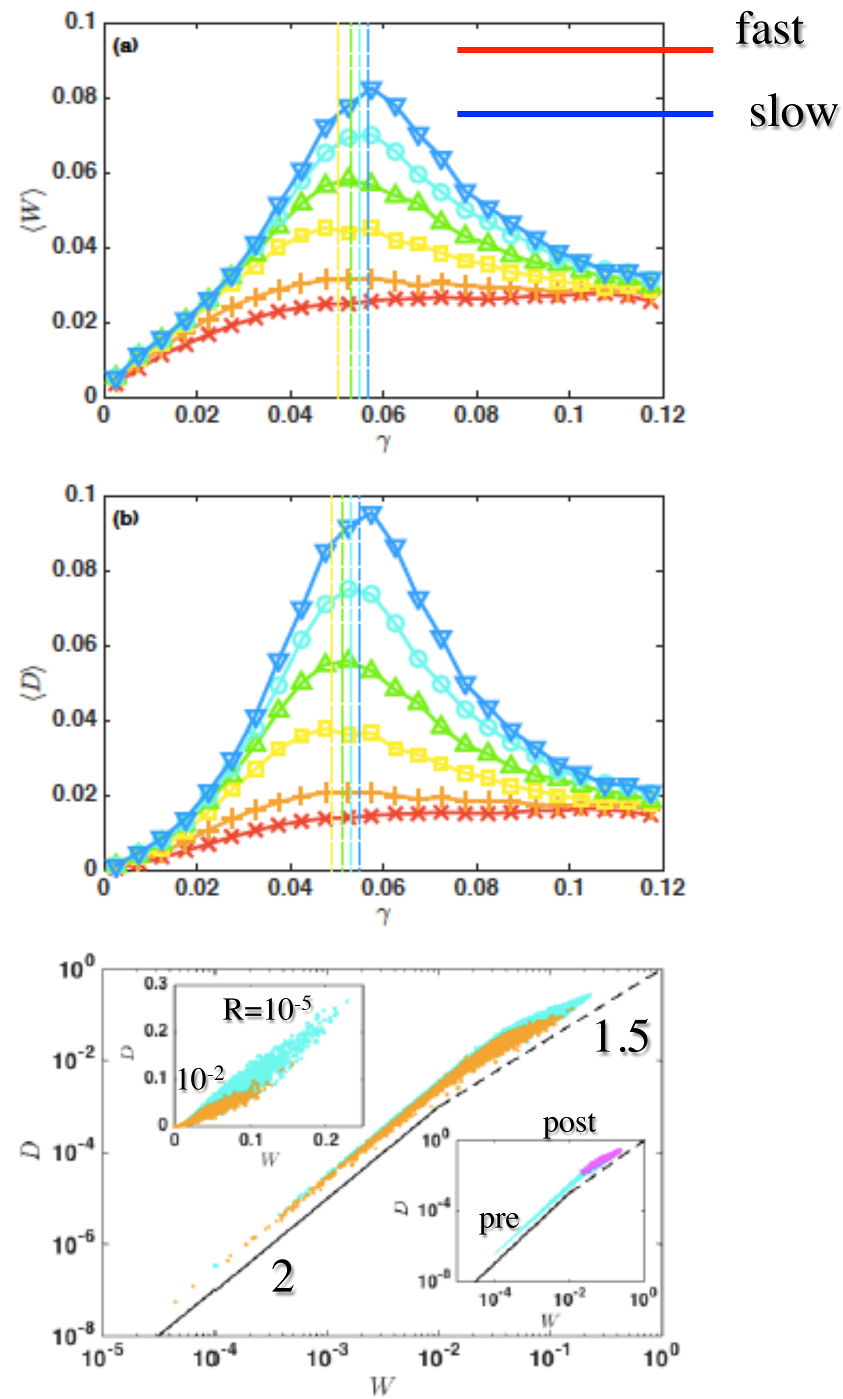


Figure 7: Ensemble-averaged (a) elastic stress $\sigma_{\rm elastic}(\gamma)$ (solid), rearrangement-induced stress loss $\sigma_{\rm loss}(\gamma)$ (dashed), and softening-induced stress loss $\sigma'_{\rm loss}(\gamma)$ (dotted) plotted versus strain γ. (b) Ensemble-averaged stress $\langle\sigma(\gamma)\rangle$ and the stress $\sigma_{\rm total}$ obtained by combining the elastic stress, and the rearrangement- and softening-induced stress losses (Eq. 3) plotted versus γ. In both (a) and (b), the system size $N = 2000$, and six cooling rates, $R = 10^{-1}$ (red), 10^{-2} (orange), 10^{-3} (yellow), 10^{-4} (green), 10^{-5} (cyan), and 10^{-6} (blue) are shown.

Extracting elastic segments

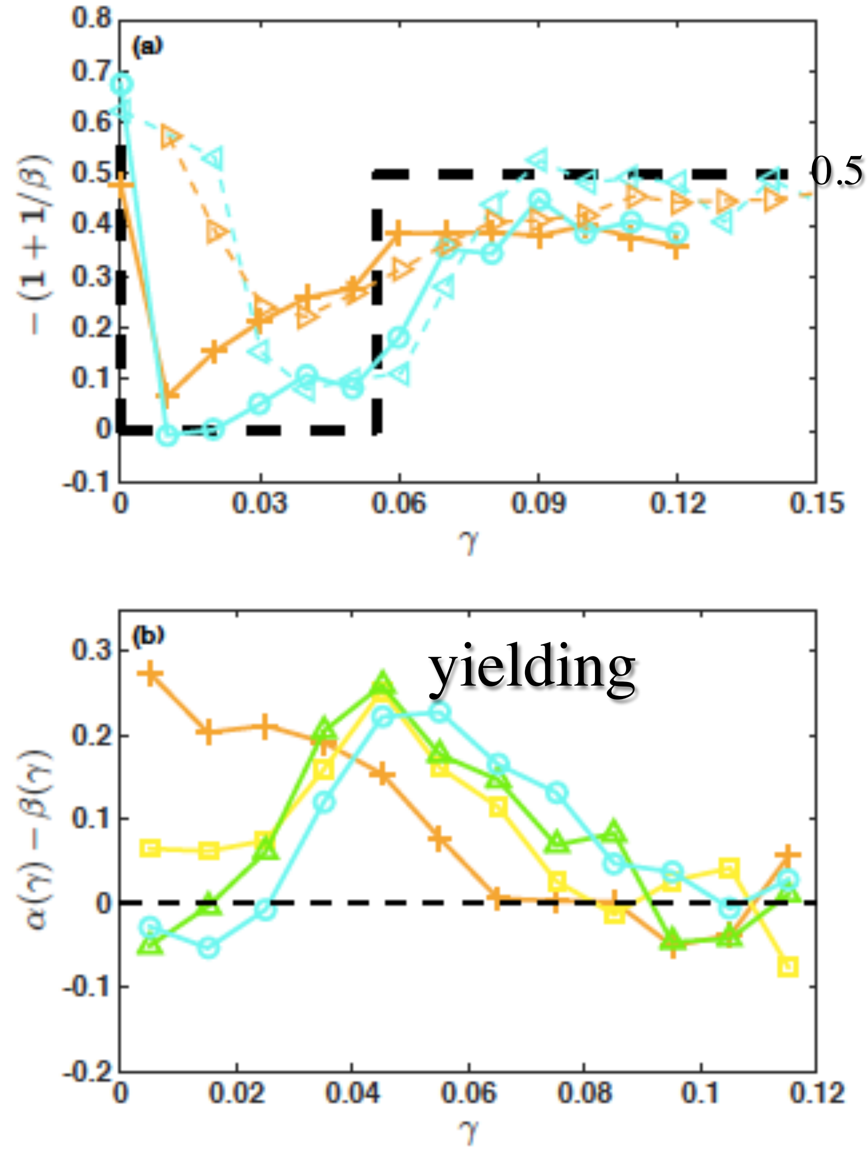


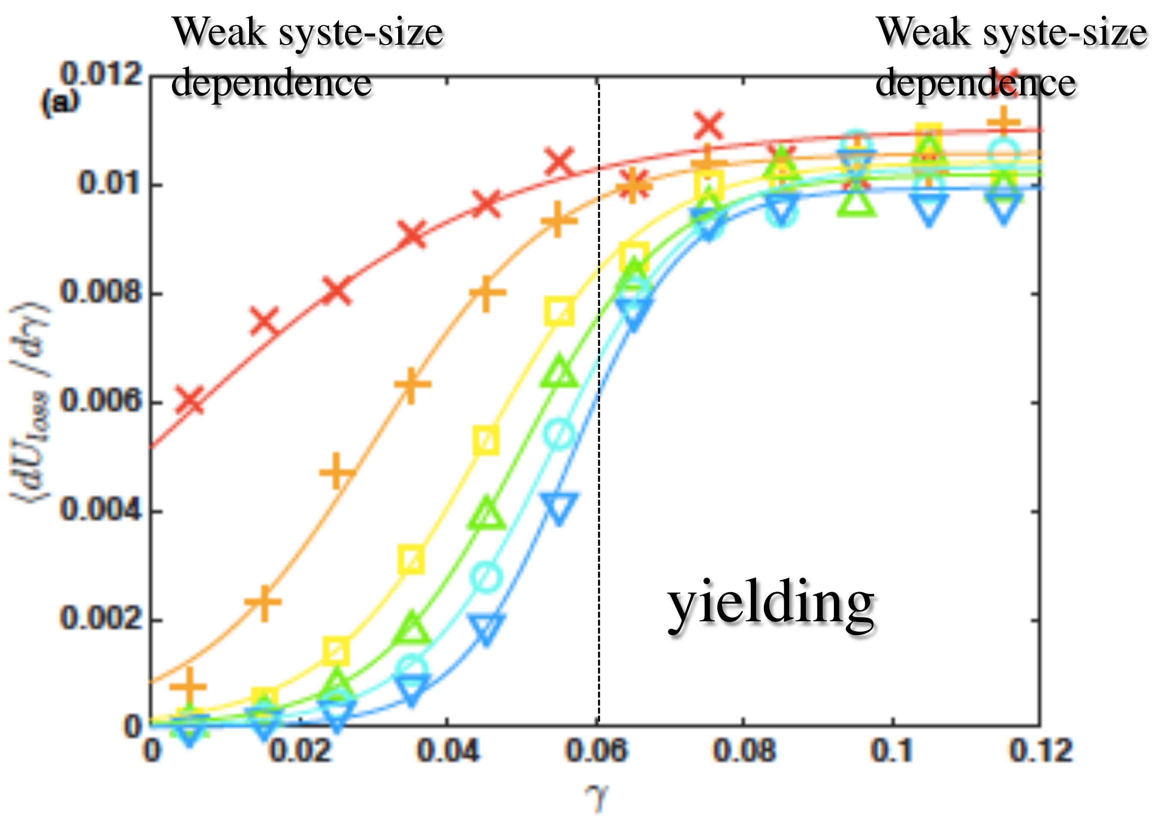


System-size scaling of rearrangements

$$\langle dU_{\mathrm{loss}}/dN_r \rangle \sim N^{\alpha(\gamma)}$$

$$\langle dN_r/d\gamma \rangle \sim N^{-\beta(\gamma)}$$




Weak syste-size
dependence
Weak syste-size
dependence
(a)
yielding
0.012
0.01
0.008
0.006
0.004
0.002
0
0
0.02
0.04
0.06
0.08
0.1
0.12
$\langle dU_{loss}/d\gamma \rangle$
γ

Athermal, quasistatic simple shear at constant pressure in granular materials

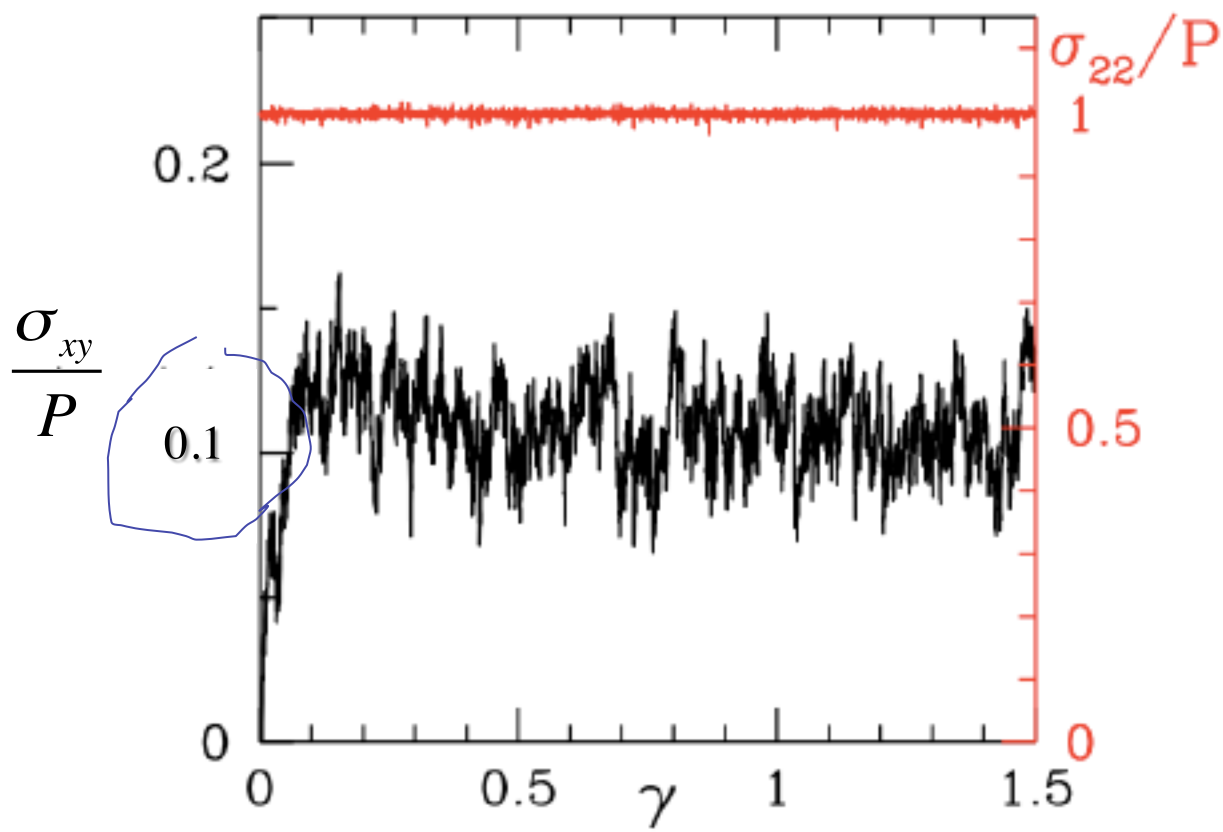
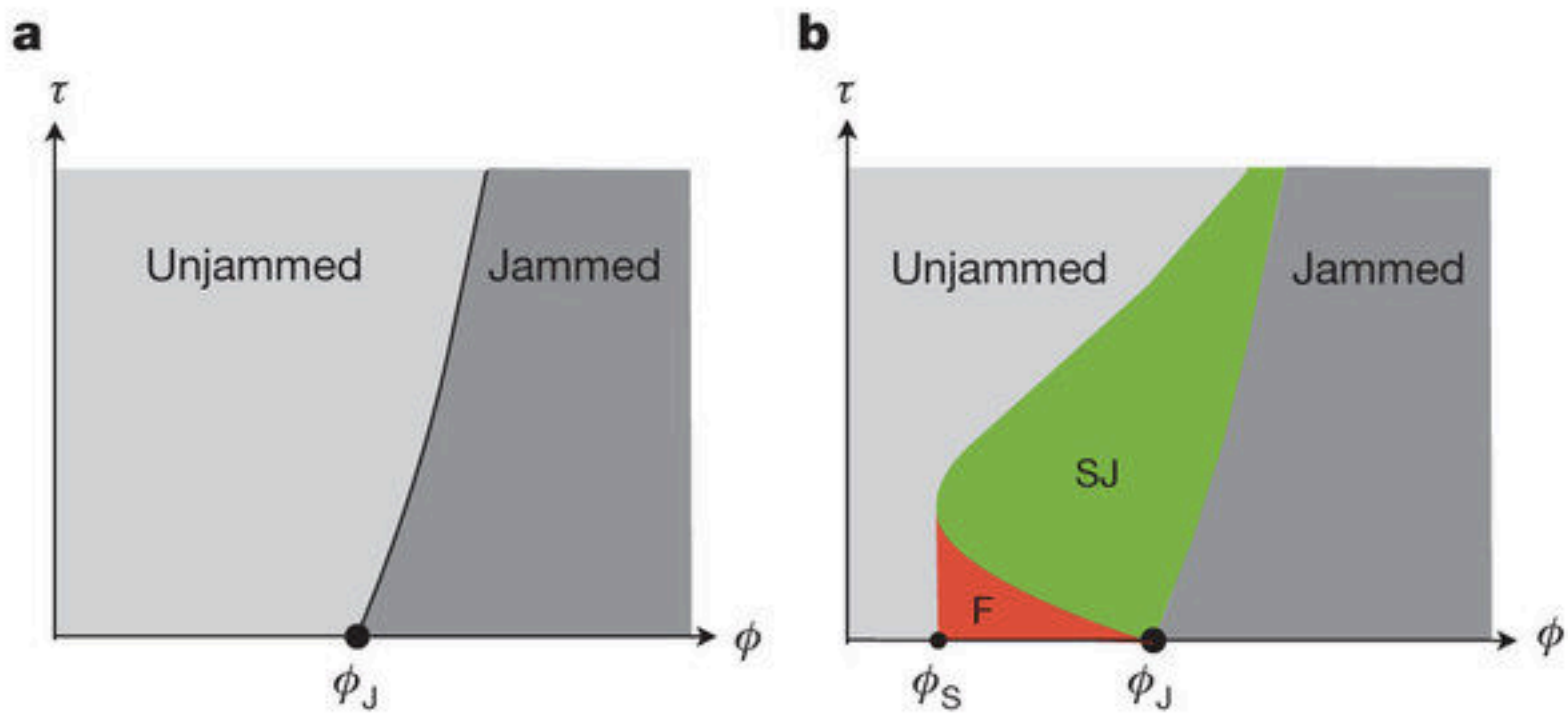


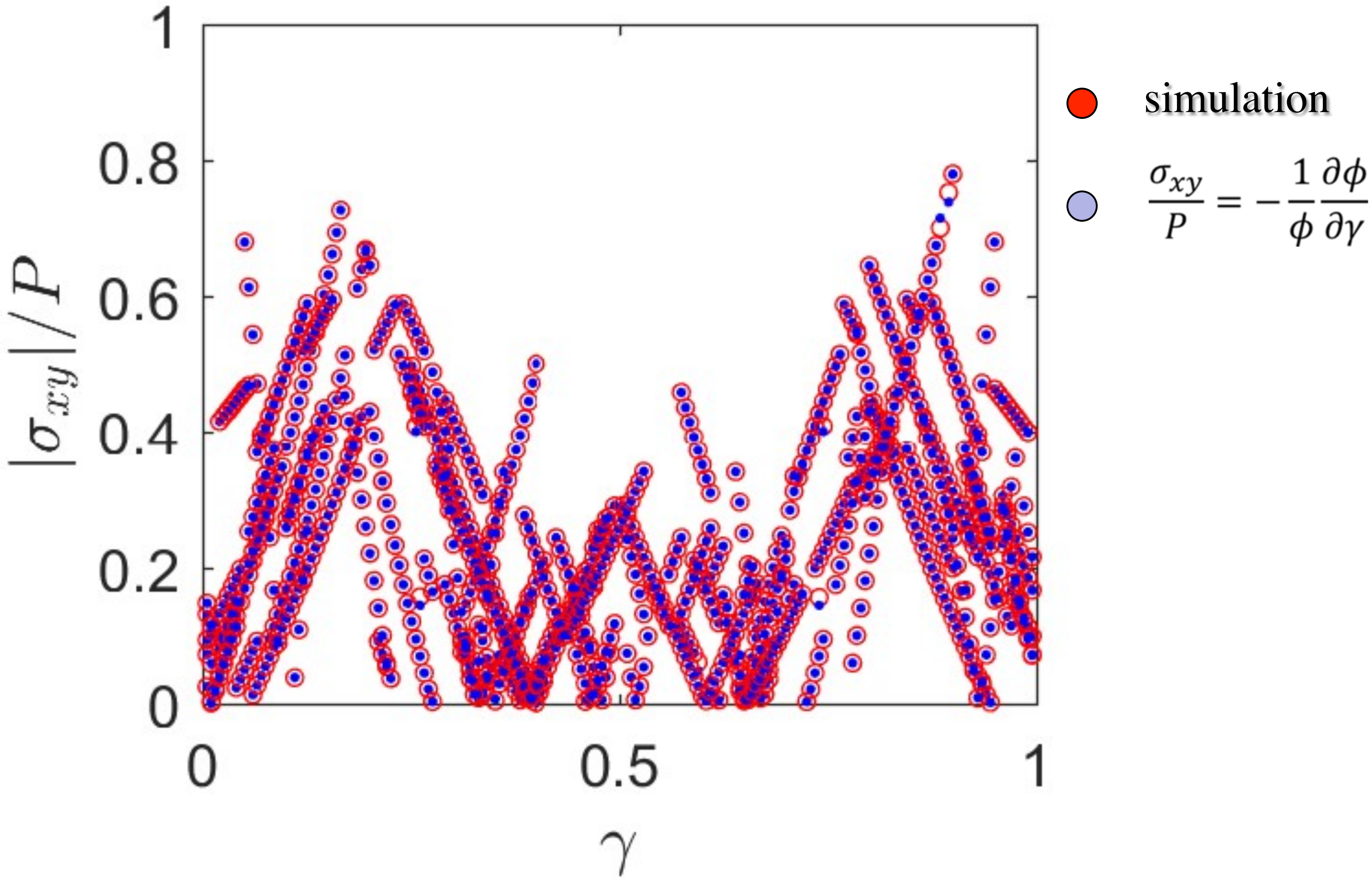
Figure 1: Jamming phase diagrams in the $T = 0$ plane.



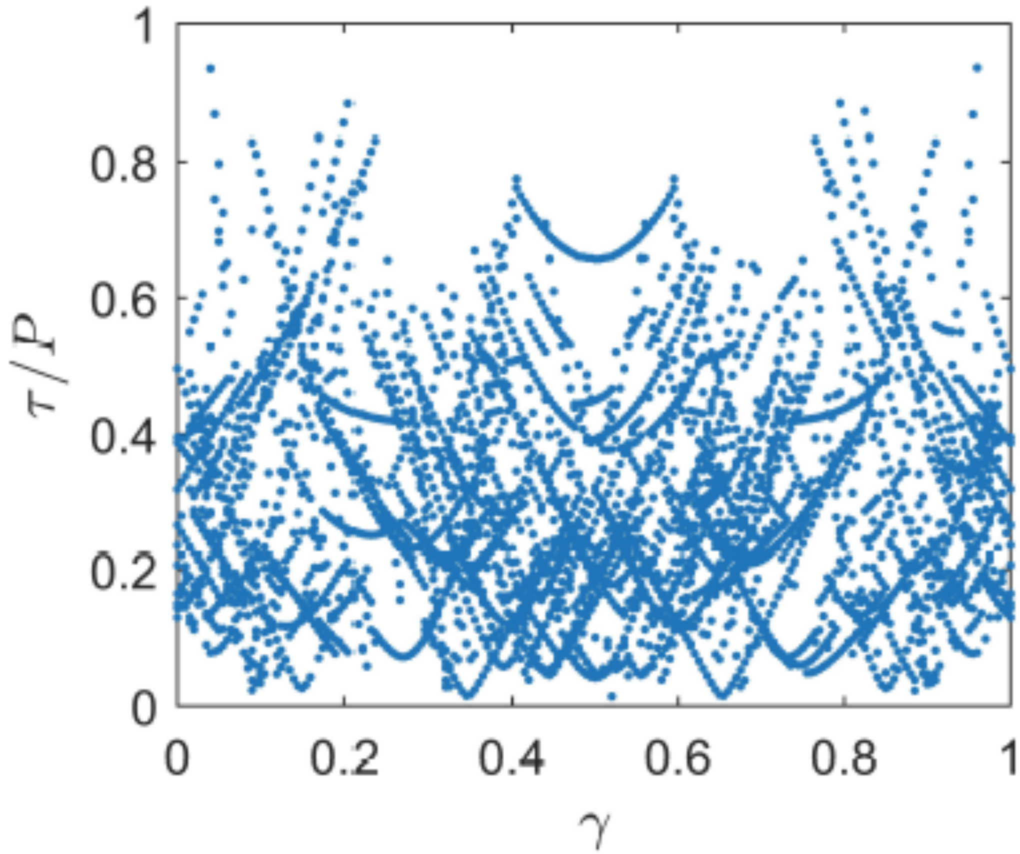
a, Original Liu–Nagel jamming phase diagram[1]. The boundary between unjammed and jammed regions is the yield stress line. Unjamming can be induced by decreasing the packing fraction or increasing the shear stress. **b**, Generalized jamming diagram including the shear-jammed (SJ) and fragile (F) states. Along the φ axis, there are two special densities: φ_S, below which there is no shear jamming, and φ_J, above which isotropically jammed states exist. For $\varphi_S \leq \varphi \leq \varphi_J$, jamming can occur with application of shear stress.

"Jamming by shear," D. Bi, J. Zhang, B. Chakraborty, and R. P. Behringer, Nature 480 (2011) 355.

Shear stress of jammed packings from isotropic compression



Jammed packings generated using isotropic compression

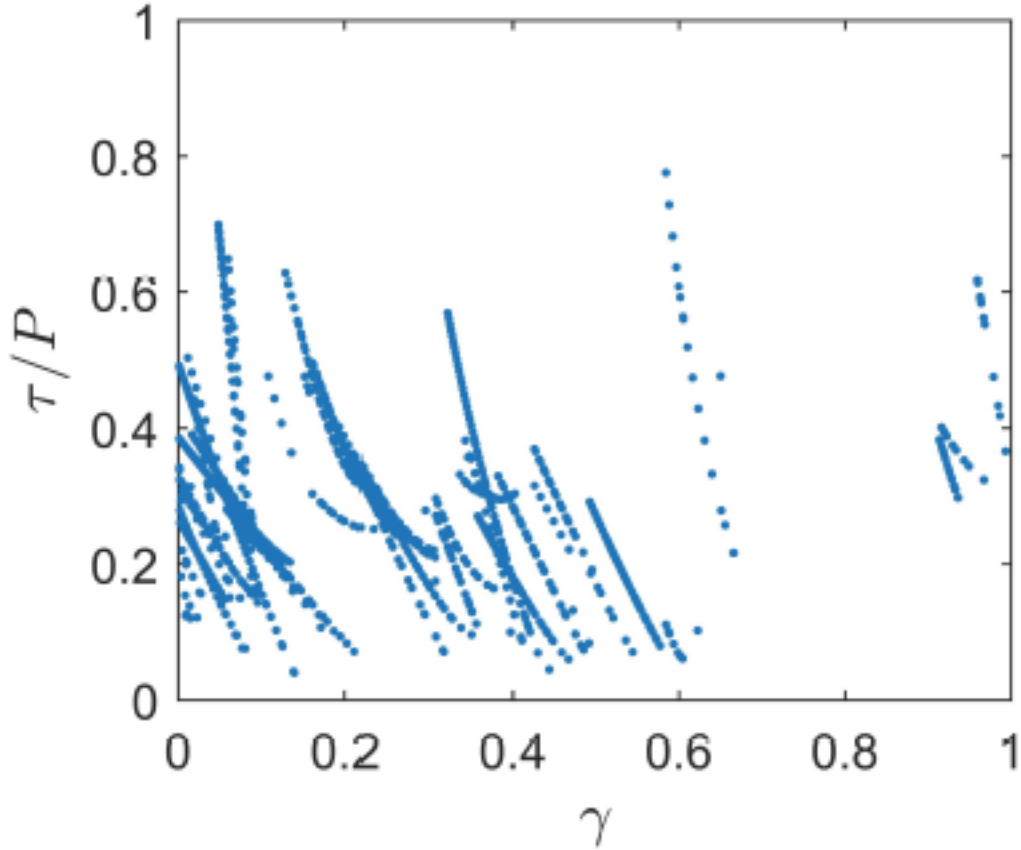


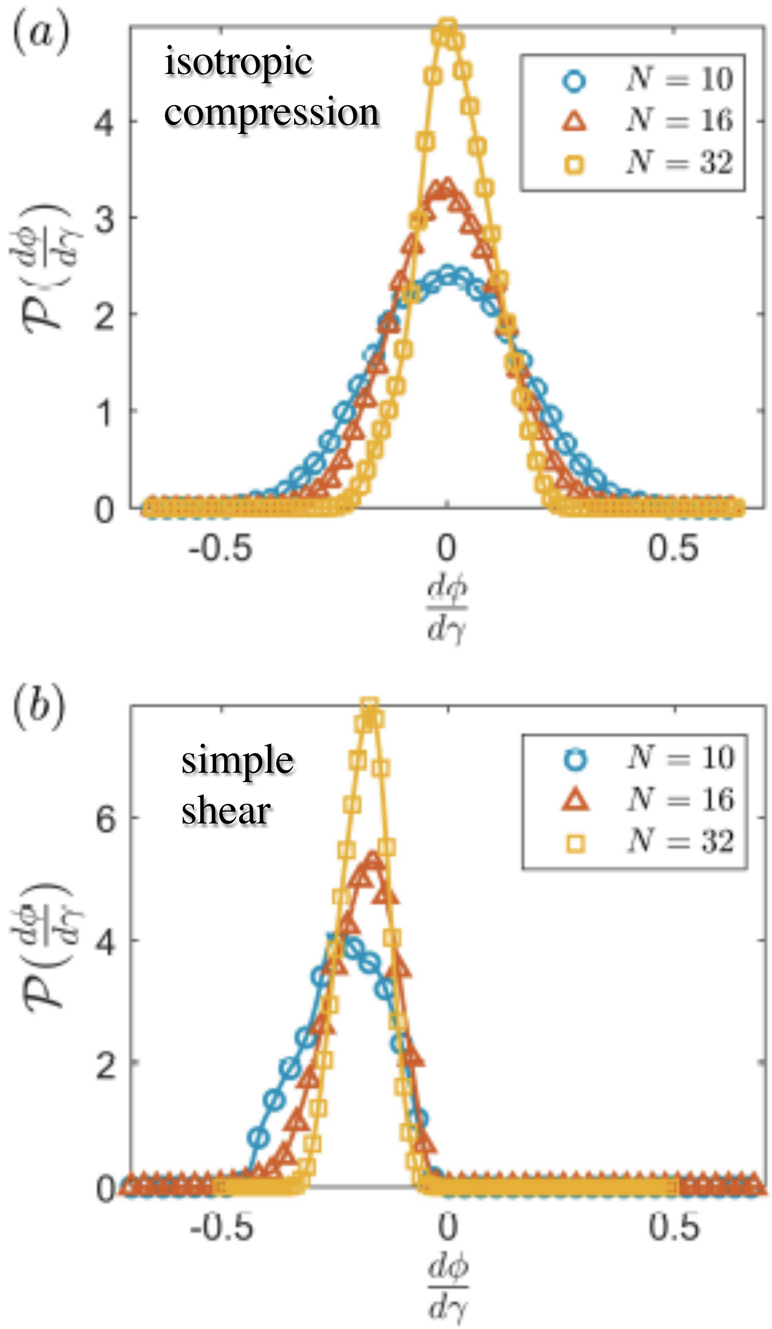
$$\frac{\tau}{P} = \frac{\sqrt{\Sigma_N^2 + \Sigma_{xy}^2}}{P}$$

$$\frac{\Sigma_{xy}}{P} = -\frac{1}{\phi}\frac{\partial \phi}{\partial \gamma}$$

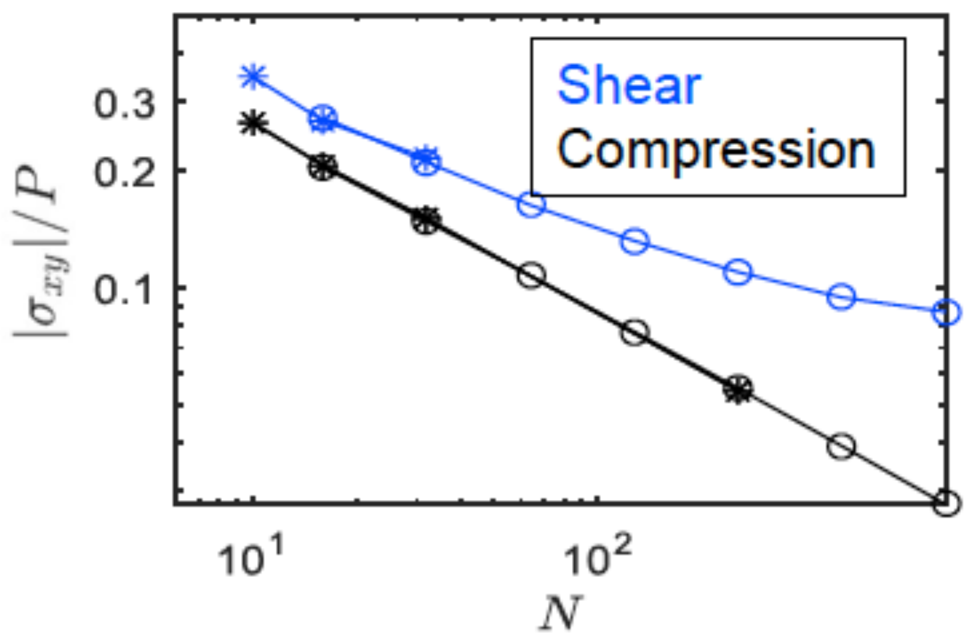
$$\frac{\Sigma_N}{P} = \frac{1+\gamma}{2\phi}\frac{\partial \phi}{\partial \gamma}$$

Jammed packings generated through simple shear





(a)
isotropic compression
N = 10
N = 16
N = 32
$\mathcal{P}\left(\frac{d\phi}{d\gamma}\right)$
$\frac{d\phi}{d\gamma}$
(b)
simple shear
N = 10
N = 16
N = 32
$\mathcal{P}\left(\frac{d\phi}{d\gamma}\right)$
$\frac{d\phi}{d\gamma}$

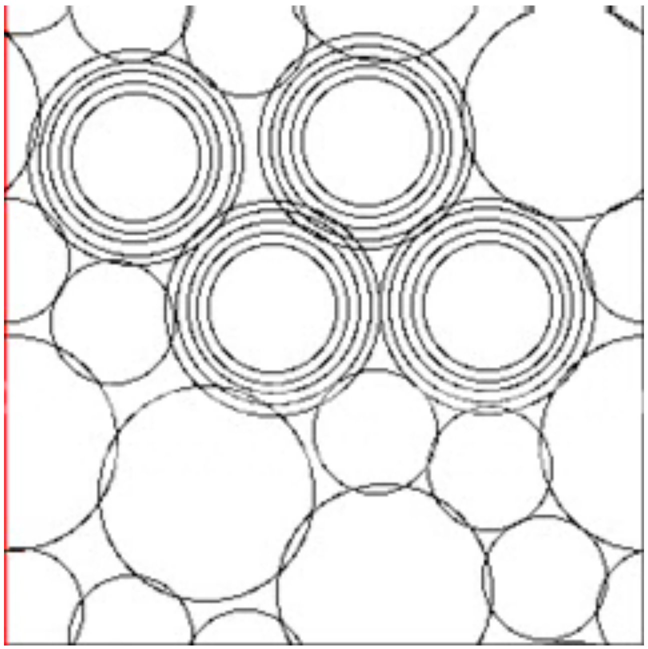


Shear
Compression
0.3
0.2
0.1
$|\sigma_{xy}|/P$
10^1
10^2
N

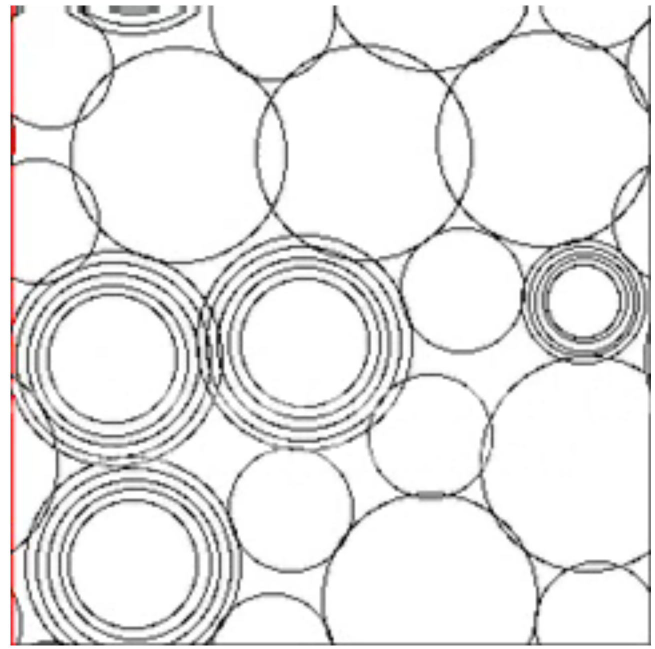
Conclusions

- Nonlinear mechanical response stems from rearrangement- and softening-induced losses
- Both are small below yield stress and increase rapidly near yielding
- Both contributions remain finite in large system limit
- Identified several signatures of yielding transition
- Develop ability to theoretically predict yield stress for a given preparation protocol

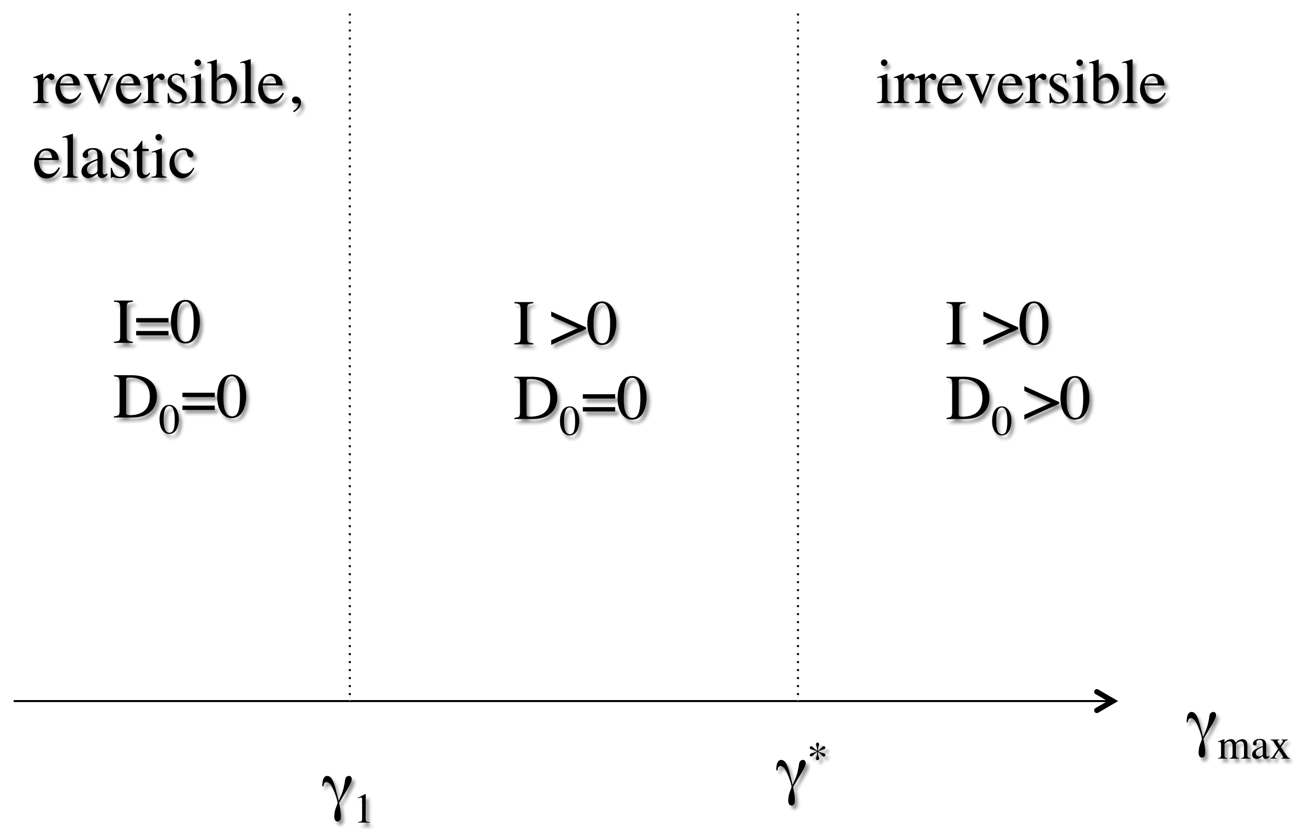
Reversibility



Reversible

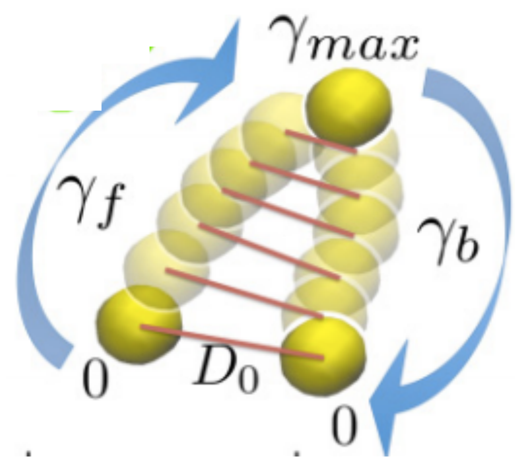


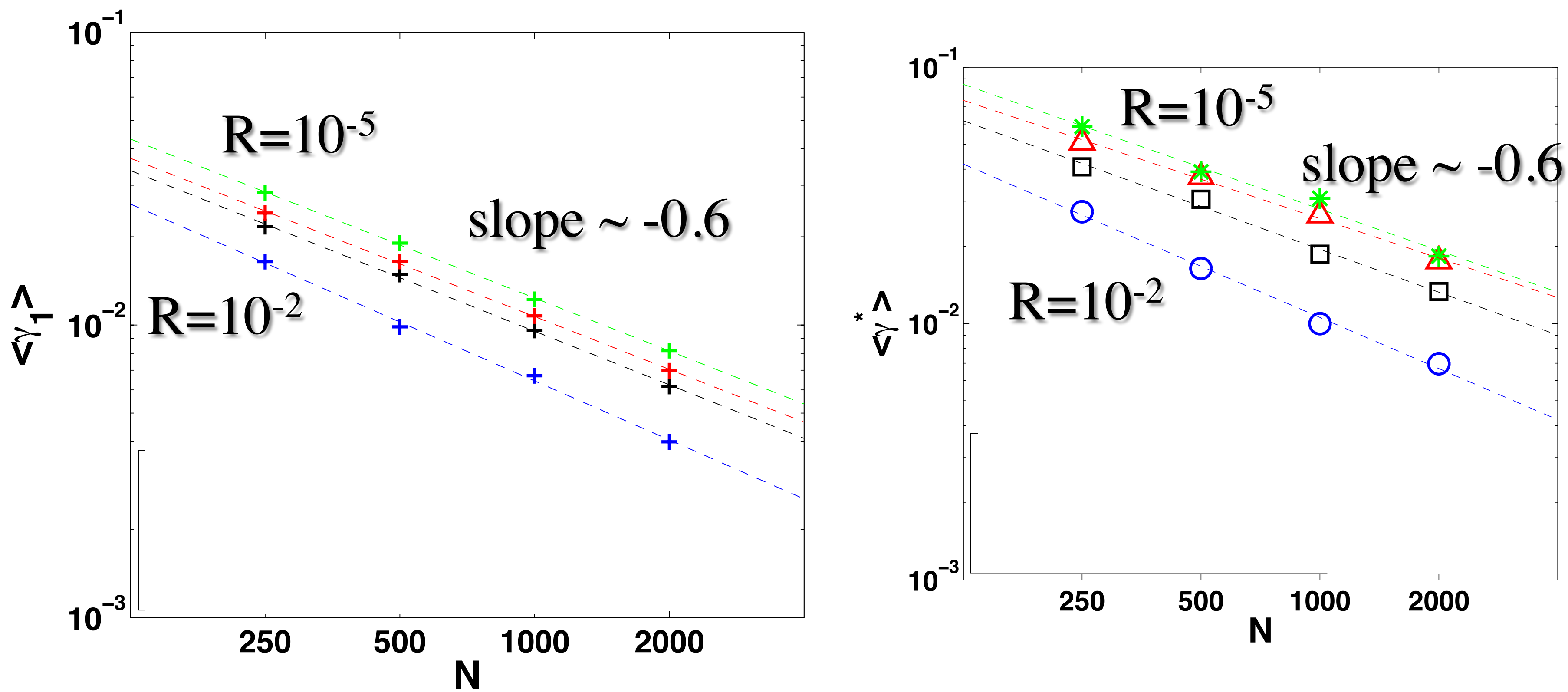
Irreversible



$$D_0(\gamma) = |\vec{R}(0,0) - \vec{R}(\gamma,\gamma)|/N.$$

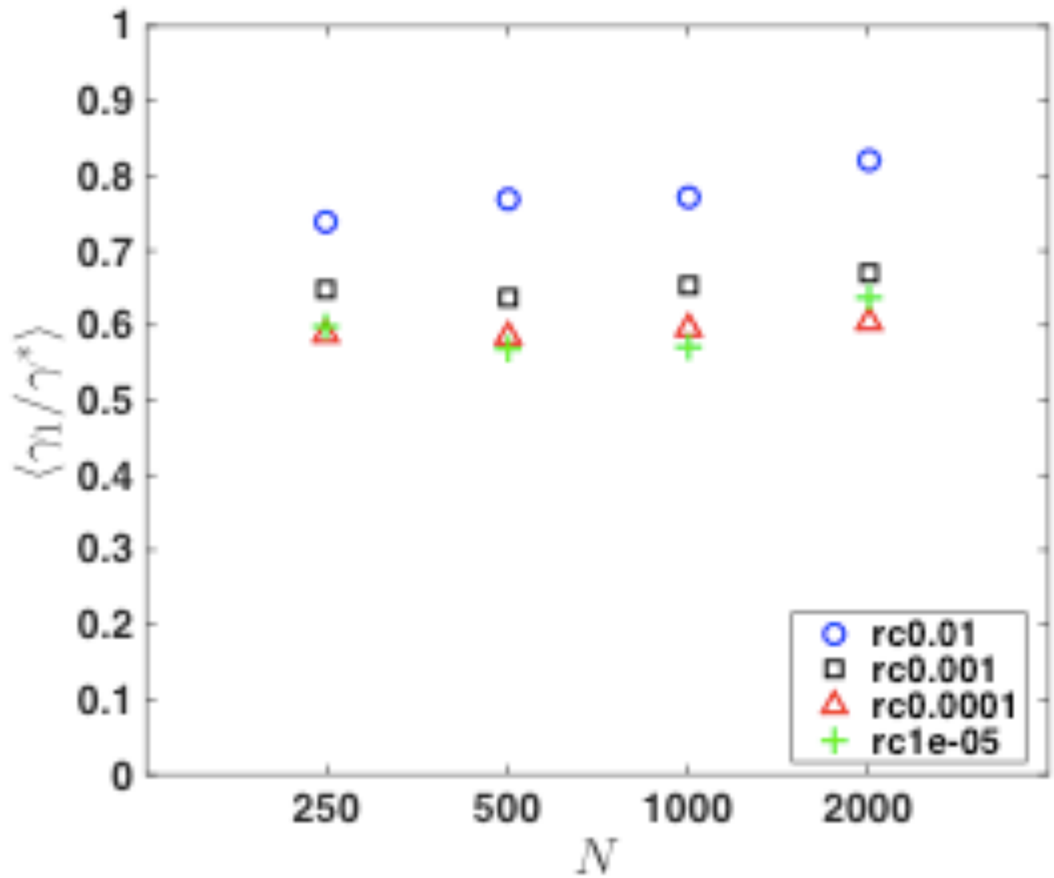
$$I(\gamma) = \frac{1}{N}\sqrt{\frac{1}{\gamma}\int_0^{\gamma} |\vec{R}(\gamma',0) - \vec{R}(\gamma,\gamma-\gamma')|^2 d\gamma'}.$$



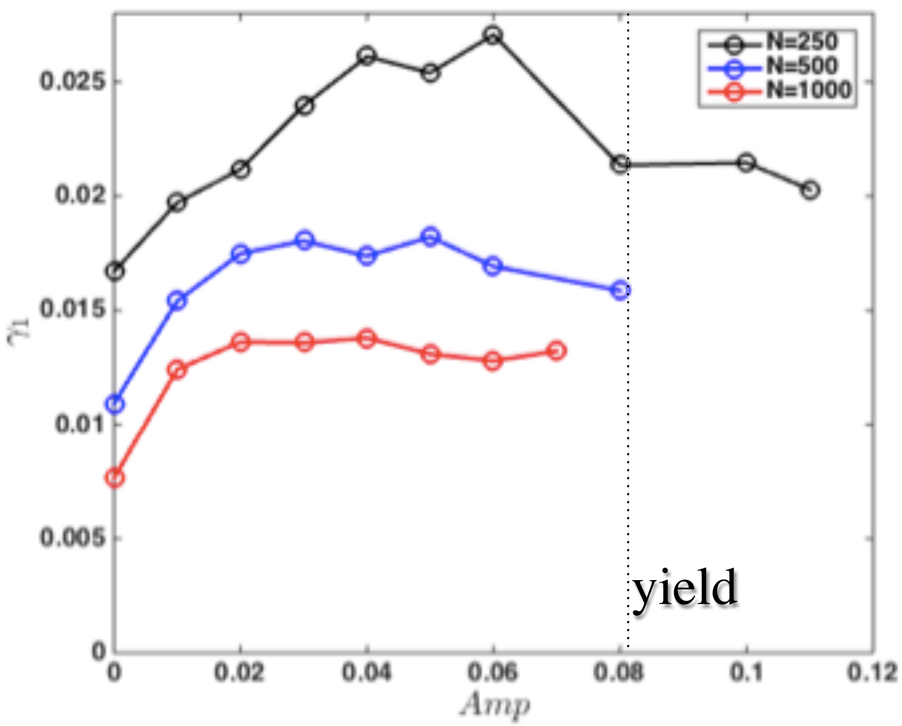


R=10-5
slope ~ -0.6
R=10-2
N
250
500
1000
2000
R=10-5
slope ~ -0.6
R=10-2
N
250
500
1000
2000

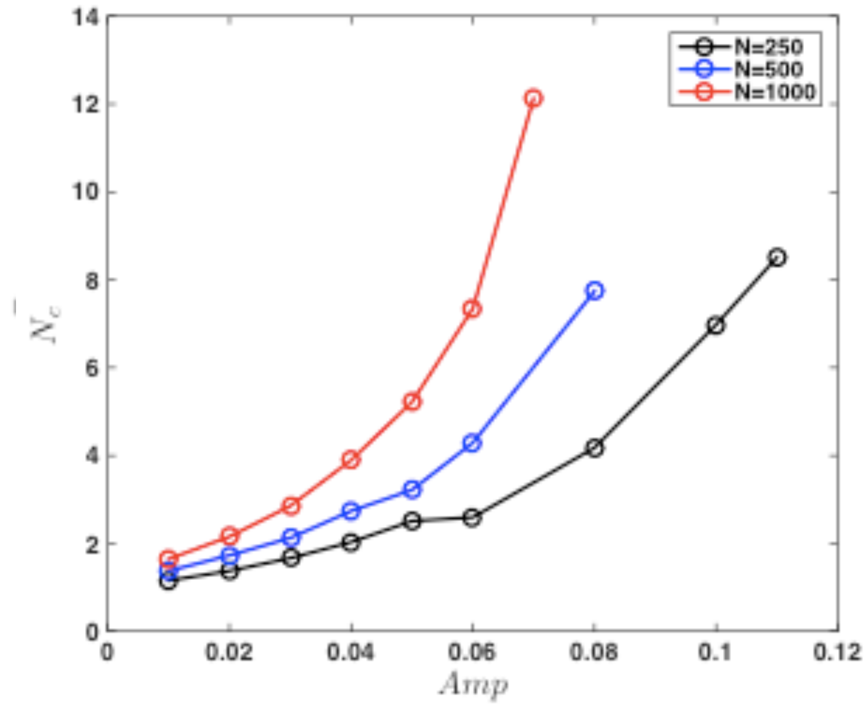
…but the critical strains still tend to zero in large-system limit.
Can we increase strain range over which system is reversible?



Cyclic shear can increase strain over which system is reversible



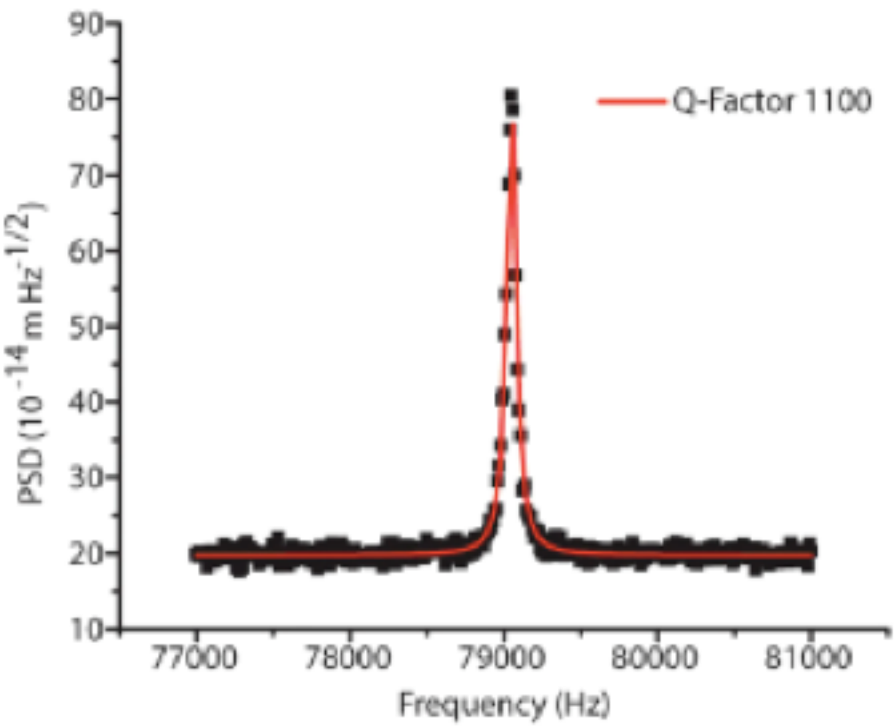
# of cycles required to reach steady state



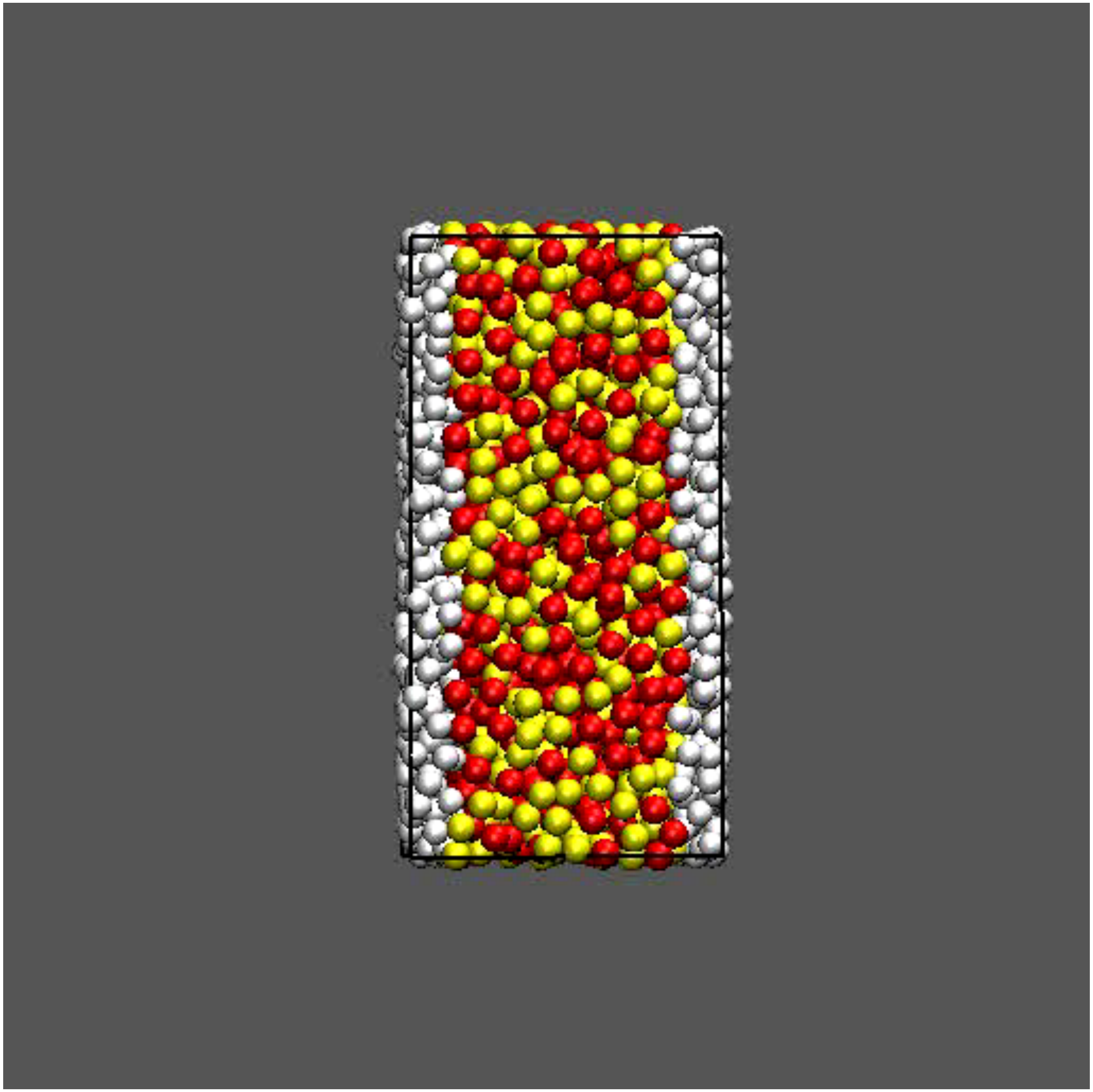
Finite region of strain where system is reversible in large-system limit

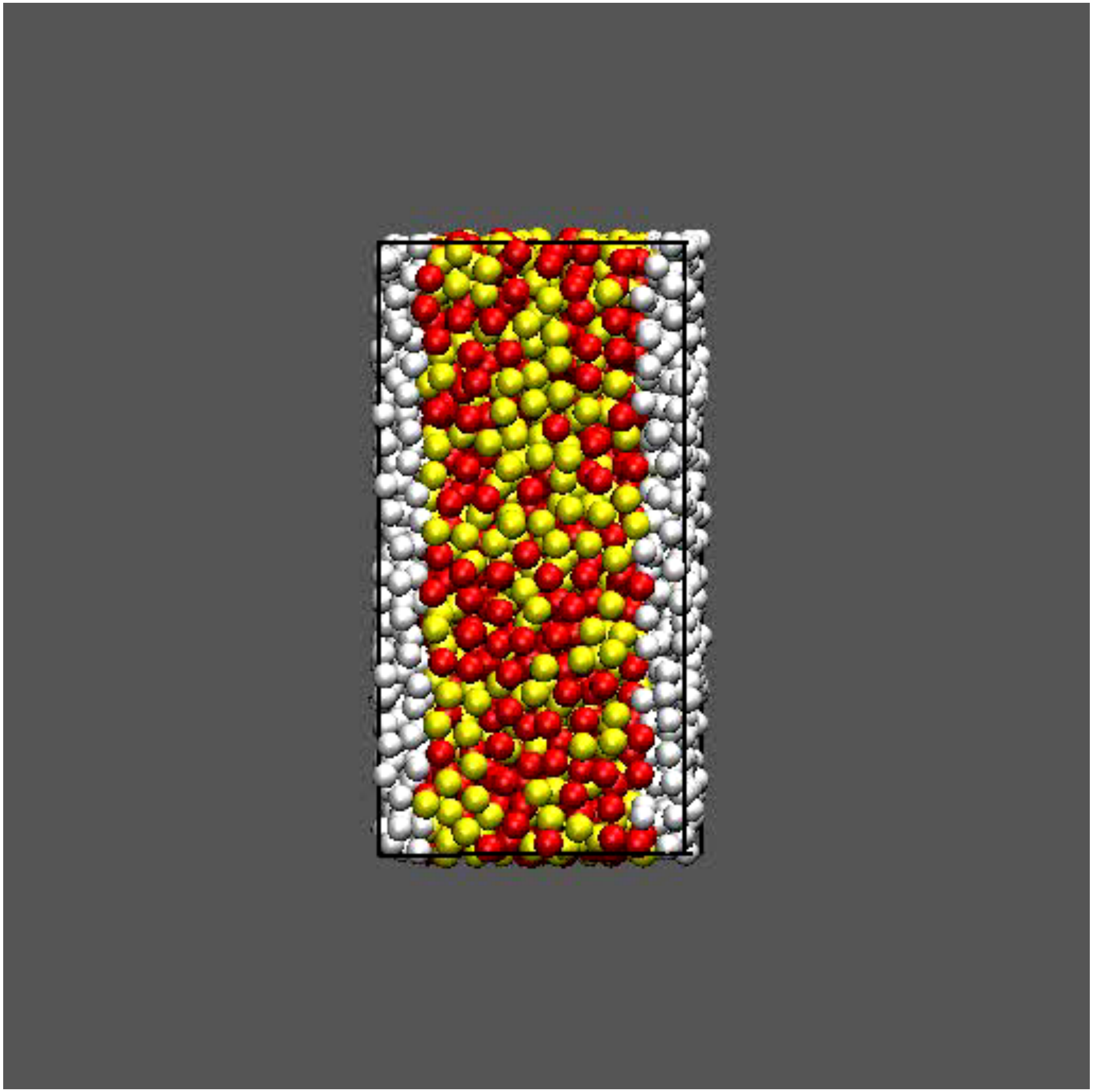
N	$(\gamma^*)_{ss}$	$(\gamma_1)_{ss}$	ratio
250	0.1126	0.02029	0.1802
500	0.08537	0.01587	0.1859
1000	0.07243	0.01322	0.1825

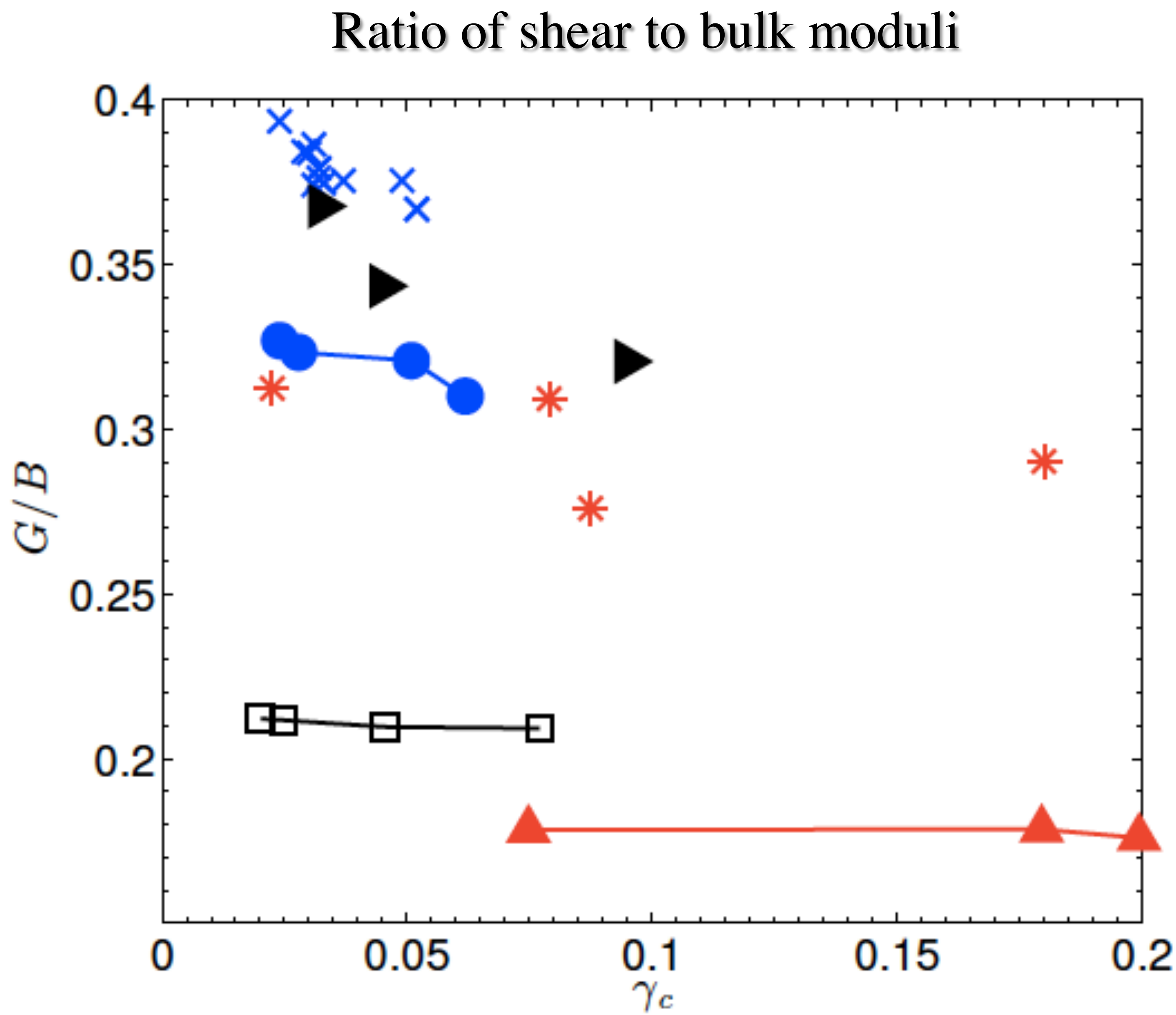
Application to high-Q metallic glasses

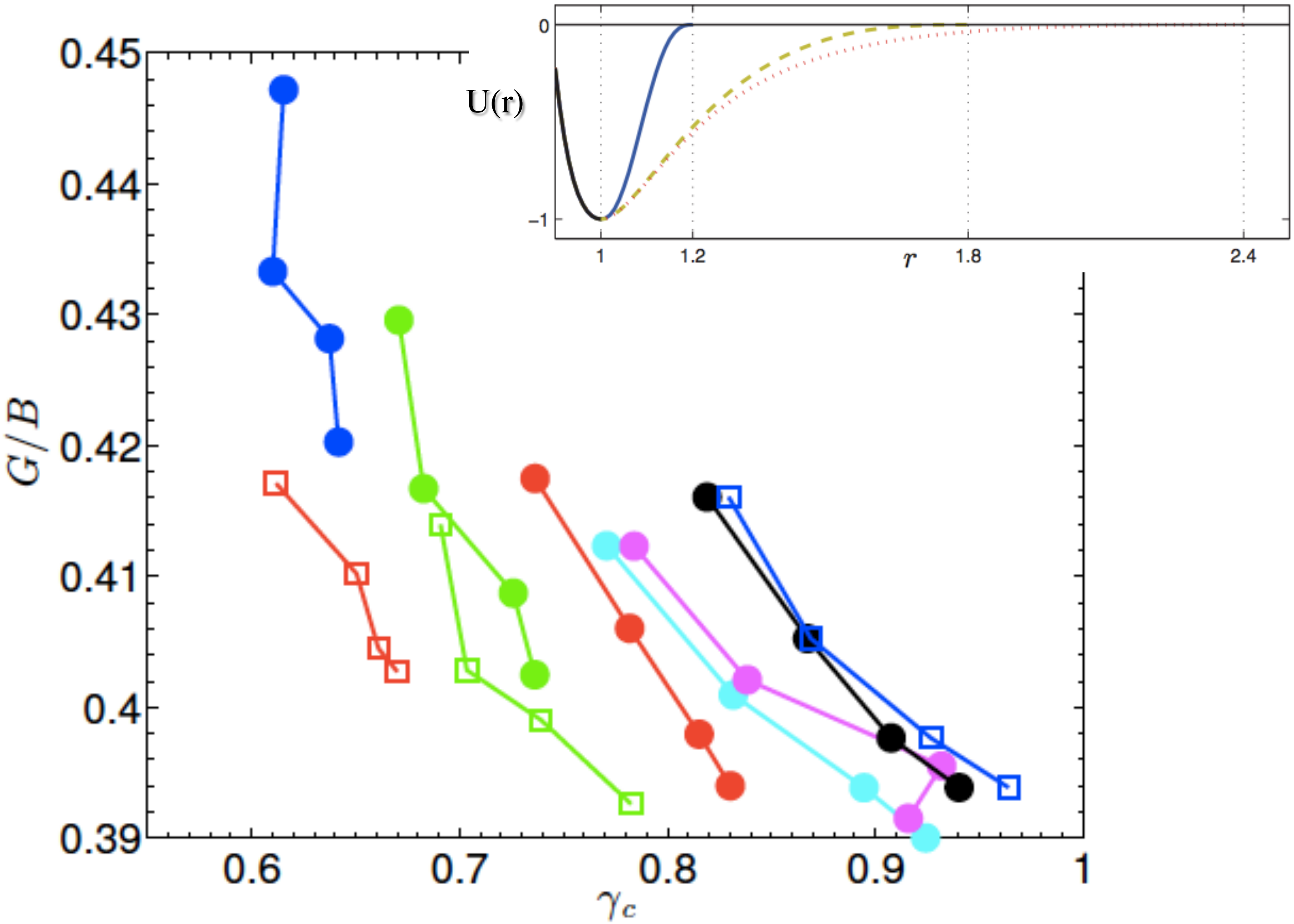


Brittle-Ductile Continuum



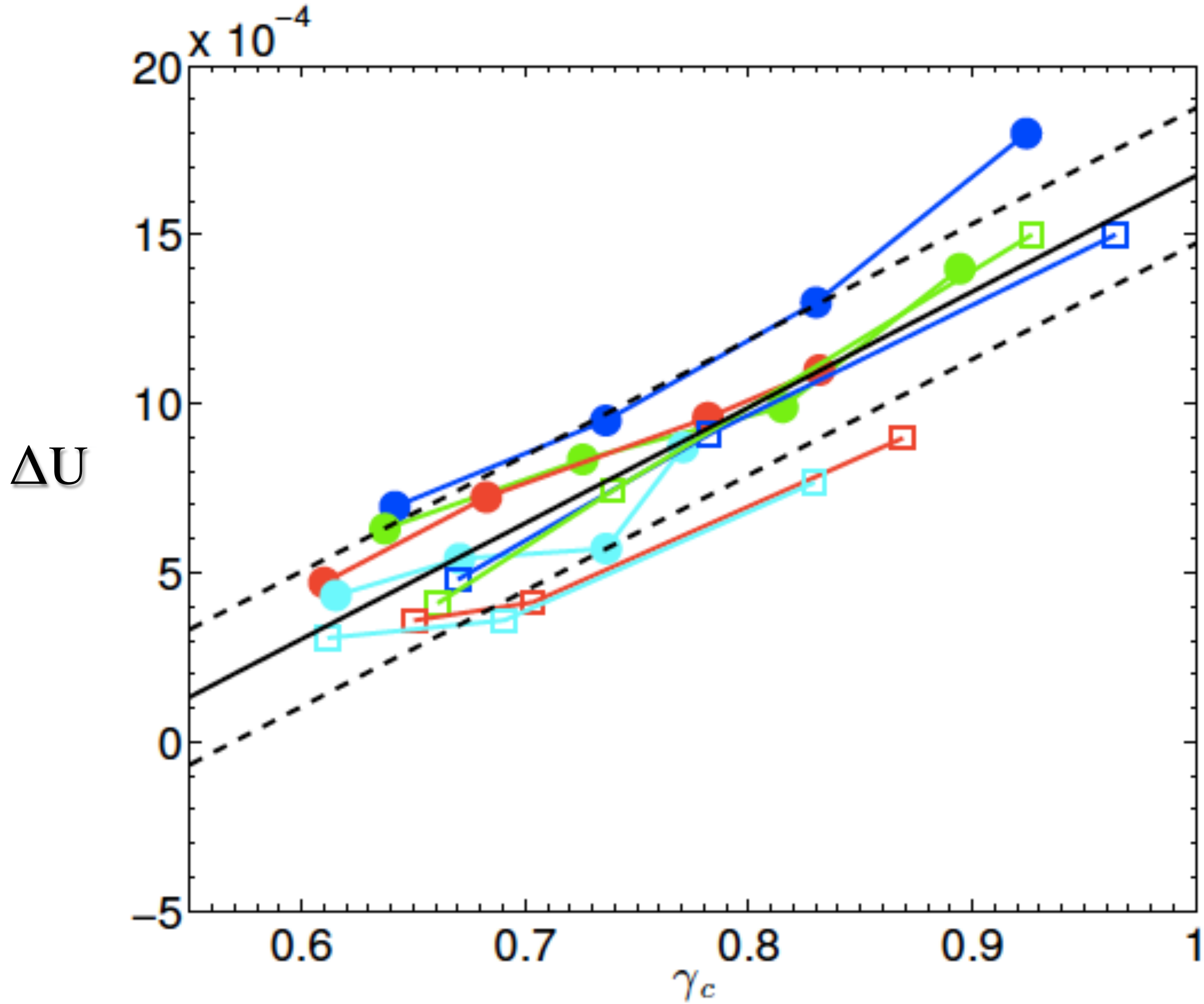



Ratio of shear to bulk moduli
0.4
0.35
0.3
0.25
0.2
G/B
0
0.05
0.1
0.15
0.2
γ_c



0.45
0.44
0.43
0.42
0.41
0.4
0.39
G/B
0.6
0.7
0.8
0.9
1
γc
U(r)
0
−1
1
1.2
r
1.8
2.4

Add energy drops prior to yield



Conclusions

- Identify precursor events that relieve stress/energy and make system less prone to failure.
- How do we make simulation samples brittle? Do we need much larger samples?