Elementary Mechanisms of Deformation in Amorphous Solids

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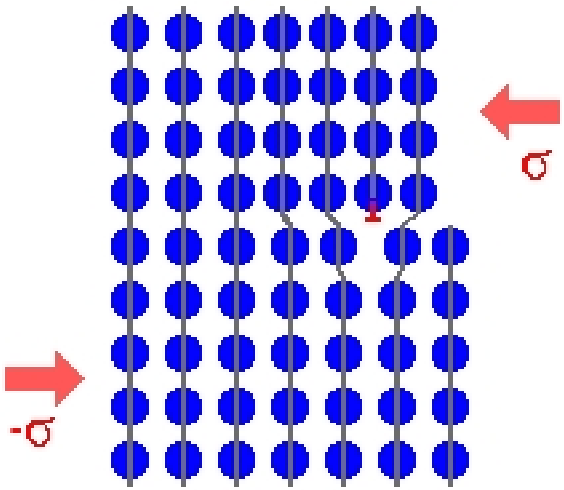
Navier

Rhéophysique

Amorphous materials are, well... disordered

<u>In crystals</u>

defects = dislocations
(Volterra, 1930; SEM, 1960)



Interaction and motion understoon
(Peierls, Nabarro, Friedel, 1950's)

Dislocation dynamics in computer
codes since the 1980's

<u>In disordered materials</u>

No topological order => defects?

What are the elementary mechanisms
of deformation?

How can we up-scale the dynamics?

Length and energy scales in amorphous materials

<u>Hard glasses</u>

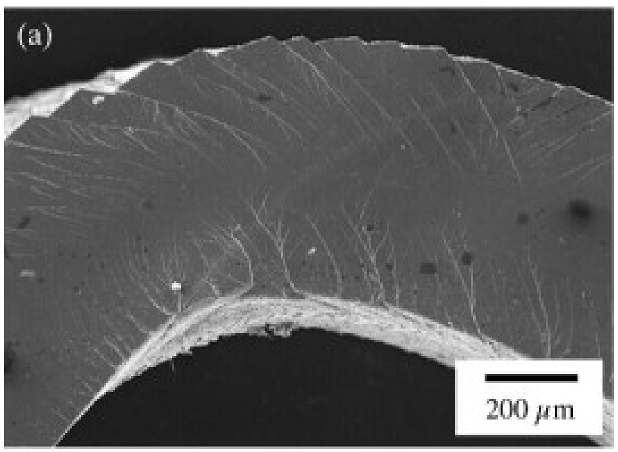
<u>Soft glasses</u>

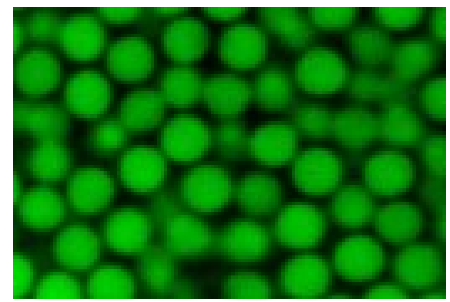
Metallic/oxyde glasses

Polymers

Colloids

Foams





Length scales nm's

Energies ~ 0.1—1 eV

Stresses ~ GPa

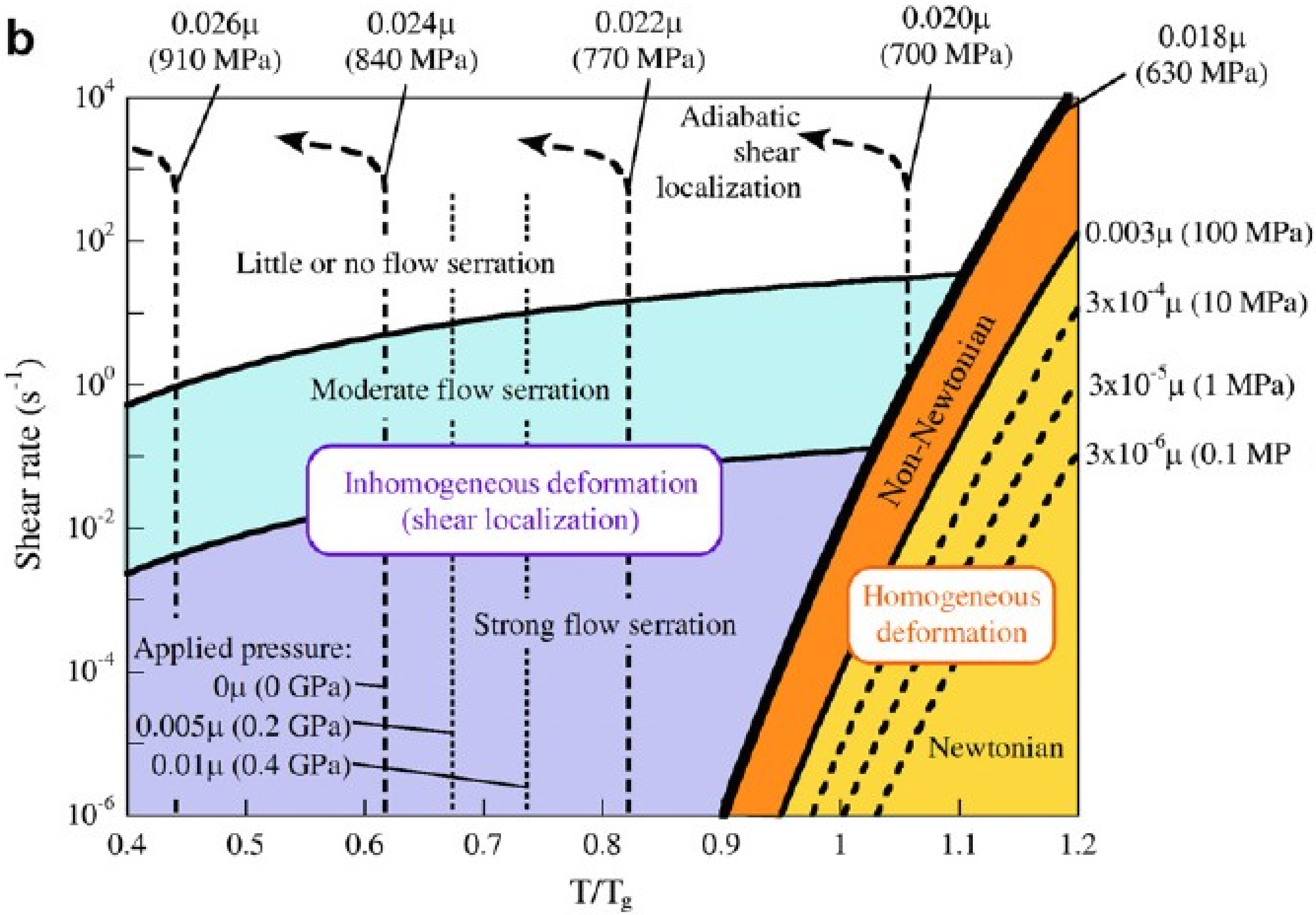
Length scales 0.1 µm's

Energies ~ kT = 1/40 eV

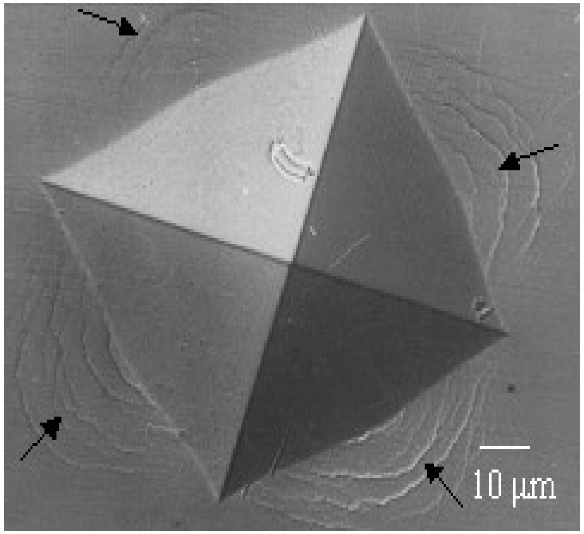
Stresses ~ Pa—kPa

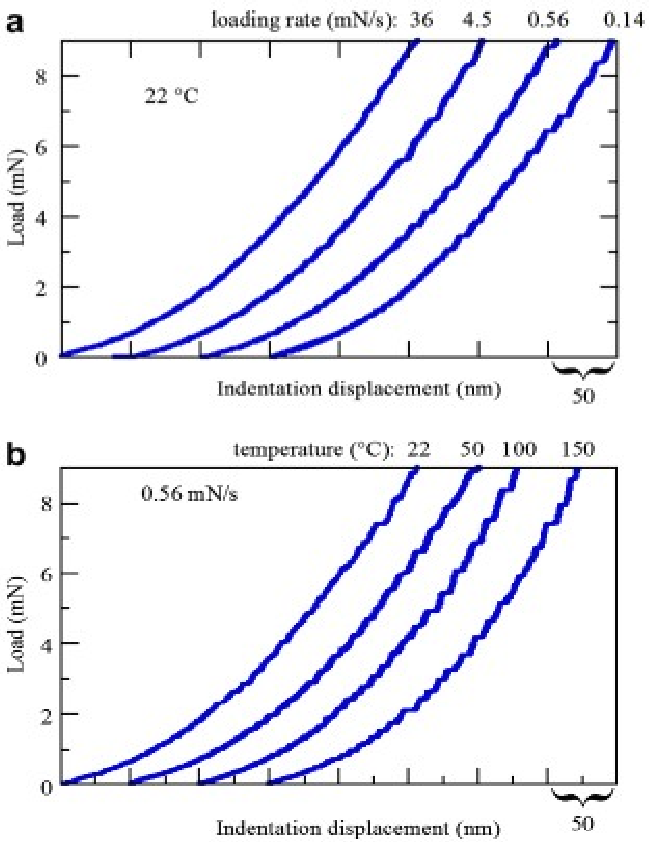
Can we identify some mechanisms of deformation, at least for broad classes of materials, or time-, energy-, length-scales?

Deformation map for a metallic glass



Schuh *et al*, Acta Mat. 55, 4067 (2007)





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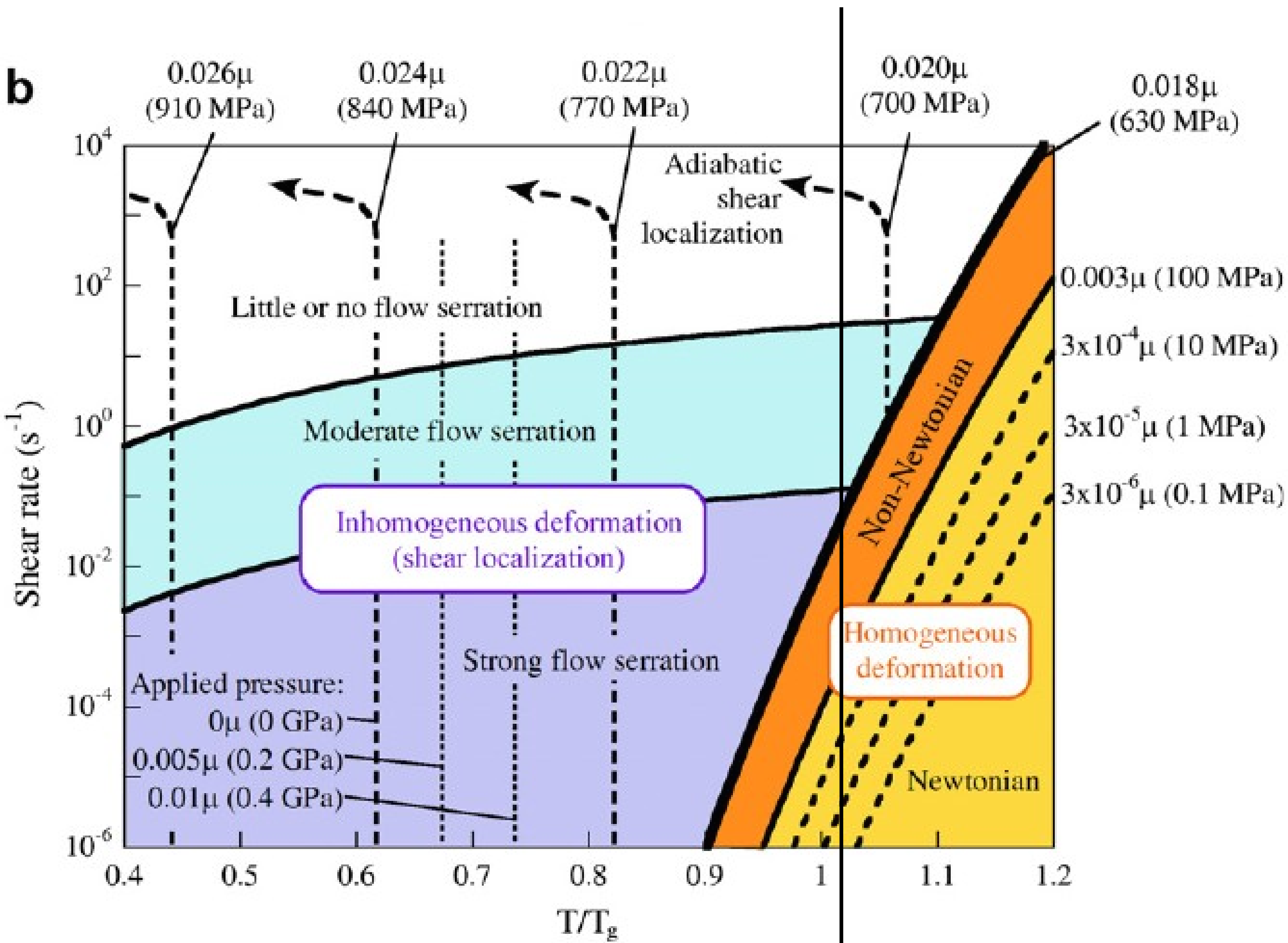
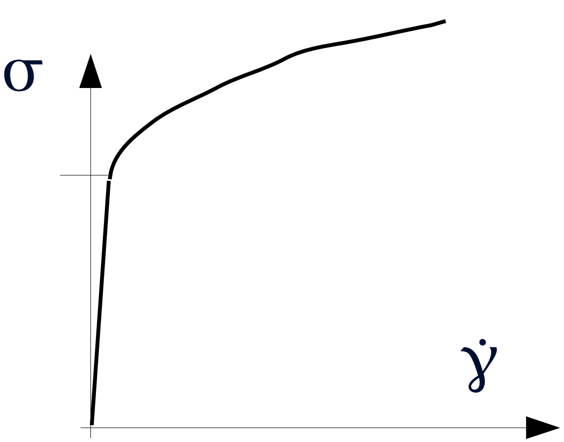


Schuh *et al*, Acta Mat. 55, 4067 (2007)



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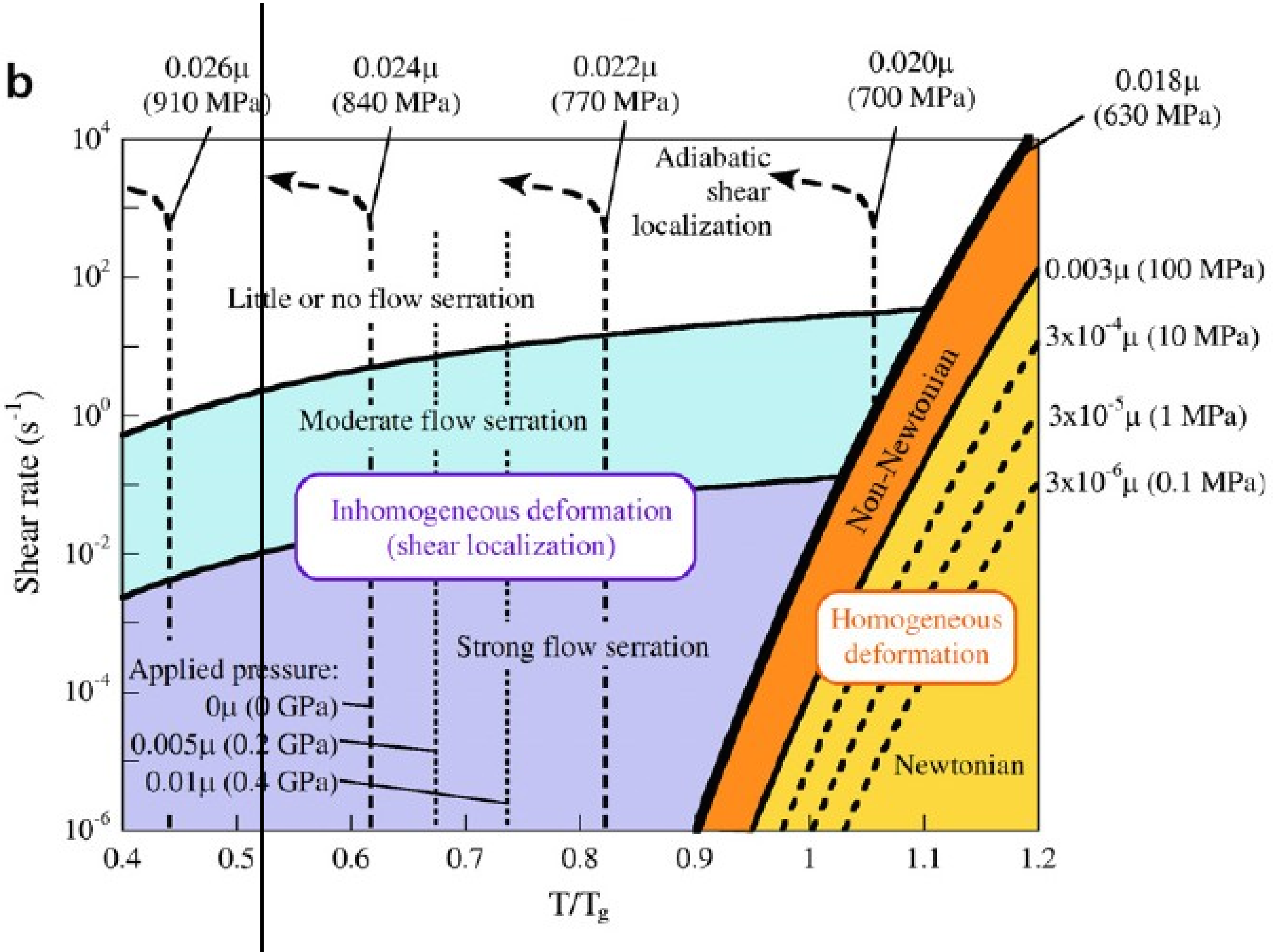

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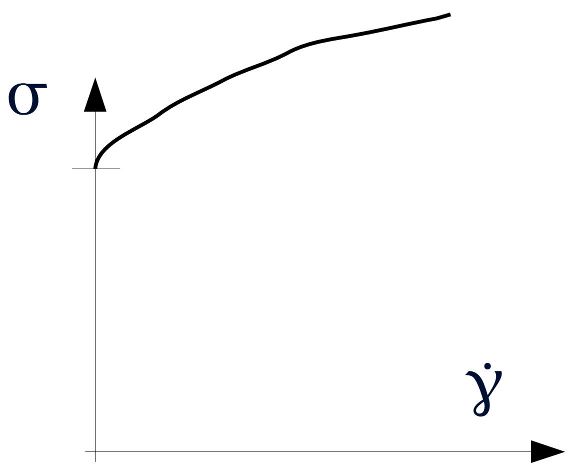
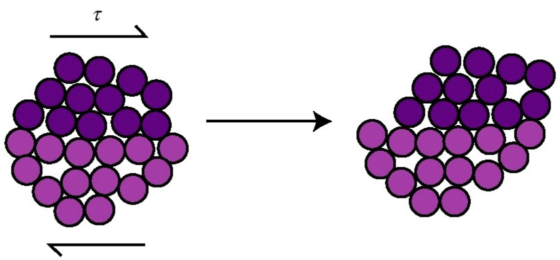


What are the elementary mechanisms of deformation in amorphous solids?

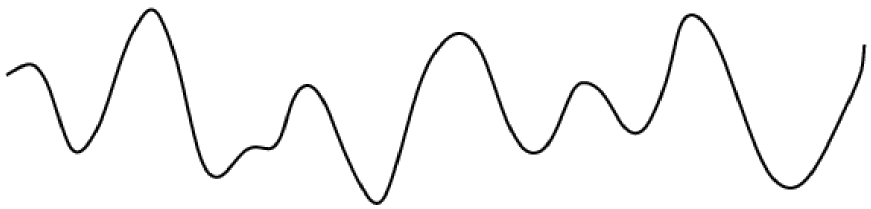
Argon (1979):

local shear transformations



= flips

stress-induced
hopping among inherent states



In real space

In PEL

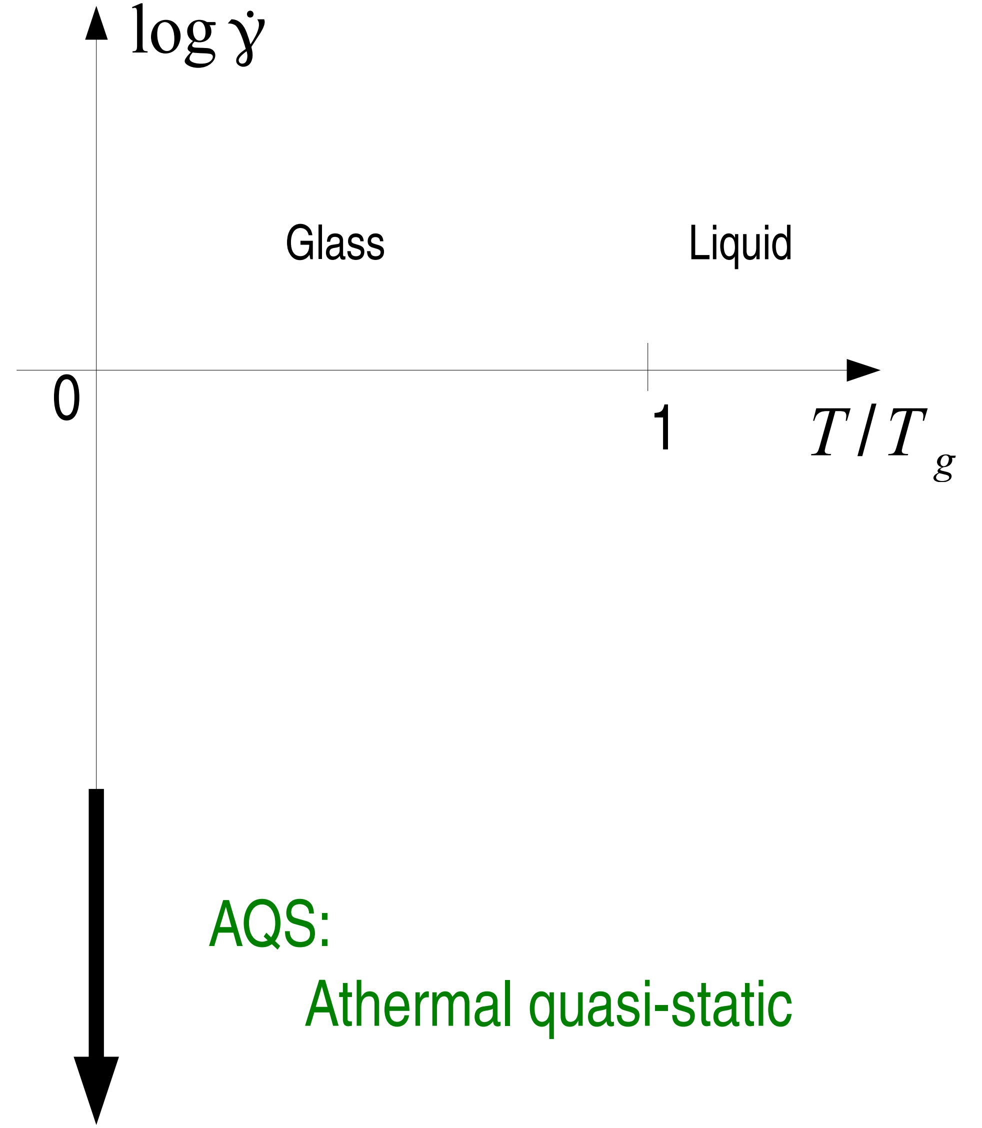
The AQS limit

<u>Low temperature:</u>

$$T < T_g$$

$$\dot{\gamma} \ll 1/\tau_\alpha$$

Neglect any thermally activated process



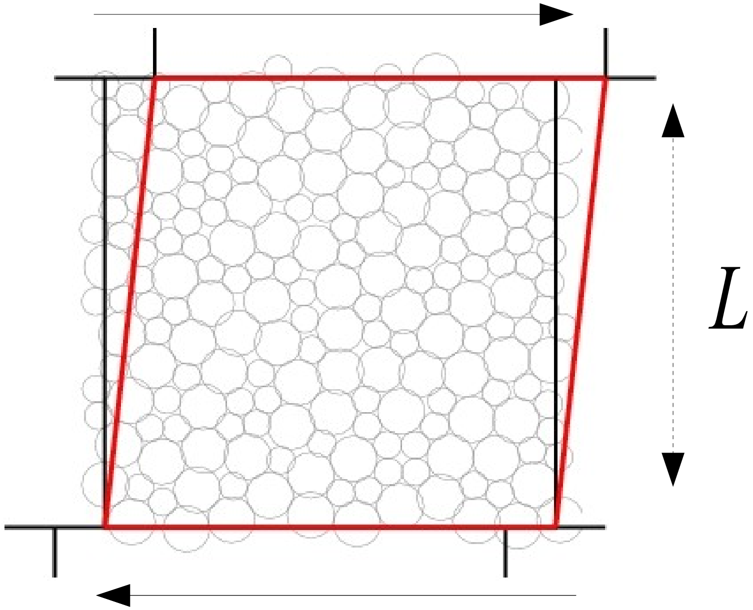
AQS:

Athermal quasi-static

$$\tau_\alpha^{-1} \ll \dot{\gamma} \ll \tau_{irr.}^{-1}$$

Plasticity in a low-T (finite-sized) glass:

The system resides at all times in local energy minima



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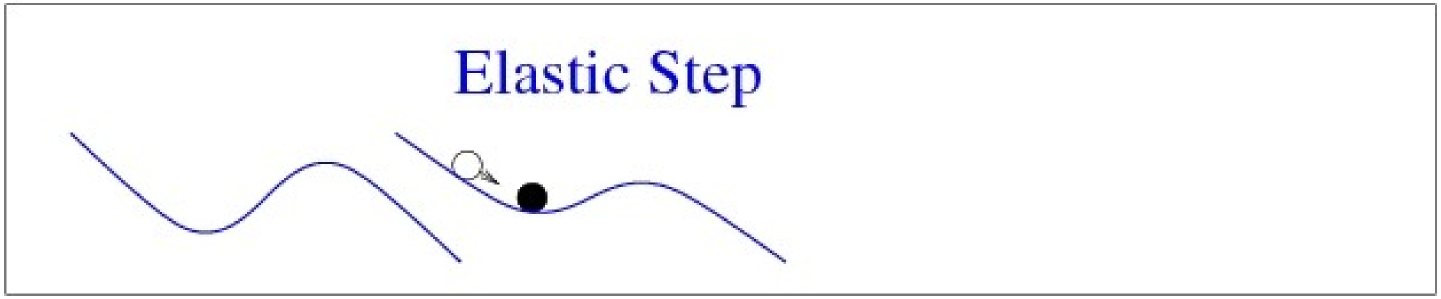
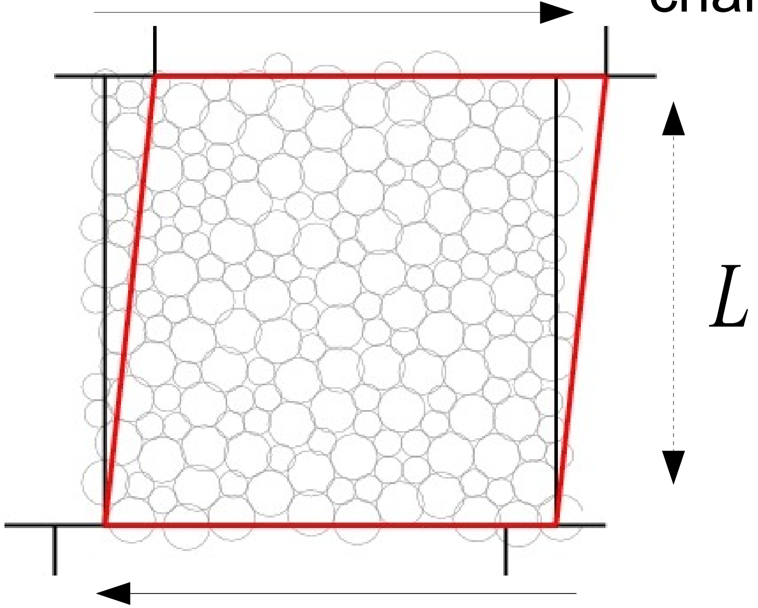


The system resides at all times in local energy minima

It track reversibly strain-induced changes in minima



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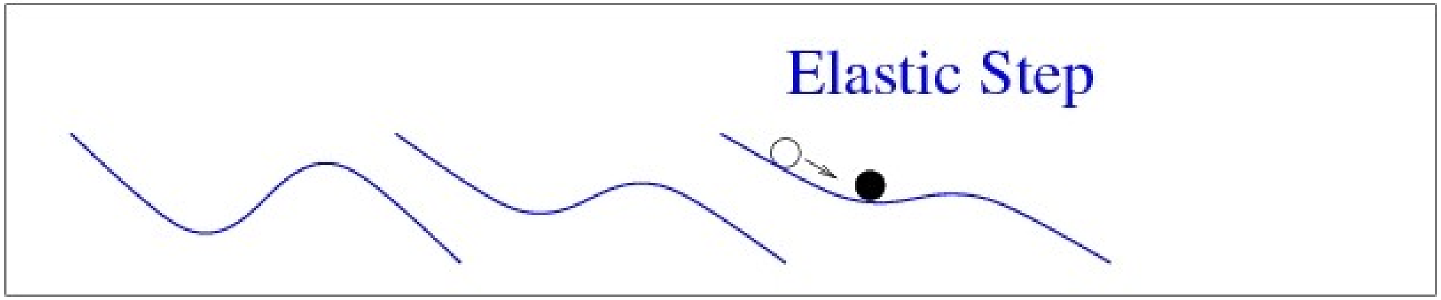

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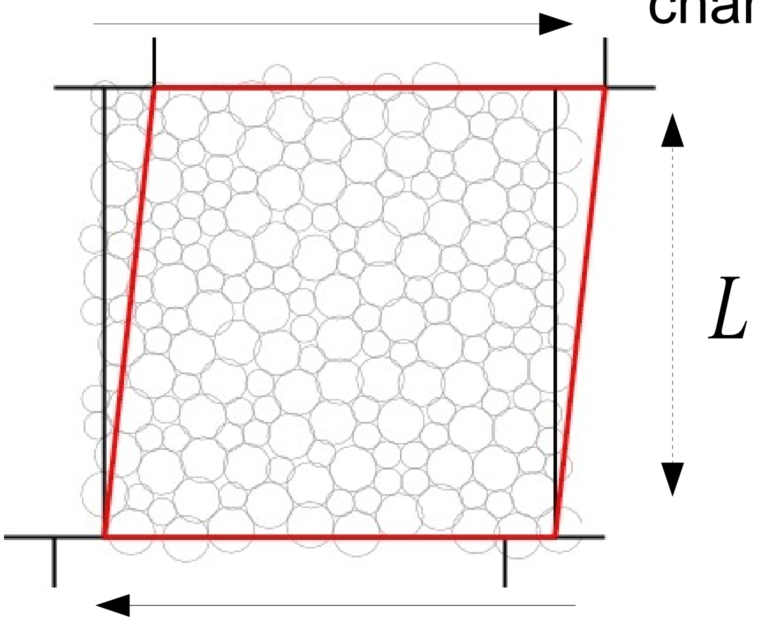

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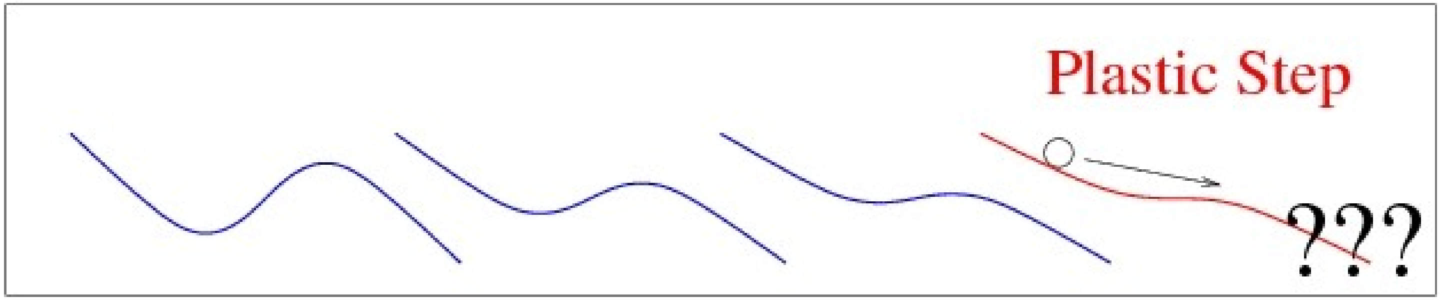

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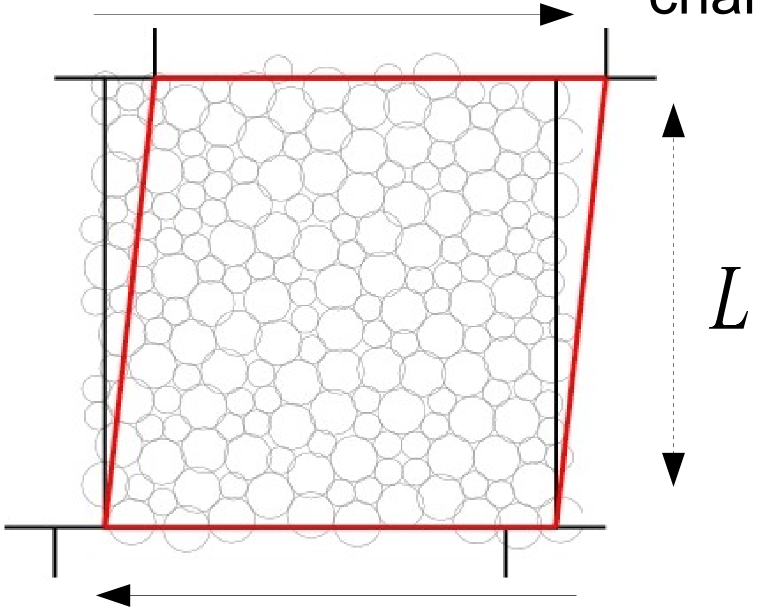


It track reversibly strain-induced changes in minima

Occasionally the occupied minimum becomes unstable:

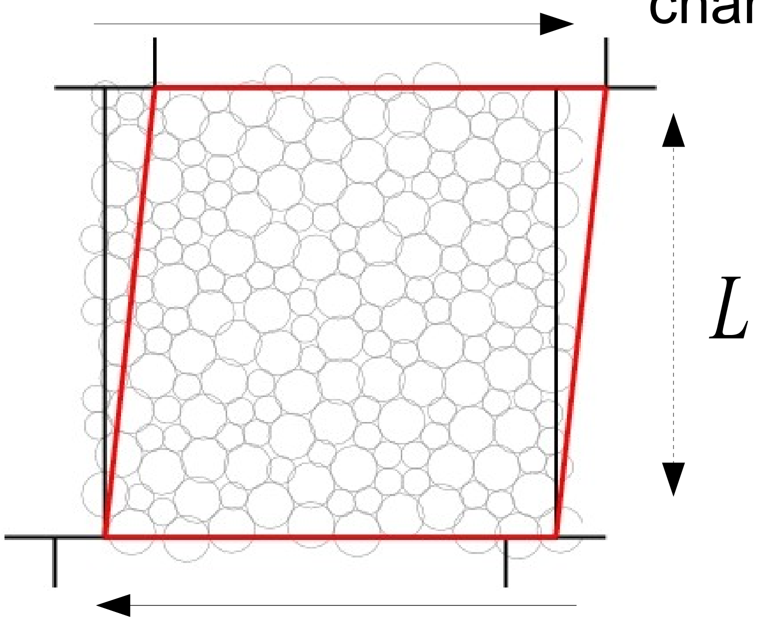
A plastic event then occurs leading to a new local minimum

Athermal, quasi-static protocol:

- Minimize energy
- Apply a small increment of strain (homogeneously)
- Repeat

The system resides at all times in local energy minima

It track reversibly strain-induced changes in minima



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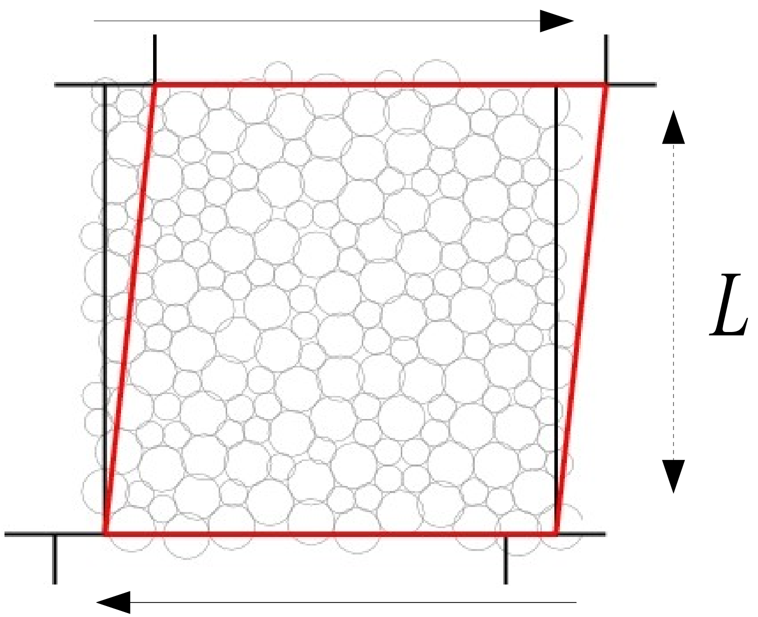
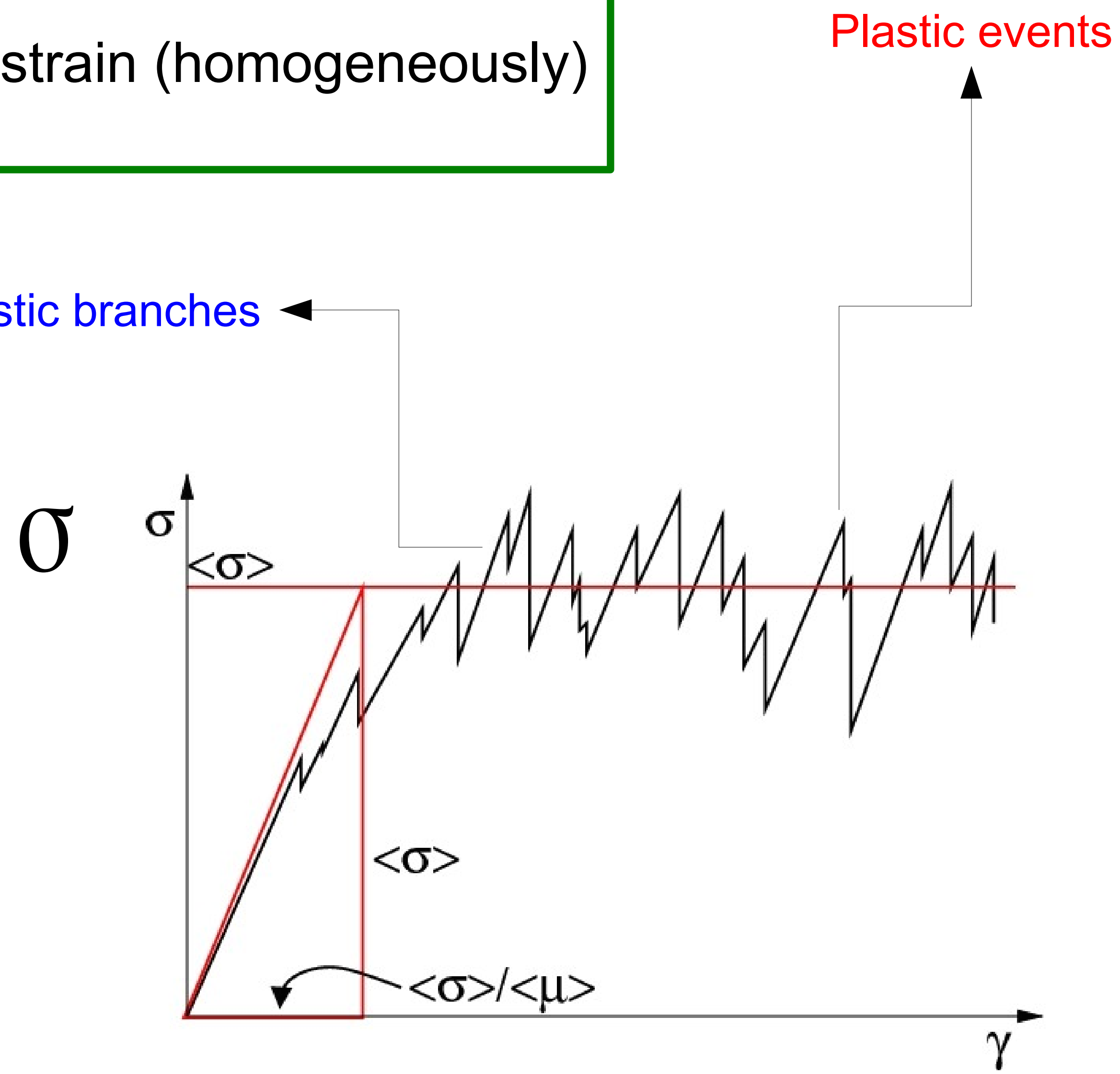
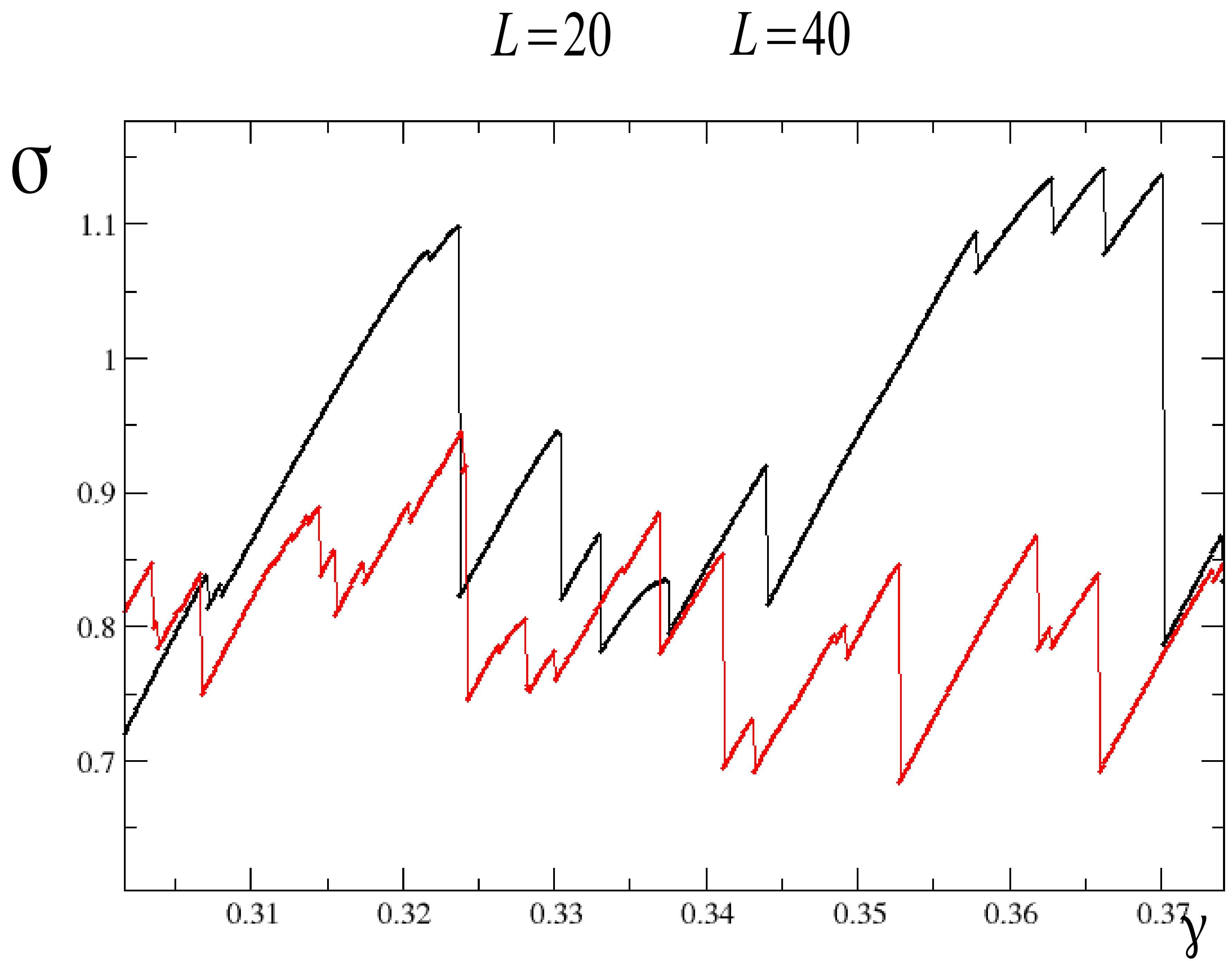
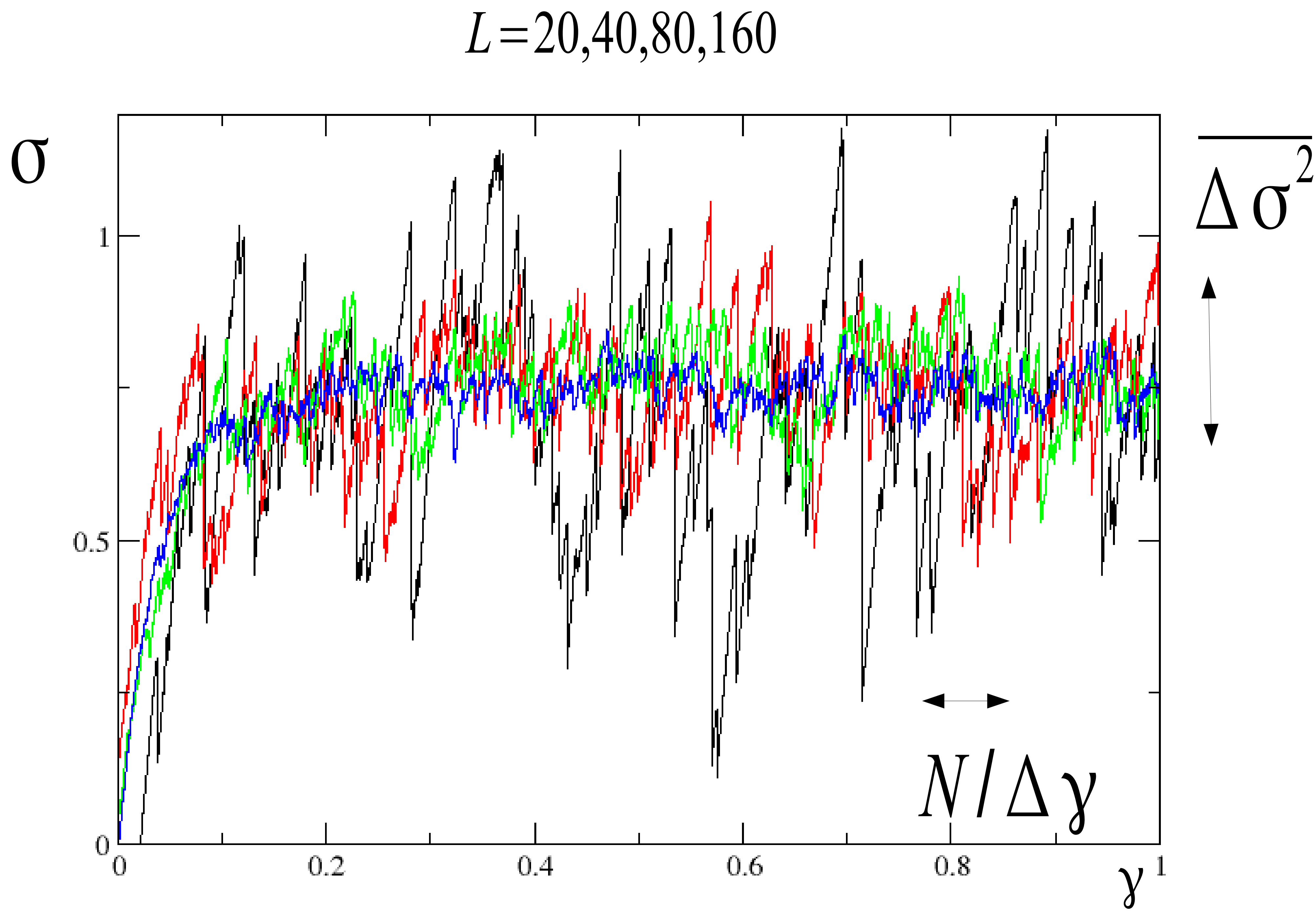




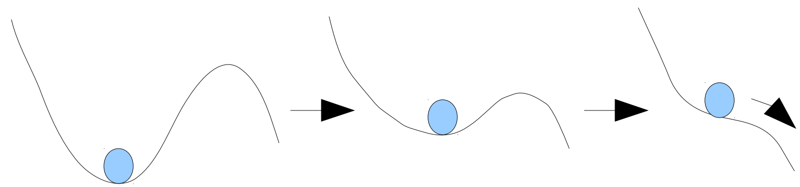


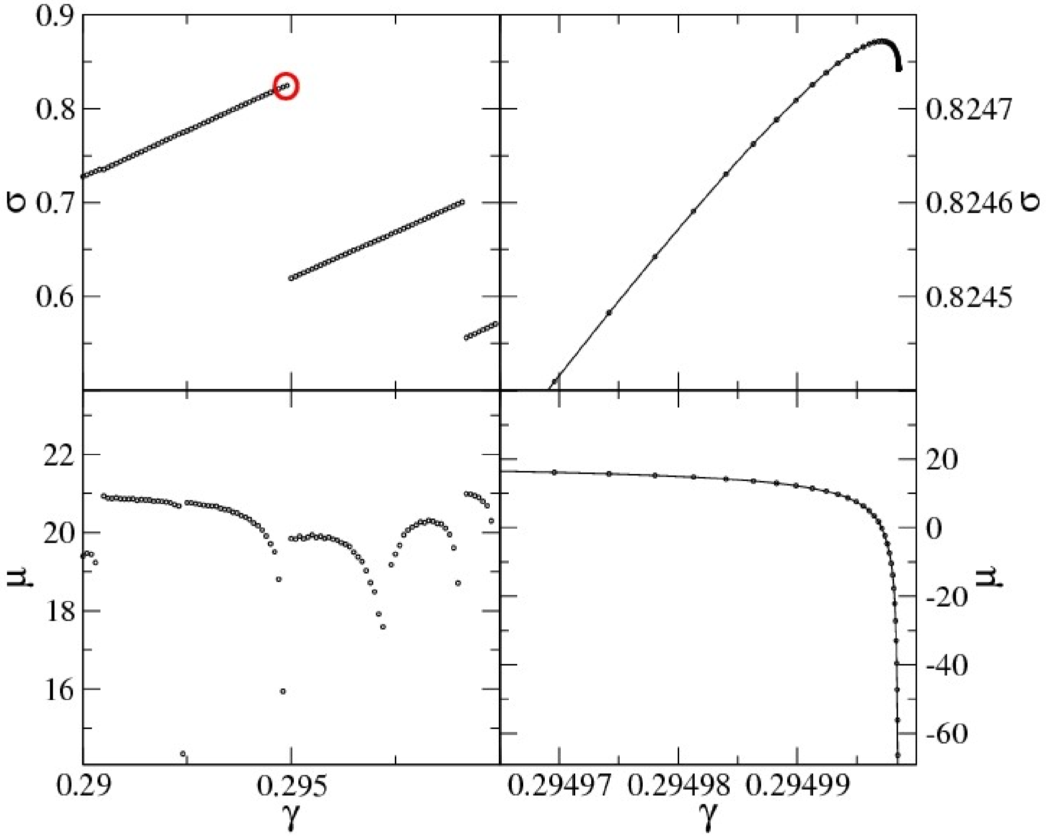
L=20 L=40
σ
1.1
1
0.9
0.8
0.7
0.31
0.32
0.33
0.34
0.35
0.36
0.37
γ



L=20,40,80,160
σ
$\overline{\Delta\sigma^2}$
1
0.5
0
0
0.2
0.4
0.6
0.8
1
γ
N/Δγ

AQS I: Saddle-node bifurcation





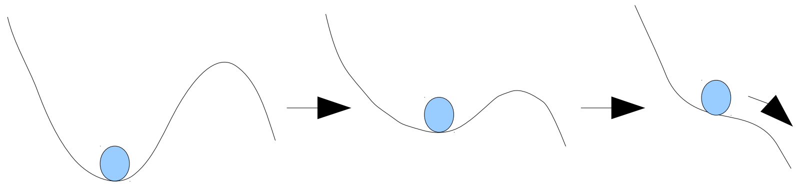
C. Maloney et al, PRL 93, 195501 (2004)

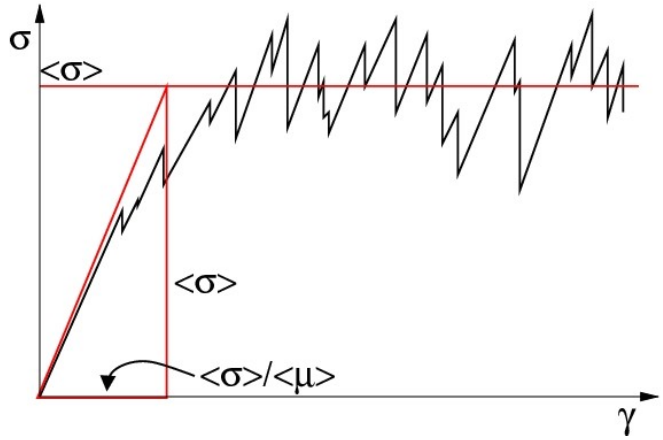
$$\sigma \sim -A\sqrt{\gamma_c - \gamma}$$

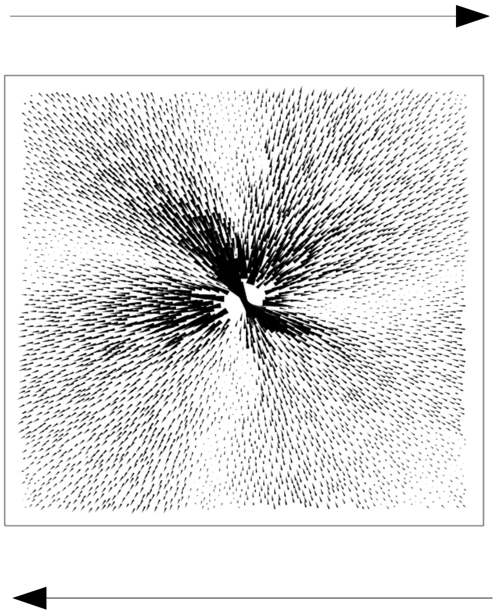
$$\mu \sim -A/\sqrt{\gamma_c - \gamma}$$

$$\Delta E \sim (\gamma_c - \gamma)^{3/2}$$

AQS II: Eshelby quadrupolar events

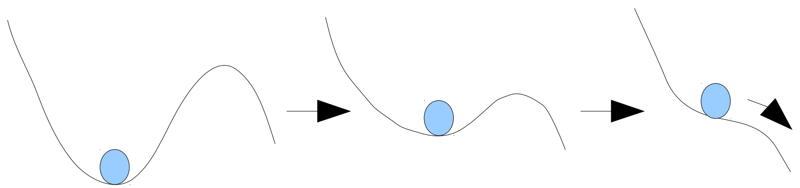


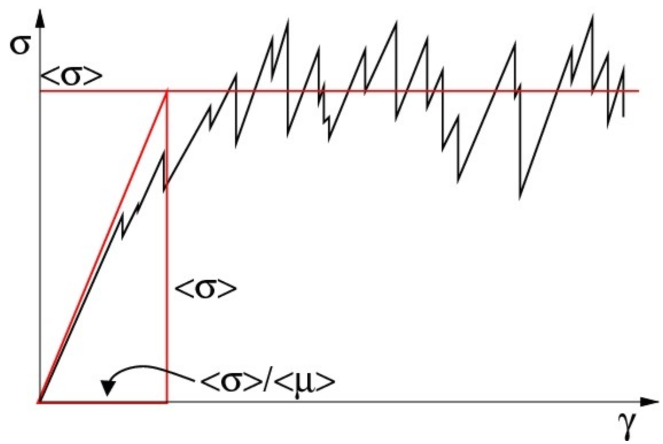




Onset of an event

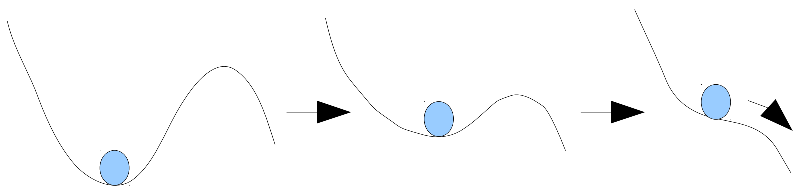
AQS III: Avalanches

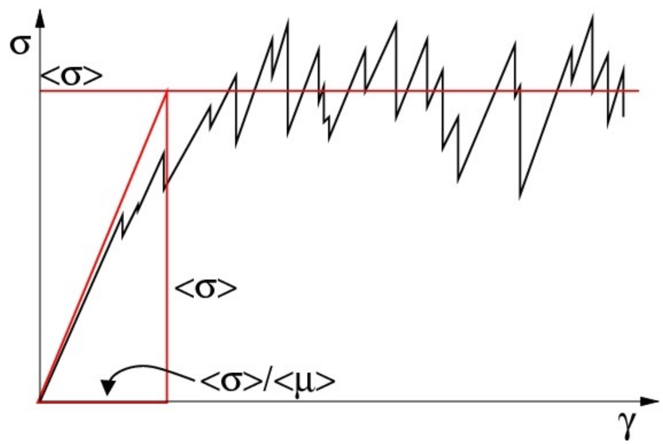




Full plastic event = avalanche

AQS III: Avalanches





In 2D

C. Maloney and AL,
PRL 93, 016001 (2004);

PRE 74, 016118 (2006) $\Delta E \sim L$

E. Lerner and I. Procaccia,
PRE 79, 066109 (2009)

$$\Delta E \sim L^{\beta}, \beta = 0.74$$

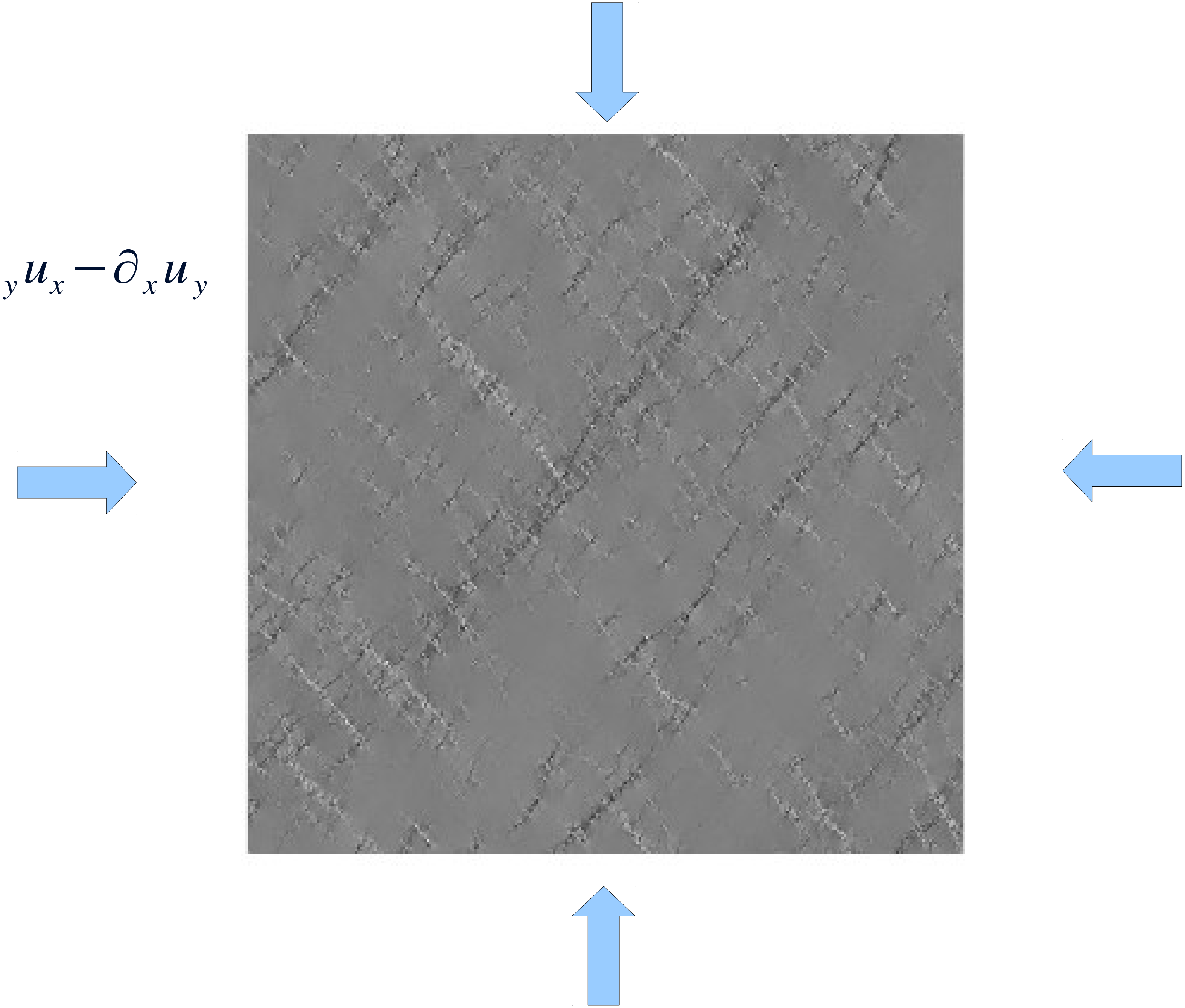
In 3D

N. Bailey et al
PRL 98, 095501 (2007)

$$\Delta E \sim L^{1.4}$$

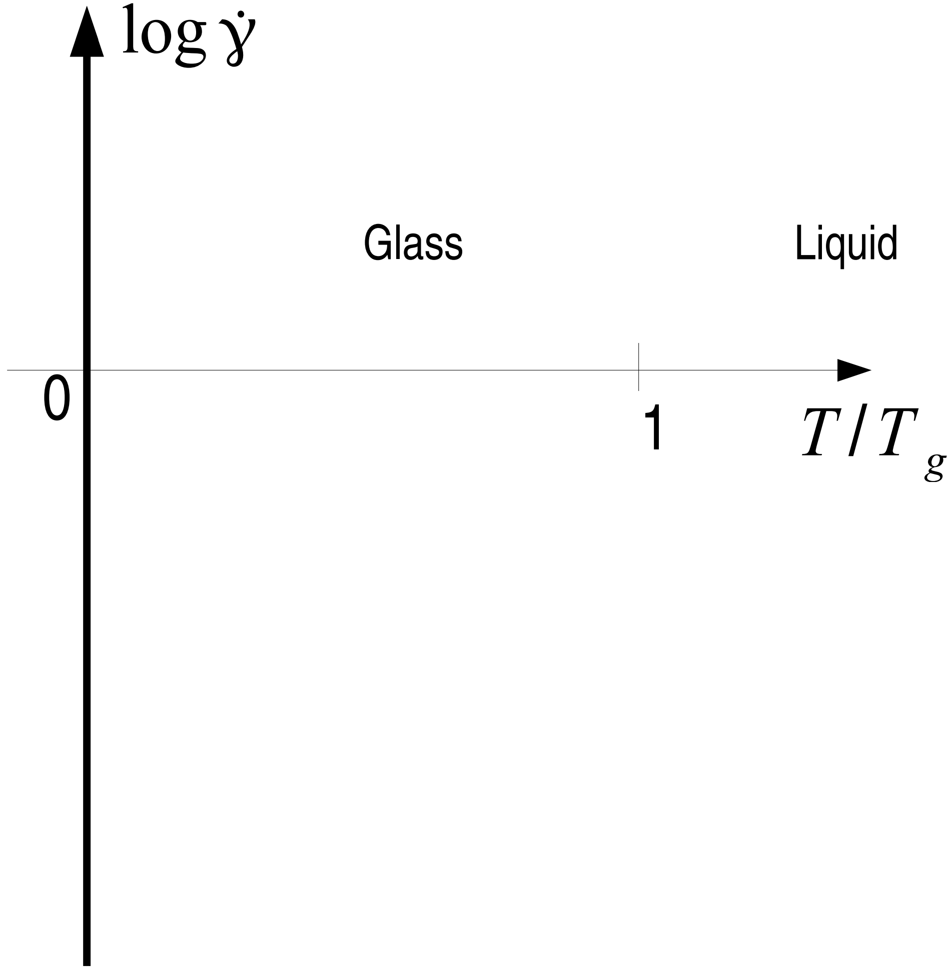
Particle displacement distribution in AQS

$$\omega = \partial_y u_x - \partial_x u_y$$



Maloney & Robbins, J. Phys. Cond. Mat. 20, 244128 (2008)

Athermal, finite-strain rate



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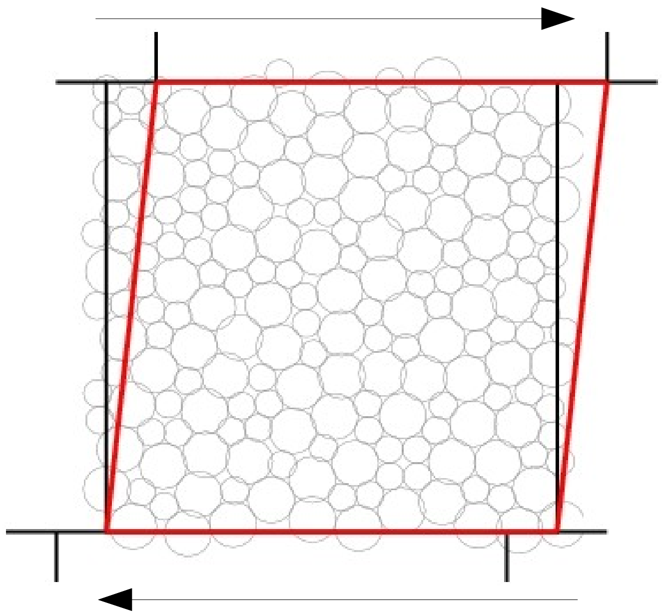
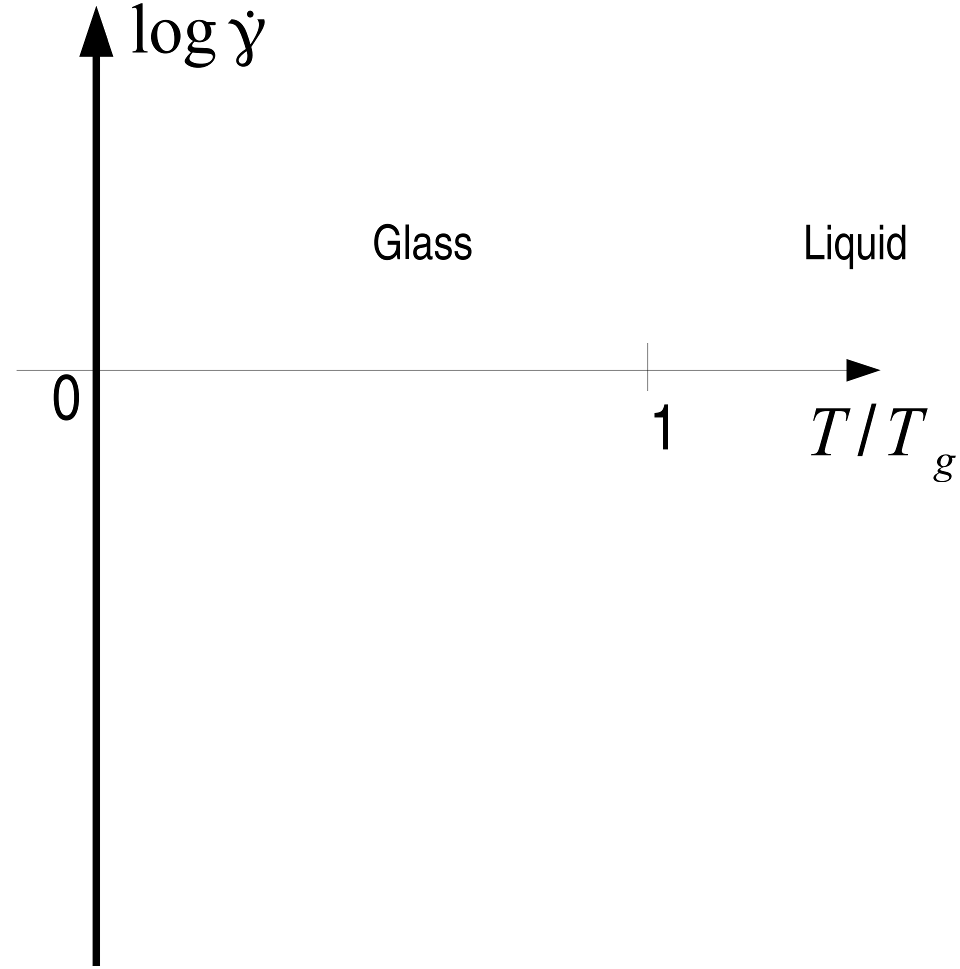


$$U = k\left(r^{-12} - 2r^{-6}\right)$$

Binary Lennard-Jones



AL and C. Caroli, PRL 103, 065501 (2009)

<u>Athermal, finite strain-rate simulations:</u> $T=0 \quad \dot{\gamma} \neq 0$

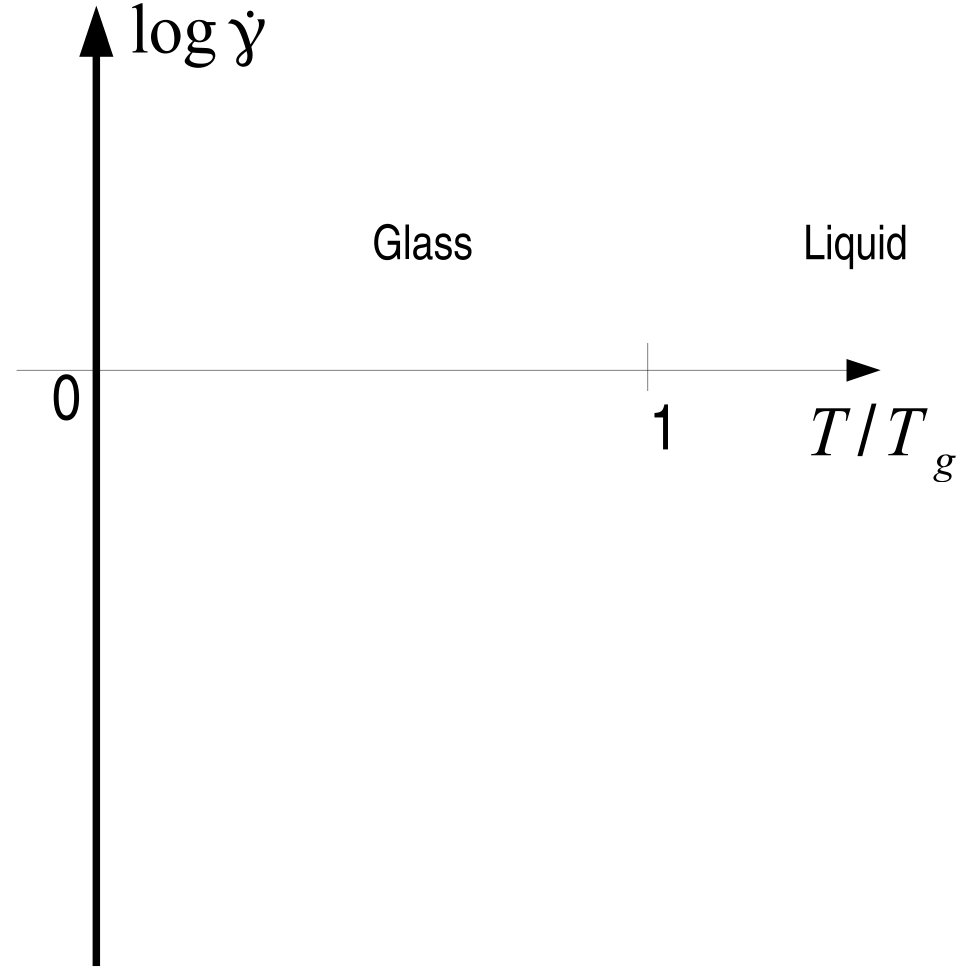
- Standard MD simulation
- Damping forces

$$f_{ij} = \frac{m}{\tau}\phi(r)\left(\vec{v}_j - \vec{v}_i\right)$$

Athermal, finite-strain rate

Non-affine velocity

$$\vec{v}_i - \dot{\gamma}\, y_i \vec{e}_x$$



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Athermal, finite strain-rate

Non-affine velocity

$$\vec{v}_i - \dot{\gamma}\, y_i \vec{e}_x$$

$L = 160$

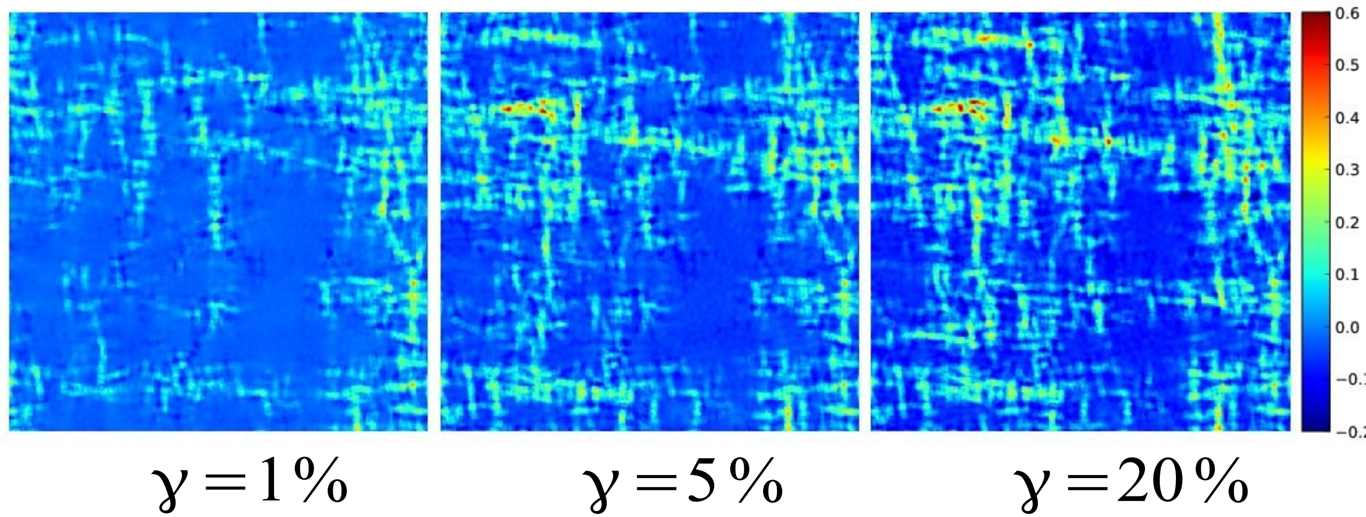
$\dot{\gamma} = 5.10^{-5}$

PRL 103, 065501 (2009)

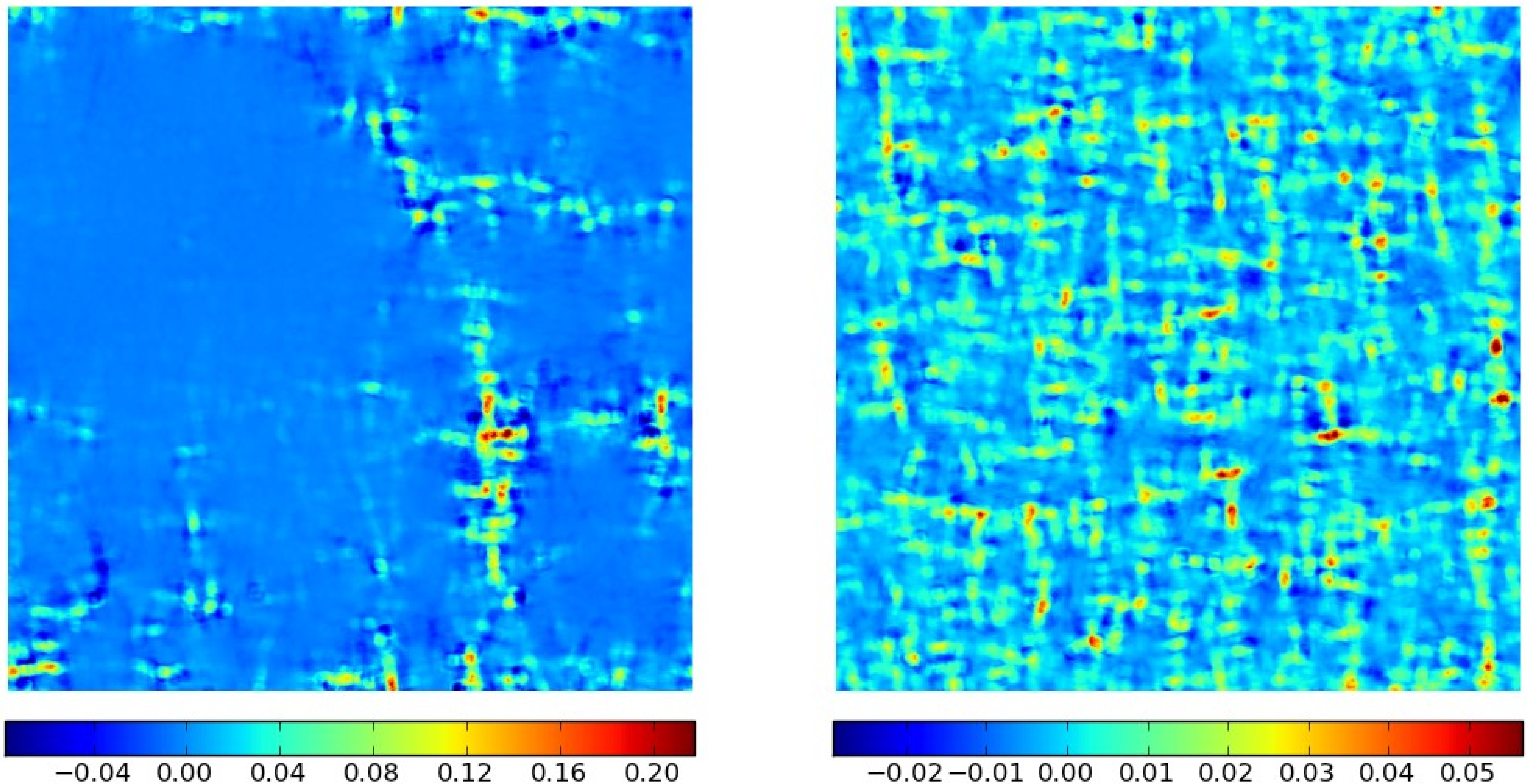
$T < 10^{-4}$

Deformation maps

$\epsilon_{xy}(\vec{r})$

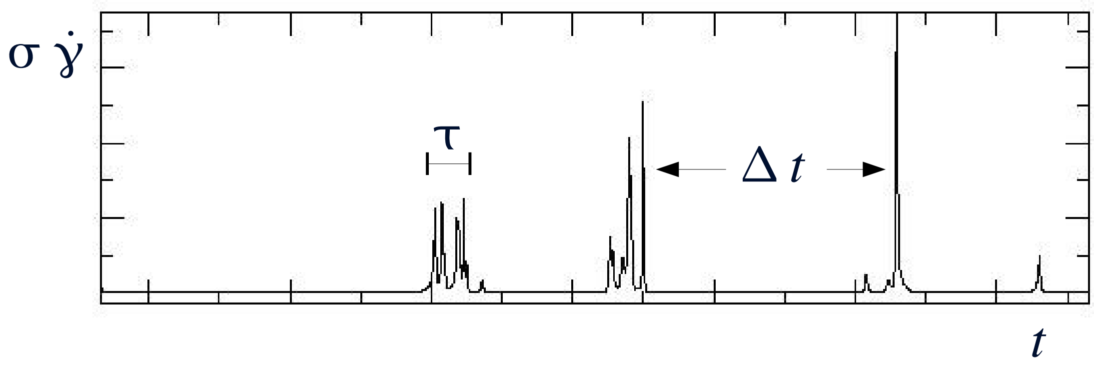


$\dot{\gamma}=10^{-4}$ $\dot{\gamma}=10^{-2}$



$\Delta\gamma=1\%$

How slow should we drive an athermal system to reach the AQS limit?



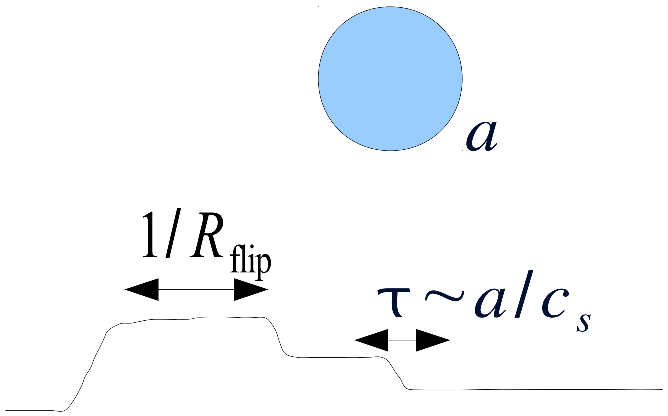
$$\langle \Delta t \rangle \gg \tau$$

Average interval — event duration

What is the noise received by a weak zone?

System size: L

Total flip rate: $R_{\text{flip}} = \frac{L^2 \dot{\gamma}}{a^2 \Delta \epsilon_0}$



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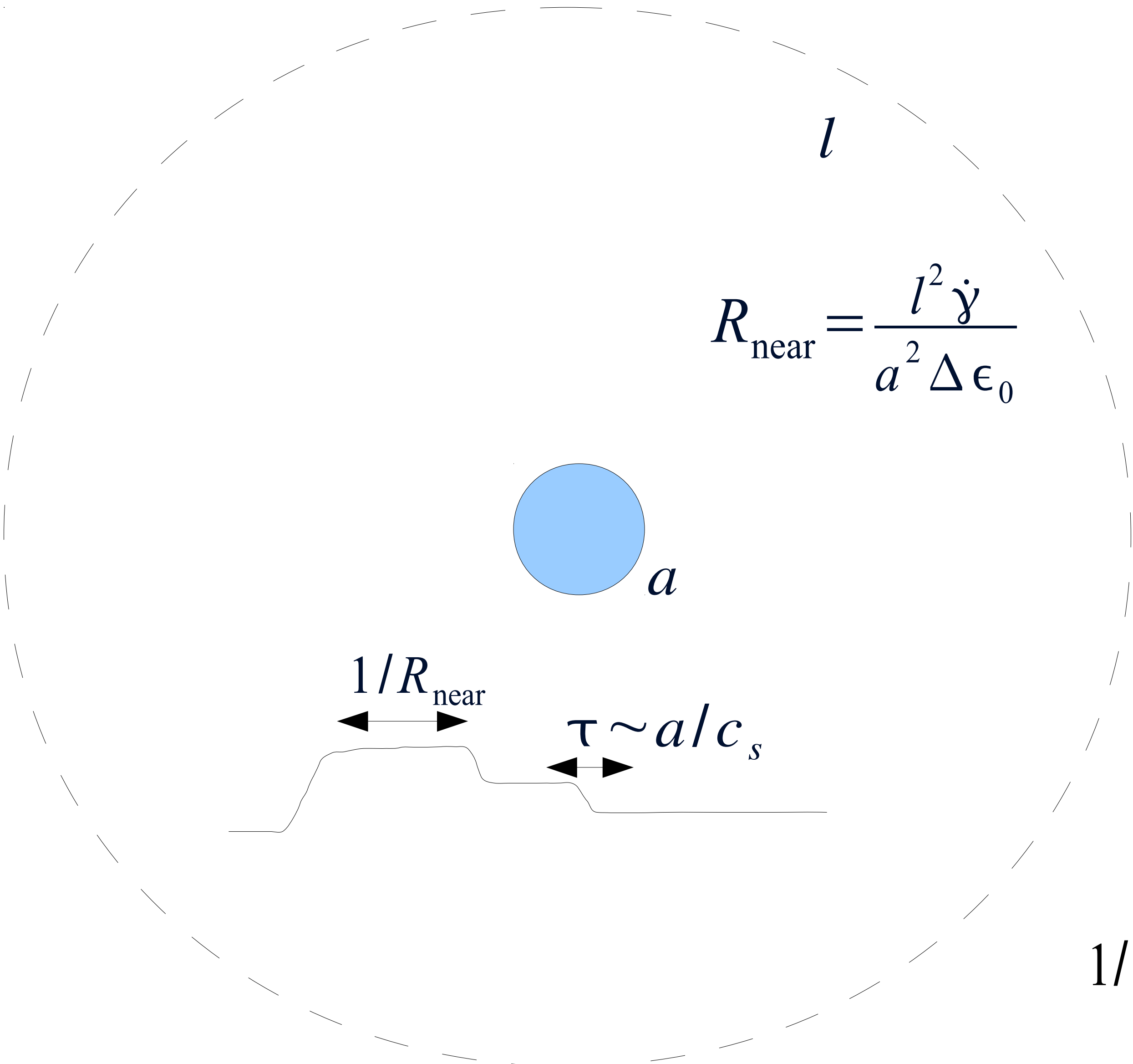

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Now isolate a nearby region of size l

Near field signals are separated iff:

$$1/R_{\text{near}} \gg \tau \;\Leftrightarrow\; l \ll \sqrt{a^2 \Delta \epsilon_0 / \dot{\gamma} \tau_{\text{flip}}}$$

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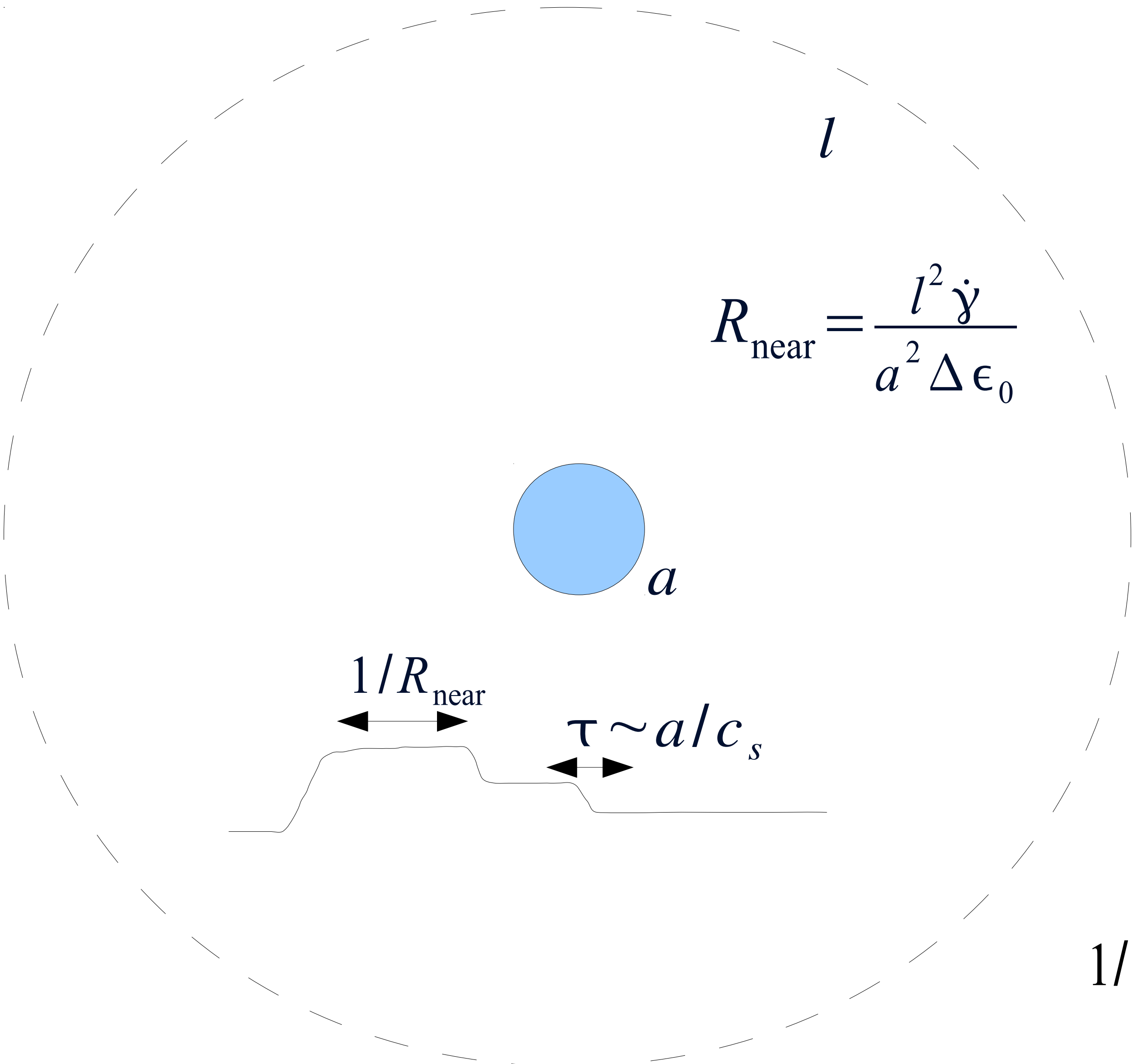

System size: L

Total flip rate: $R_{\text{flip}} = \frac{L^2 \dot{\gamma}}{a^2 \Delta \epsilon_0}$

Background noise:

$$R_{\text{back}} = \frac{(L^2 - l^2)\dot{\gamma}}{a^2 \Delta \epsilon_0}$$

During time τ

Local stress diffuses by:

$$\langle \Delta \sigma^2 \rangle \sim \dot{\gamma} \tau (\mu^2 a^2 \Delta \epsilon_0 / l^2)$$

Now isolate a nearby region of size l

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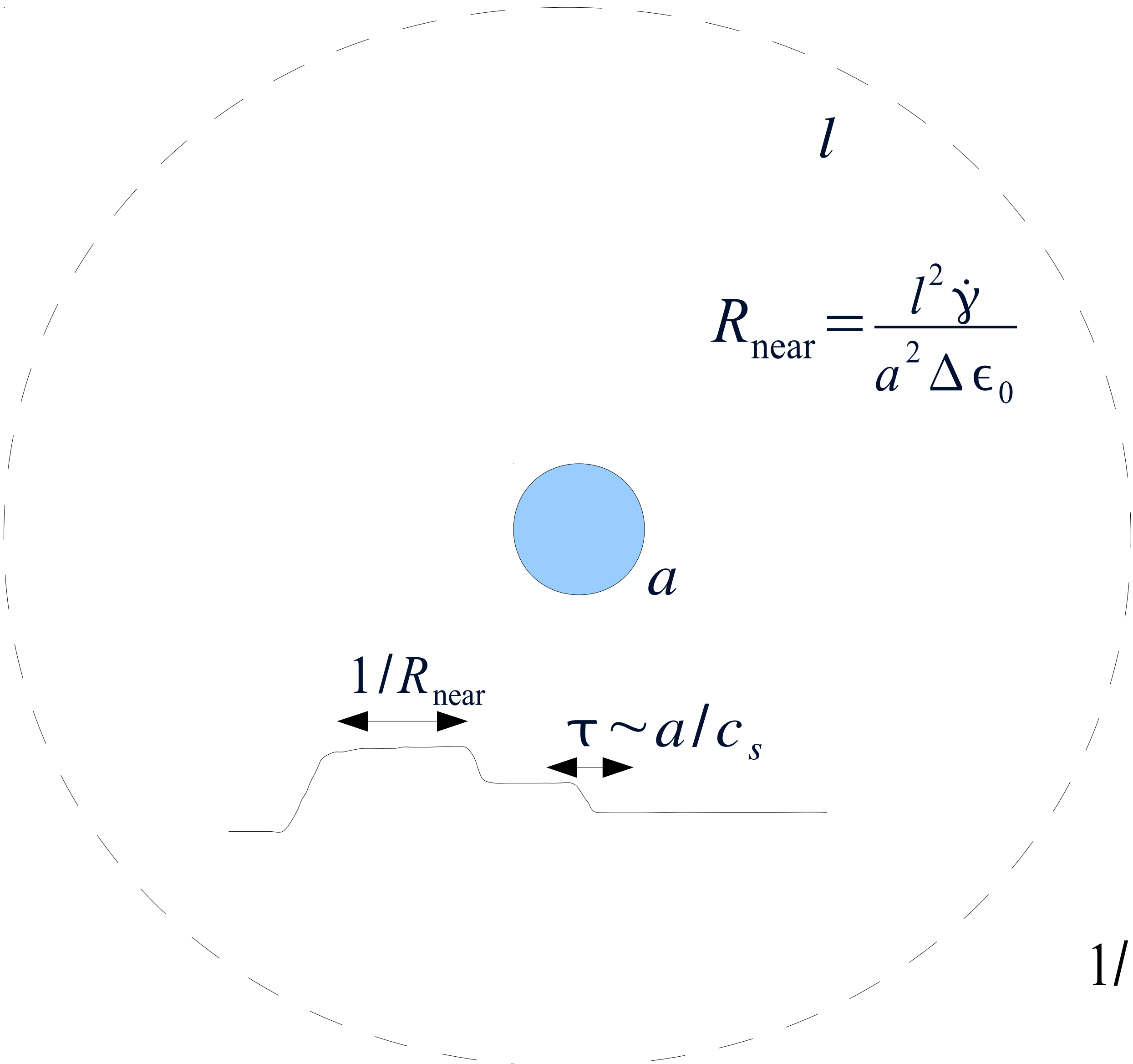

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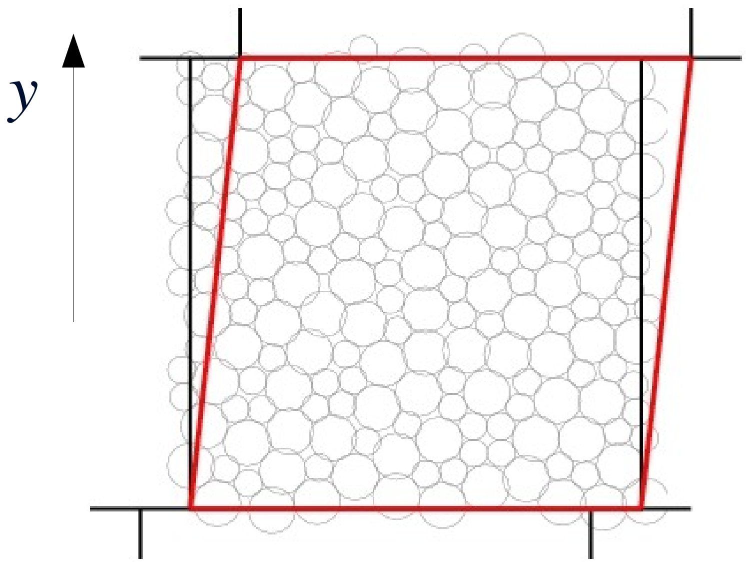
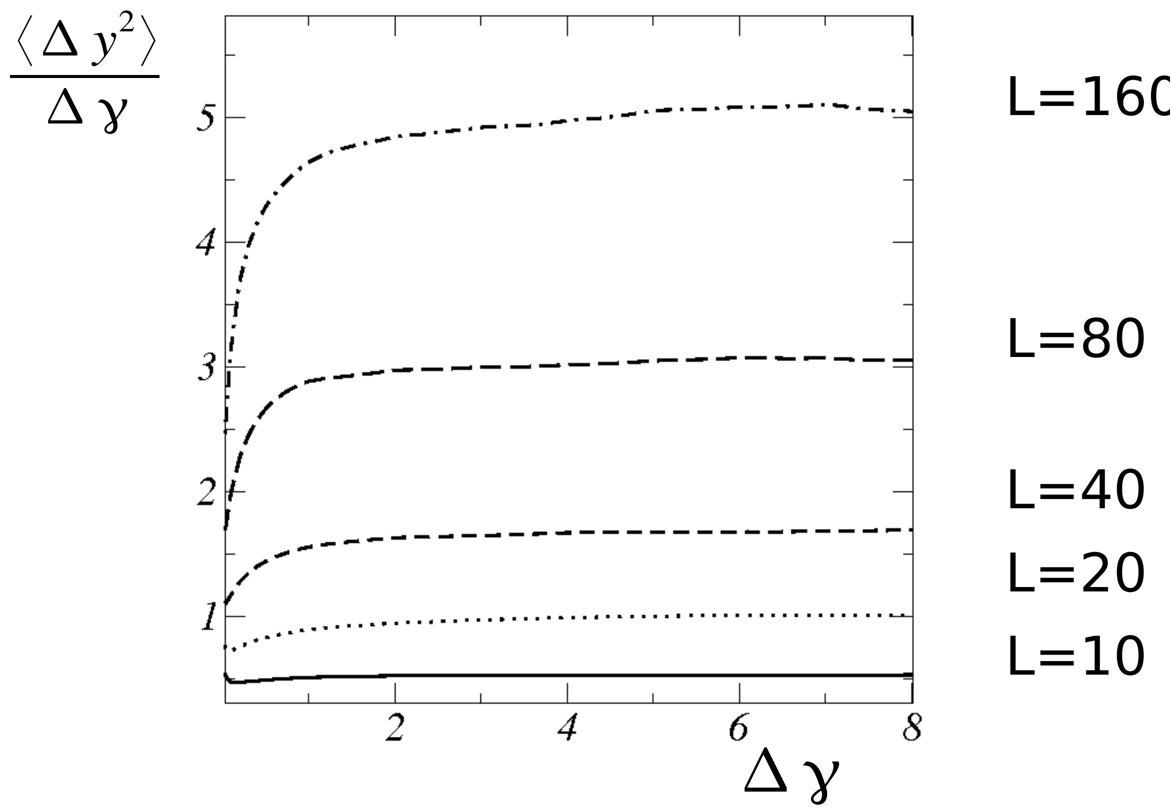
$$\sqrt{\langle \Delta \sigma^2 \rangle} \ll \mu (a^2 \Delta \epsilon_0 / l^2)$$

How to characterize avalanches?

Transverse diffusion coefficient





$$\frac{\langle \Delta y^2 \rangle}{\Delta \gamma} \longrightarrow \widehat{D} = D/\dot{\gamma}$$

with L

Plasticity-induced diffusion

Over a large strain interval: $\Delta y_i = \sum_f u_y^e(\vec{r}_i - \vec{r}_f) \Rightarrow \langle \Delta y^2 \rangle = N_e(\Delta\gamma)\ \langle u_y^2 \rangle_e$

<u>Events = single flips</u>

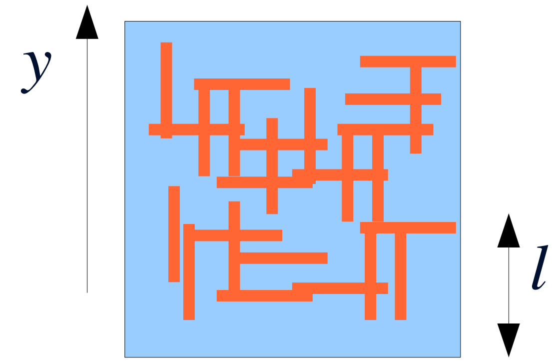
$$N_f(\Delta\gamma) = \frac{L^2 \Delta\gamma}{a^2 \Delta\epsilon_0}$$

Eshelby: $\vec{u} = \frac{2a^2\Delta\epsilon_0}{\pi} \frac{xy}{r^4}\vec{r}$

$$\langle u_y^2 \rangle_f = \frac{a^4 \Delta\epsilon_0^2}{4\pi} \ln(L/a)$$

$$\frac{\langle \Delta y^2 \rangle}{\Delta\gamma} = \frac{a^2\Delta\epsilon_0}{4\pi}\ln(L/a)$$

<u>Events = linear avalanches</u>



$$N_a(\Delta\gamma) = N_f(\Delta\gamma)/\nu l$$

$$\langle u_y^2 \rangle_a = \frac{a^4 \Delta\epsilon_0^2 \nu^2}{2\pi}\left(\frac{l}{L}\right)^2 \ln(L/l)$$

$$\frac{\langle \Delta y^2 \rangle}{\Delta\gamma} = \frac{a^2\Delta\epsilon_0}{4\pi}\nu l \ln(L/l)$$

AL and C. Caroli, PRL 103, 065501 (2009)
Chattoraj *et al*, PRE 011501 (2011)

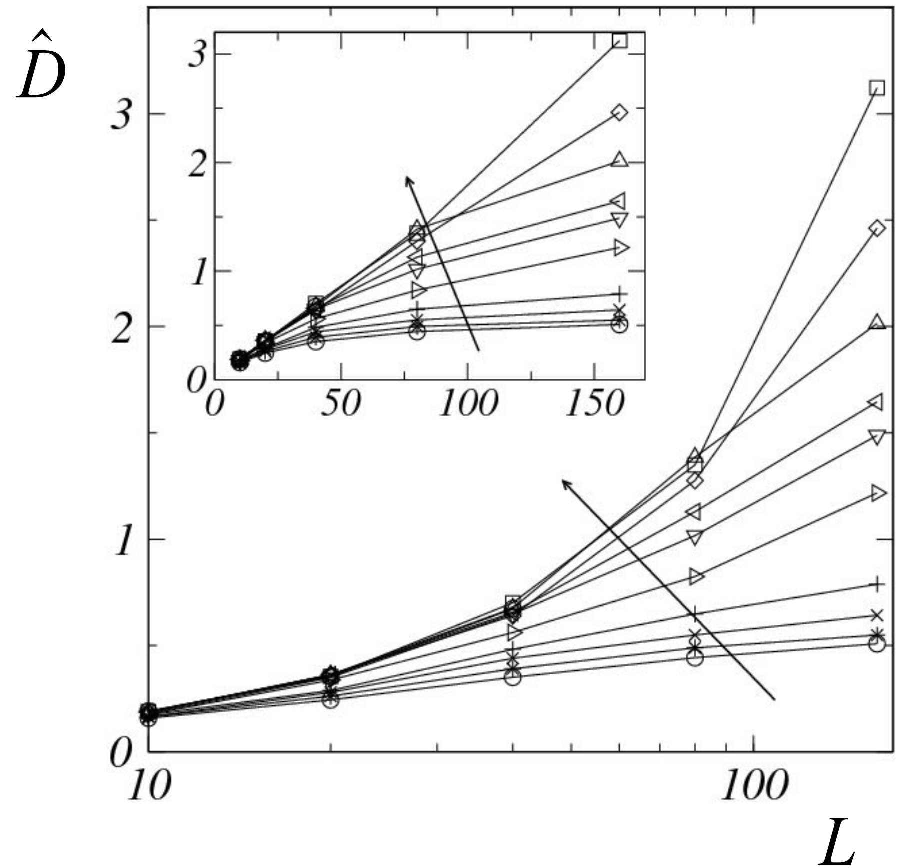
Athermal, finite strain rate: transverse diffusion

$$\hat{D} \equiv \frac{\langle \Delta y^2 \rangle}{\Delta \gamma} = \frac{a^2 \Delta \epsilon_0}{4\pi} \nu\, l \ln(L/l)$$

Large $\dot{\gamma} \Rightarrow l \sim a \qquad \hat{D} \sim \ln L$

$\dot{\gamma} \to 0 \Rightarrow l \sim L \qquad \hat{D} \sim L$

QS regime



Using $l(\dot{\gamma}) \propto 1/\sqrt{\dot{\gamma}} \Rightarrow \hat{D}/L = f(L\sqrt{\dot{\gamma}})$

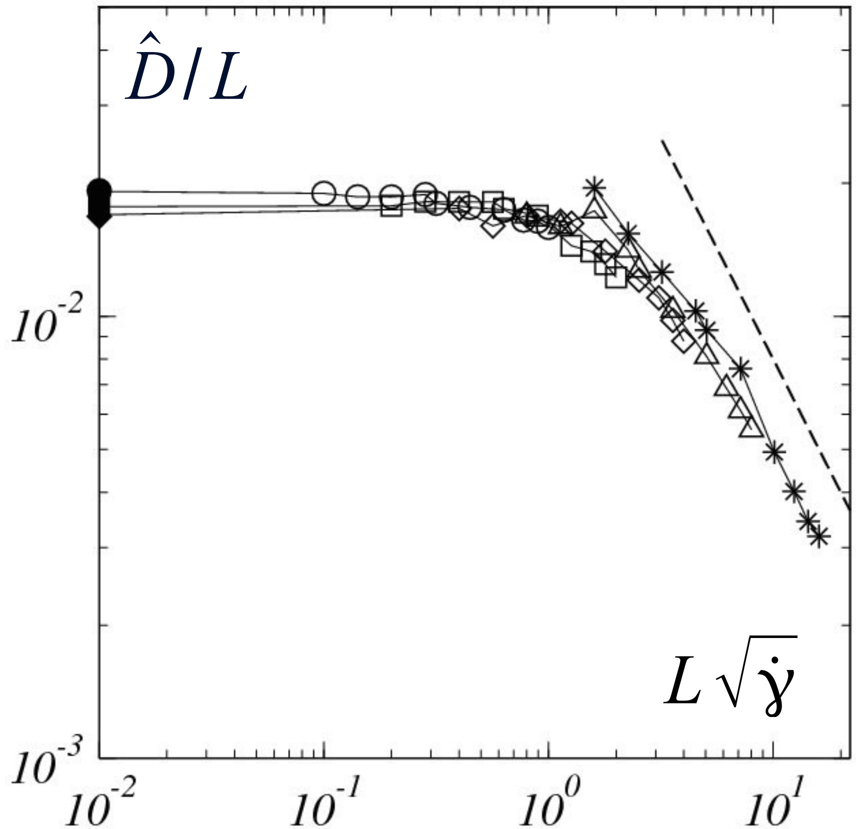
Athermal, finite strain rate: transverse diffusion

$$\hat{D} \equiv \frac{\langle \Delta y^2 \rangle}{\Delta \gamma} = \frac{a^2 \Delta \epsilon_0}{4\pi} \nu\, l \ln(L/l)$$

Large $\dot{\gamma} \Rightarrow l \sim a \qquad \hat{D} \sim \ln L$

$\dot{\gamma} \to 0 \Rightarrow l \sim L \qquad \hat{D} \sim L$

QS regime



Using $l(\dot{\gamma}) \propto 1/\sqrt{\dot{\gamma}} \Rightarrow \hat{D}/L = f(L\sqrt{\dot{\gamma}})$

Relevance of avalanche size

- Extension to 3D $l(\dot\gamma) \sim a(\Delta\epsilon_0/\dot\gamma\tau_{\mathrm{flip}})^{1/3}$

  $\Rightarrow$ For atomic glass, with $\tau_{\mathrm{LJ}} \sim 10^{-13}\,\mathrm{sec}$ $\quad a \sim 1\,\mathrm{nm}$ $\quad \Delta\epsilon_0 \sim 5\,\%$

  For $\dot\gamma \le 10^{-3}\,\mathrm{s}^{-1}$ $\quad l \ge 1\,\mu\mathrm{m}$ (see: Nieh *et al* (2002))

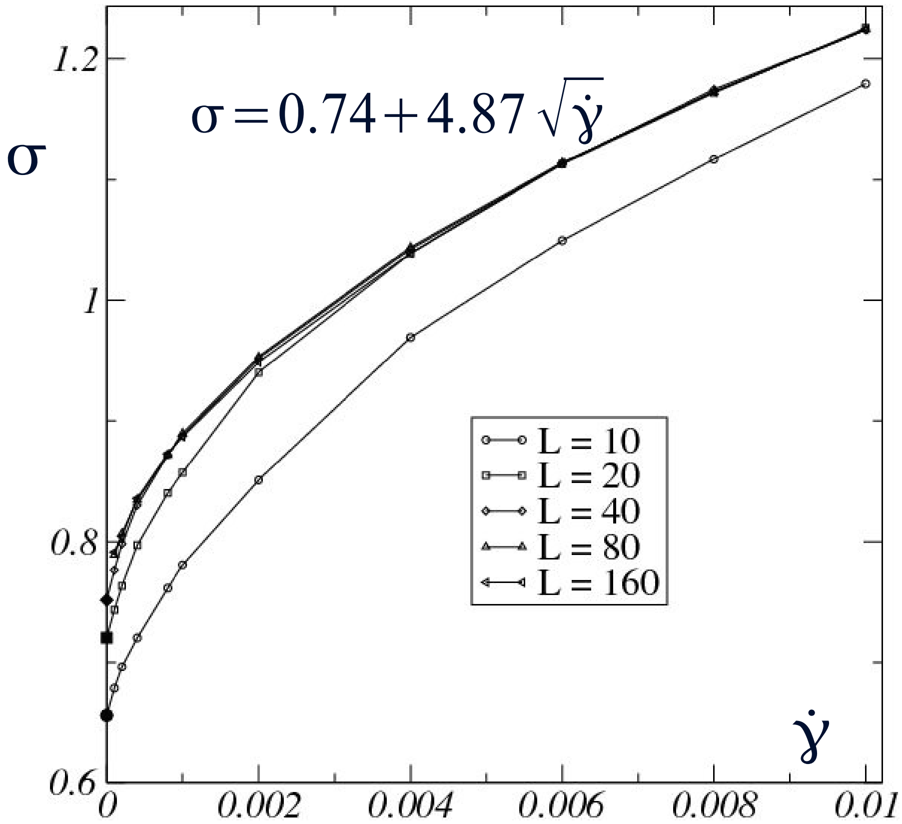
- 2D flow curve $\sigma(\dot\gamma)$

guess: $\sigma - \sigma_y \approx \mu\dot\gamma\tau_{\mathrm{av}}$

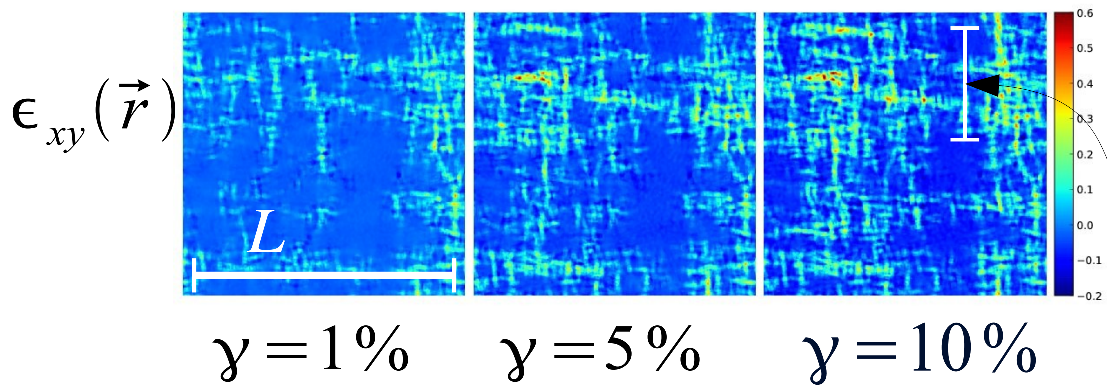
event duration: $\tau_{\mathrm{av}} \sim l/c_s$
(domino-like avalanches)

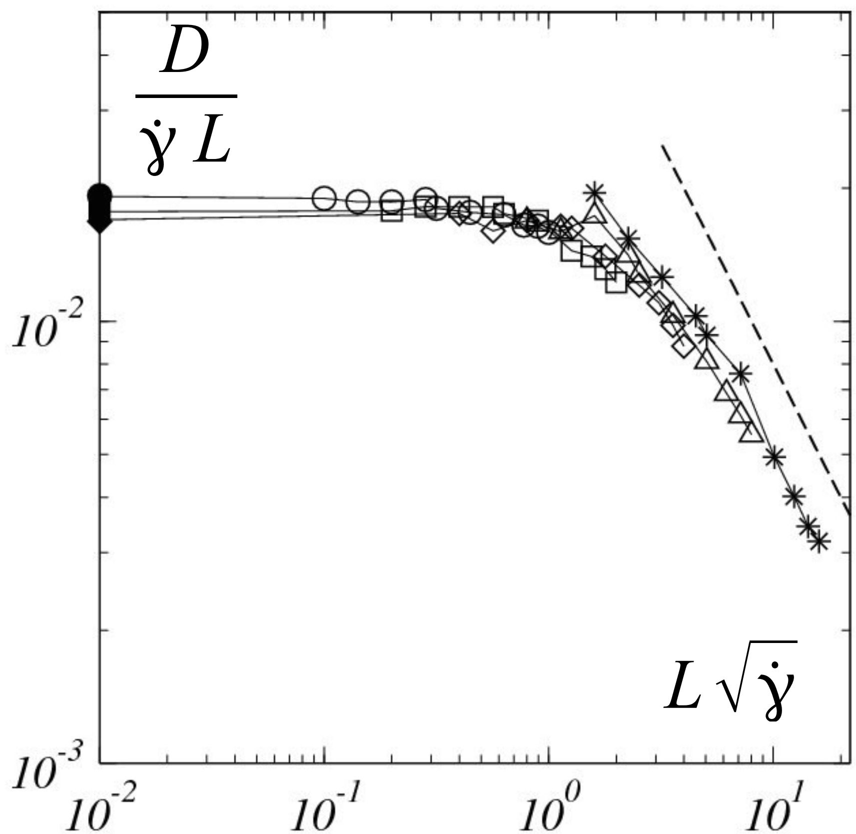
$$\Rightarrow \sigma = \sigma_y + C\sqrt{\dot\gamma}$$

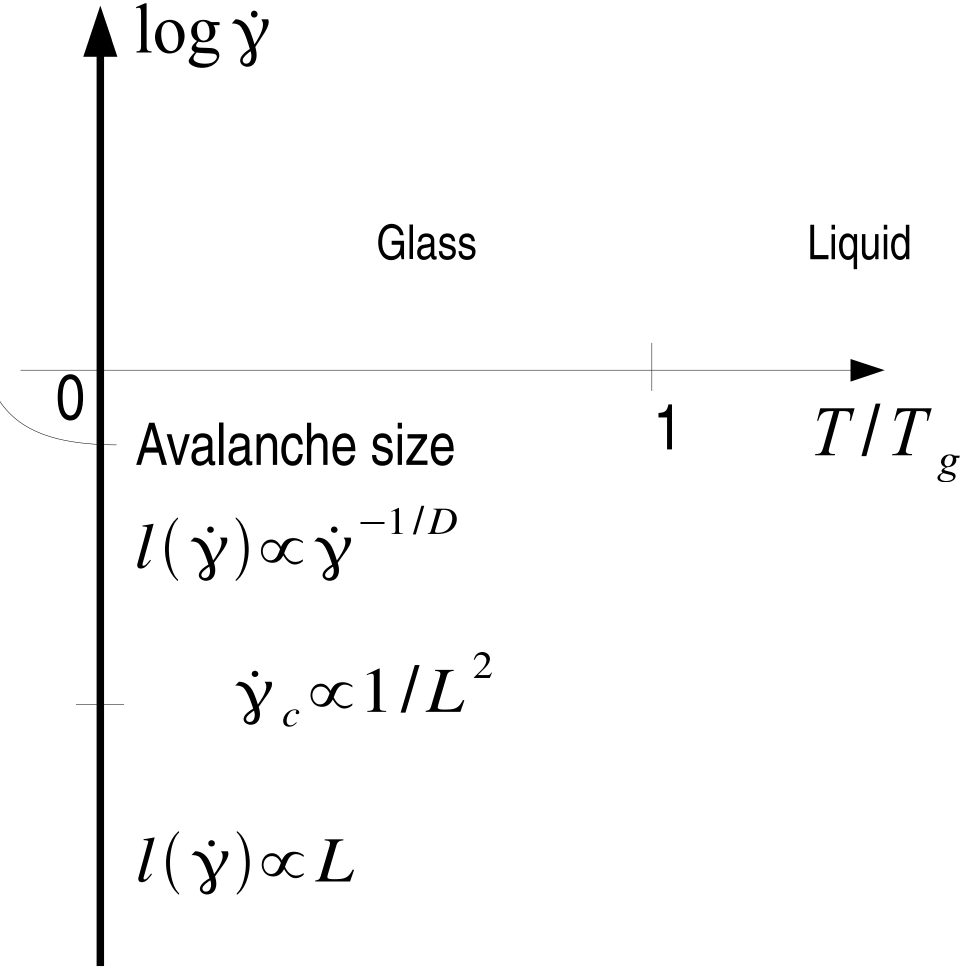
$$C = \frac{\mu}{c_s} a^2 \frac{\Delta\epsilon_0}{\tau} \approx 13$$



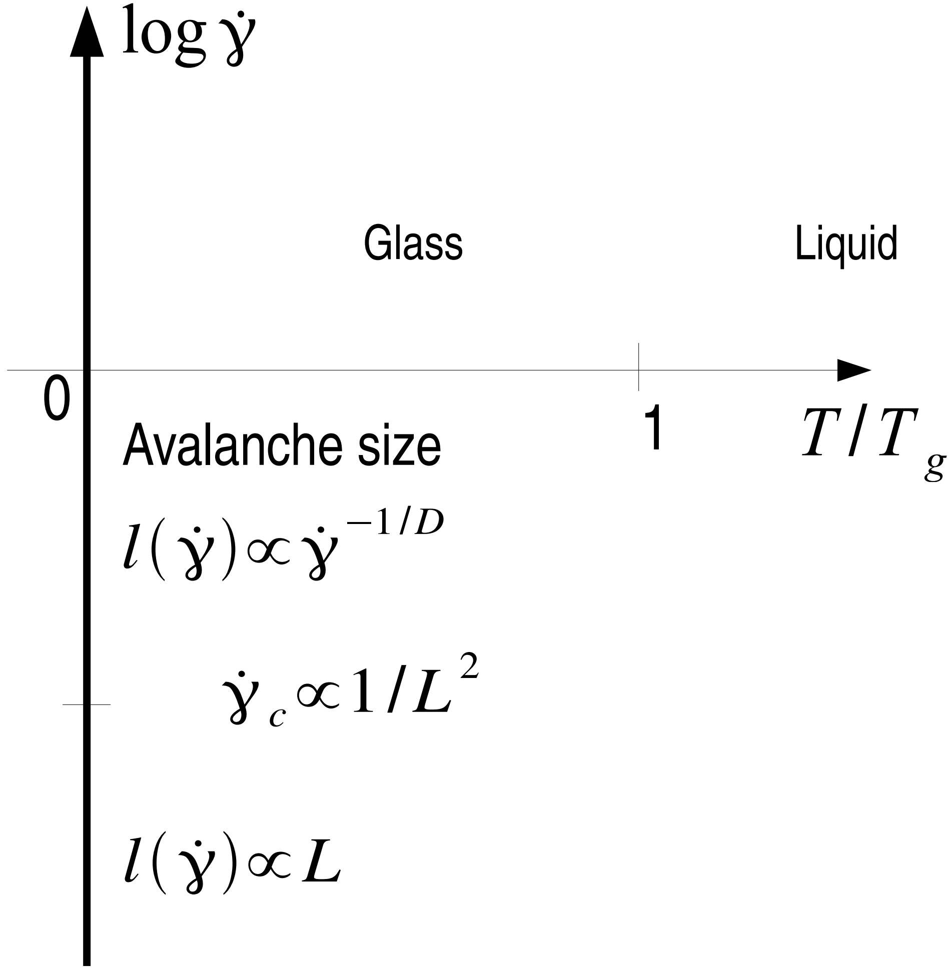
Athermal, finite-strain rate



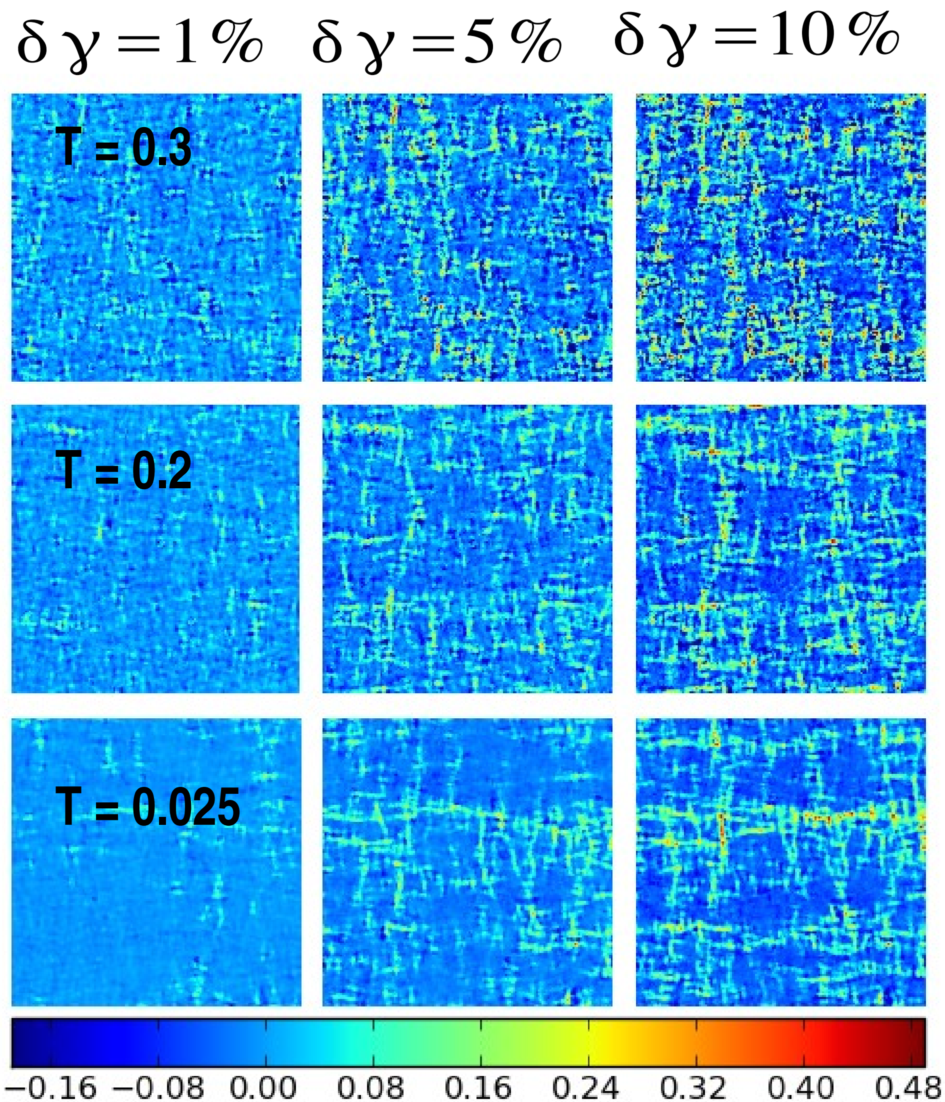


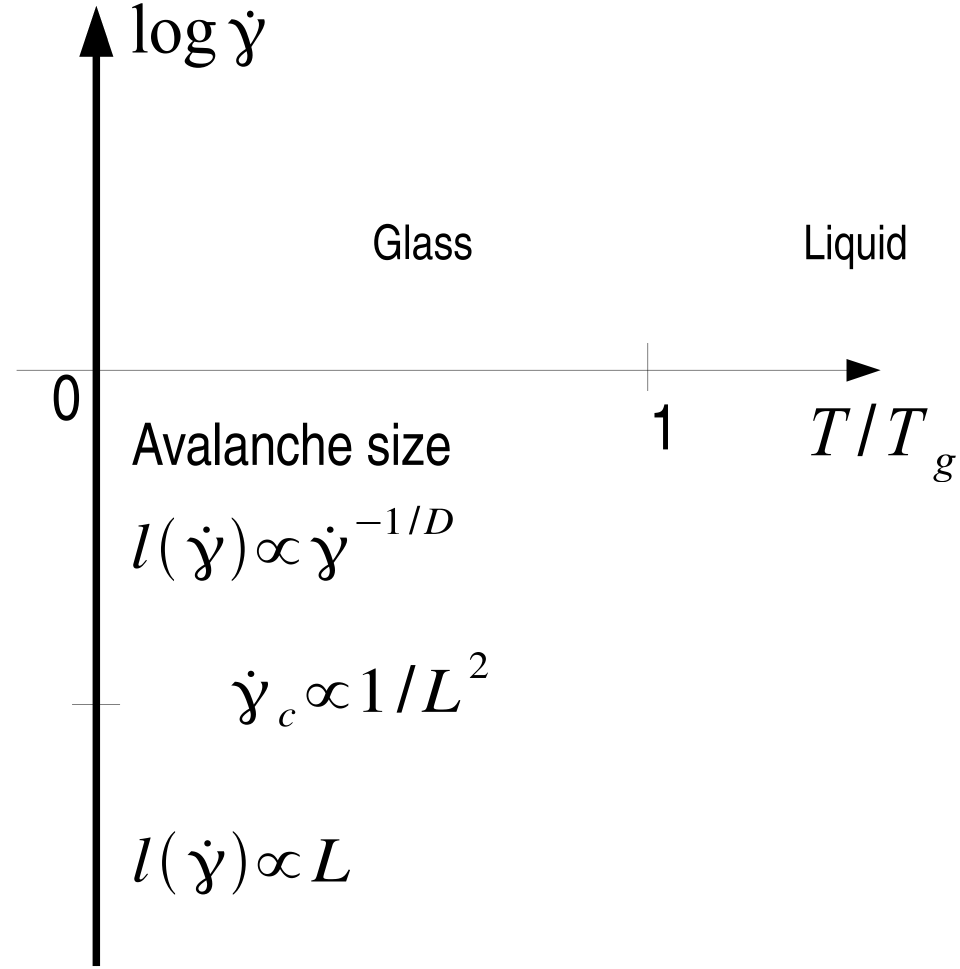


At finite temperature



At finite temperature





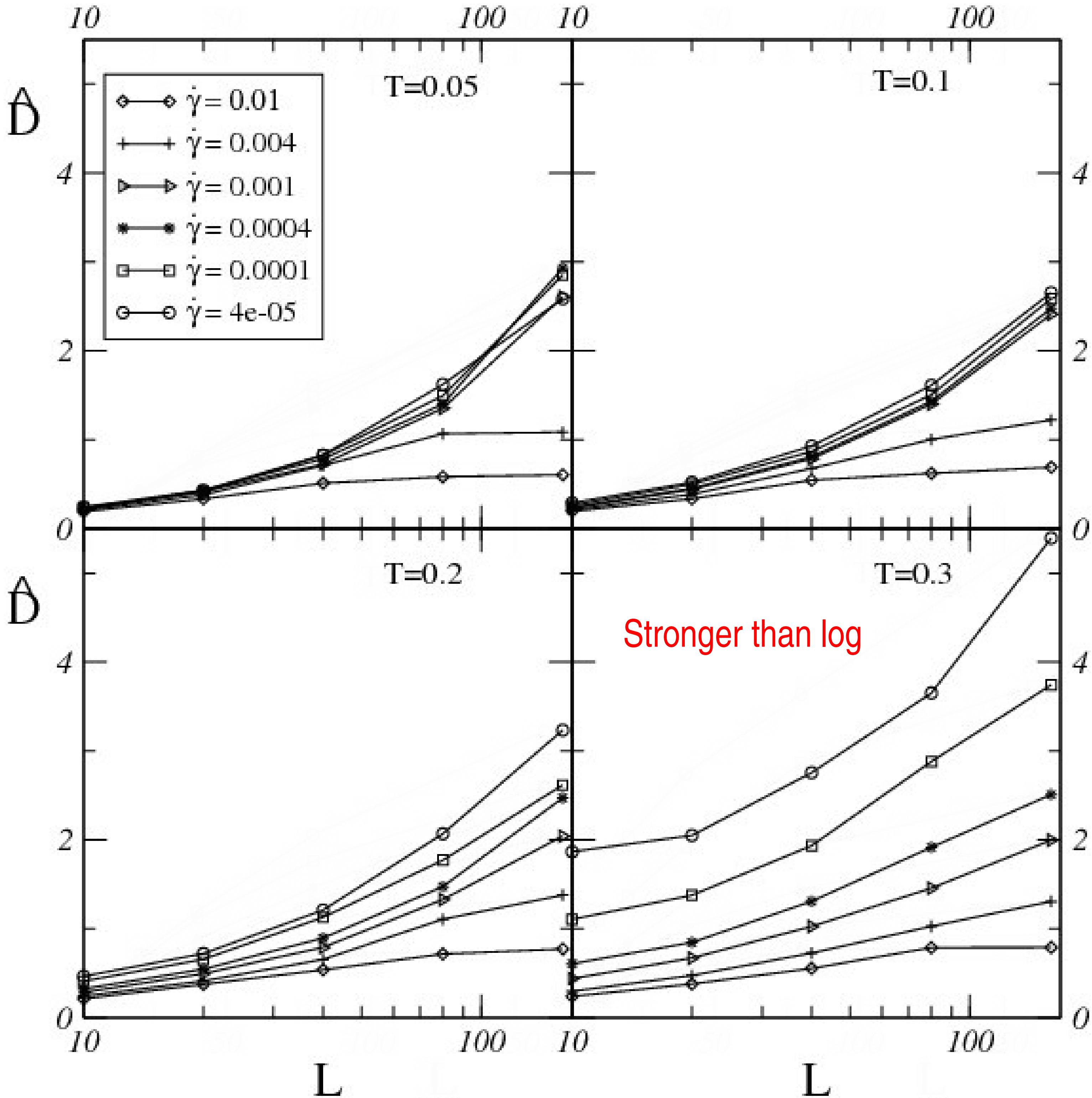
Chattoraj *et al* PRL 105, 266001 (2010)

<u>Finite T, finite strain-rate simulations:</u> $T \neq 0 \quad \dot{\gamma} \neq 0$

- Standard MD simulation
- Velocity rescaling

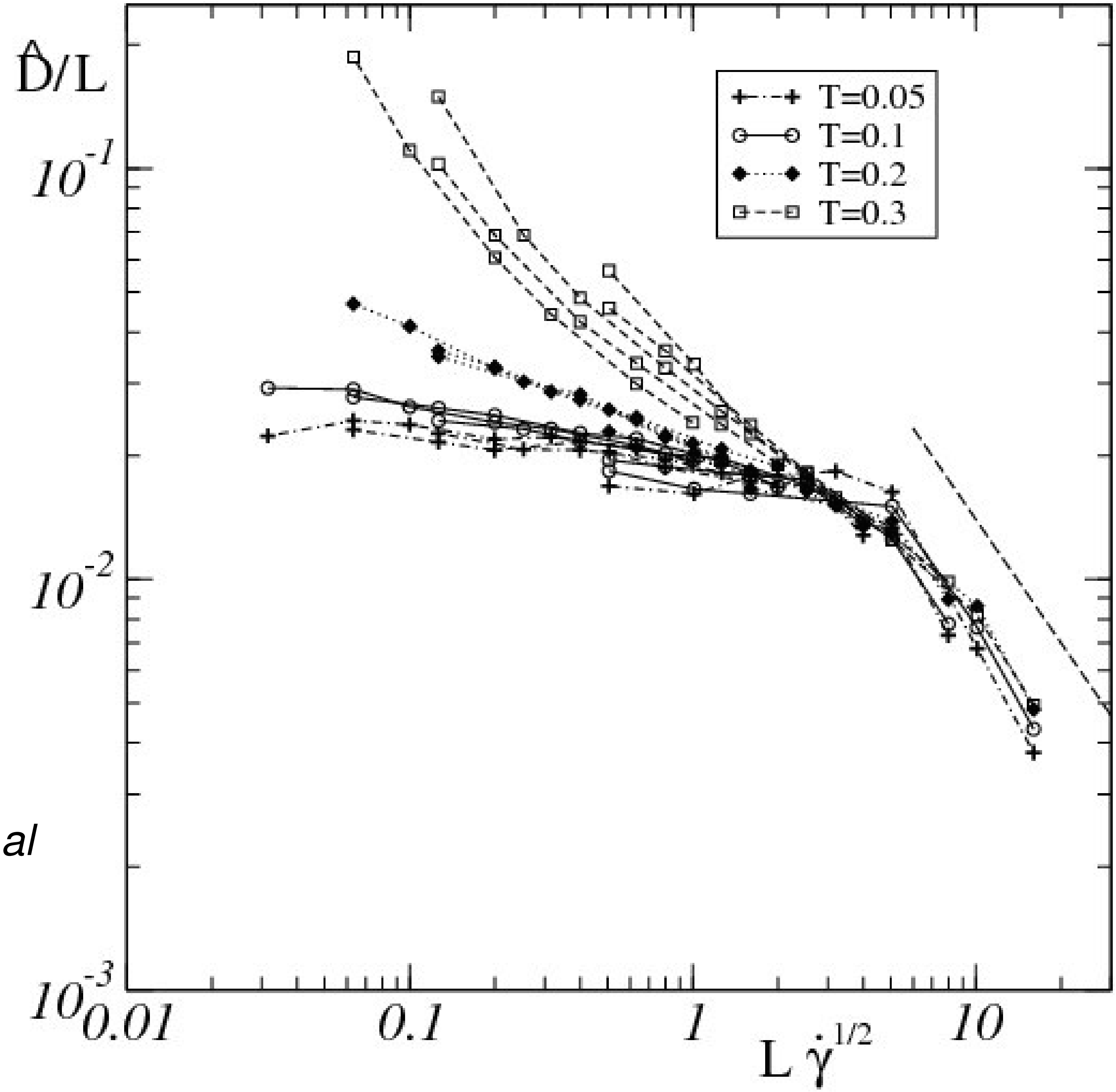
At finite T

For independent events: $\widehat{D} \sim \ln L$



Chattoraj *et al*
PRE (2011)

At finite T

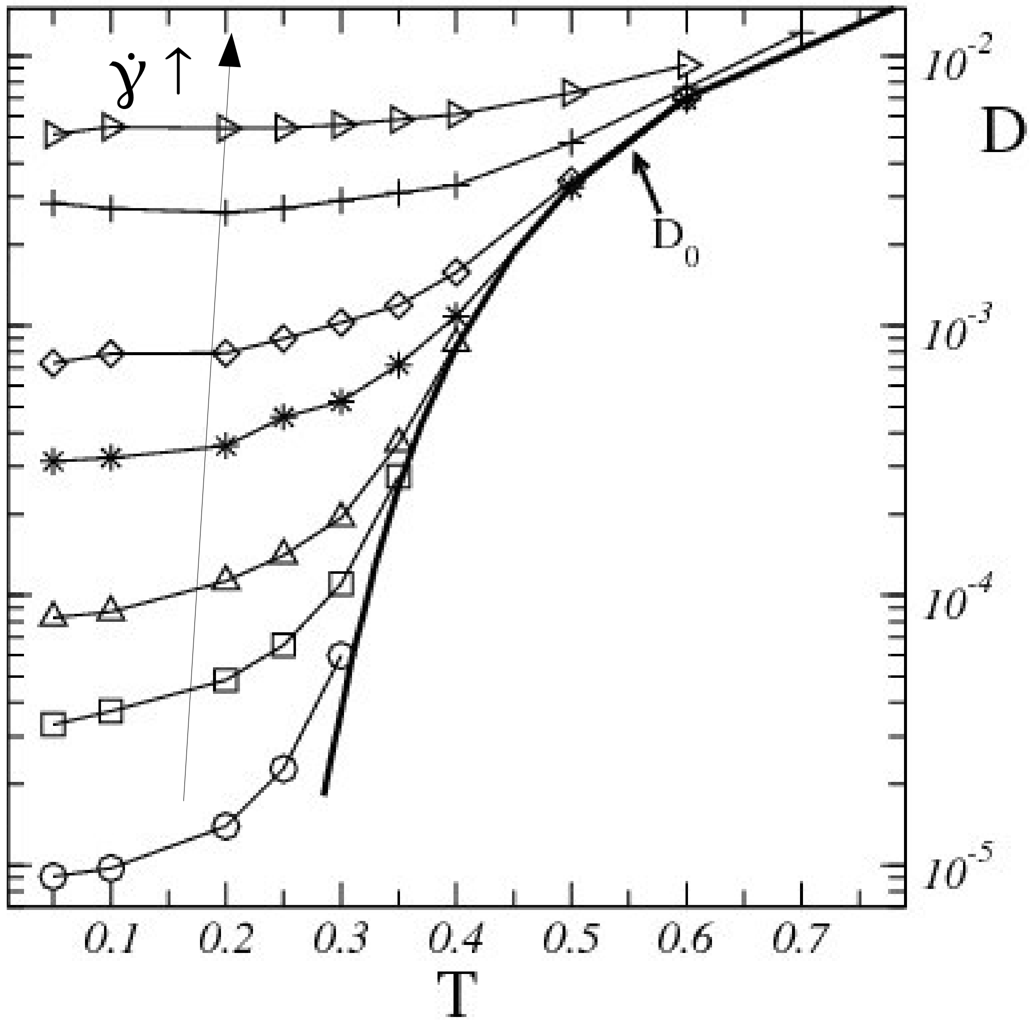


$l(\dot{\gamma}) \propto 1/\sqrt{\dot{\gamma}}$

Chattoraj *et al*
PRE (2011)

At finite T

$$D = \lim_{\Delta\gamma \to \infty} \frac{\langle \Delta y^2 \rangle}{\Delta t}$$



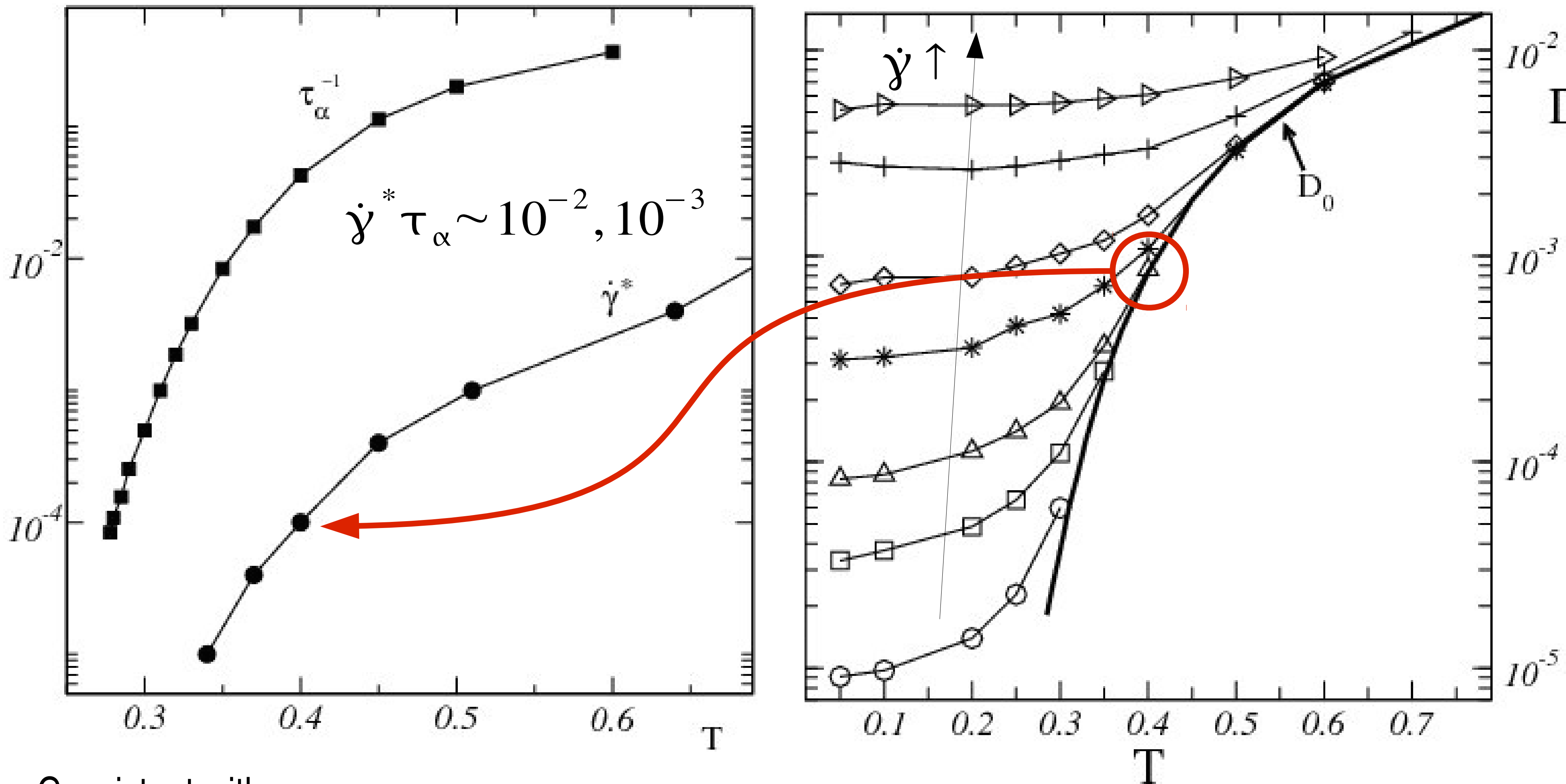
Finite T, finite strain-rate simulations: $T \neq 0 \quad \dot{\gamma} \neq 0$

- Standard MD simulation
- Velocity rescaling

Chattoraj *et al, PRE 2011*

At finite T

$$D = \lim_{\Delta\gamma \to \infty} \frac{\langle \Delta y^2 \rangle}{\Delta t}$$



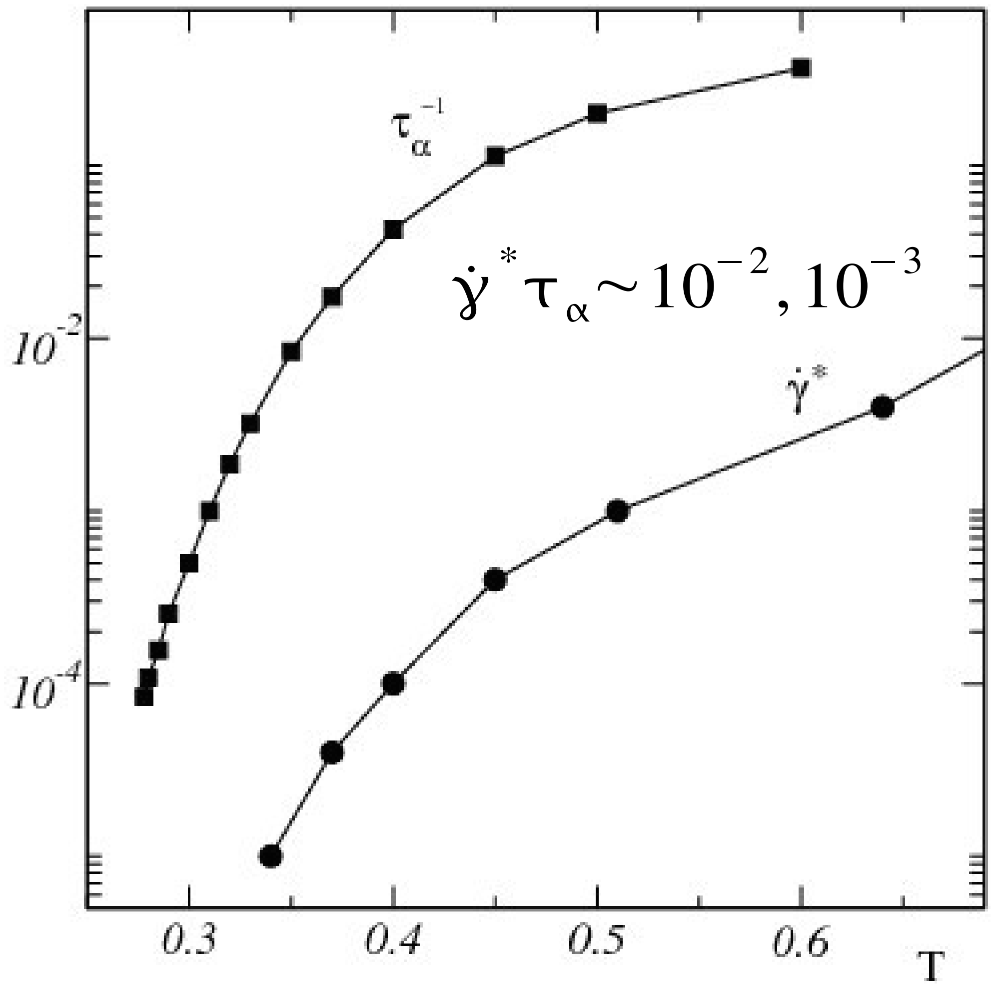
Consistent with Furukawa et al, PRL (2009)

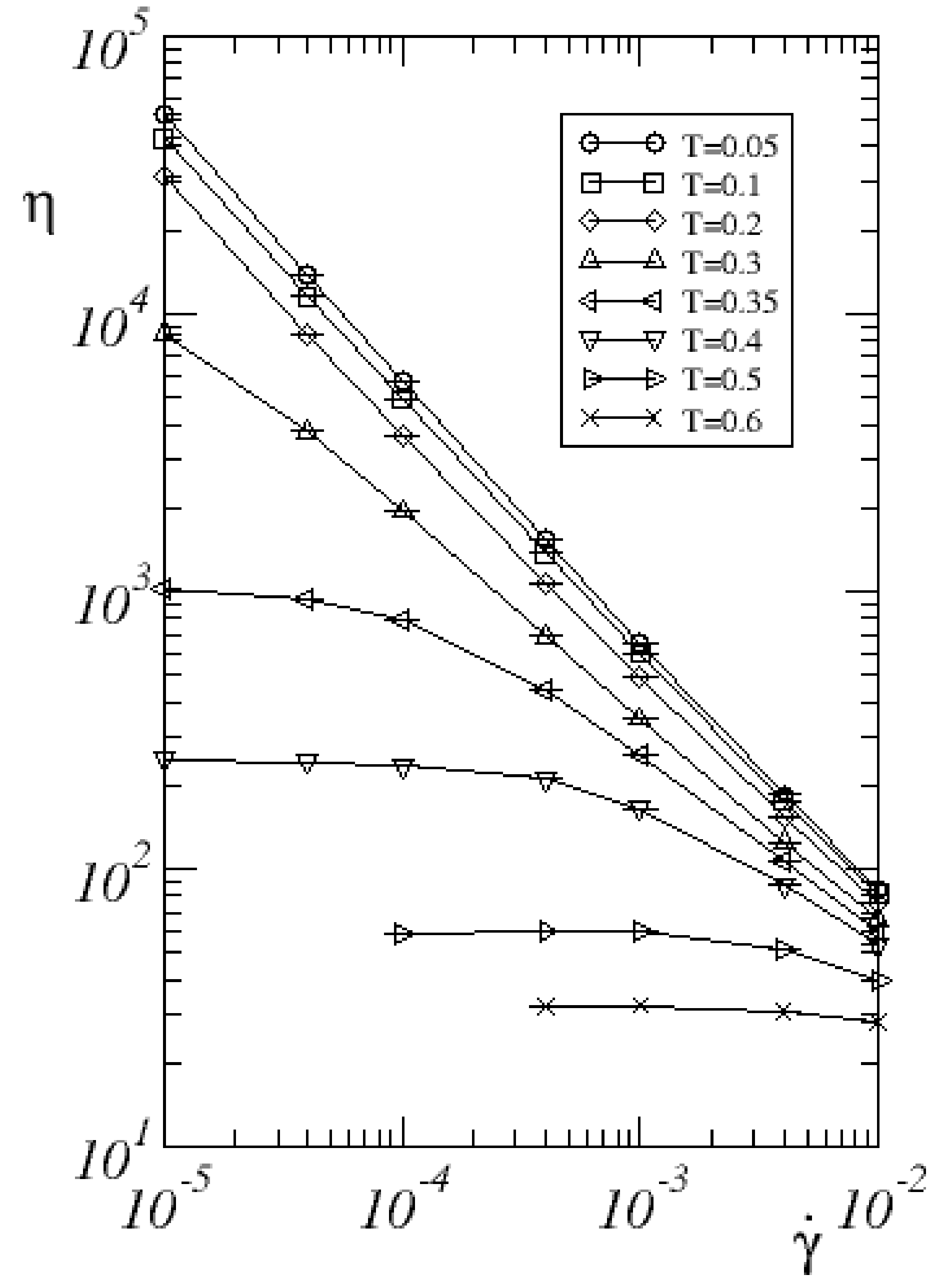
<u>Finite T, finite strain-rate simulations:</u> $T \neq 0 \quad \dot{\gamma} \neq 0$

- Standard MD simulation
- Velocity rescaling

Chattoraj *et al, PRE 2011*

At finite T





Consistent with Furukawa et al, PRL (2009)

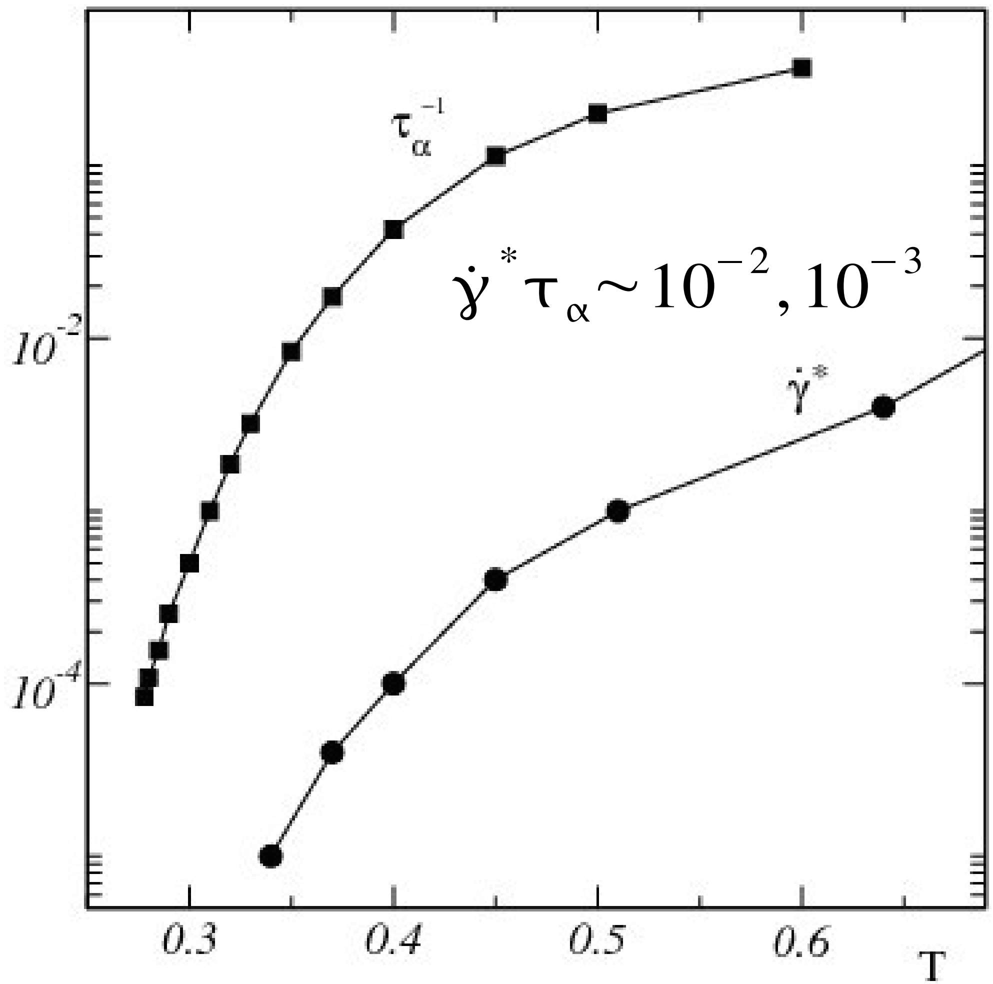
<u>Finite T, finite strain-rate simulations:</u>

$T \neq 0 \quad \dot{\gamma} \neq 0$

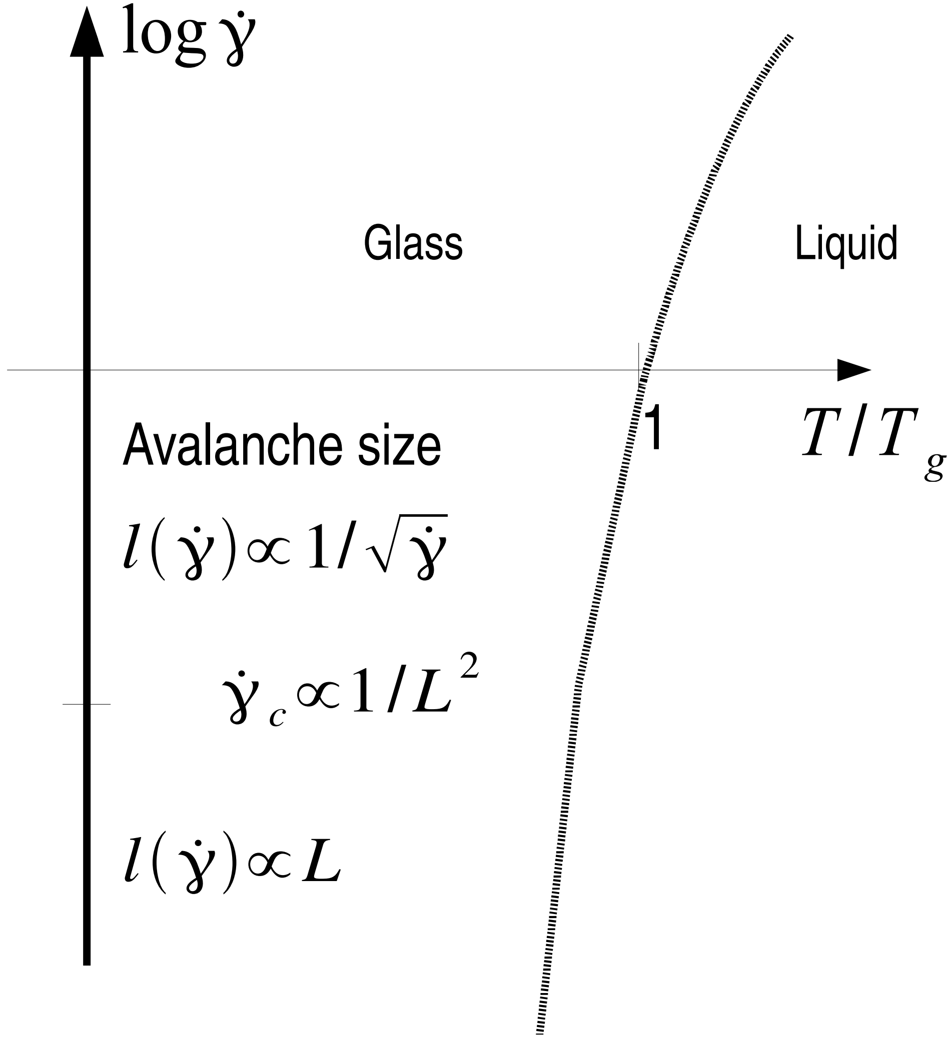
- Standard MD simulation
- Velocity rescaling

Chattoraj *et al, PRE 2011*

At finite T



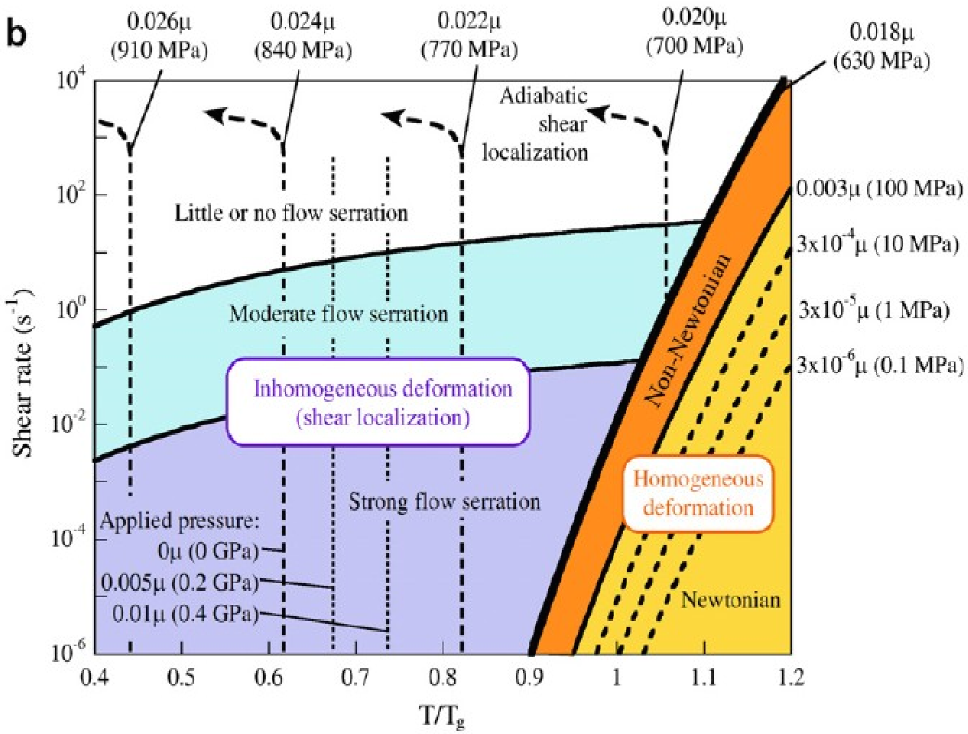
τ_α^{-1}
$\dot\gamma^* \tau_\alpha \sim 10^{-2}, 10^{-3}$
$\dot\gamma^*$
10^{-2}
10^{-4}
0.3
0.4
0.5
0.6
T

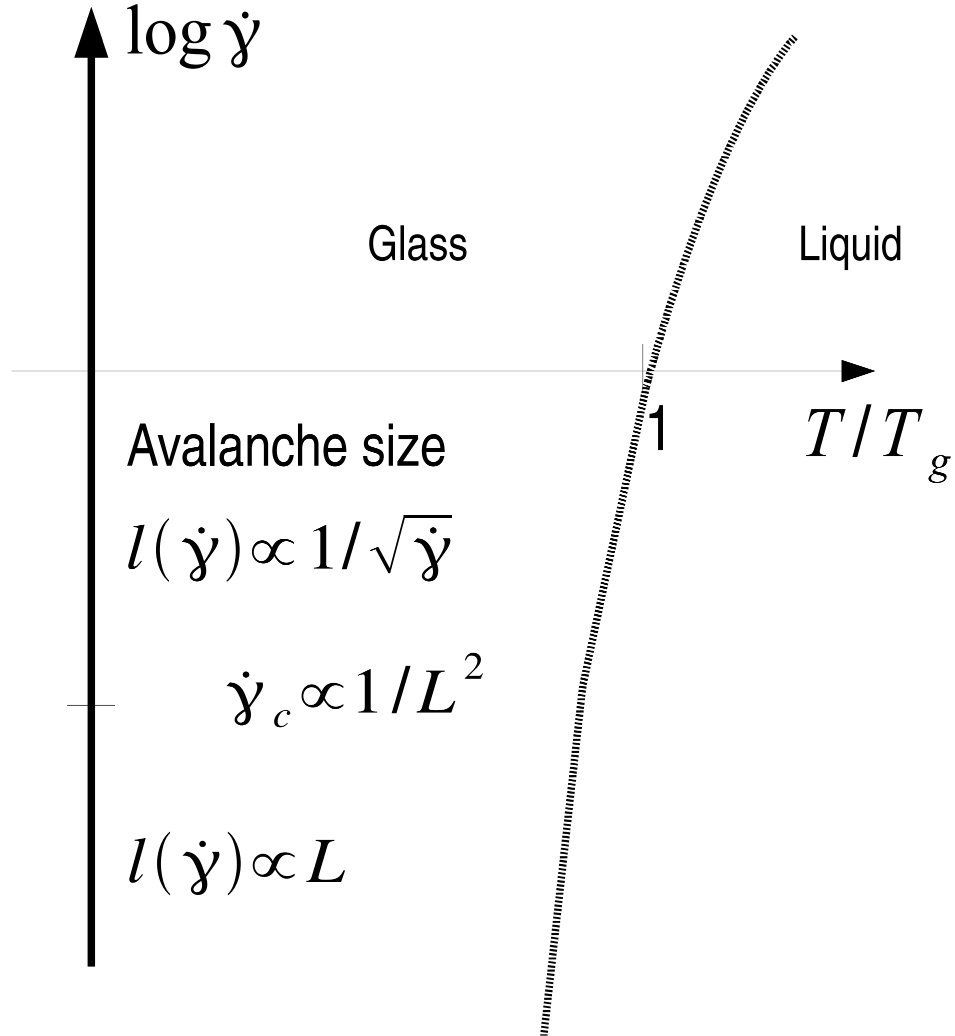


$\log \dot\gamma$
Glass
Liquid
1
T/T_g
Avalanche size
$l(\dot\gamma) \propto 1/\sqrt{\dot\gamma}$
$\dot\gamma_c \propto 1/L^2$
$l(\dot\gamma) \propto L$

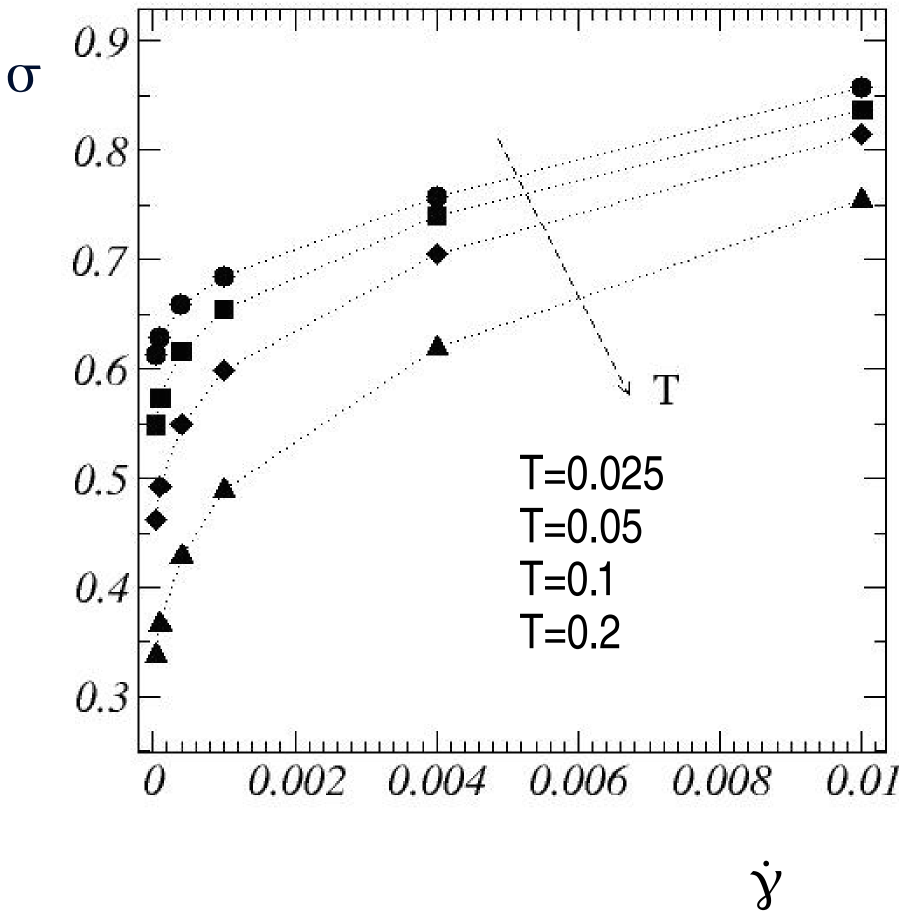
At finite T

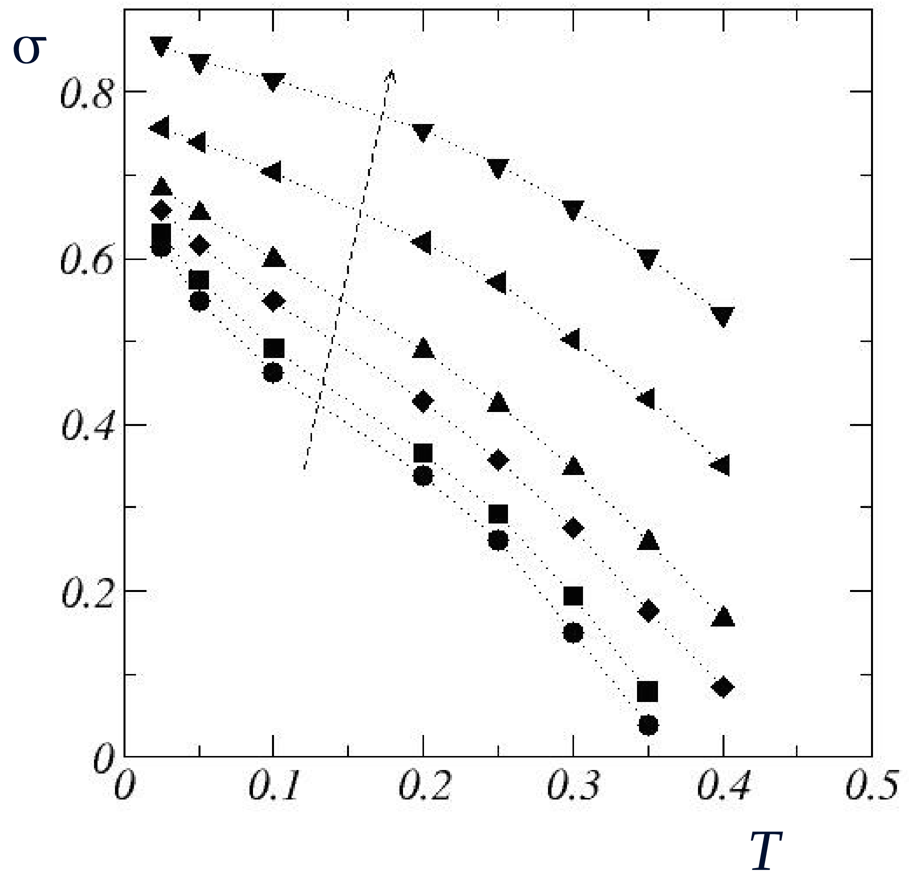
Schuh *et al*,
Acta Mat. 55, 4067 (2007)





Stress data



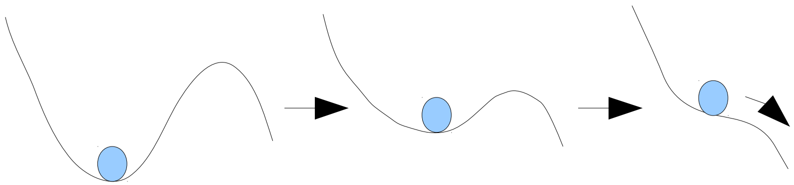


$\sigma(\dot{\gamma})$

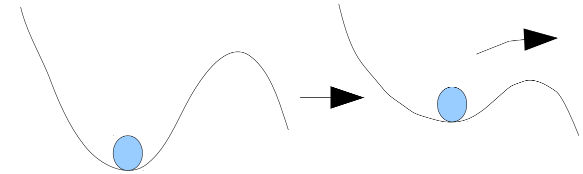
- Decreases strongly with T
- No longer fits Hershel Bulkley law

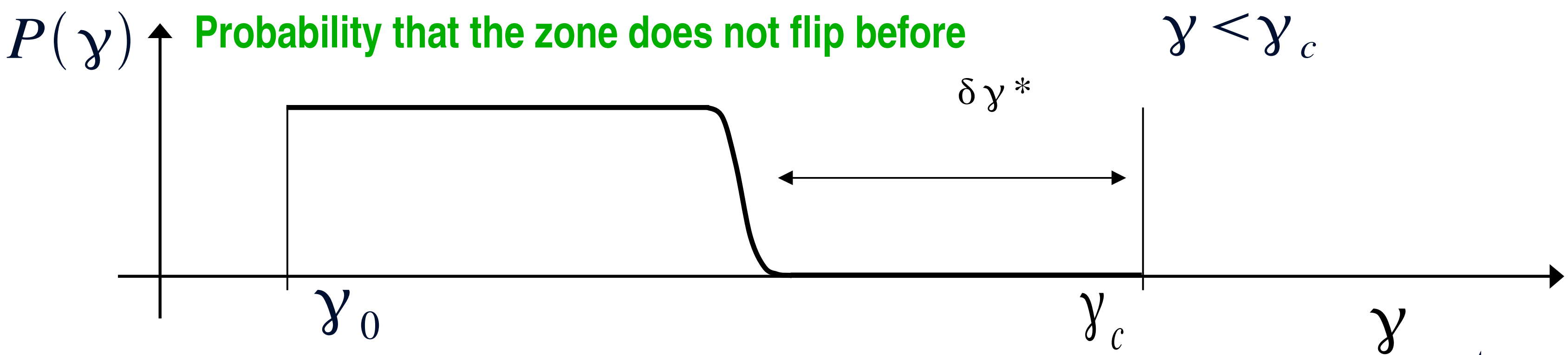
Activation and driven zones

$T=0$



$T\neq 0$





$$\frac{\partial P}{\partial \gamma}=-\frac{1}{\dot{\gamma}}P\,R(\gamma)$$

rate of activated jumps: $$R=\omega\exp\left(-\frac{\Delta E}{T}\right)$$

$$\Rightarrow P(\gamma;\gamma_0)=\exp\left(-\frac{1}{\dot{\gamma}}\int_{\gamma_0}^{\gamma}R(\gamma')\,d\gamma'\right)$$

with:
$$\begin{cases}\omega\propto(\gamma_c-\gamma)^{1/4}\\ \Delta E\propto(\gamma_c-\gamma)^{3/2}\end{cases}$$

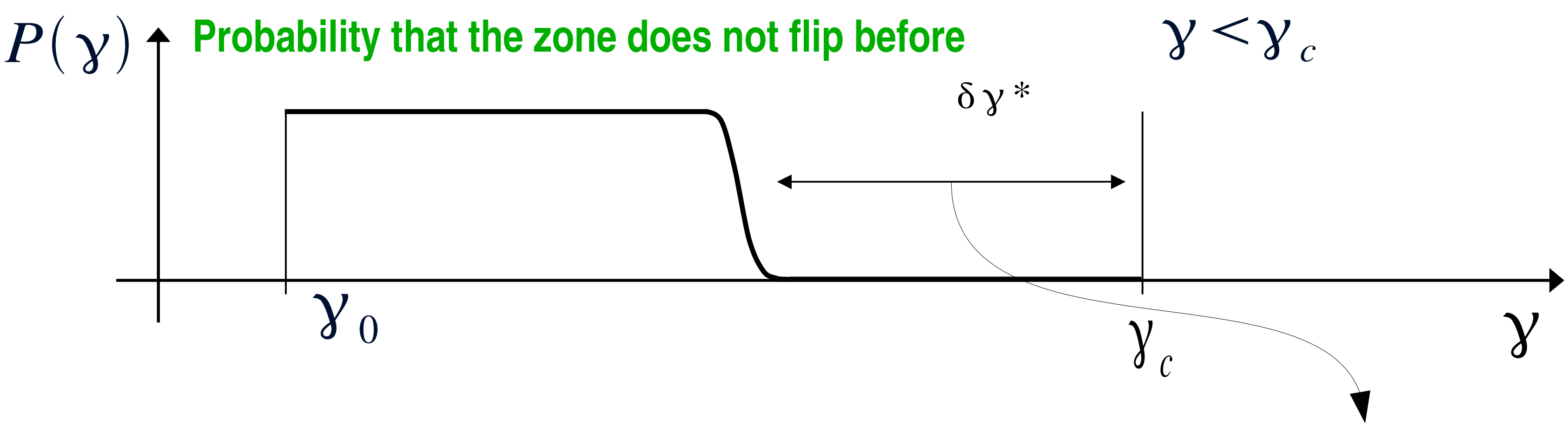
$$\boxed{P(\gamma)=\exp\left(-\frac{2}{3}\frac{\nu}{\dot{\gamma}}\left(\frac{T}{B}\right)^{5/6}\left(Q(\delta\gamma)-Q(\delta\gamma_0)\right)\right)}$$

$$Q(\delta\gamma)=\Gamma\left(\frac{5}{6};\frac{B}{T}\delta\gamma^{3/2}\right)$$

Chattoraj et al, PRL 105, 26601 (2010)

Activation and driven zones

Chattoraj et al, PRL 105, 26601 (2010)



$$\delta\gamma^* \sim \left[\frac{T}{B} \ln\left(\frac{2}{3} \frac{\nu}{\dot\gamma} \left(\frac{T}{B} \right)^{5/6} \right) \right]^{2/3}$$

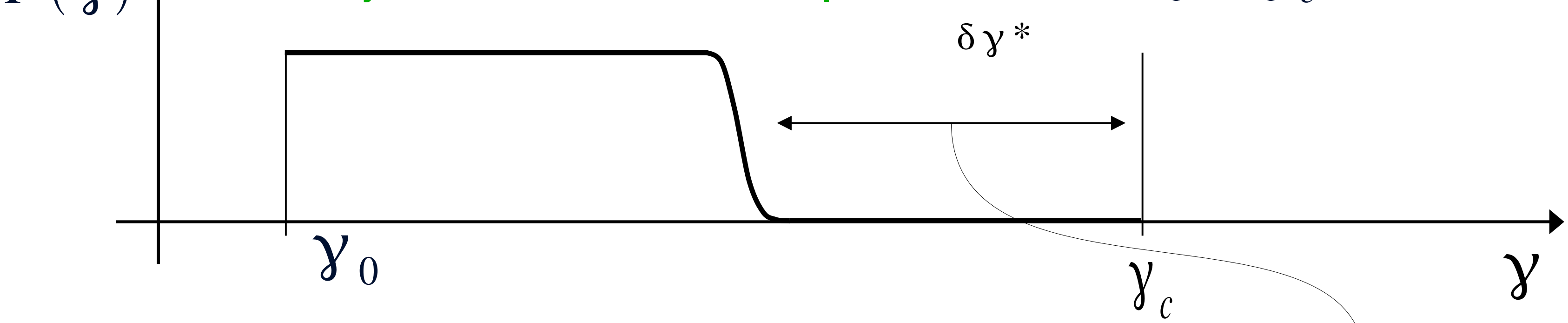
- Argue: Mechanical noise and thermal noise can be separated
- Yields: Average shift of occurrence of plastic events

$$\sigma(\dot\gamma ; T) = \sigma(\dot\gamma ; T = 0) - 2\mu \overline{\delta\gamma^*}$$

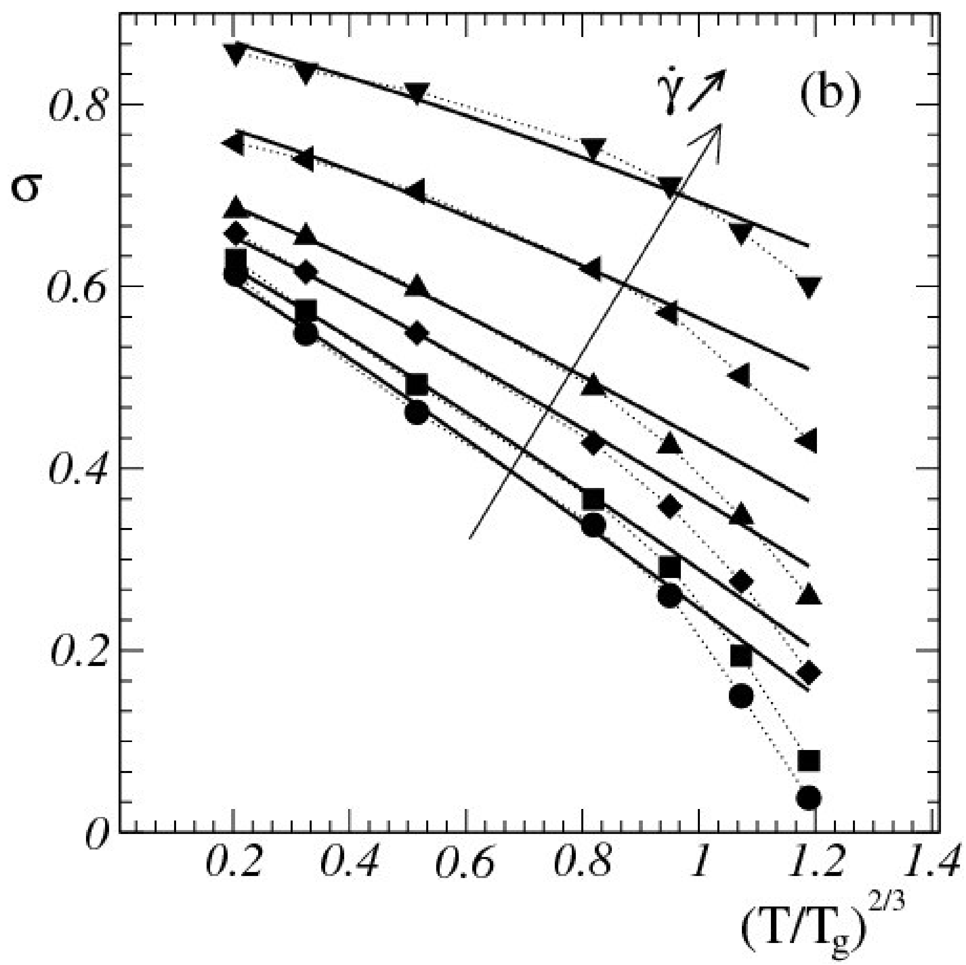
Activation and driven zones

Chattoraj et al, PRL 105, 26601 (2010)

Probability that the zone does not flip before $\gamma < \gamma_c$



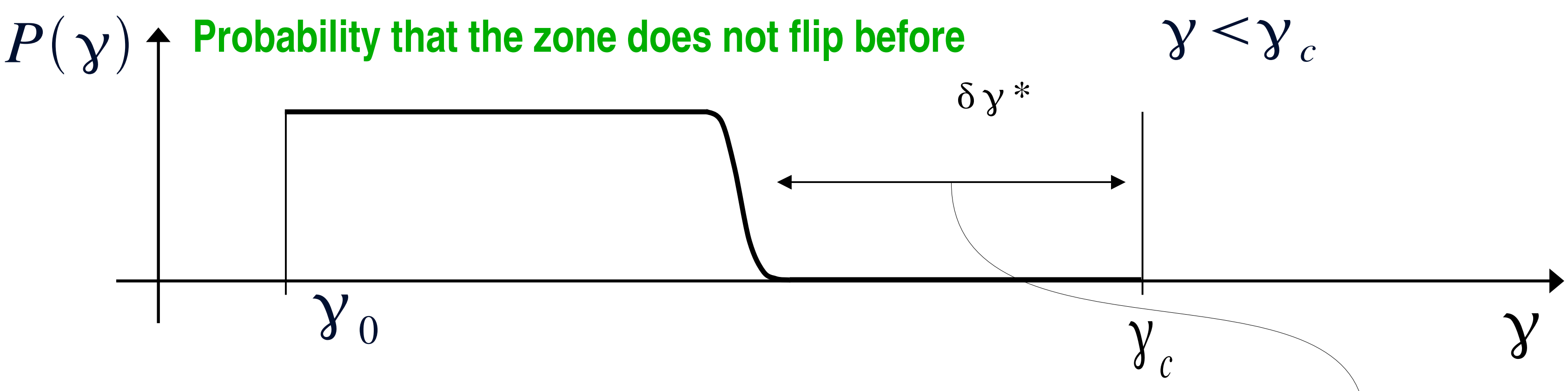
$$\delta\gamma^* \sim \left[\frac{T}{B}\ln\left(\frac{2}{3}\frac{\nu}{\dot\gamma}\left(\frac{T}{B}\right)^{5/6}\right)\right]^{2/3}$$

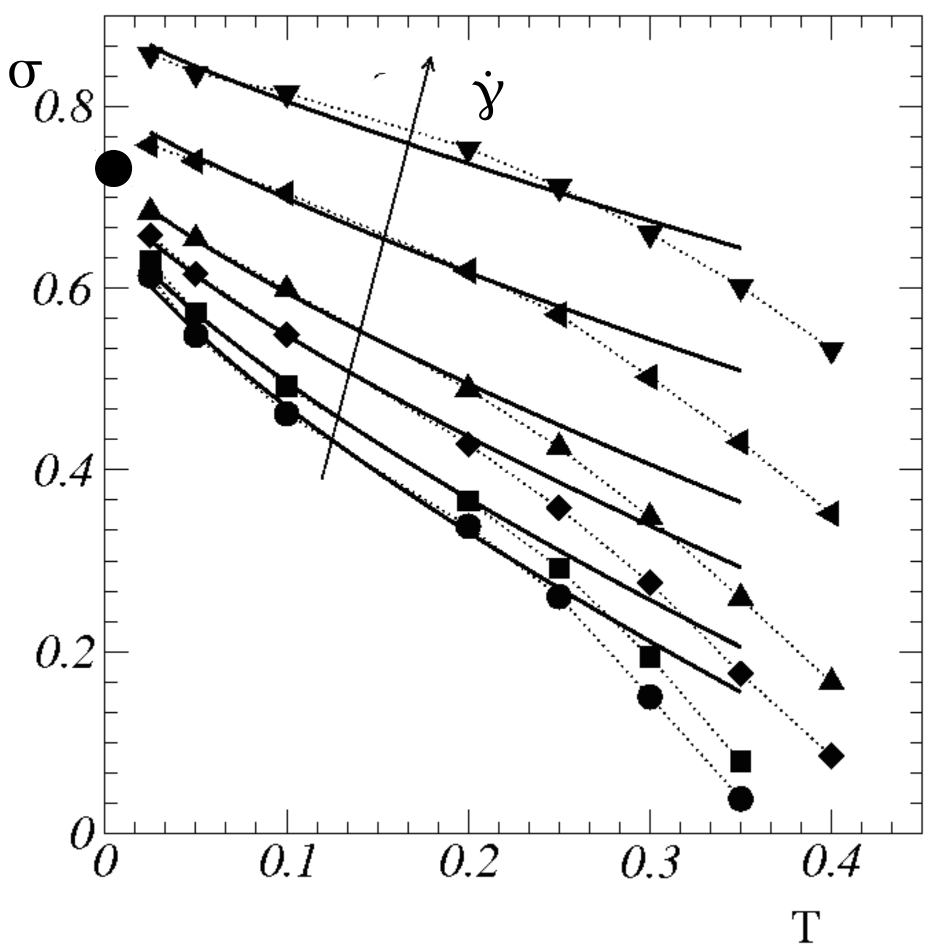


$$\sigma(\dot\gamma;T) = \sigma(\dot\gamma;T=0) - 2\mu\,\overline{\delta\gamma^*}$$

Activation and driven zones

Chattoraj et al, PRL 105, 26601 (2010)



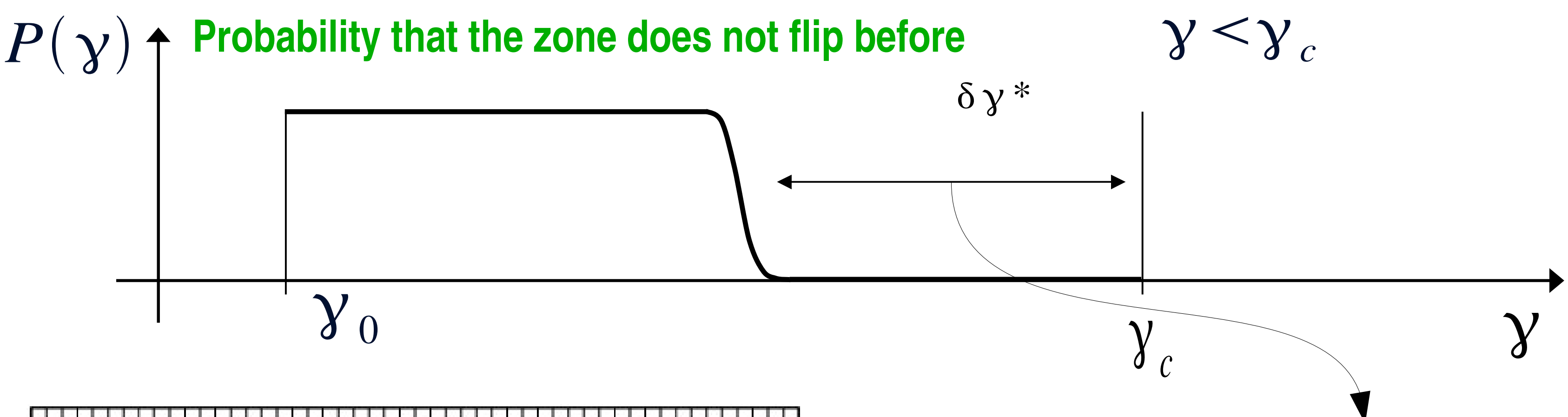


$$\delta\gamma^* \sim \left[\frac{T}{B}\ln\left(\frac{2}{3}\frac{\nu}{\dot{\gamma}}\left(\frac{T}{B}\right)^{5/6}\right)\right]^{2/3}$$

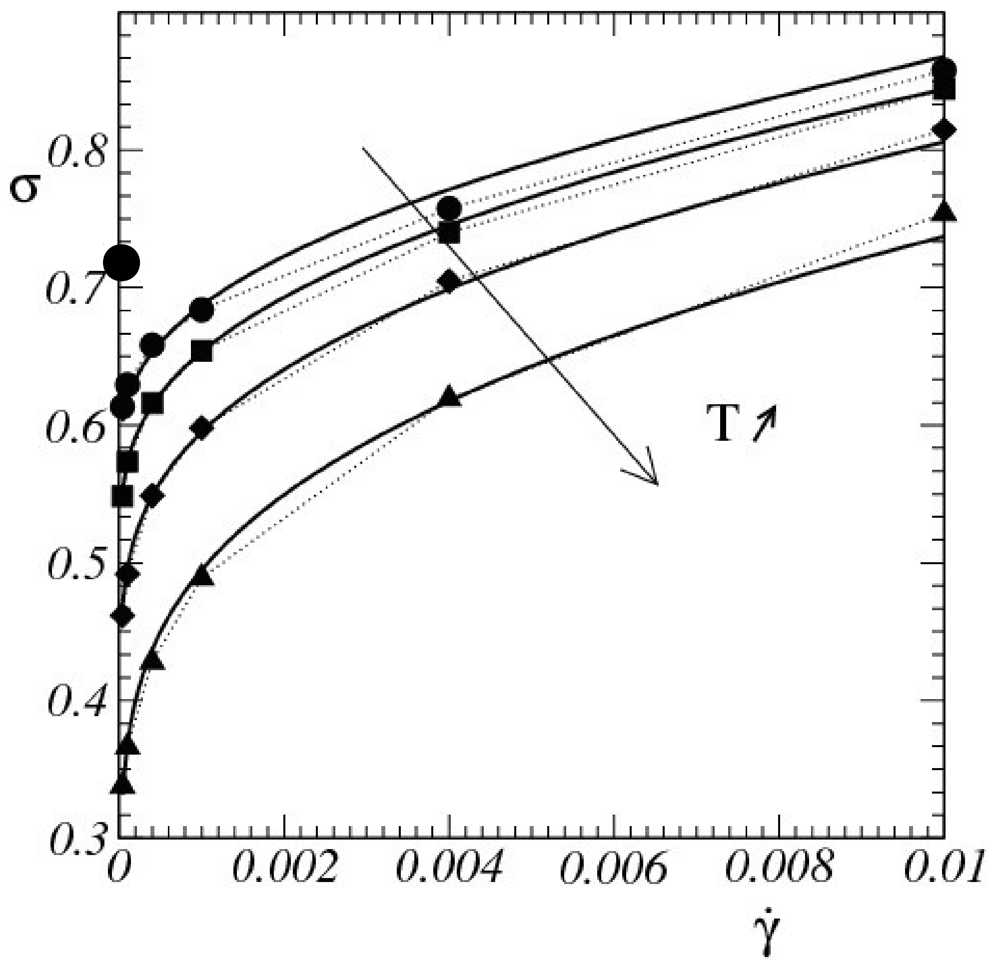
$$\sigma(\dot{\gamma};T) = \sigma(\dot{\gamma};T=0) - 2\mu\,\overline{\delta\gamma^*}$$

Activation and driven zones

Chattoraj et al, PRL 105, 26601 (2010)



$$\delta\gamma^* \sim \left[\frac{T}{B} \ln\left(\frac{2}{3} \frac{\nu}{\dot{\gamma}} \left(\frac{T}{B} \right)^{5/6} \right) \right]^{2/3}$$



$$\sigma(\dot{\gamma}; T) = \sigma(\dot{\gamma}; T=0) - 2\mu \overline{\delta\gamma^*}$$

Metallic glass yield stress

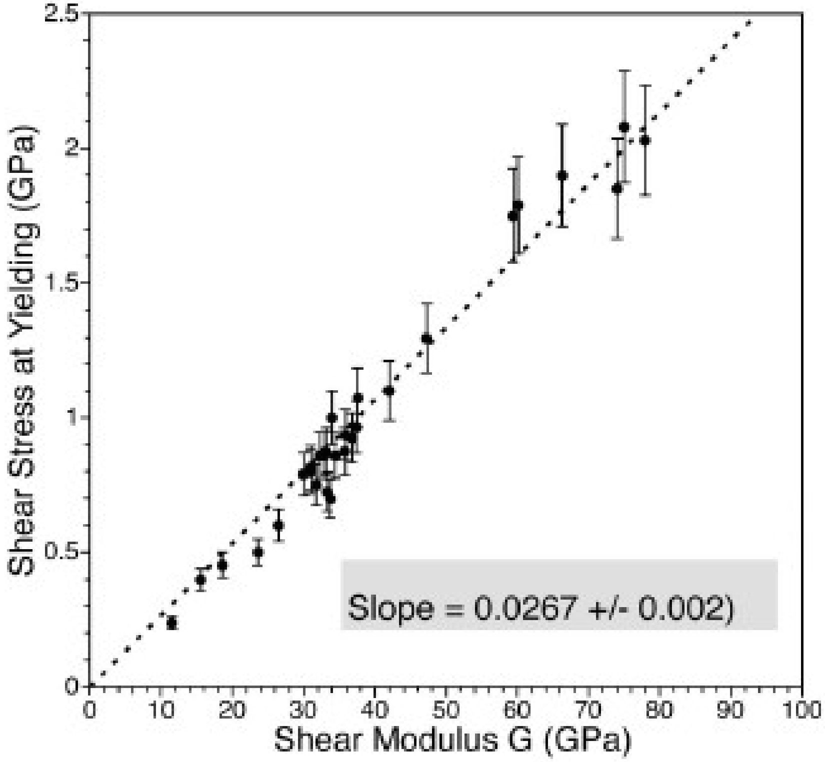
Johnson & Samwer 95, 195501 (2005)

TABLE I. Summary of data on alloy compositions and properties used in this Letter.

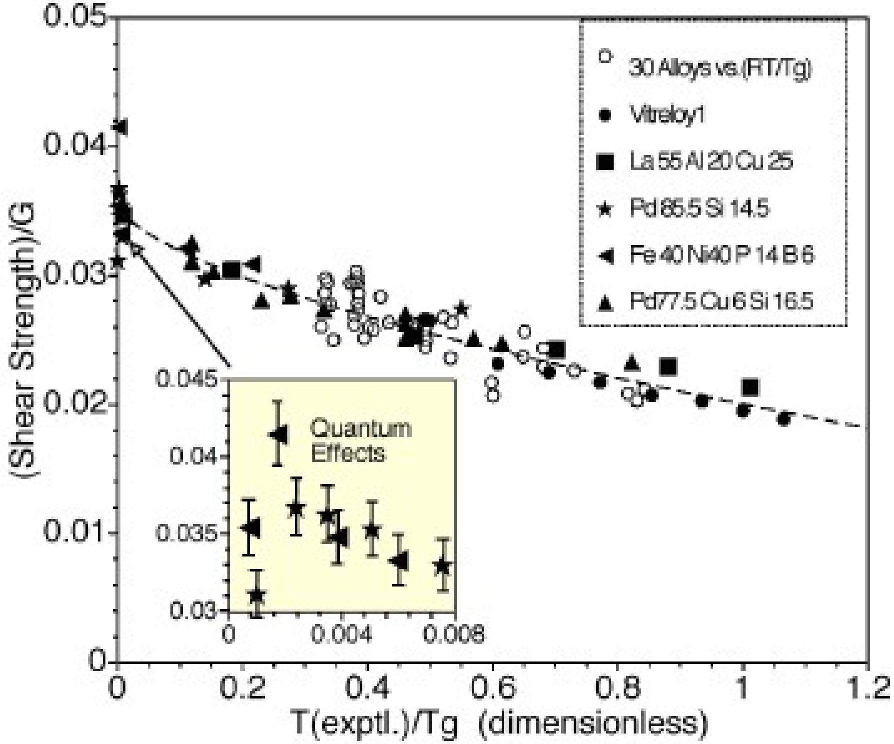
Alloy	ρ (g/cc)	Y) (GPa)	G (GPa)	B (GPa)	ν	σ_y (GPa)	T_g (K)	σ_y/Y	Ref.
1. $Zr_{41.2}Ti_{13.8}Ni_{10}Cu_{12.5}Be_{22.5}$	5.9	95	34.1	114.1	0.352	1.86	618	0.0196	[13–15]
		97.2	35.9	111.2	0.354	1.85	613	0.0190	
2. $Zr_{48}Nb_8Ni_{12}Cu_{14}Be_{18}$	6.7	93.9	34.3	118	0.367	1.95	620	0.0208	[15]
3. $Zr_{55}Ti_5Cu_{20}Ni_{10}Al_{10}$	6.62	85	31	118	0.375	1.63	625	0.0192	[15]
4. $Zr_{57.5}Nb_5Cu_{15.4}Ni_{12}Al_{10}$	6.5	84.7	30.8	117.6	0.379	1.58	663	0.0187	[15]
5. $Zr_{55}Al_{19}Co_{19}Cu_7$	6.2	101.7	37.6	114.9	0.352	2.2	733	0.0216	[16]
6. $Pd_{40}Cu_{30}Ni_{10}P_{20}$	9.28	92	34.5	151.8	0.399	1.72	593	0.0187	[17]
7. $Pd_{40}Cu_{30}Ni_{10}P_{20}$	9.28	92	33	146	0.394	1.72	593	0.0187	[18]
8. $Pd_{40}Cu_{30}Ni_{10}P_{20}$	9.30	92	35.8	144.7	0.394	1.75	595	0.0190	[17]
9. $Pd_{60}Cu_{20}P_{20}$	9.78	91	32.3	167	0.409	1.70	604	0.0187	[15]
10. $Pd_{40}Cu_{40}P_{20}$	9.30	93	33.2	158	0.402	1.75	548	0.0188	[15]
11. $Ni_{45}Ti_{20}Zr_{25}Al_{10}$	6.4	109.3	40.2	129.6	0.359	2.37	791	0.0217	[19]
12. $Ni_{40}Ti_{17}Zr_{28}Al_{10}Cu_5$	6.48	127.6	47.3	140.7	0.349	2.59	862	0.0203	[19]
13. $Ni_{60}Nb_{35}Sn_5$	8.64	183.7	66.32	267	0.385	3.85	885	0.0210	[20]
14. $Ni_{60}Sn_6(Nb_{0.8}Ta_{0.2})_{34}$	9.24	161.3	59.41	189	0.357	3.50	875	0.0217	[16]
15. $Ni_{60}Sn_6(Nb_{0.6}Ta_{0.4})_{34}$	9.80	163.7	60.1	197.6	0.361	3.58	882	0.0219	[16]
16. $Cu_{64}Zr_{36}$	8.07	92	34	104.3	0.352	2.0	787	0.0217	[21]
17. $Cu_{46}Zr_{54}$	7.62	83.5	30.0	128.5	0.391	1.40	696	0.0168	[22]
18. $Cu_{46}Zr_{42}Al_7Y_5$	7.23	84.6	31	104.1	0.364	1.60	713	0.0189	[23]
19. $Pd_{77.5}Cu_6Si_{16.5}$	10.4	89.7	31.8	166	0.409	1.5	550	0.0167	[24]
20. $Pt_{60}Ni_{15}P_{25}$	15.7	96.1	33.8	202	0.420	1.4	488	0.0146	[25]
21. $Pt_{57.5}Cu_{14.7}Ni_5P_{22.8}$	15.2	95.7	33.4	243.2	0.434	1.45	490	0.0151	[26]
22. $Pd_{64}Ni_{16}P_{20}$	10.1	91.9	32.7	166	0.405	1.55	452	0.0169	[24]
23. $MgGd_{10}Cu_{25}$	4.04	49.1	18.6	46.3	0.32	0.98	428	0.020	[16]
24. $La_{55}Al_{25}Cu_{10}Ni_5Co_5$	6.0	41.9	15.6	44.2	0.342	0.85	430	0.0203	[15]
25. $Ce_{70}Al_{10}Ni_{10}Cu_{10}$	6.67	30.3	11.5	27	0.313	0.65	359	0.0215	[27]
26. $Cu_{50}Hf_{43}Al_7$	11.0	113	42	132.8	0.358	2.2	774	0.0195	[16]
27. $Cu_{57.5}Hf_{27.5}Ti_{15}$	9.91	103	37.3	117.5	0.356	1.94	729	0.0188	[16]
28. $Fe_{61}Mn_{10}Cr_4Mo_6Er_1C_{15}B_6$	6.89	193	75	146	0.280	4.16	870	0.0216	[28]
29. $Fe_{53}Cr_{15}Mo_{14}Er_1C_{15}B_6$	6.92	195	75	180	0.32	4.2	860	0.0215	[28]
30. $Au_{49.5}Ag_{5.5}Pd_{2.3}Cu_{26.9}Si_{16.3}$	11.6	74.4	26.5	132.3	0.406	1.20	405	0.0141	[29]
31. $Au_{55}Cu_{25}Si_{20}$	12.2	69.8	24.6	139.8	0.417	1.00	348	0.0143	[29]

Metallic glass yield stress

Johnson & Samwer 95, 195501 (2005)



$$\sigma - \sigma_Y \propto T^{2/3}$$



Conclusion

Low T

- <u>Activation over driven barriers</u>
  - thermal fluctuations primarily trigger activation above driven barriers
  - the avalanche dynamics is unchanged: mere shift of the occurrence of plastic events
  - permits to predict $\sigma(\dot{\gamma}, T)$
- <u>Diffusion measurements</u>
  - particle displacements dominated by shearing effect when with $\dot{\gamma}^* \tau_\alpha \sim 10^{-2}, 10^{-3}$
  - in this region and for $\dot{\gamma} > \dot{\gamma}^*$ $\dot{\gamma} > \dot{\gamma}_c(L)$

$$l(\dot{\gamma}) \propto 1/\sqrt{\dot{\gamma}}$$