Elementary Mechanisms of Deformation in Amorphous Solids: From Zero to Low Temperature

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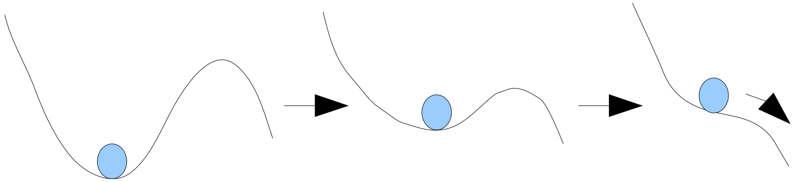
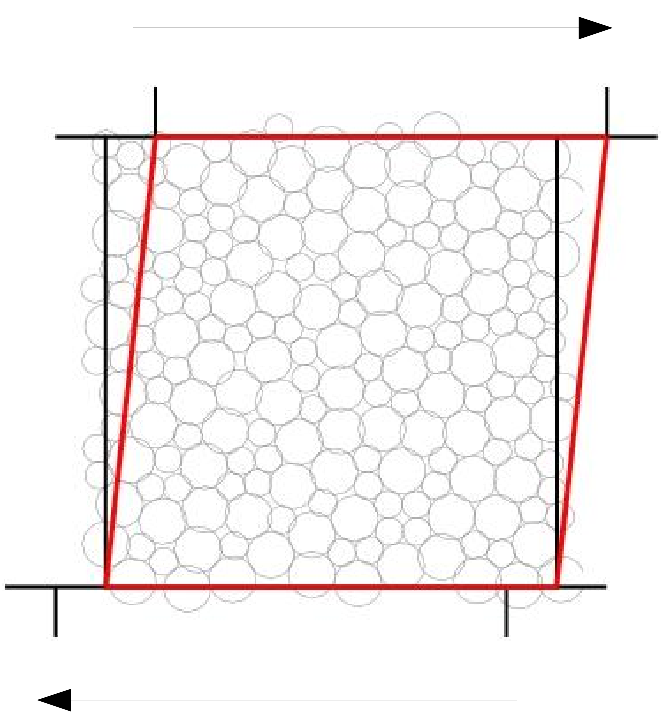
The zero temperature glass

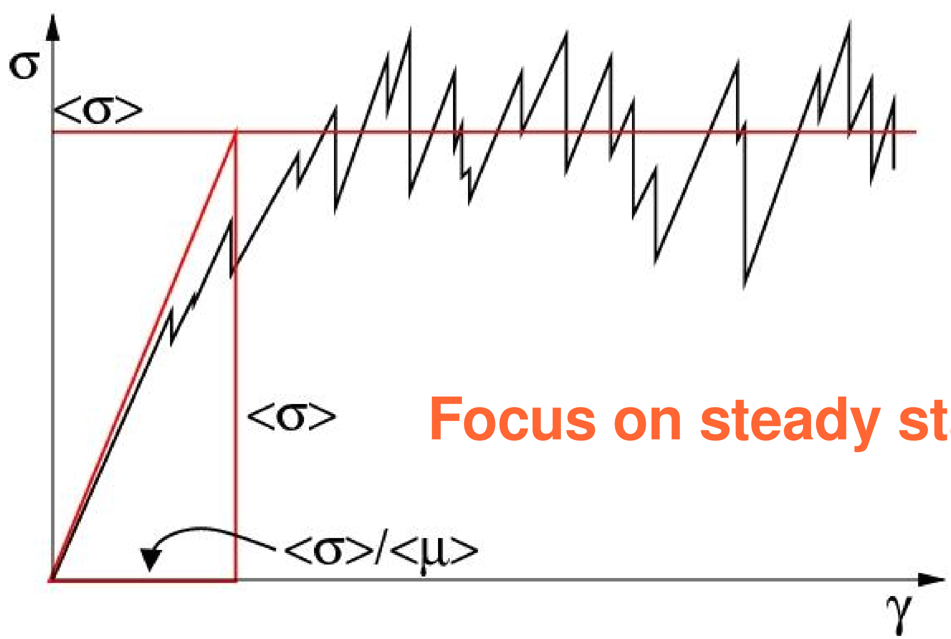
At low T, a glass lives in inherent states:



<u>Athermal, quasi-static protocol:</u> $T=0 \quad \dot{\gamma} \rightarrow 0$

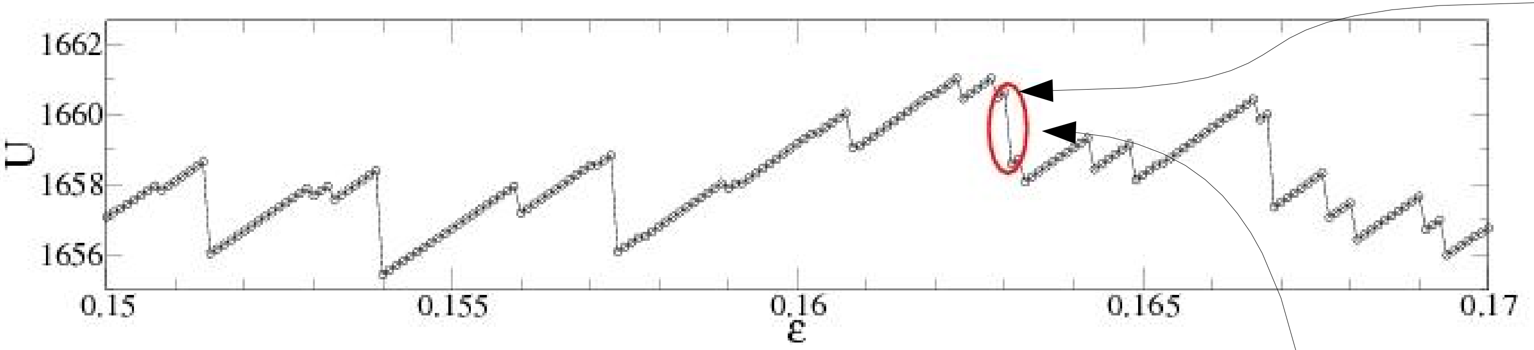
- Minimize energy
- Apply a small increment of strain (homogeneously)
- Repeat

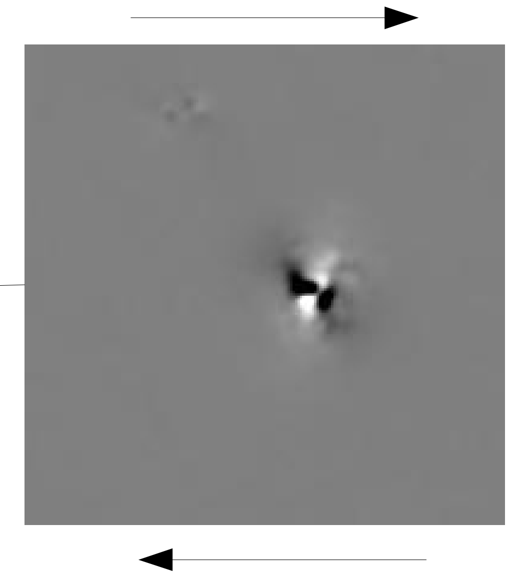




Focus on steady state

AQS I: plastic events are avalanches of flips





In 2D

C. Maloney and AL,
PRL 93, 016001 (2004);
PRE 74, 016118 (2006)

$$\Delta E \sim L$$

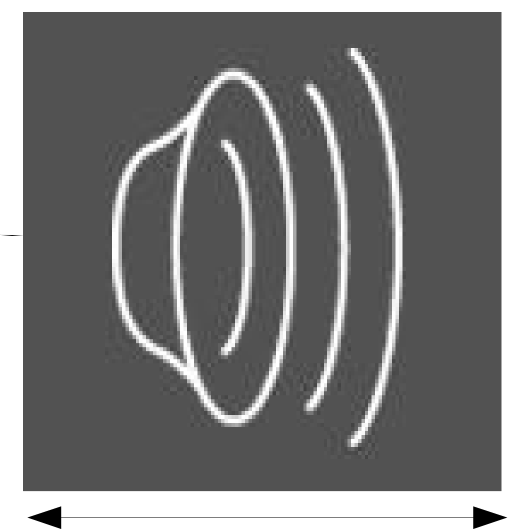
In 3D

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

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

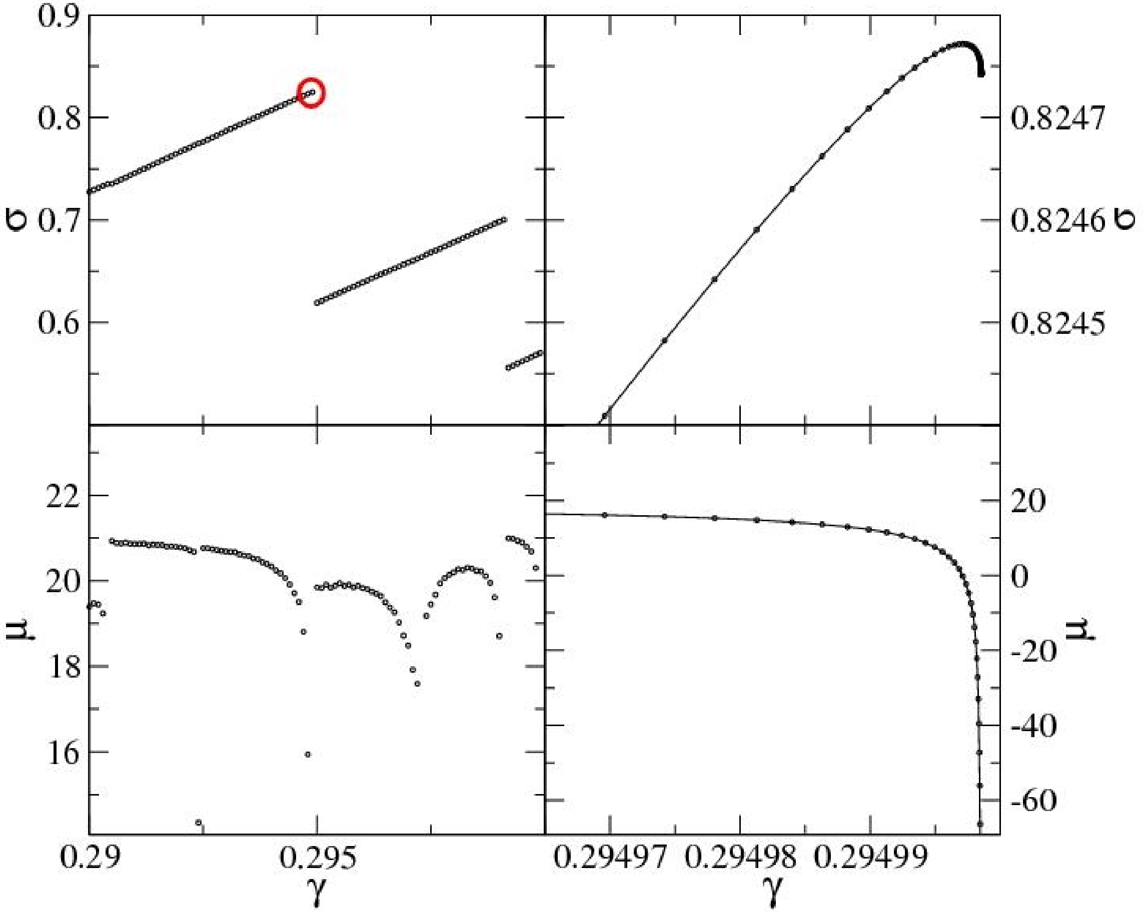
E. Lerner and I. Procaccia,
PRE 79, 066109 (2009)

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



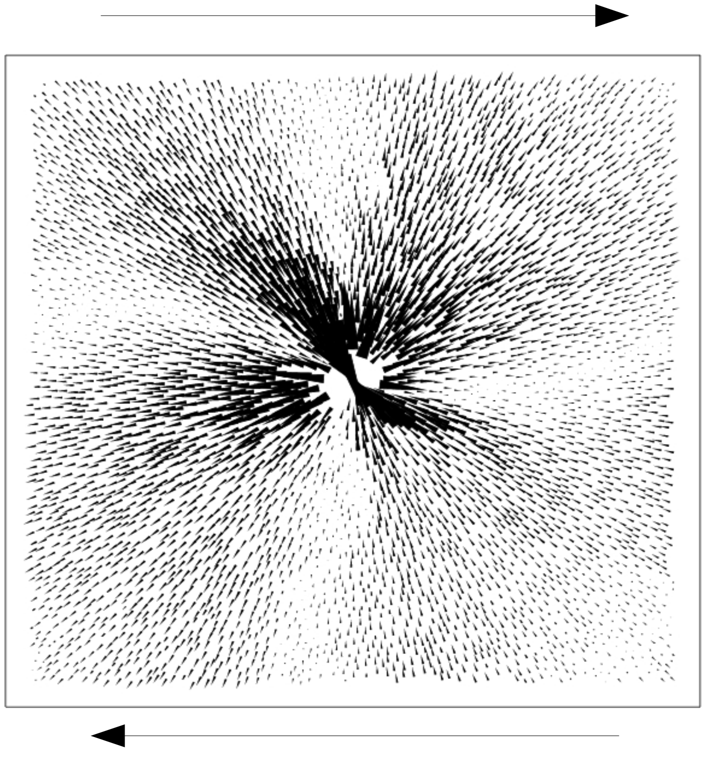
L

AQS II: plastic events occur via saddle-node bifurcations



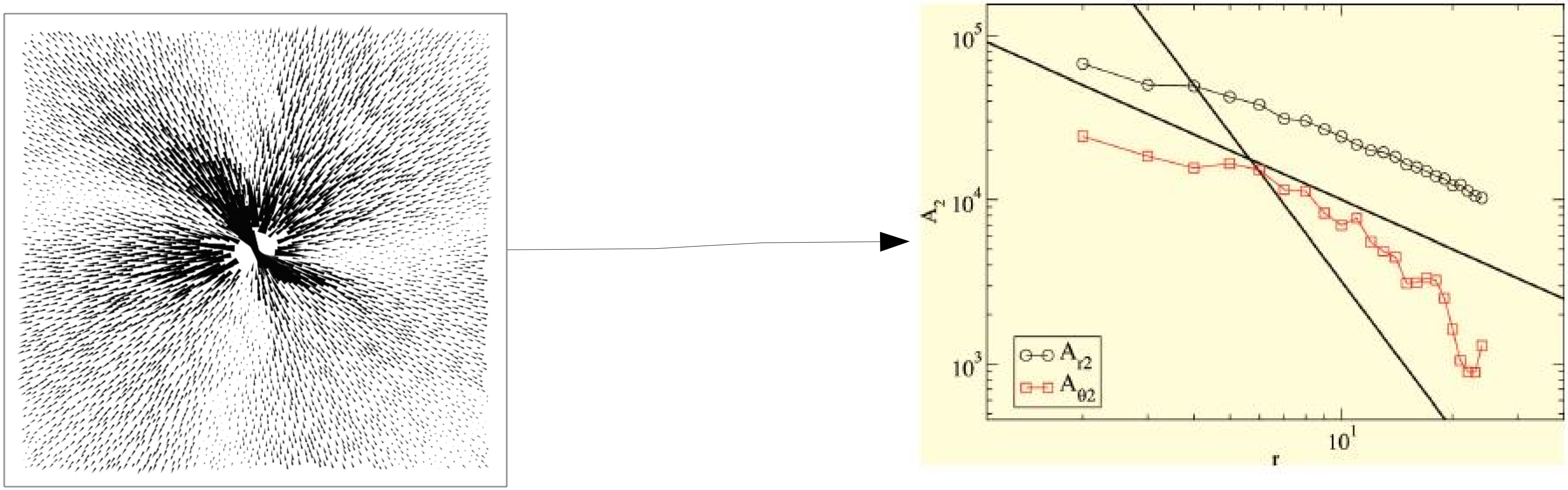
$$\sigma \sim \mu_\infty (\gamma - \gamma_0) - A\sqrt{\gamma_c - \gamma}$$

Zero mode

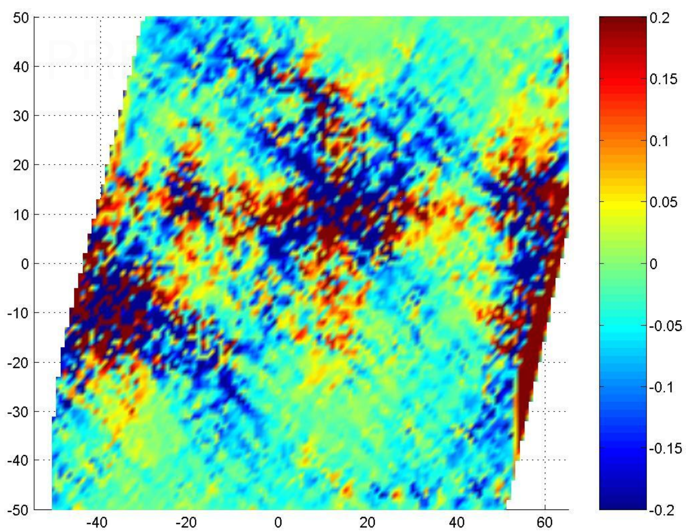


PRL 93, 195501 (2004)

AQS III: flips are analogous to Eshelby transformations



C. Maloney and AL, PRE 74, 016118 (2006)



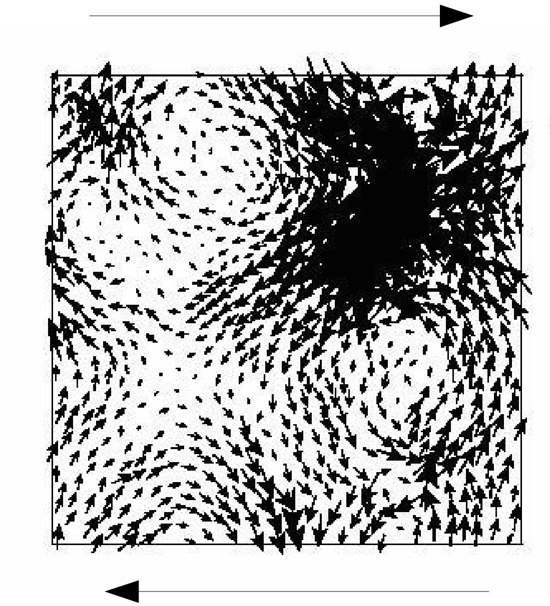
A. Tanguy *et al,* EPJE 20, 355 (2006)

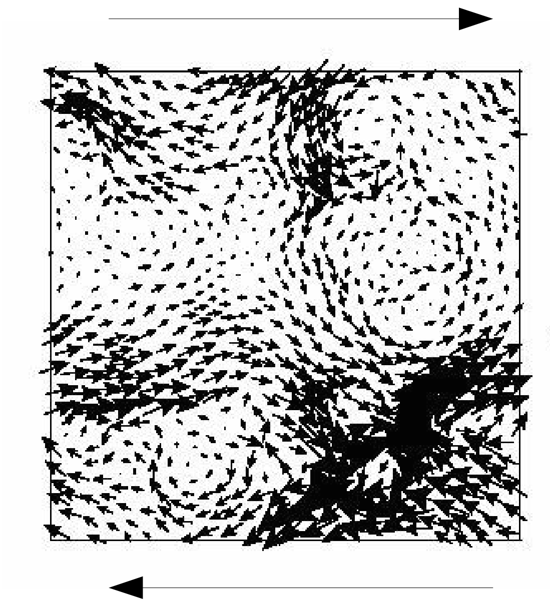
$$\vec{u} = \frac{2a^2 \Delta \epsilon_0}{\pi} \frac{x\,y}{r^4} \vec{r}$$

$$\sigma_{xy} = \frac{2\mu\, a^2 \Delta \epsilon_0}{\pi} \frac{\cos(4\theta)}{r^2}$$

AQS IV: zones are progressively loaded and interact

$$\gamma = 5.56 \,\&\, 5.58\,\%$$





PRE 76, 036104 (2007)

AQS phenomenology:

- Progressive convection of shear zones towards instability
- Each flip produces an Eshelby-like field likely to trigger secondary flips

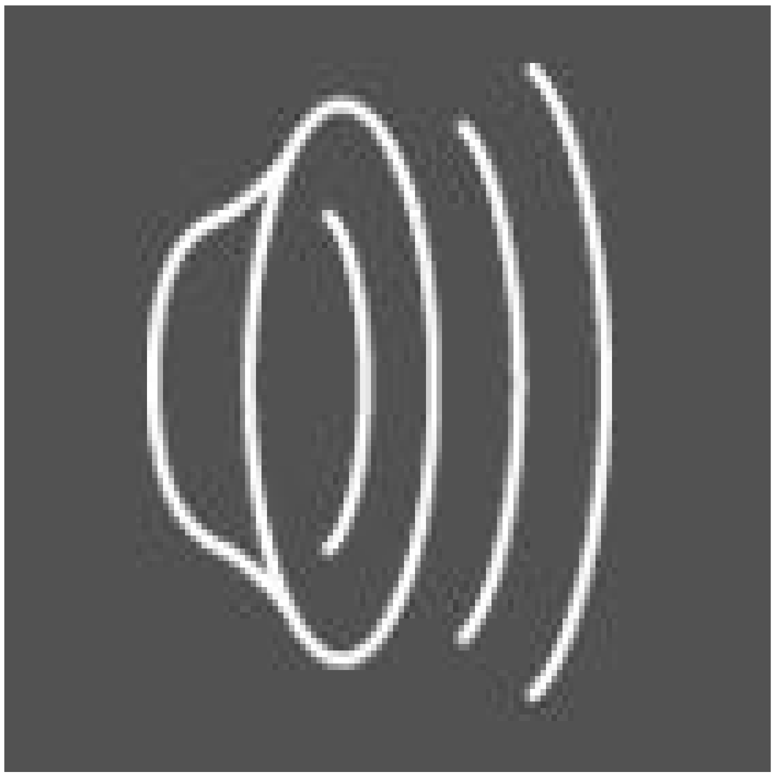
$\Rightarrow$

system-spanning avalanches

What happens at finite strain-rate?

Athermal systems $T = 0$

Near QS regime $\dot{\gamma} \neq 0$



$$\lambda_c = 5d$$
$$\tau = 0.2\,\tau_{LJ}$$

Pair potential:

$$U = k(r^{-12} - 2r^{-6})$$ Lennard-Jones

Dissipative forces:

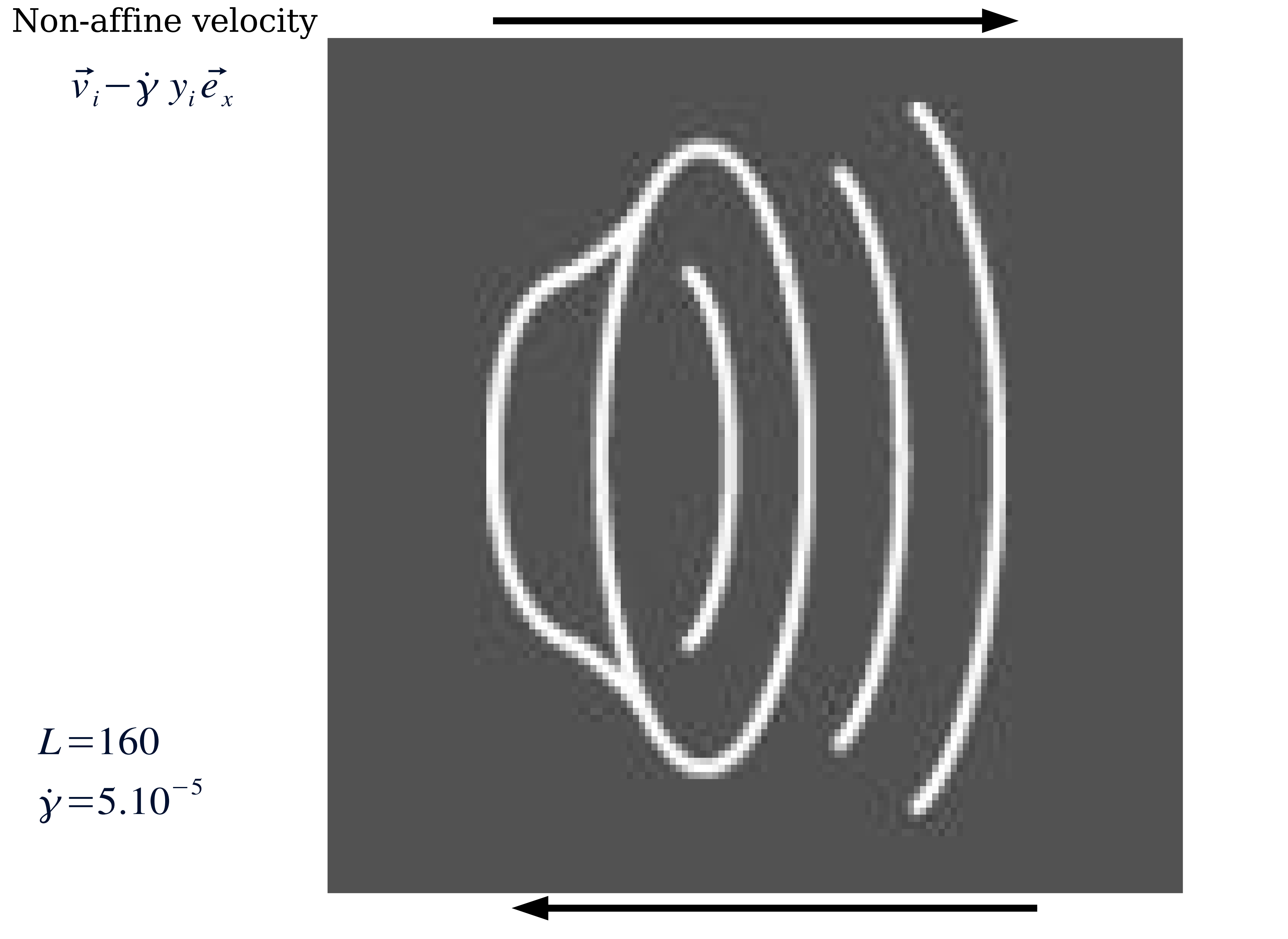
$$f_{ij} = \frac{m}{\tau}\phi(r)(\vec{v}_j - \vec{v}_i)$$ Viscous drag

$$\phi(r) = 1 - 2(r/2)^4 + (r/2)^8$$

This form of dissipation guarantees that:

- long wavelength are not damped
- short wavelength are, for:

$$\lambda < \lambda_c = \frac{\pi d^2}{\tau c_s}$$


Non-affine velocity
$\vec{v}_i - \dot{\gamma}\, y_i \vec{e}_x$
$L = 160$
$\dot{\gamma} = 5.10^{-5}$

The strain field

Dynamics of non-affine velocity field show:

Flips retain same nature (progressive softening)

Acoustic propagation of long range signals observable

But:

- Are flips correlated?
- Are there avalanches?

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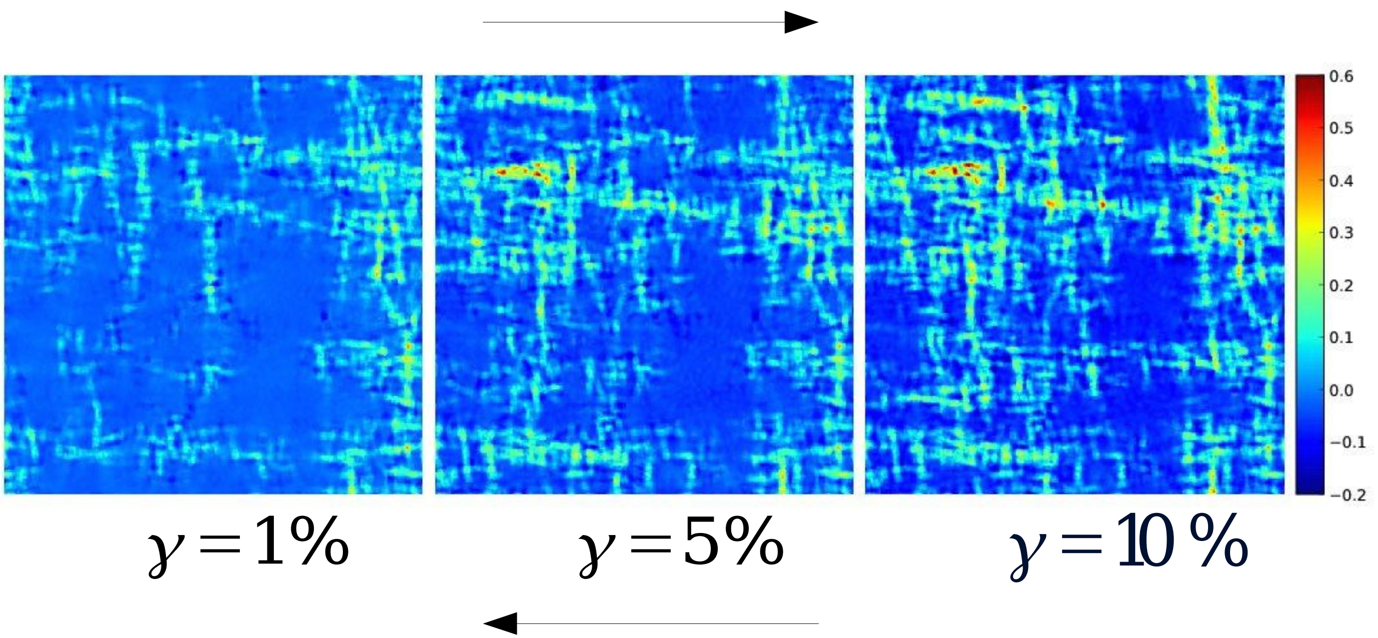
Deformation maps $\epsilon_{xy}(\vec{r})$



$\gamma = 1\%$ $\gamma = 5\%$ $\gamma = 10\%$

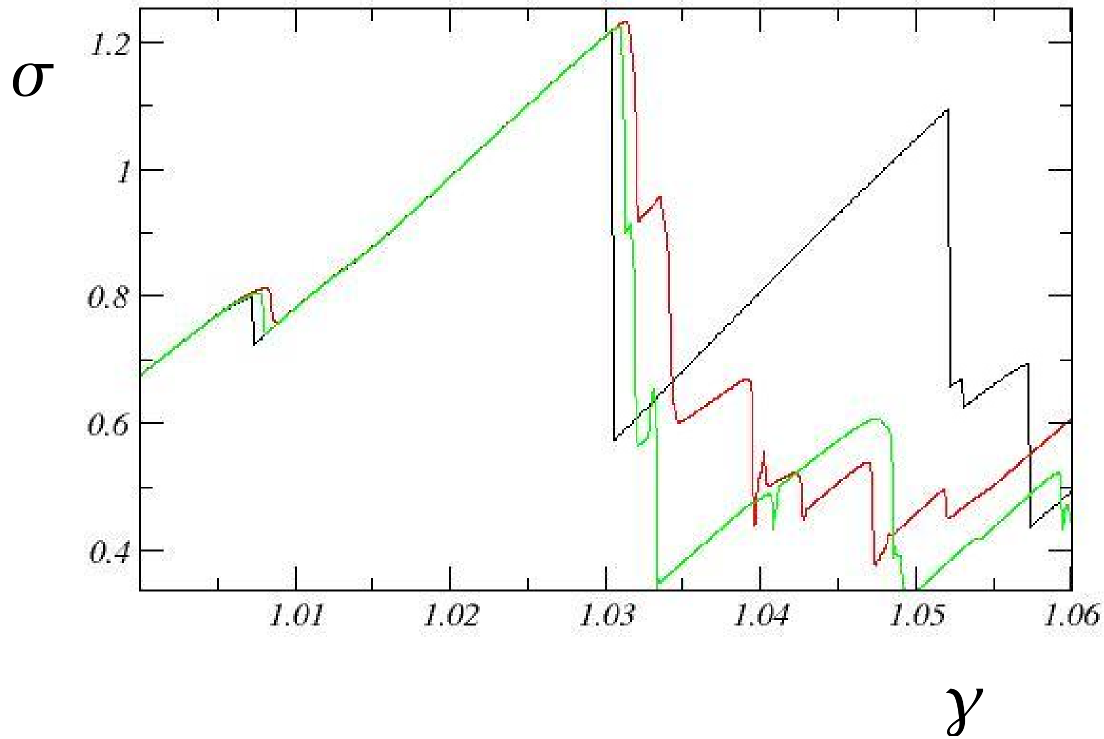
Looking for robust observables

In AQS limit:

Plastic events = discontinuous drops
= avalanches

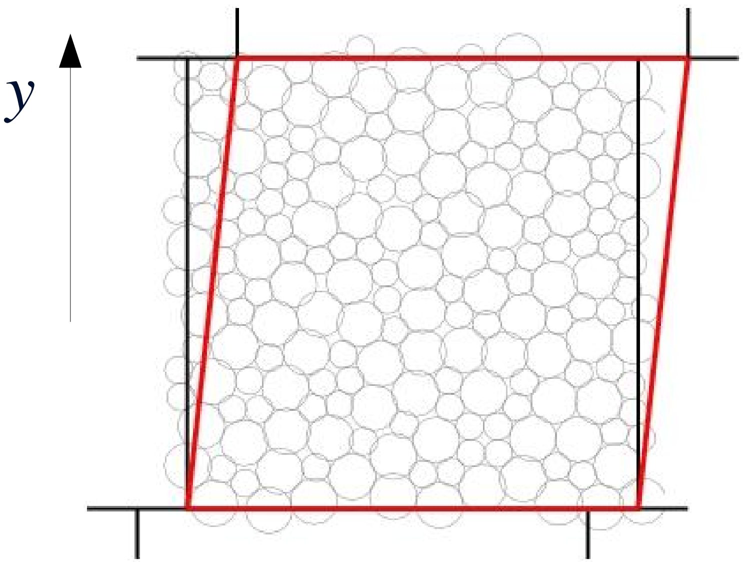
At finite strain rates:

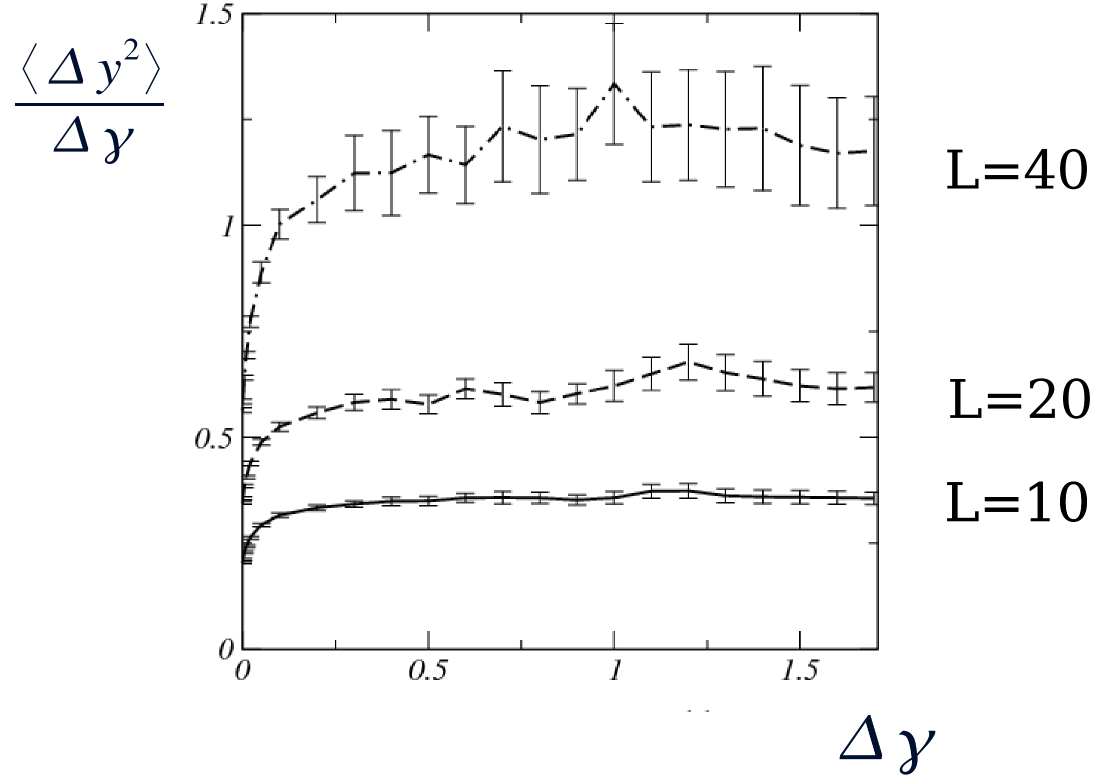
Flips and avalanches have a finite duration



What observables should we look at to characterize flip-flip correlations?

AQS V: Transverse diffusion is system size dependent





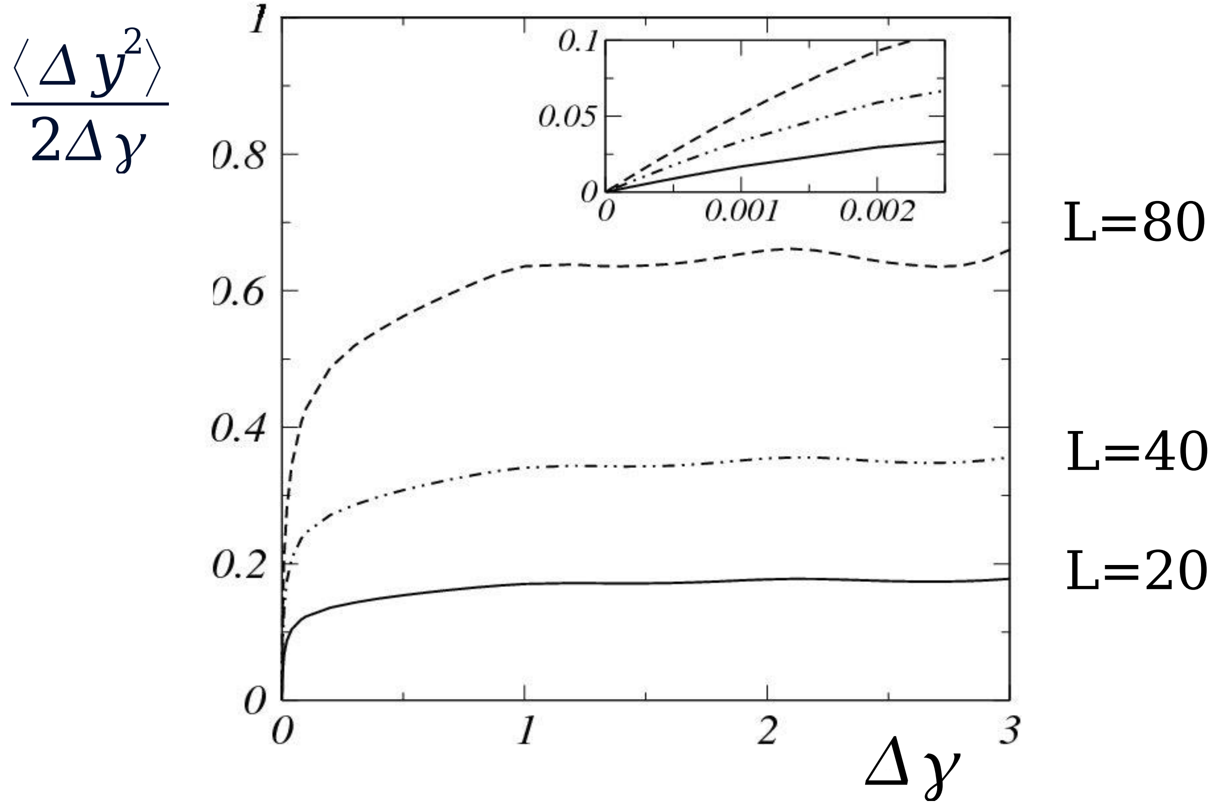
$$\frac{\langle \Delta y^2 \rangle}{\Delta \gamma} \longrightarrow \hat{D} \qquad (\Delta \gamma > 0.5)$$

with L

PRE 76, 036104 (2007)

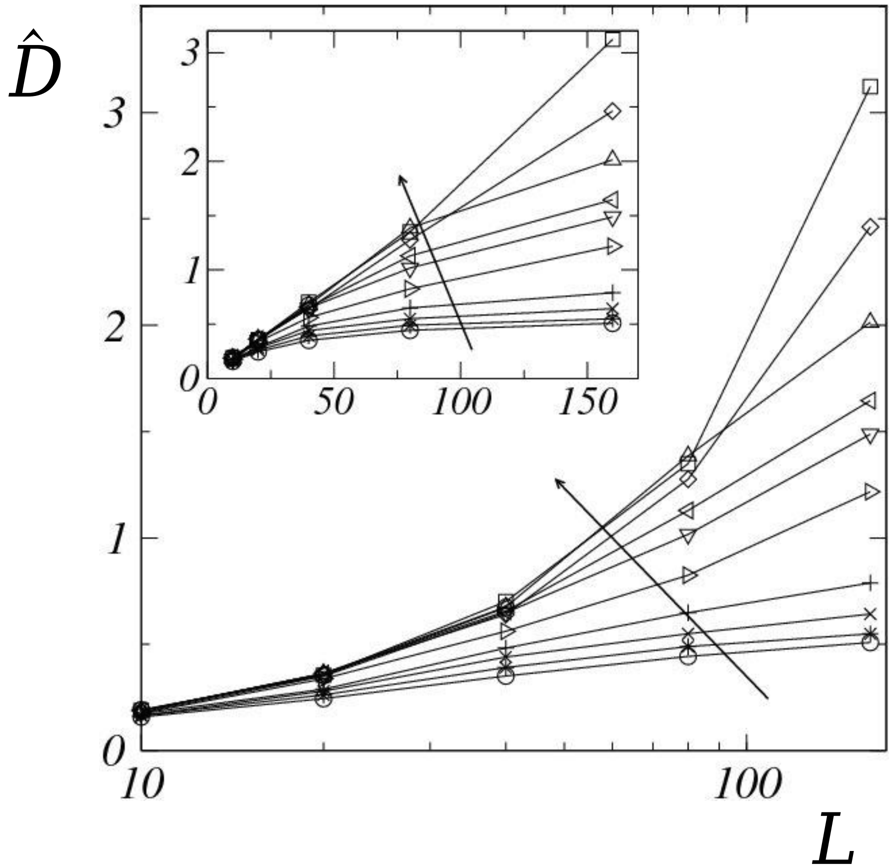
Transverse diffusion at finite strain rate

$$\dot{\gamma} = 10^{-3}$$



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

Transverse diffusion at finite strain rate



$$\widehat{D}(\dot{\gamma}, L) \sim \ln L \qquad (\dot{\gamma} = 10^{-2})$$

$$\sim L \qquad (\dot{\gamma} = 10^{-4})$$

Decomposing the plastic response in terms of flips

Characteristic flip strain: $\Delta \epsilon_0$

Characteristic flip size: a^2

Eshelby: $\Delta \overline{\sigma_{xy}} = \dfrac{2\mu a^2 \Delta \epsilon_0}{L^2}$

Over a long strain interval $\Delta \gamma$:

the average number of flips verifies: $N_f(\Delta\gamma)\Delta\overline{\sigma_{xy}} = 2\mu\Delta\gamma$

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

$$R_f = \frac{L^2 \dot{\gamma}}{a^2 \Delta\epsilon_0}$$

Assume flips independent

Over a large strain interval: $\Delta y_i = \sum_f u_y(\vec{r}_i - \vec{r}_f)$

$$\Rightarrow \langle \Delta y^2 \rangle = N_f(\Delta\gamma)\ \langle u_y^2 \rangle$$

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

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

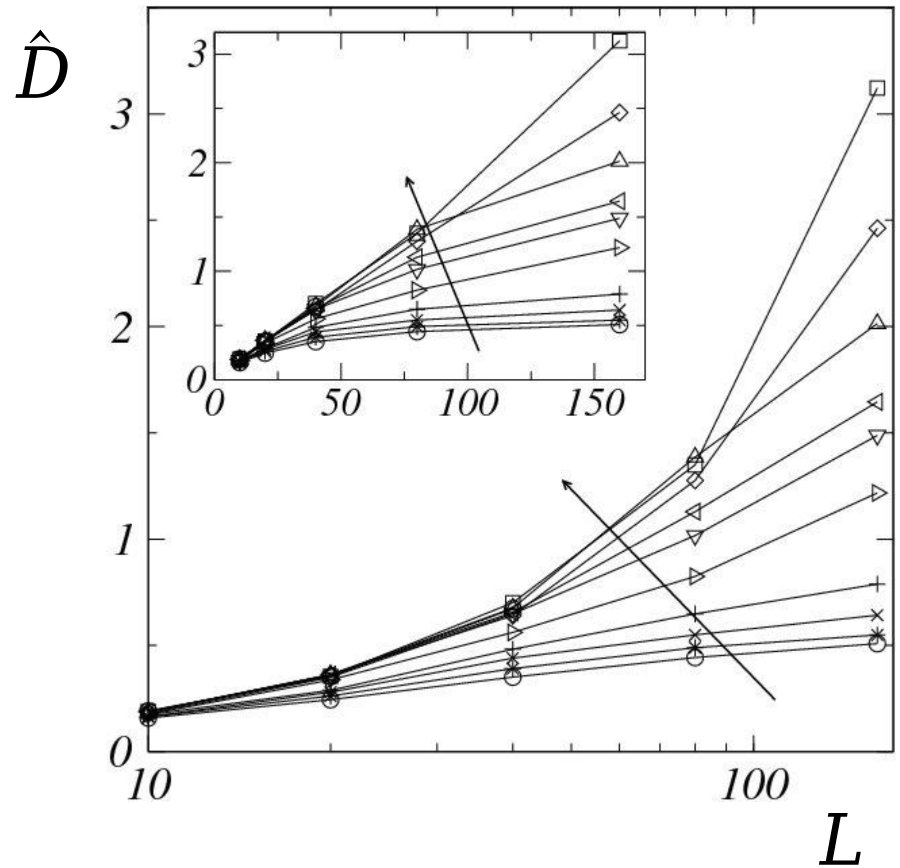
$$\langle u_y^2 \rangle = \frac{1}{L^2} \int_a^L u_y^2 \, d\vec{r} = \frac{a^4 \Delta\epsilon_0^2}{4\pi L^2} \ln(L/a)$$

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

Transverse diffusion at finite strain rate

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

$$a^2 \Delta \epsilon_0 \sim 1 \quad \begin{cases} \Delta \epsilon_0 \sim 4\% \\ a \sim 5 \end{cases}$$

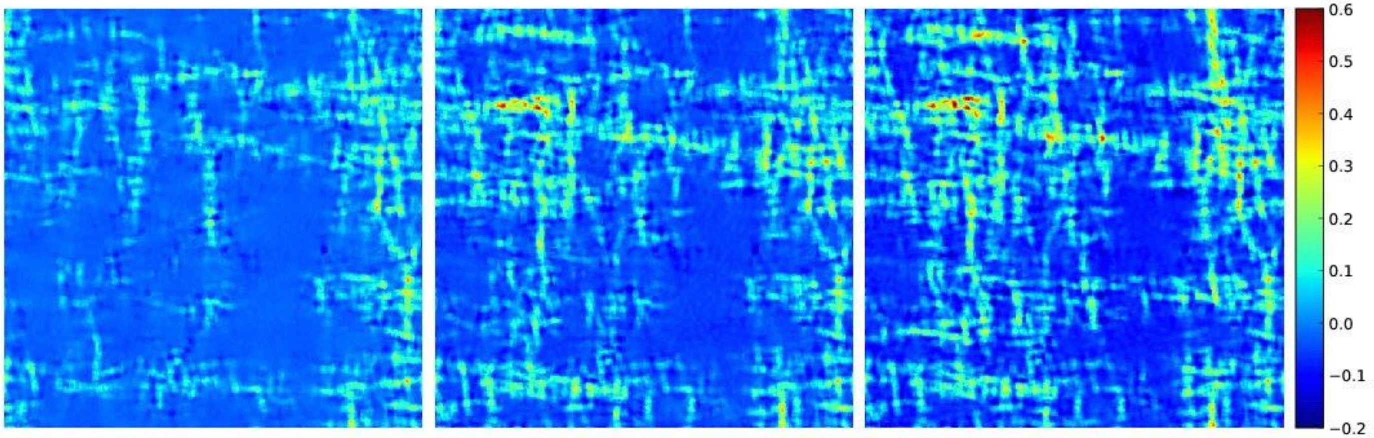


Very high strain rates $(\dot{\gamma} = 10^{-2})$
~ no flip correlations

Decreasing $\dot{\gamma}$: growing departure from $\ln L$
= growing correlation length (avalanche size)?

Assume events = correlated flips = linear avalanches

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



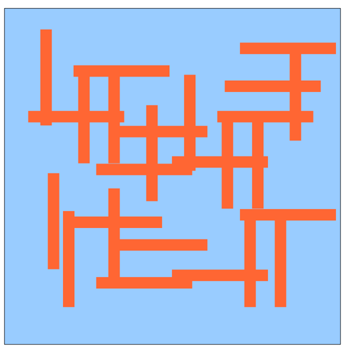
$\gamma = 1\%$ $\gamma = 5\%$ $\gamma = 10\%$

Assume events = correlated flips = linear avalanches

Avalanches:

- linear extension: l (= flip correlation length)
- density of flips in an avalanche, ν constant

$$N_{av}(\Delta\gamma) = N_f(\Delta\gamma)/\nu l$$



$$\langle \Delta y^2 \rangle_{av} = \nu^2 \int_0^l \int_0^l ds\, ds' \langle u_y(\vec{r} - \vec{r}_s) u_y(\vec{r} - \vec{r}_{s'}) \rangle$$

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

$$\equiv \langle u_y^2 \rangle_A$$

Particles diffusion

$$\Delta y_i = \sum_A u_y^A(\vec{r}_i - \vec{r}_A)$$

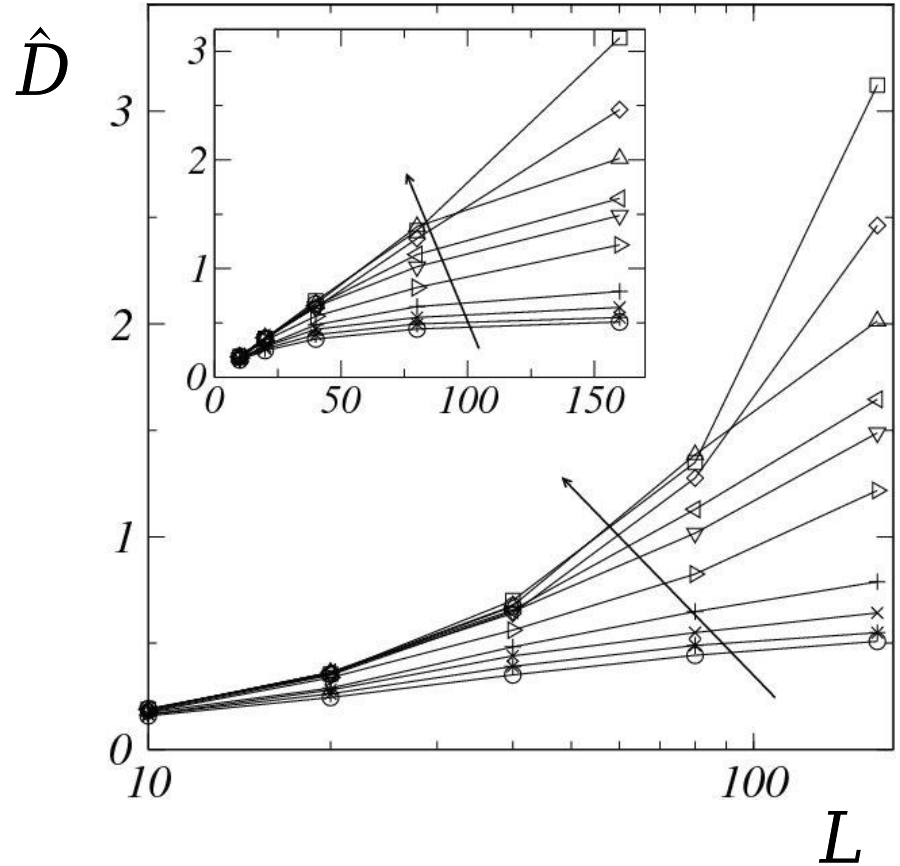
Assuming avalanches independent:

$$\langle \Delta y^2 \rangle = N_A(\Delta\gamma) \langle u_y^2 \rangle_A$$

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

Transverse diffusion at finite strain rate

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



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

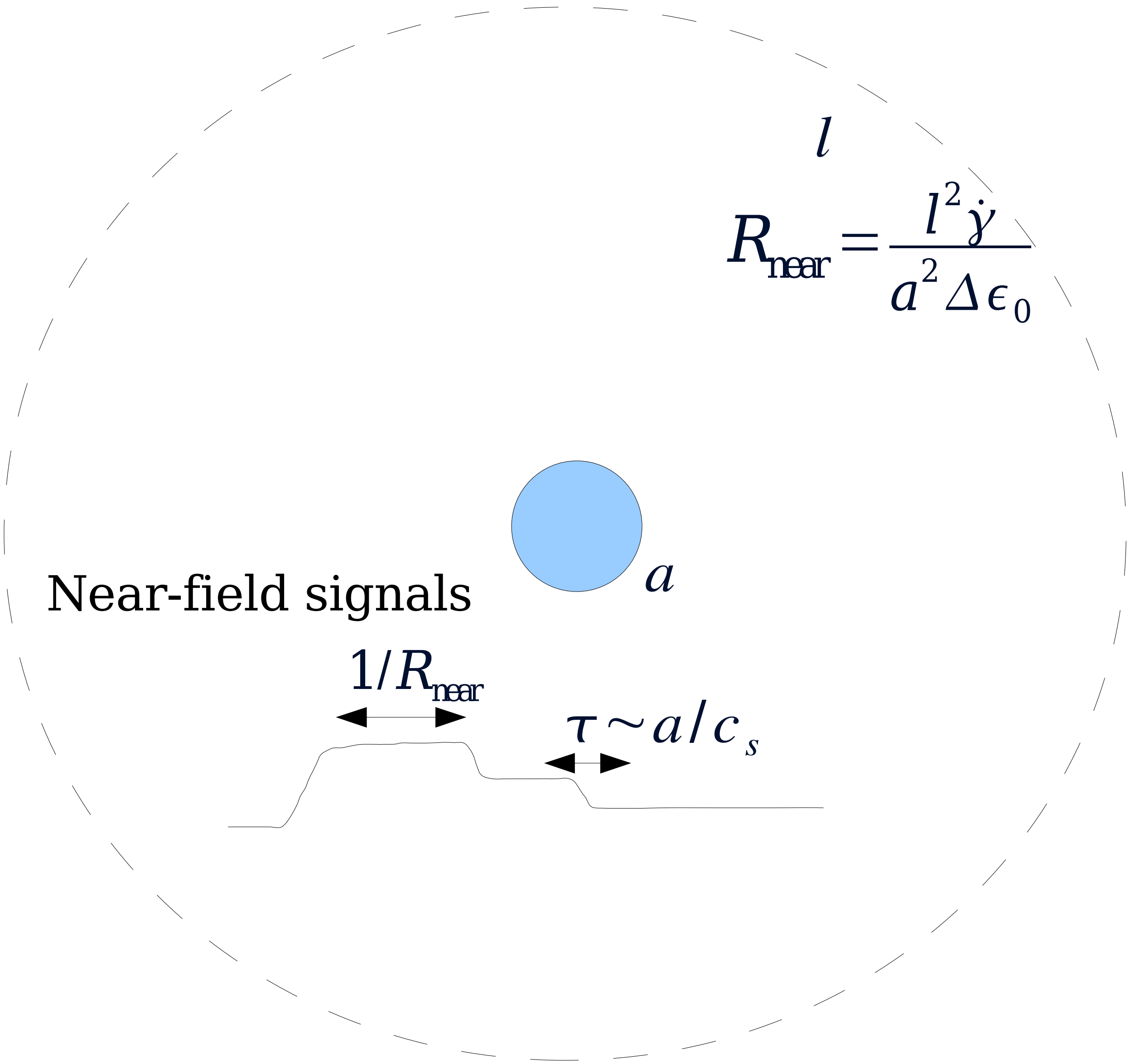
$\dot{\gamma} \to 0$ $\Rightarrow$ $l \sim L$ $\hat{D} \sim L$ QS regime

In between, evaluate $l(\dot{\gamma})$?

What is the noise received by a zone?

L

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



Near-field signals are separated iff: $1/R_{\text{near}} \gg \tau \iff l \ll \sqrt{a^2 \Delta \epsilon_0 / \dot{\gamma} \tau_{\text{flip}}}$

What is the noise received by a zone?

L

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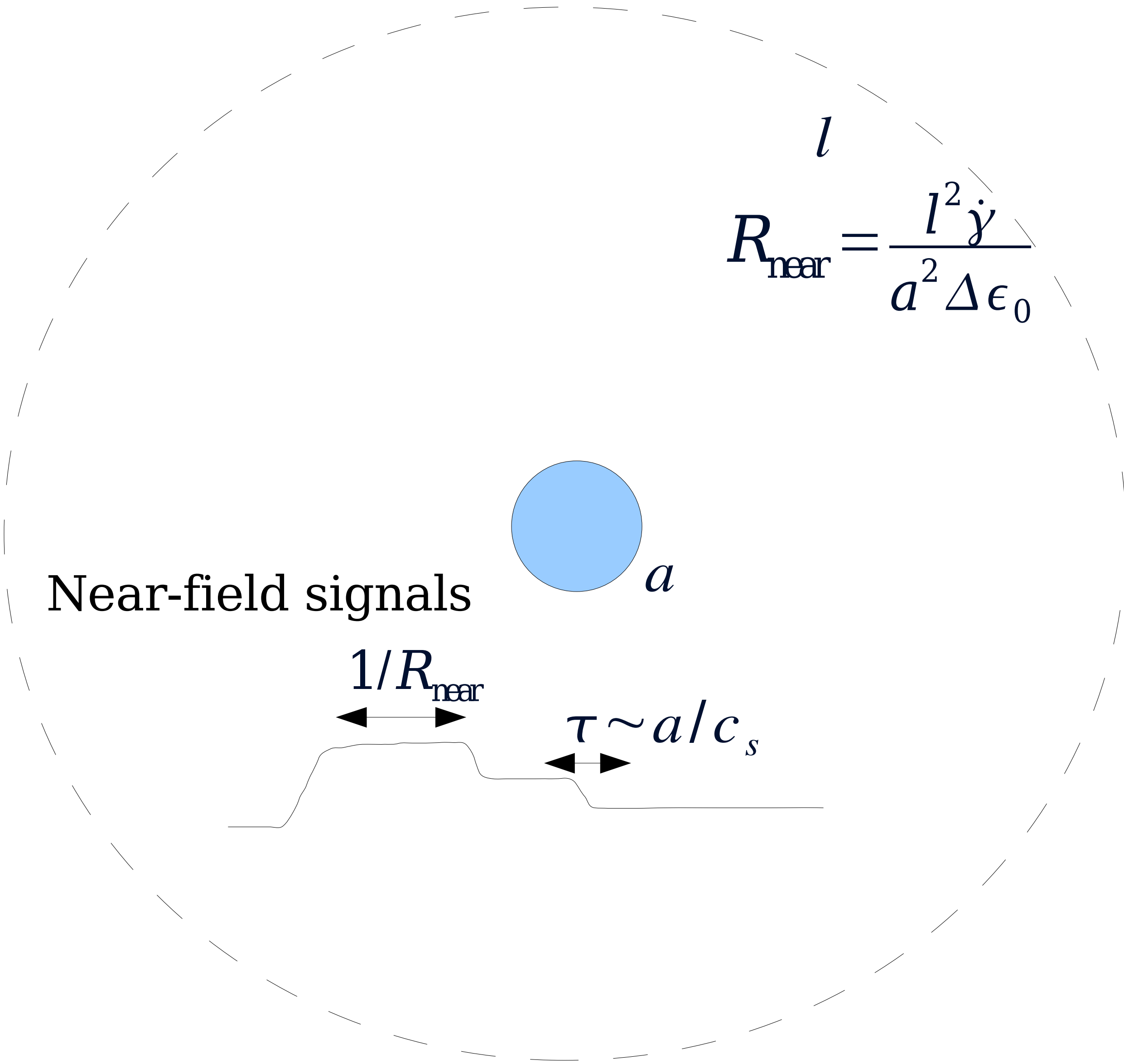


Background noise

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

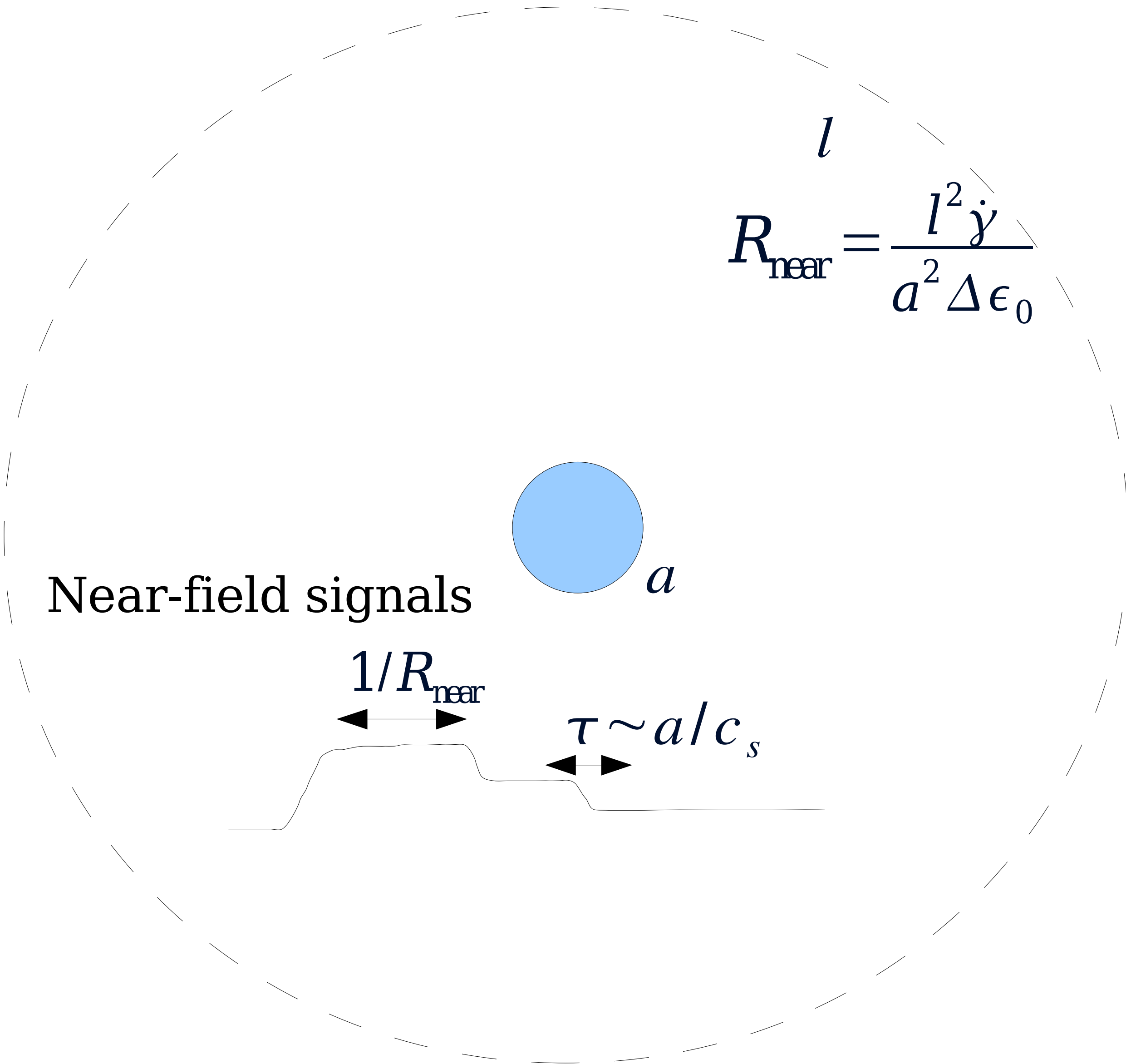
During time τ, stress diffus

$$\langle \Delta \sigma^2 \rangle \sim R_{\text{back}} \tau \langle \Delta \sigma^2 \rangle_{\text{Esh.}}$$

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

Near-field signals are separated iff: $1/R_{\text{near}} \gg \tau \Leftrightarrow l \ll \sqrt{a^2 \Delta \epsilon_0 / \dot{\gamma} \tau_{\text{flip}}}$

What is the noise received by a zone?



L

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

Background noise

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

During time τ , stress diffus

$$\langle \Delta \sigma^2 \rangle \sim R_{back} \tau \langle \Delta \sigma^2 \rangle_{Esh.}$$

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

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

Near-field signals are separated iff: $1/R_{near} \gg \tau \Leftrightarrow l \ll \sqrt{a^2 \Delta \epsilon_0 / \dot{\gamma} \tau_{flip}}$

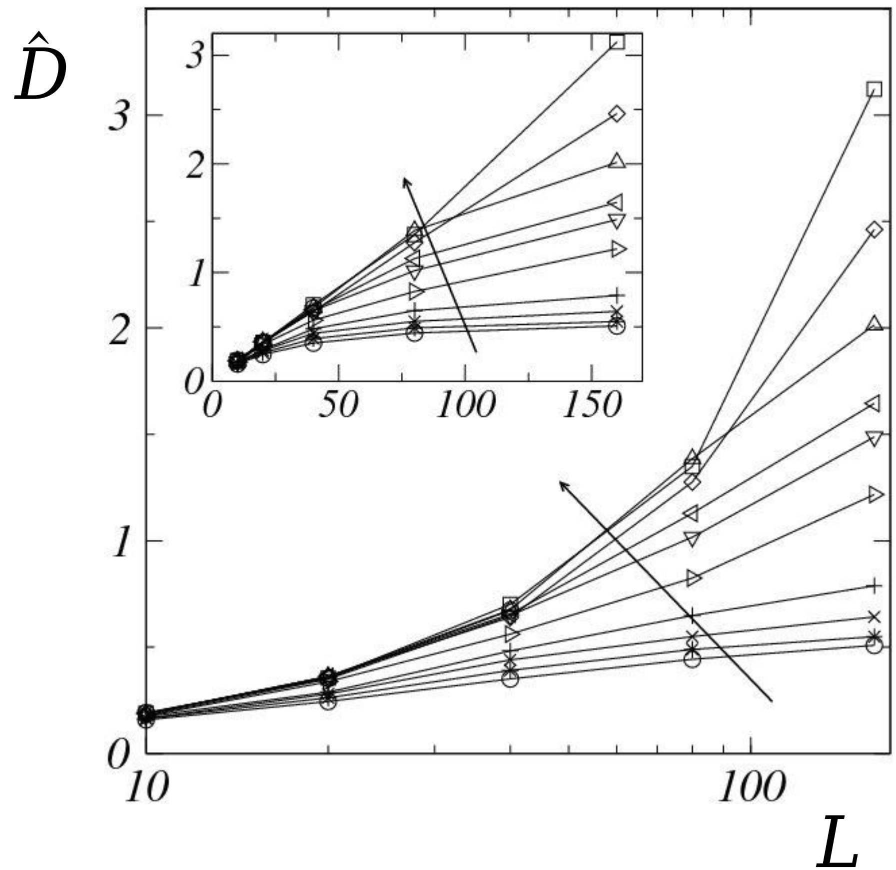
Back to diffusion data

PRL 103, 065501 (2009)

$$\hat{D} = \frac{a^2 \Delta \epsilon_0^2}{2\pi} \nu l \ln(L/l)$$

$$l \sim \sqrt{a^2 \Delta \epsilon_0 / \dot{\gamma} \tau_{\mathrm{flip}}}$$

$$\hat{D}/L \sim f(L\sqrt{\dot{\gamma}})$$



Back to diffusion data

PRL 103, 065501 (2009)

$$\hat{D} = \frac{a^2 \Delta \epsilon_0^2}{2\pi} \nu\, l \ln(L/l)$$

$$l \sim \sqrt{a^2 \Delta \epsilon_0 / \dot{\gamma} \tau_{\text{flip}}}$$

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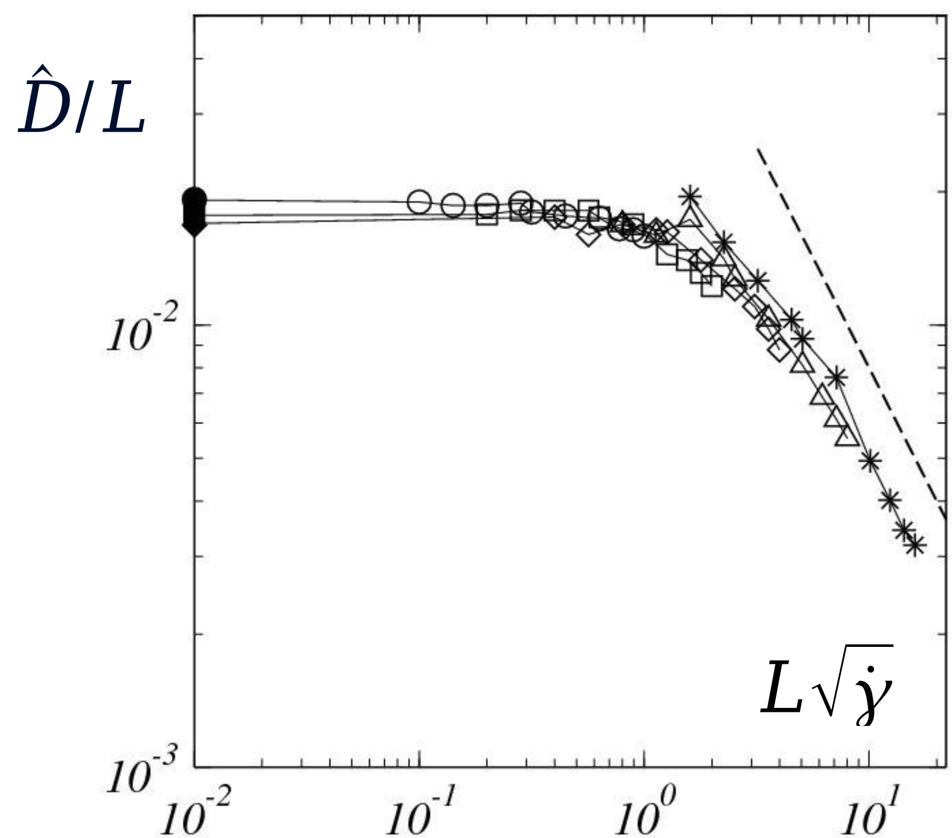


Crossover from dynamically controlled correlation length $l \sim \dot{\gamma}^{1/2}$ to QS regime $l \sim L$

For

$$\dot{\gamma} \sim \dot{\gamma}_{\infty} \approx a^2 \Delta \epsilon_0 / \tau_{\text{flip}} L^2$$

Inferences

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

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

  For $\dot{\gamma} \le 1\,\mathrm{sec}^{-1}$, $l \ge 10\,\mu\mathrm{m}$

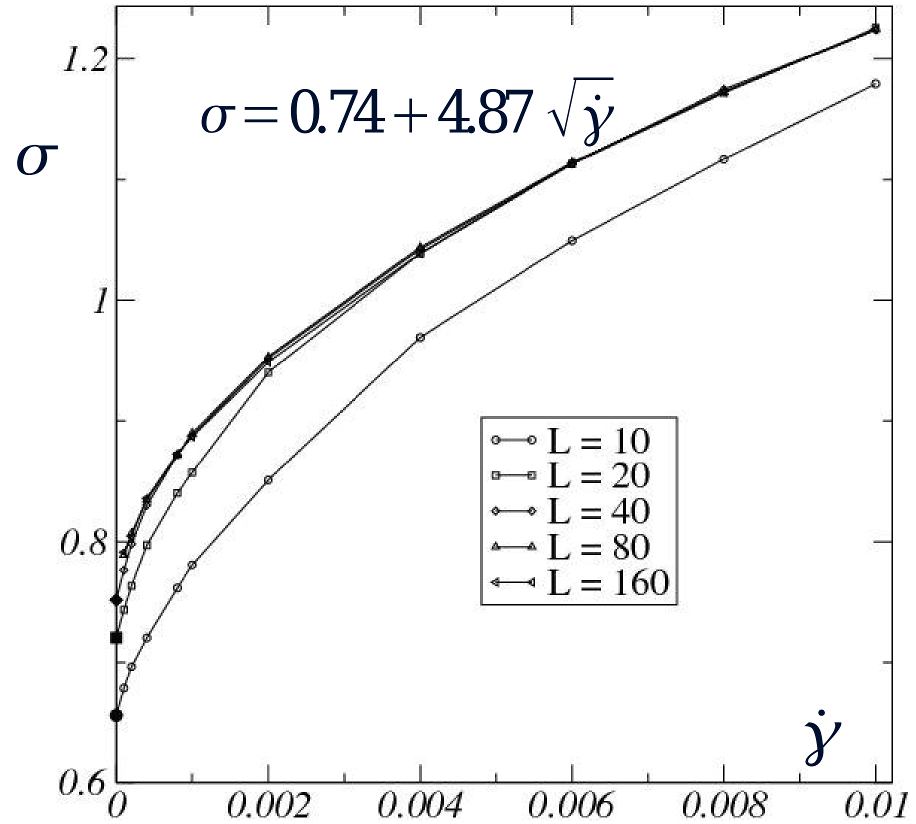
- 2D flow curve $\sigma(\dot{\gamma})$

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

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

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

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



Conclusion (partial)

AQS simulations support the following phenomenology:

- Plasticity results from local shear transformations
- Zones are progressively convected towards instability
- Each flip produces an Eshelby-like field likely to trigger secondary flips

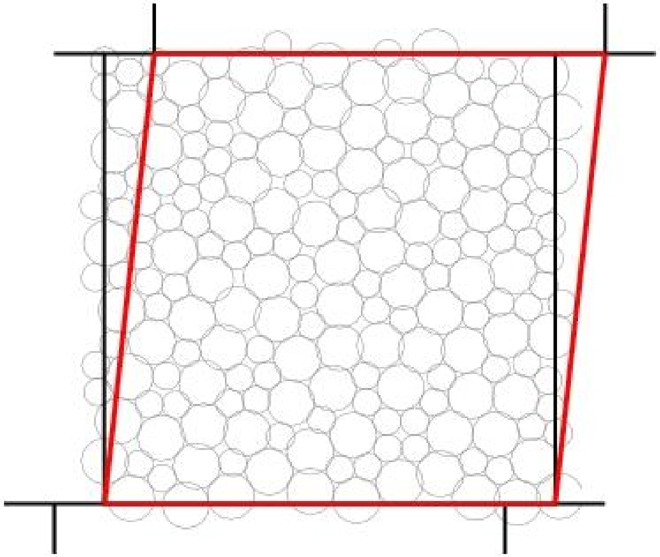
This shows up as system-spanning avalanches

At usual finite $\dot{\gamma}$, the same phenomenology continues to govern plasticity

- The size of avalanches $l \sim \dot{\gamma}^{-1/D}$
- With normal cross-over behavior when $l \sim L$
- We propose these changes govern stress/strain-rate relation

What happens at finite temperature?

Chattoraj et al,
arxiv/1005.1179



Binary LJ, radii 0.3 and 0.5

Velocity rescaling

Tg = 0.27

Data Accumulation:

T = 0.025, 0.05, 0.1, 0.2, 0.25, 0.3, 0.35, 0.4, 0.5

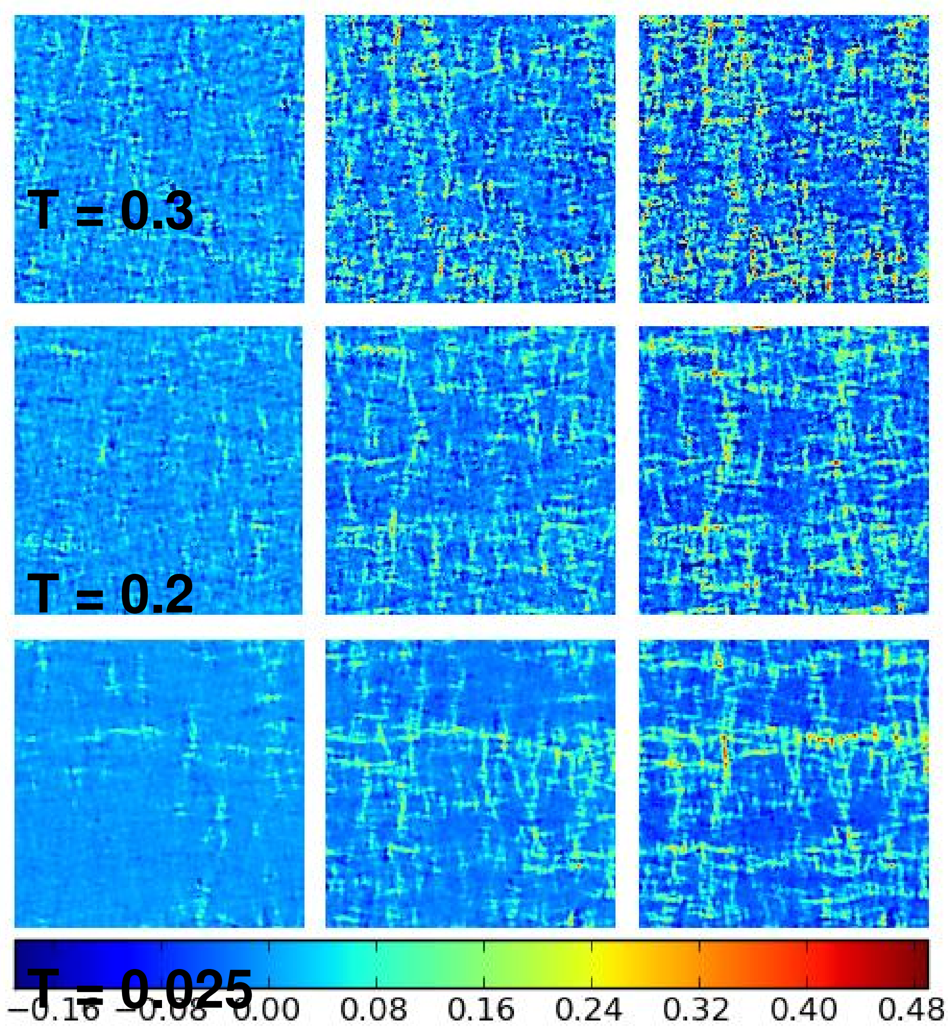
$\dot{\gamma}$ = 4e-05, 0.0001, 0.0004, 0.001, 0.004, 0.01

L = 10, 20, 40, 80, 160

Deformation Maps at T≠0

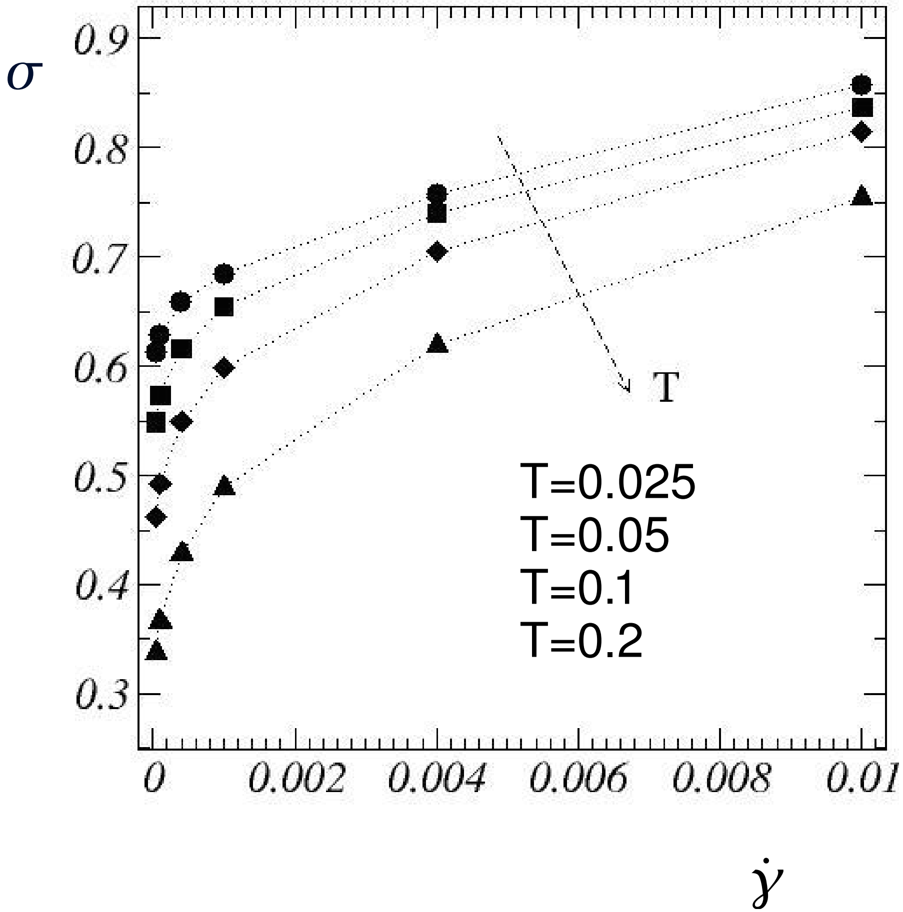
Tg=0.27

Avalanches
are clearly visible
below Tg

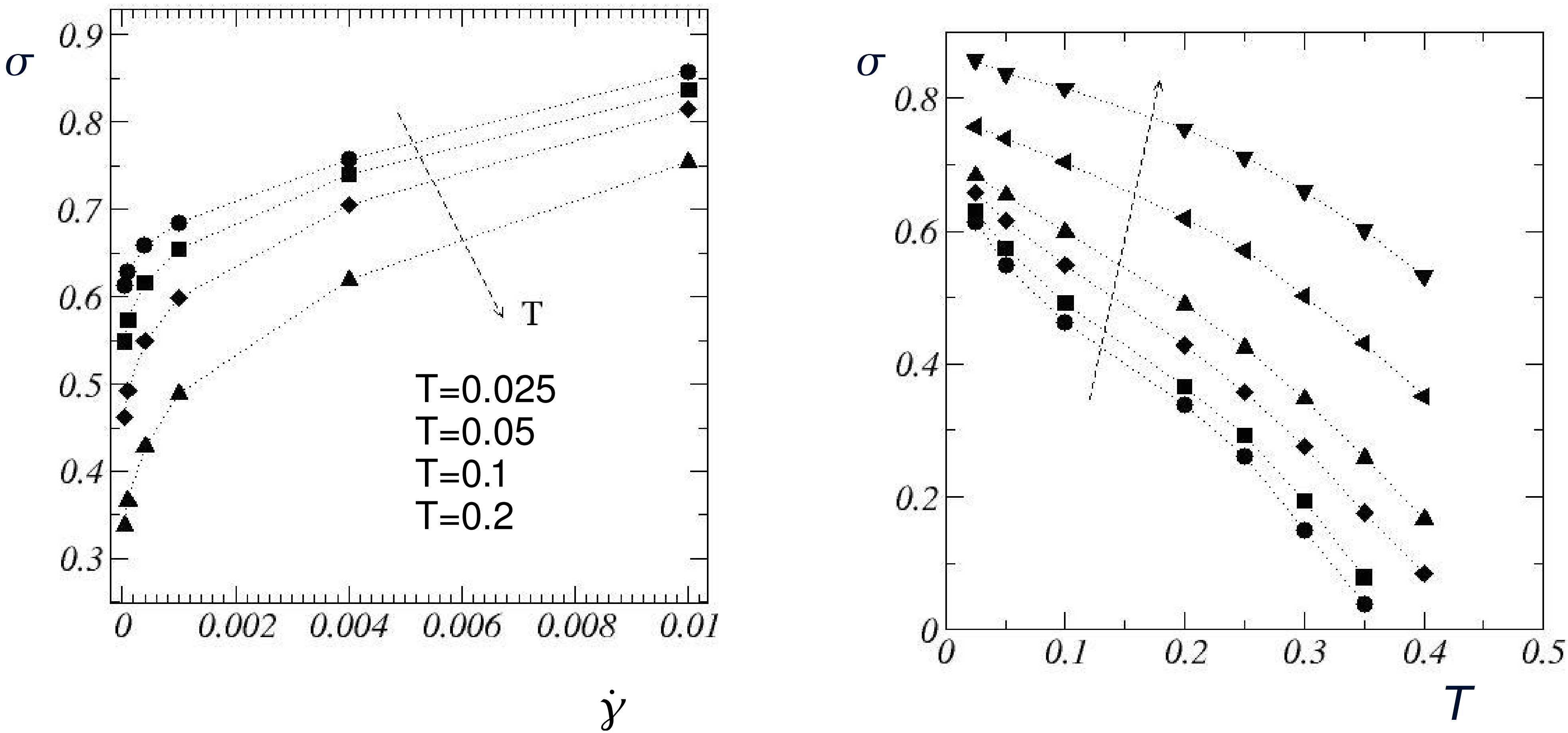


$\delta\gamma = 1\%$ $\delta\gamma = 5\%$ $\delta\gamma = 10\%$

Stress data


σ
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0
0.002
0.004
0.006
0.008
0.01
T
T=0.025
T=0.05
T=0.1
T=0.2
$\dot{\gamma}$

Stress data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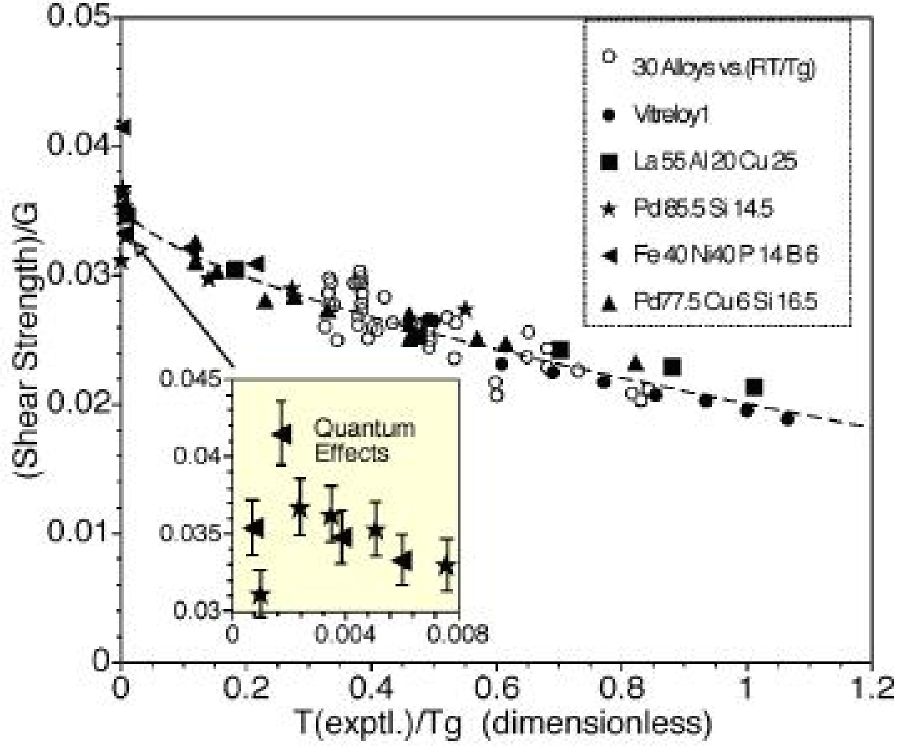
T
T=0.025
T=0.05
T=0.1
T=0.2
$\dot{\gamma}$
σ
0.8
0.6
0.4
0.2
0
0
0.1
0.2
0.3
0.4
0.5
T

Metallic glass yield stress

Johnson & Samwer 95, 195501 (2005)

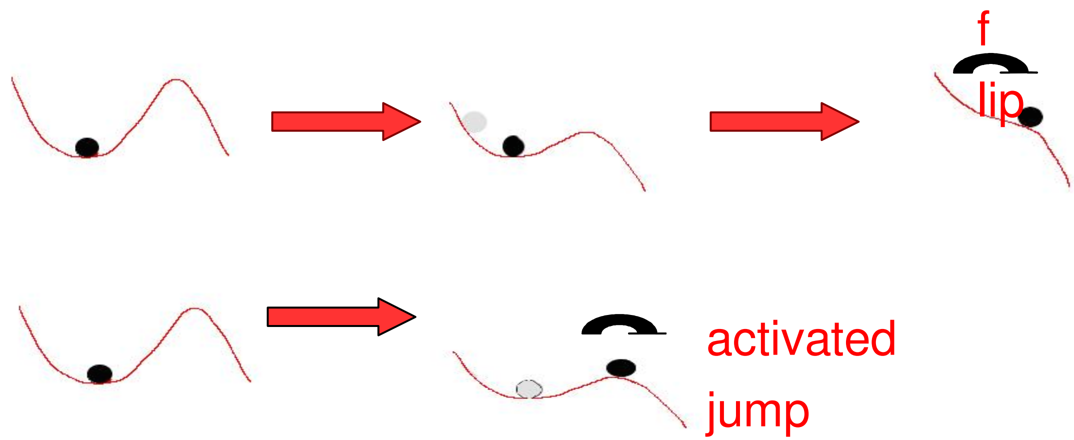
$$\sigma - \sigma_Y \propto T^{2/3}$$

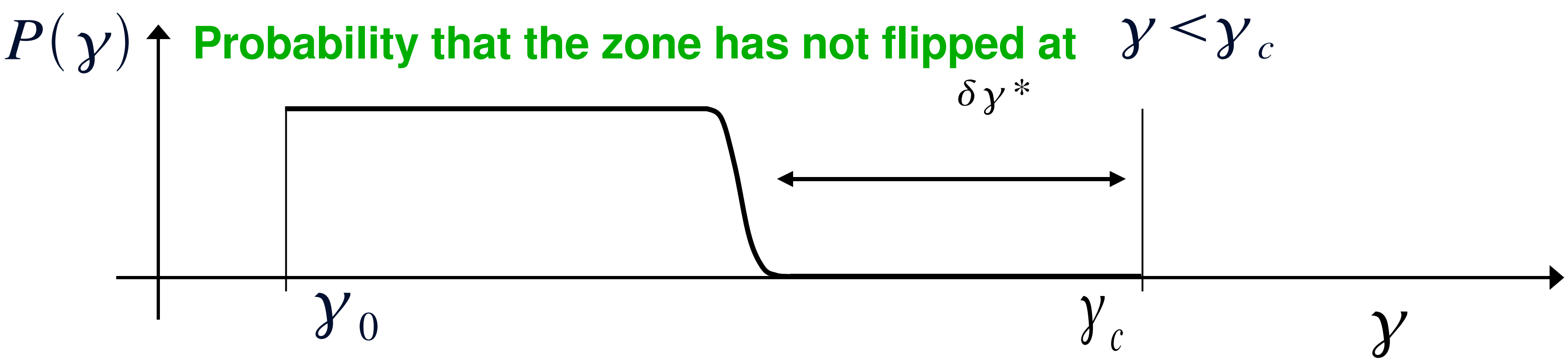


Effect of finite T on a single zone driven towards threshold

T = 0

T ≠ 0

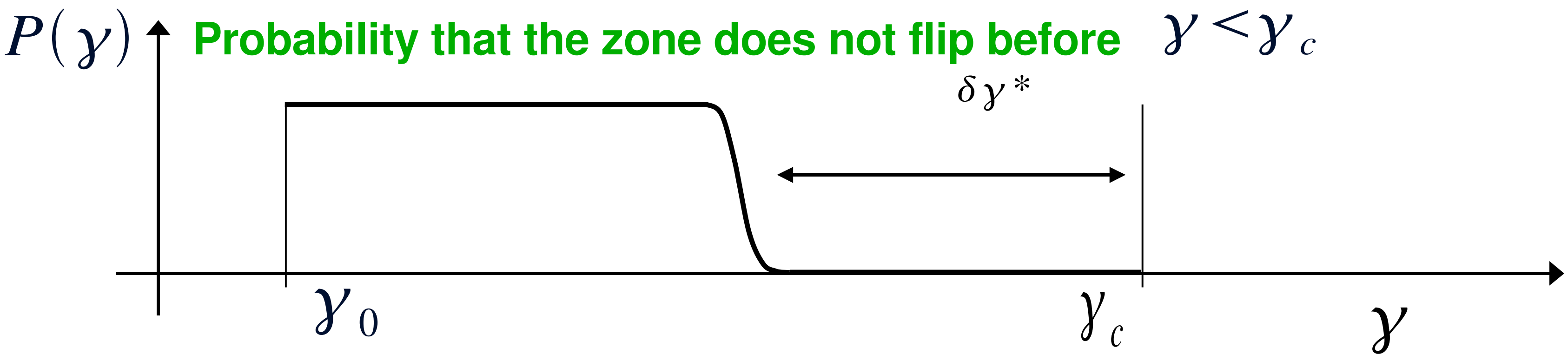




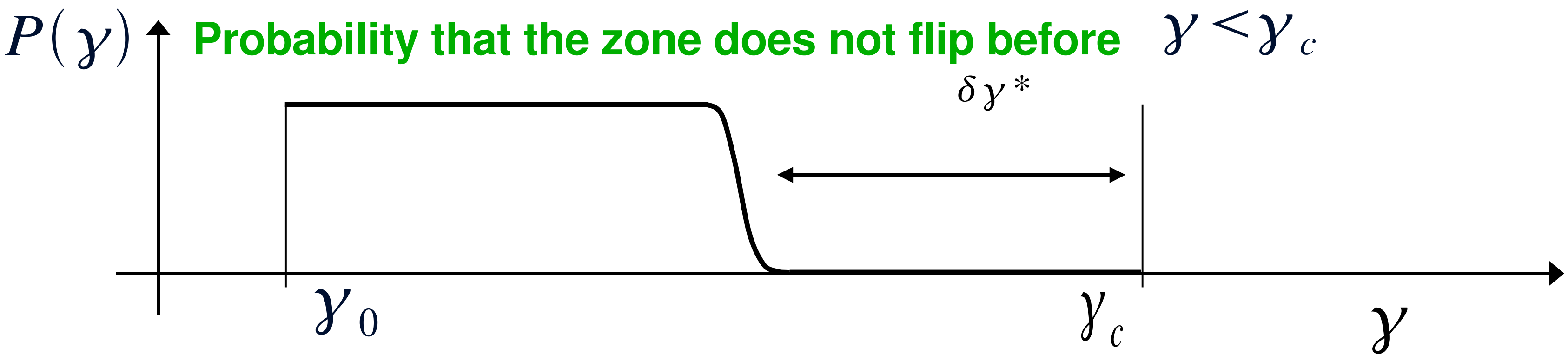
$$\sigma(\dot{\gamma};T)=\sigma(\dot{\gamma};T=0)-2\mu\delta\gamma^*$$

Effect of finite T on a single zone driven towards threshold

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



Effect of finite T on a single zone driven towards threshold



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

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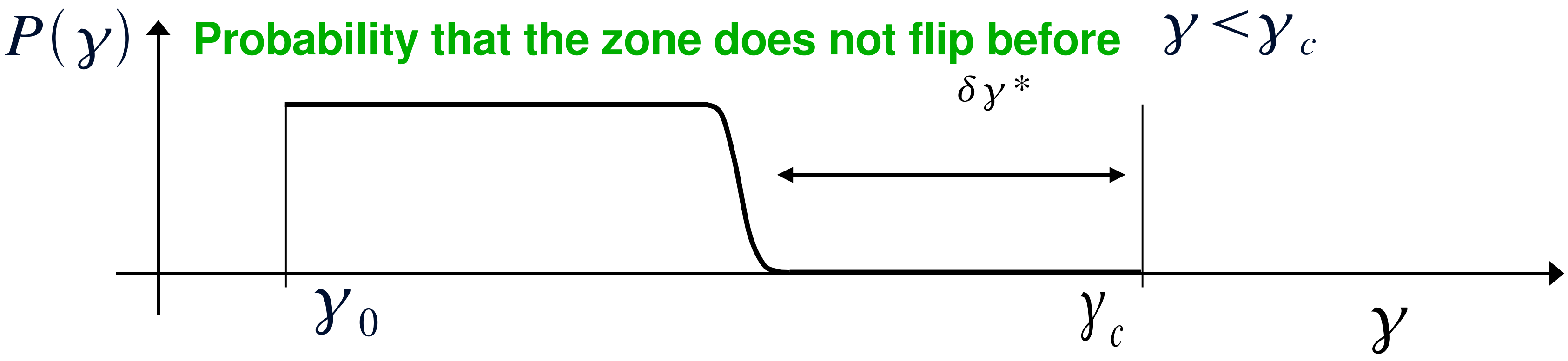

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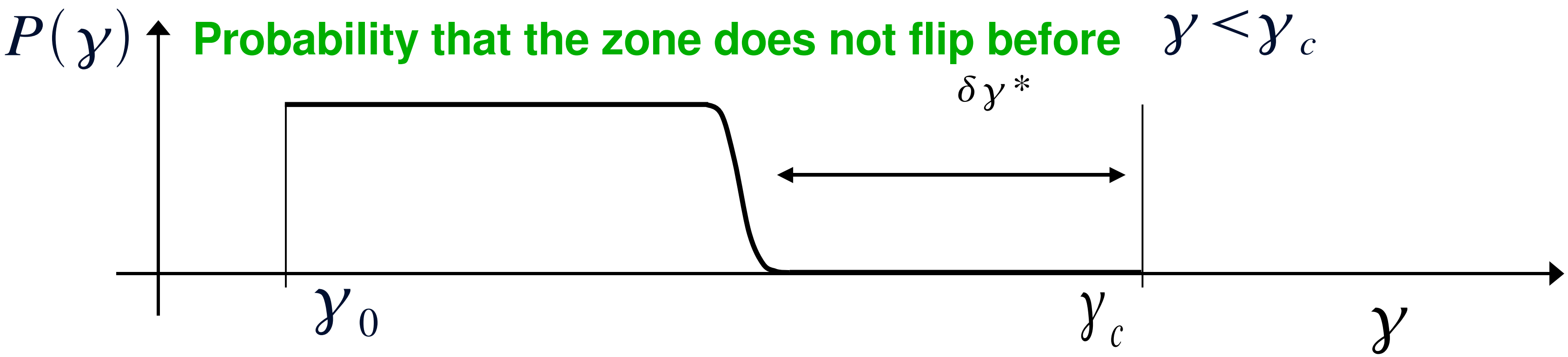

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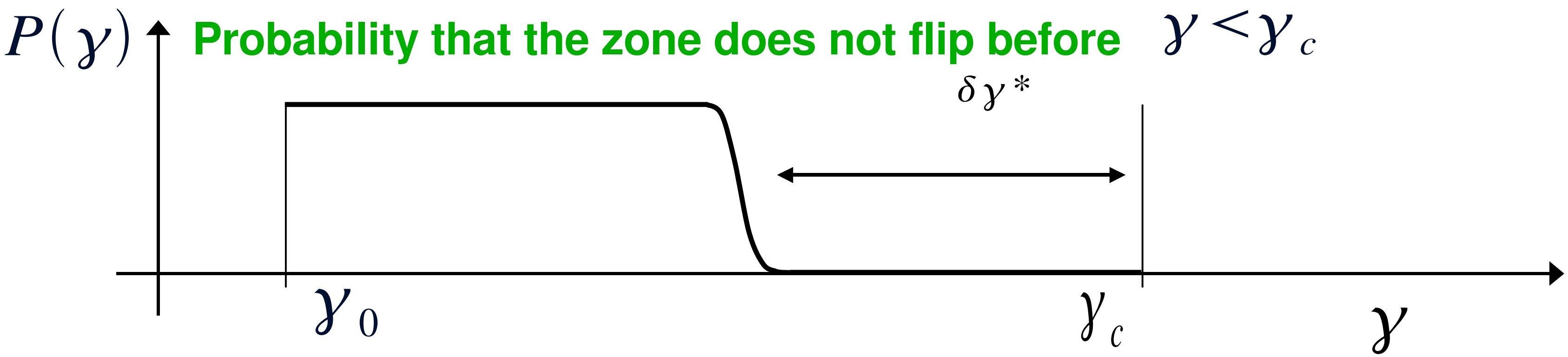

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$$P(\gamma) = \exp\left(-\frac{2}{3}\frac{\nu}{\dot{\gamma}}\left(\frac{T}{B}\right)^{5/6}\left(Q(\delta\gamma) - Q(\delta\gamma_0)\right)\right)$$

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

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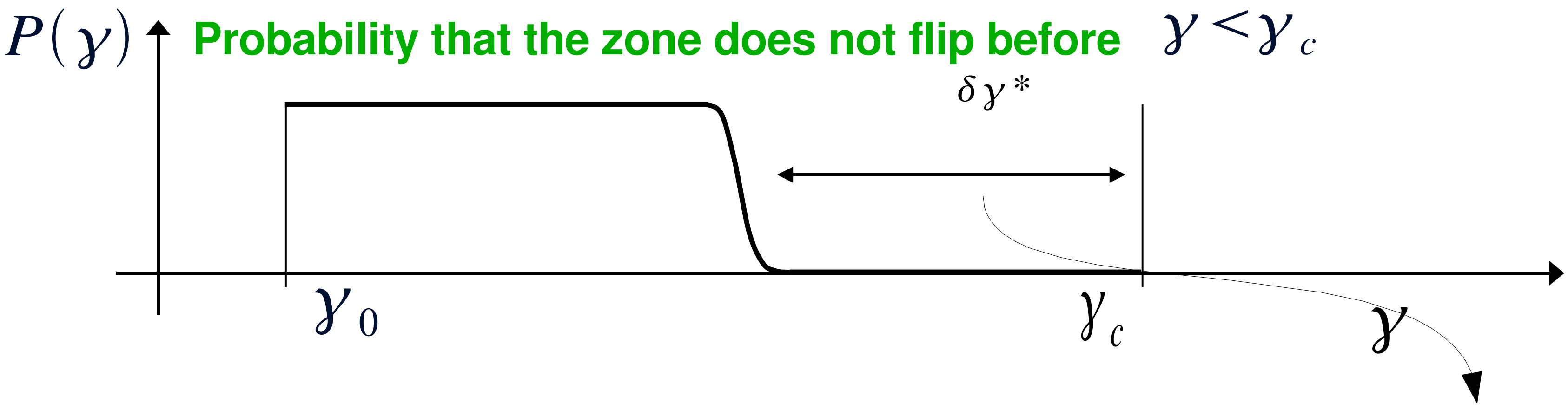

$$\delta\gamma^* \sim \left[\frac{T}{B} \ln\left(\frac{2}{3} \frac{\nu}{\dot{\gamma}} \left(\frac{T}{B} \right)^{5/6} \right) \right]^{2/3}$$

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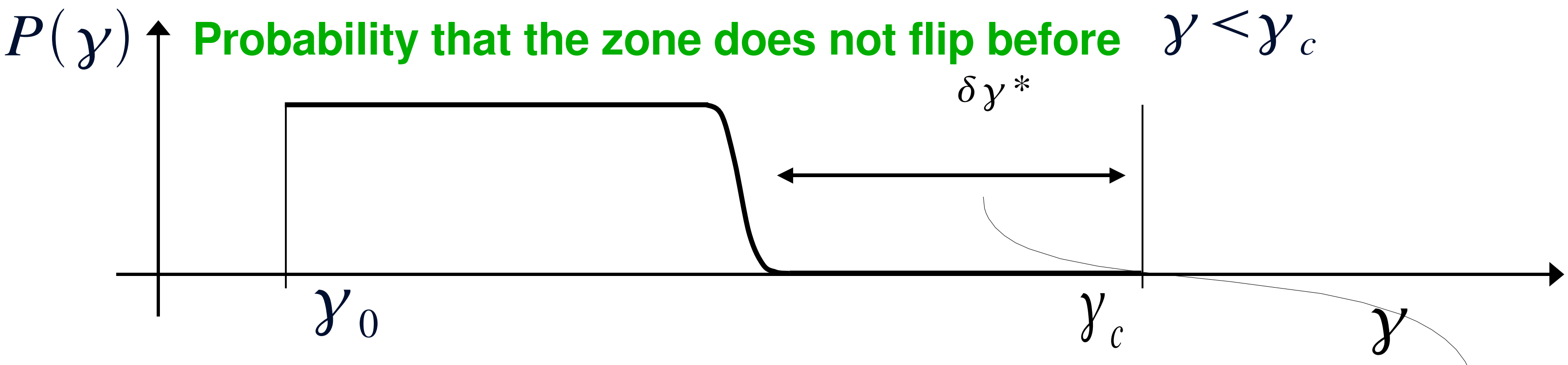

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<u>Effect of noise?</u>

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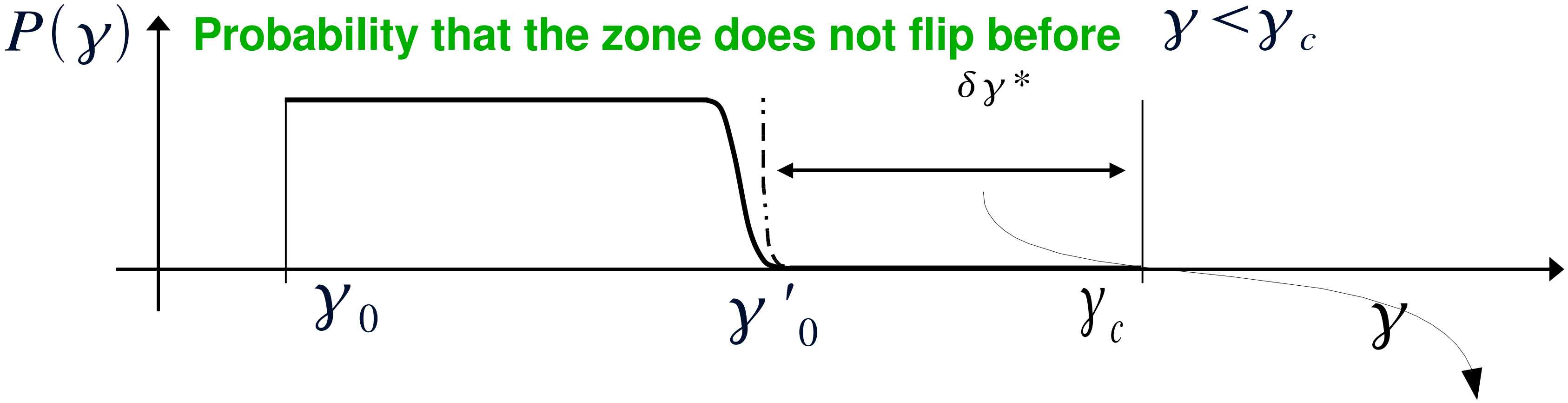

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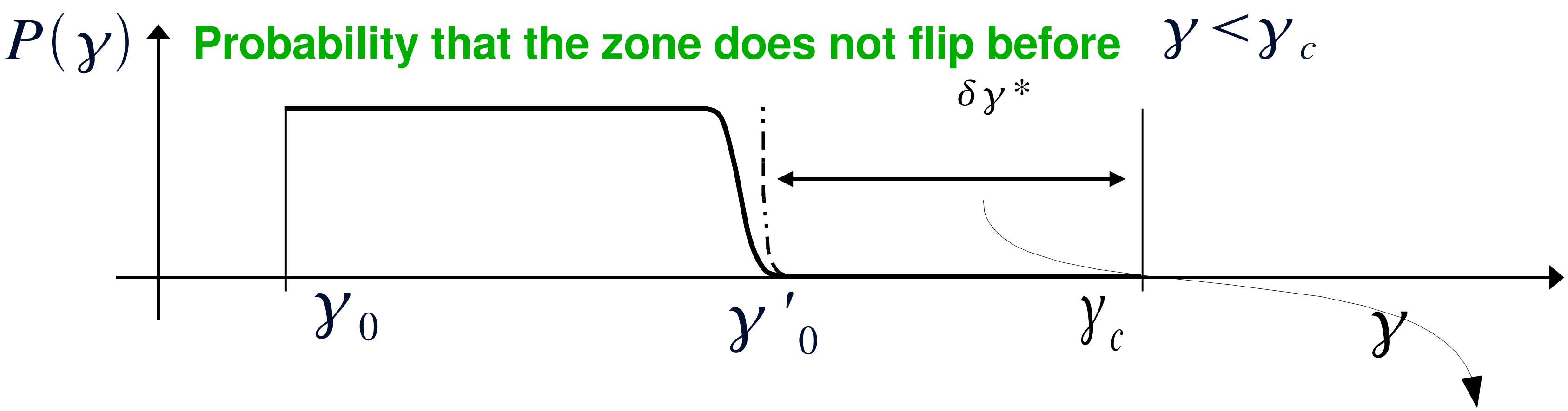

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<u>Effect of noise?</u>

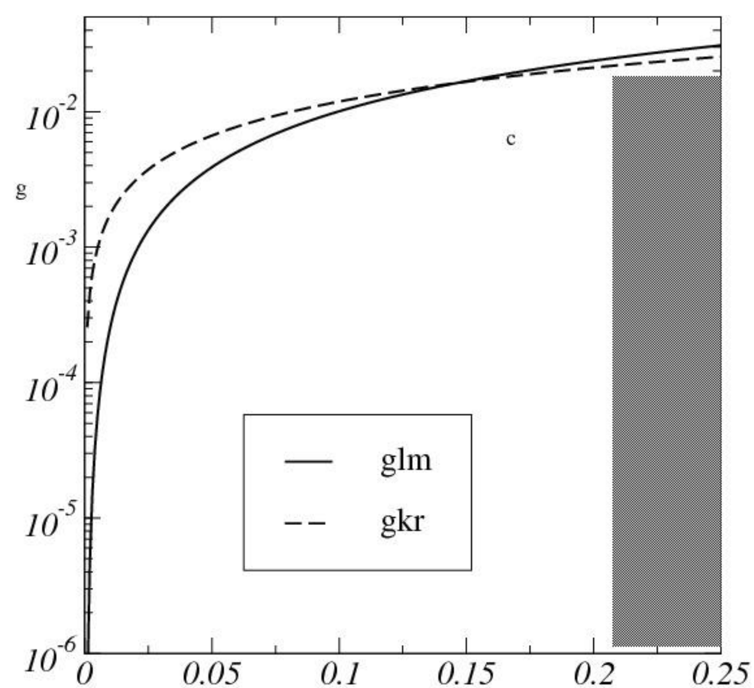
Can be separated if:

$$\frac{\Delta E}{E} \ll 1$$

during activation time

<u>Applicability of Kramers expression:</u>

$$\frac{E}{T} \gg 1$$



Consequences for stress

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

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

$$\sigma=A+B\sqrt{\dot{\gamma}}-C\left[T\ln\left(\frac{DT^{5/6}}{\dot{\gamma}}\right)\right]^{2/3}$$

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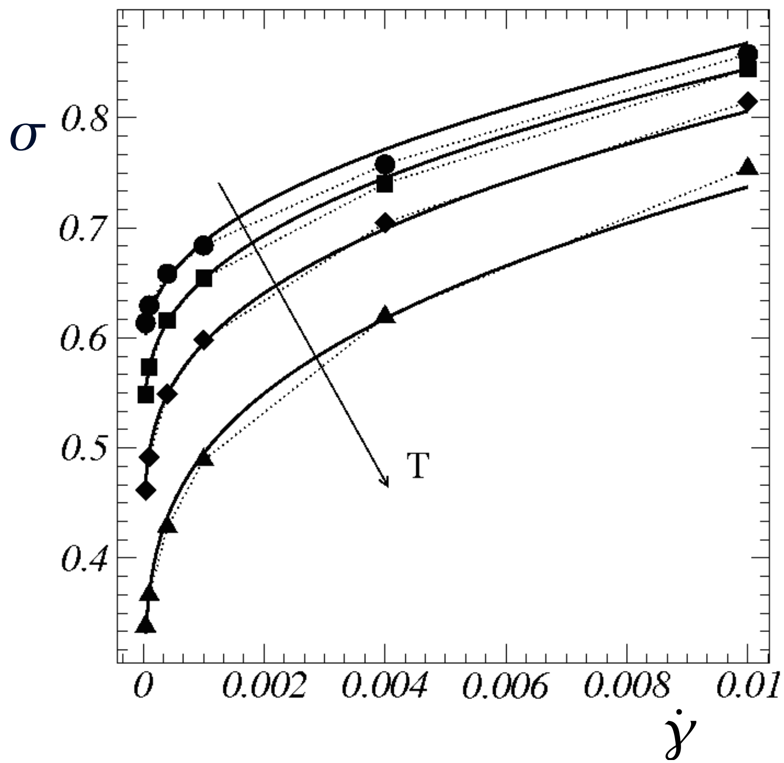

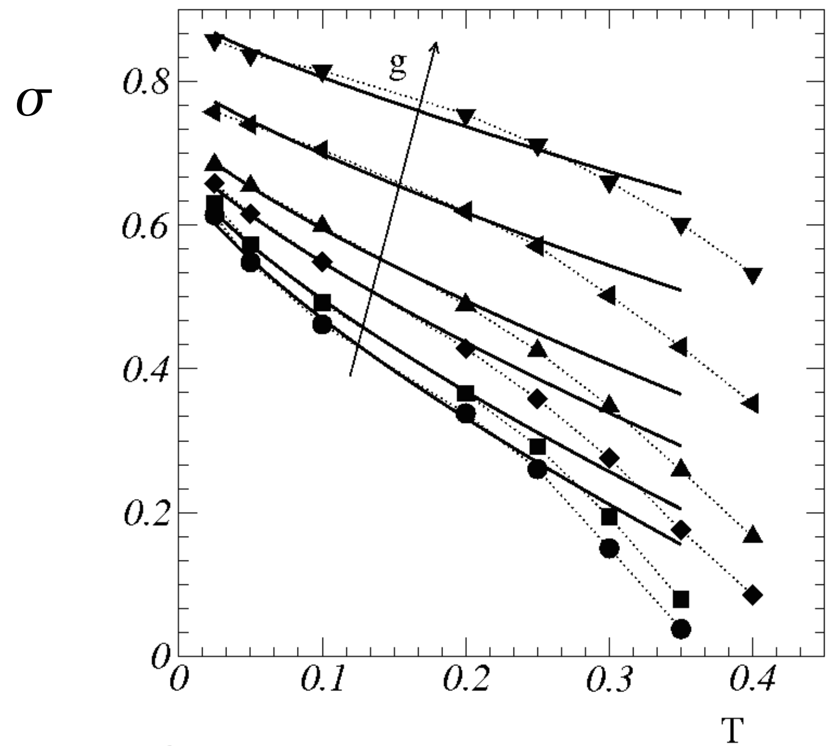

Chattoraj et al, arxiv/1005.1179

Conclusion

AQS simulations support the following phenomenology:

- Plasticity results from local shear transformations
- Zones are progressively convected towards instability
- Each flip produces an Eshelby-like field likely to trigger secondary flips

This shows up as system-spanning avalanches

At usual finite $\dot{\gamma}$, the same phenomenology continues to govern plasticity

- The size of avalanches $l \sim \dot{\gamma}^{-1/D}$
- With normal cross-over behavior when $l \sim L$
- We propose these changes govern stress/strain-rate relation

At finite T < Tg, the same phenomenology continues to hold

- Activations of driven zones leads to global lowering of the flow stress consistent with a $T^{2/3}$ stress correction
- Meanwhile, avalanche continues to be present and are only progressively blurred when approaching Tg