Elementary mechanisms of plastic deformation in amorphous materials

Anaël Lemaître

Navier

Rhéophysique

Length and energy scales in amorphous materials

Hard glasses

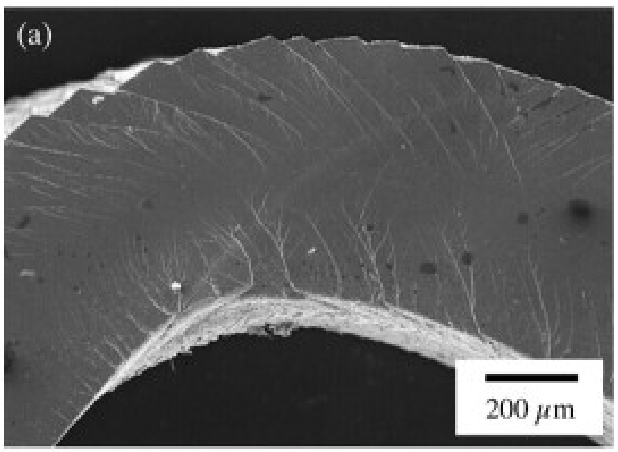
Soft glasses

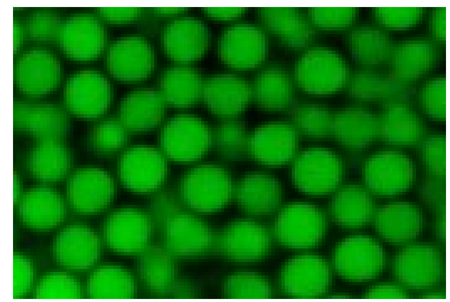
Metallic/oxyde glasses

Polymers

Colloids

Foams





Length scales ⩽ nm

Energies ~ 0.1—1 eV

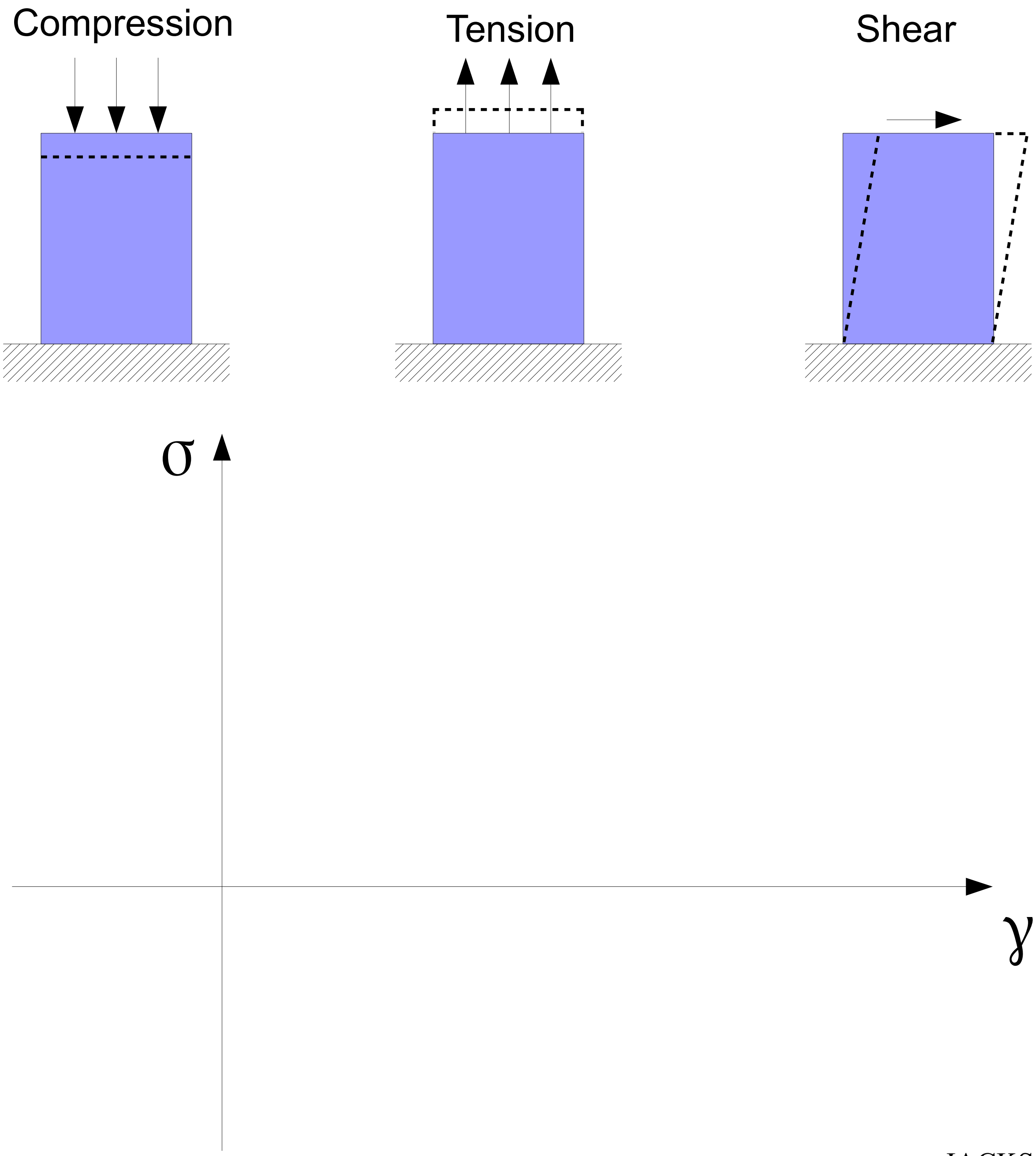
Stresses ~ GPa

Length scales ⩾ 0.1 μm

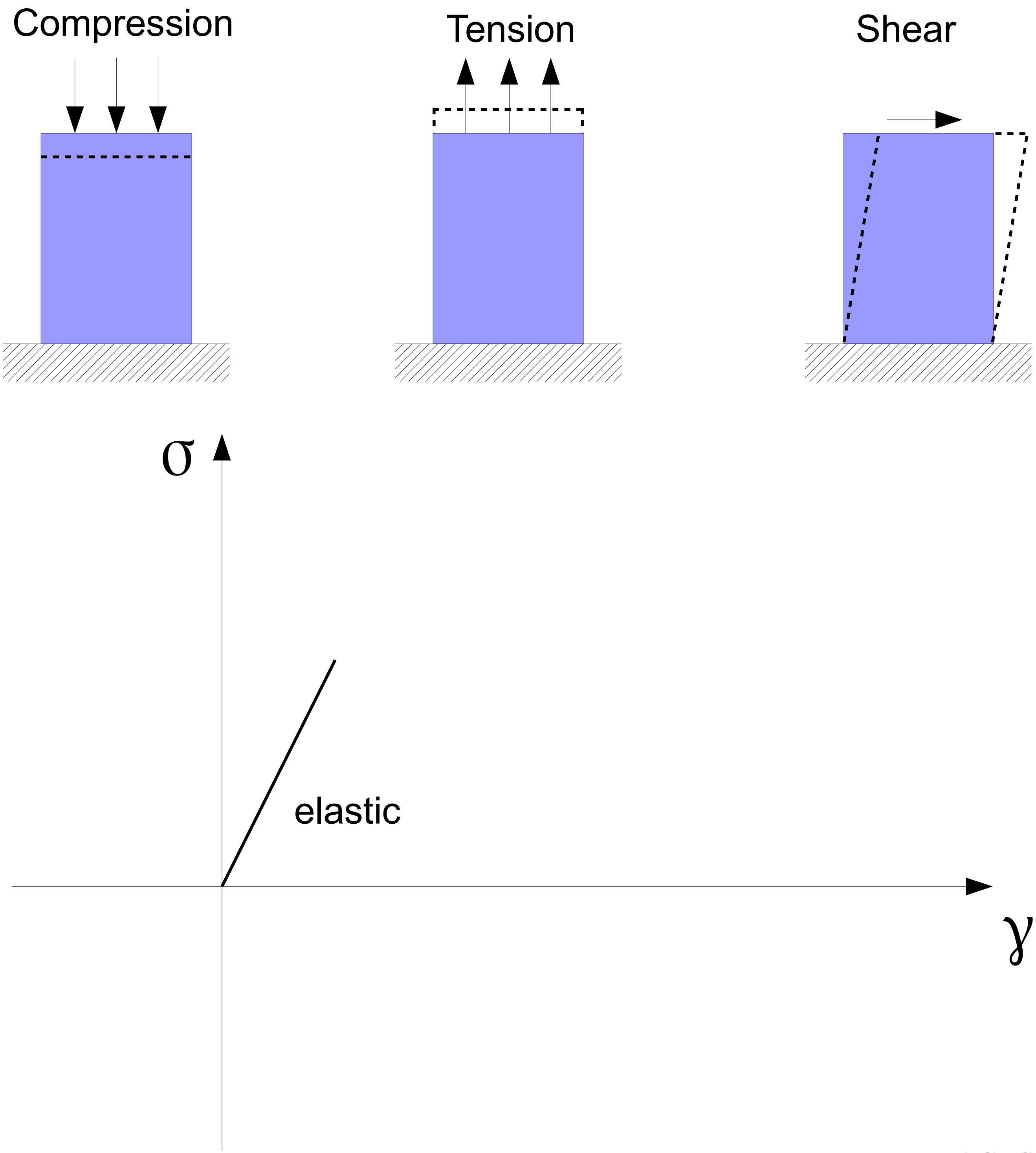
Energies ~ kT = 1/40 eV

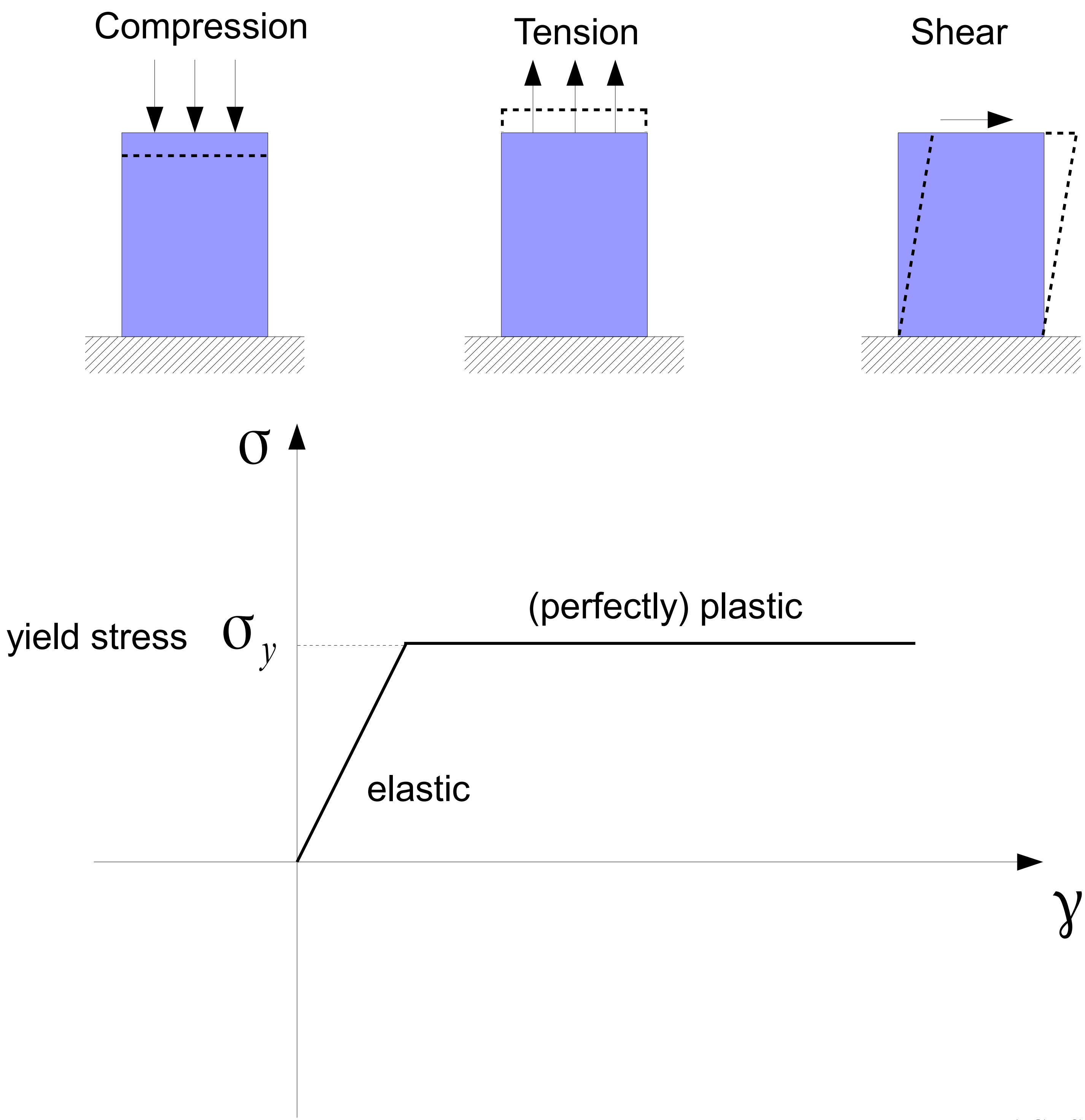
Stresses ~ Pa—kPa

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

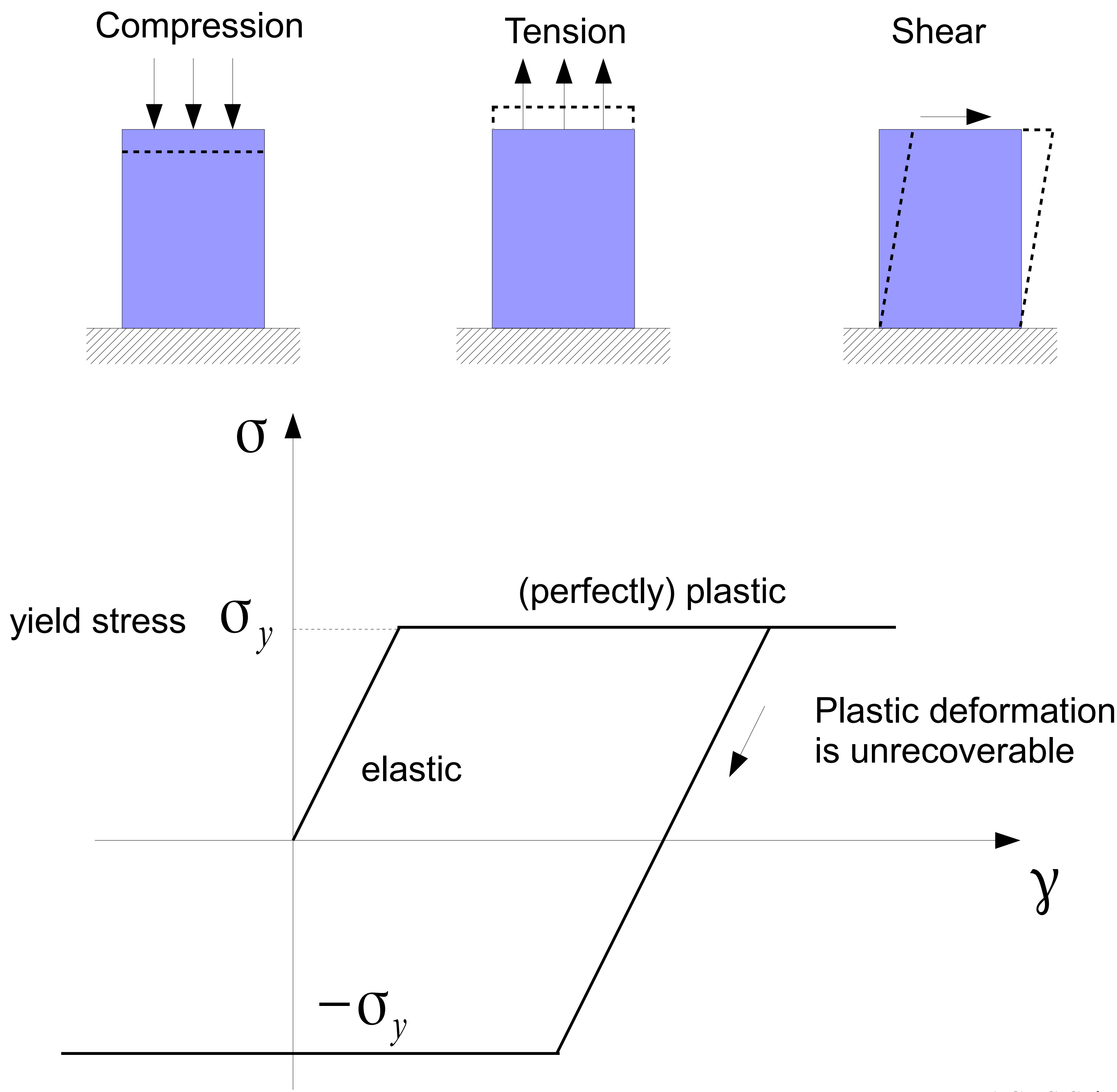


Compression
Tension
Shear
σ
γ

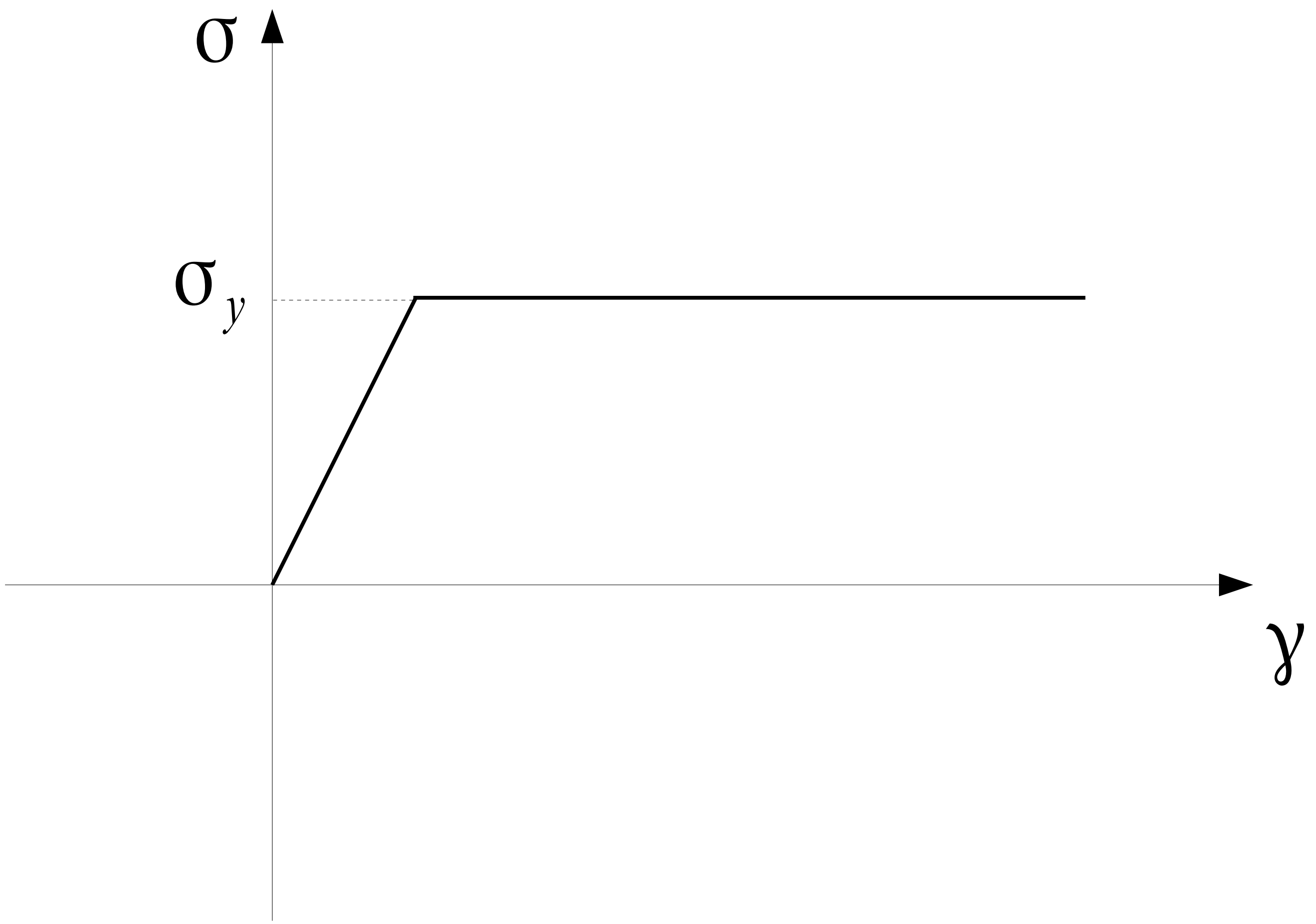

Compression
Tension
Shear
σ
elastic
γ



Compression
Tension
Shear
σ
yield stress
σ_y
(perfectly) plastic
elastic
γ


Compression
Tension
Shear
σ
yield stress σ_y
(perfectly) plastic
elastic
Plastic deformation
is unrecoverable
γ
$-\sigma_y$

Departures from elastic-perfectly-plastic behavior



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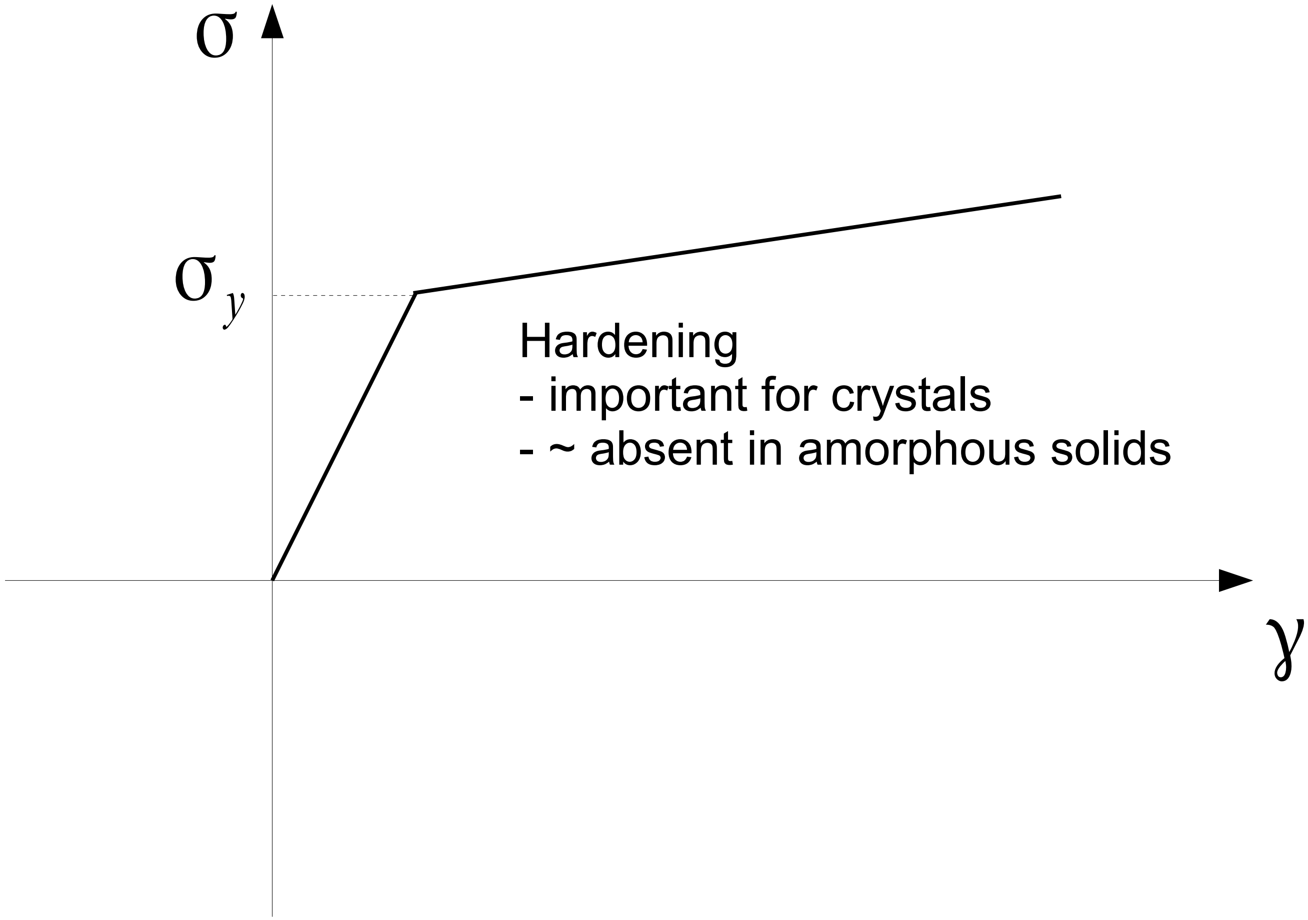
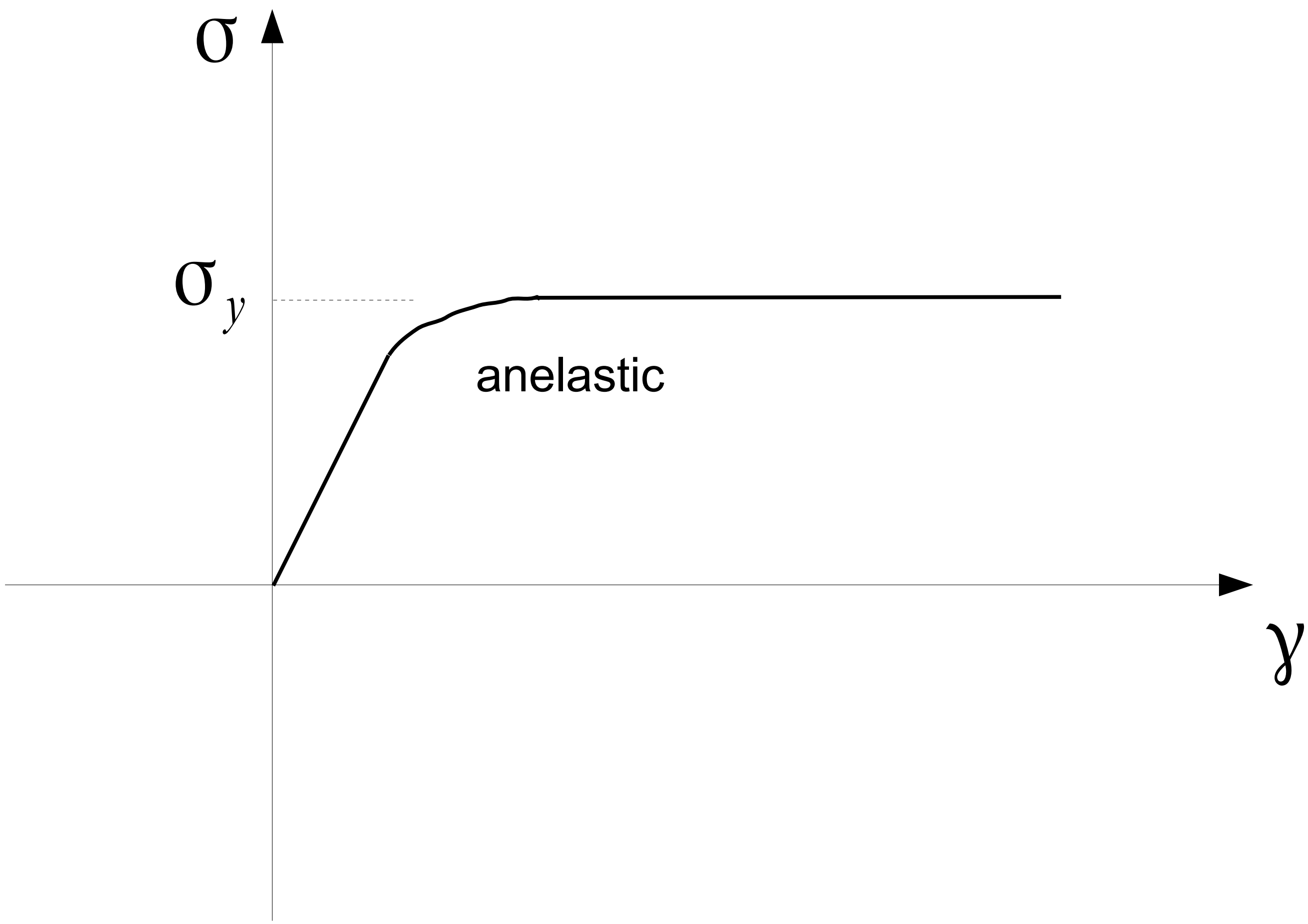
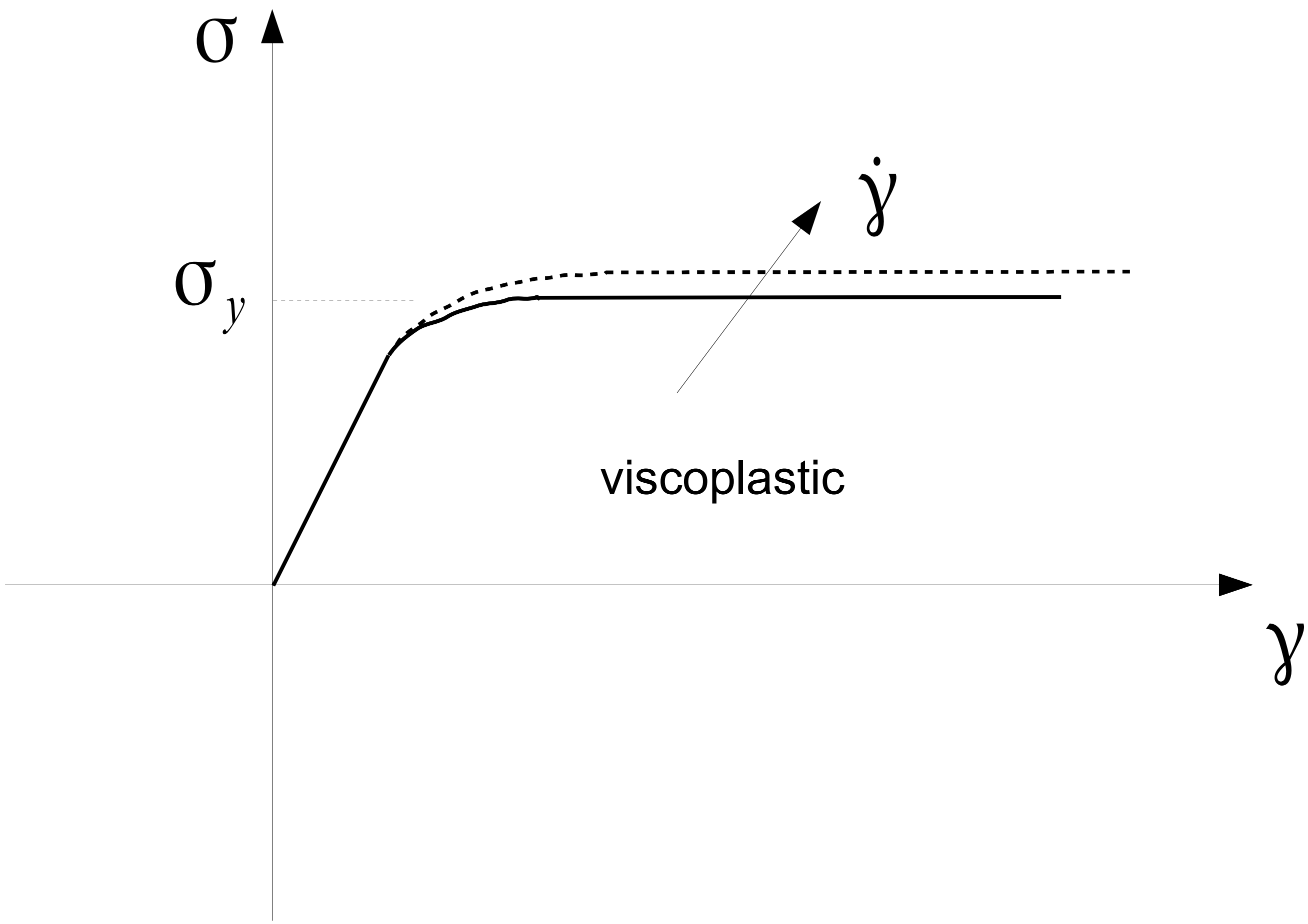


Hardening
- important for crystals
- ~ absent in amorphous solids

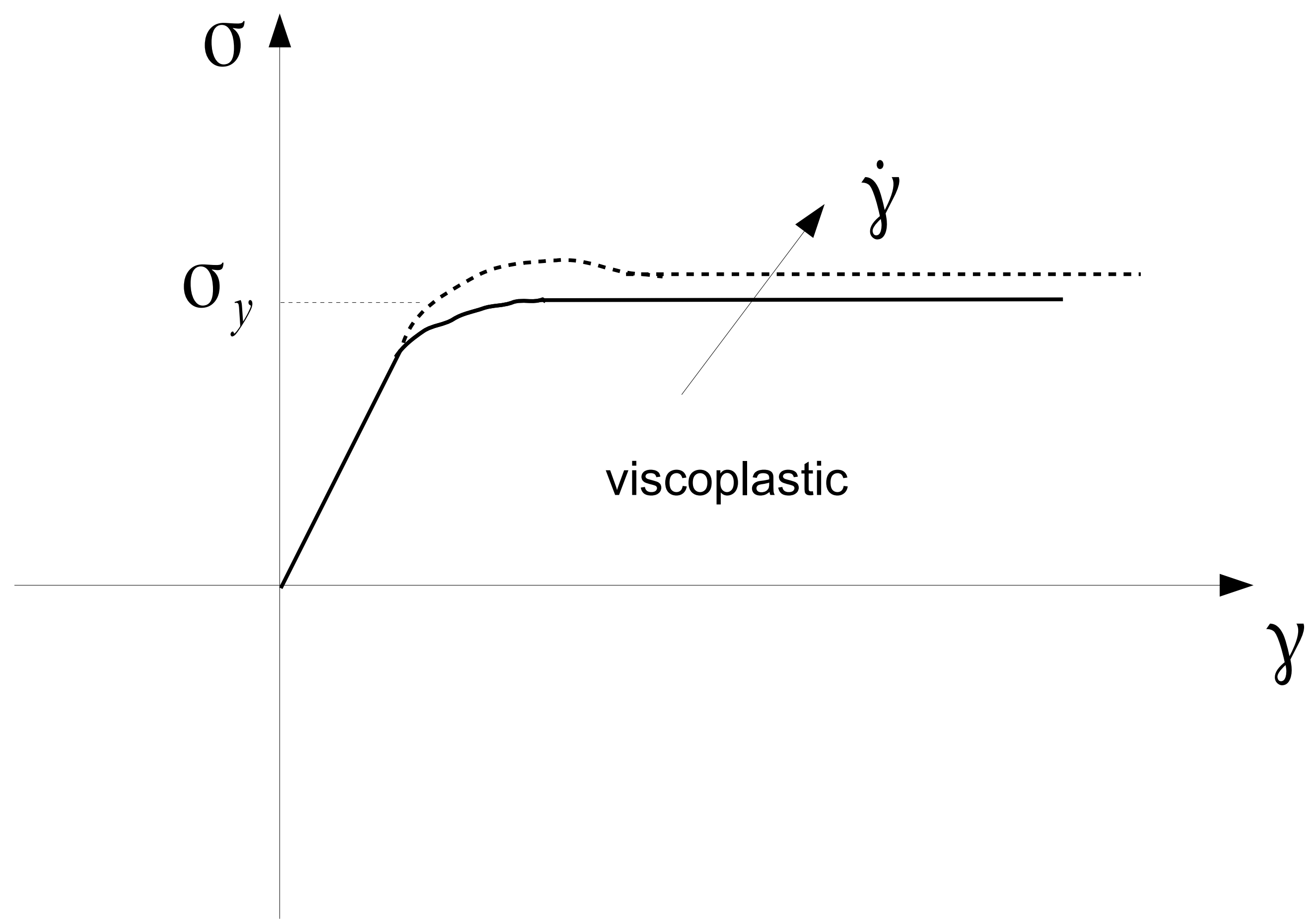
Departures from elastic-perfectly-plastic behavior



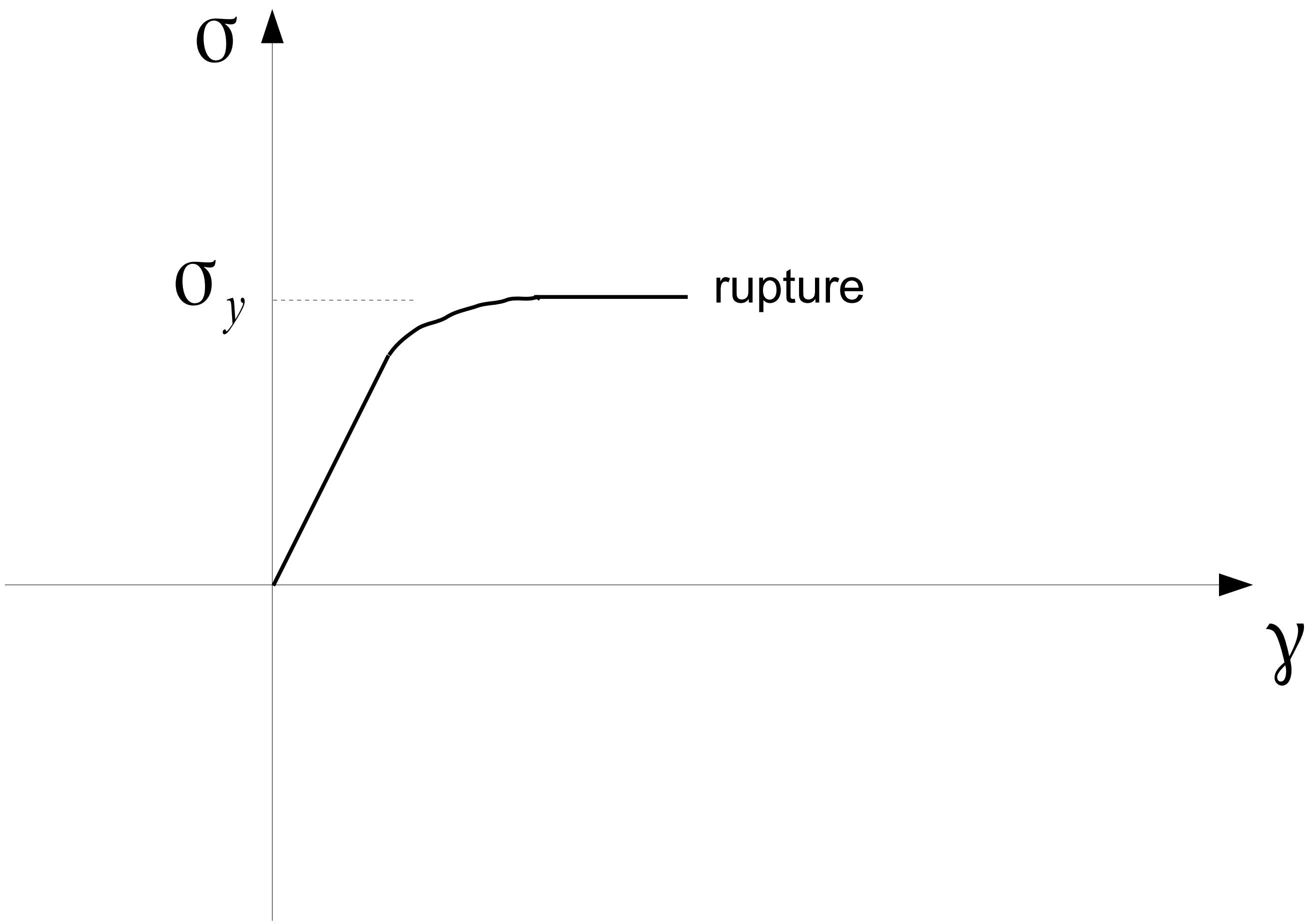
Departures from elastic-perfectly-plastic behavior



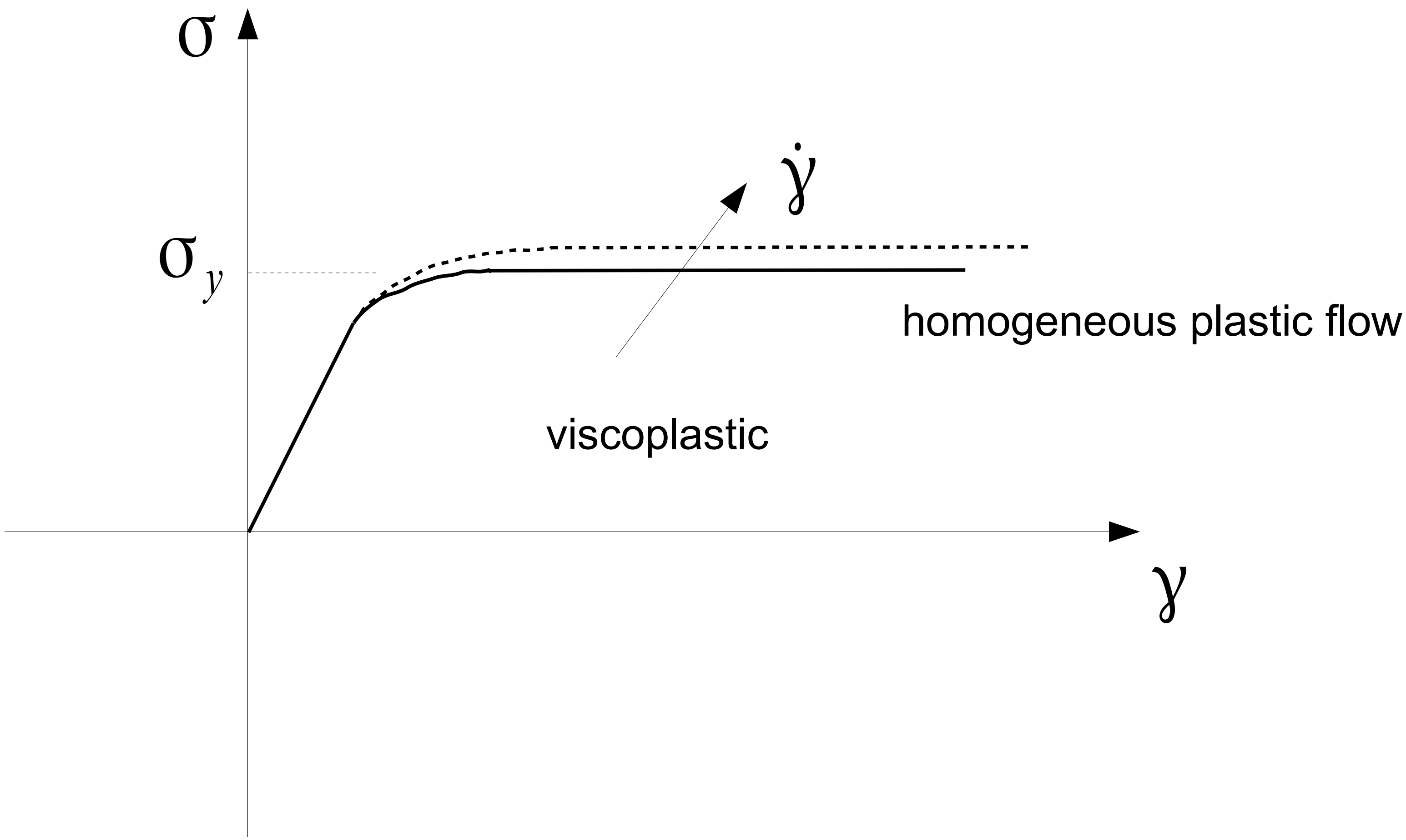
Departures from elastic-perfectly-plastic behavior



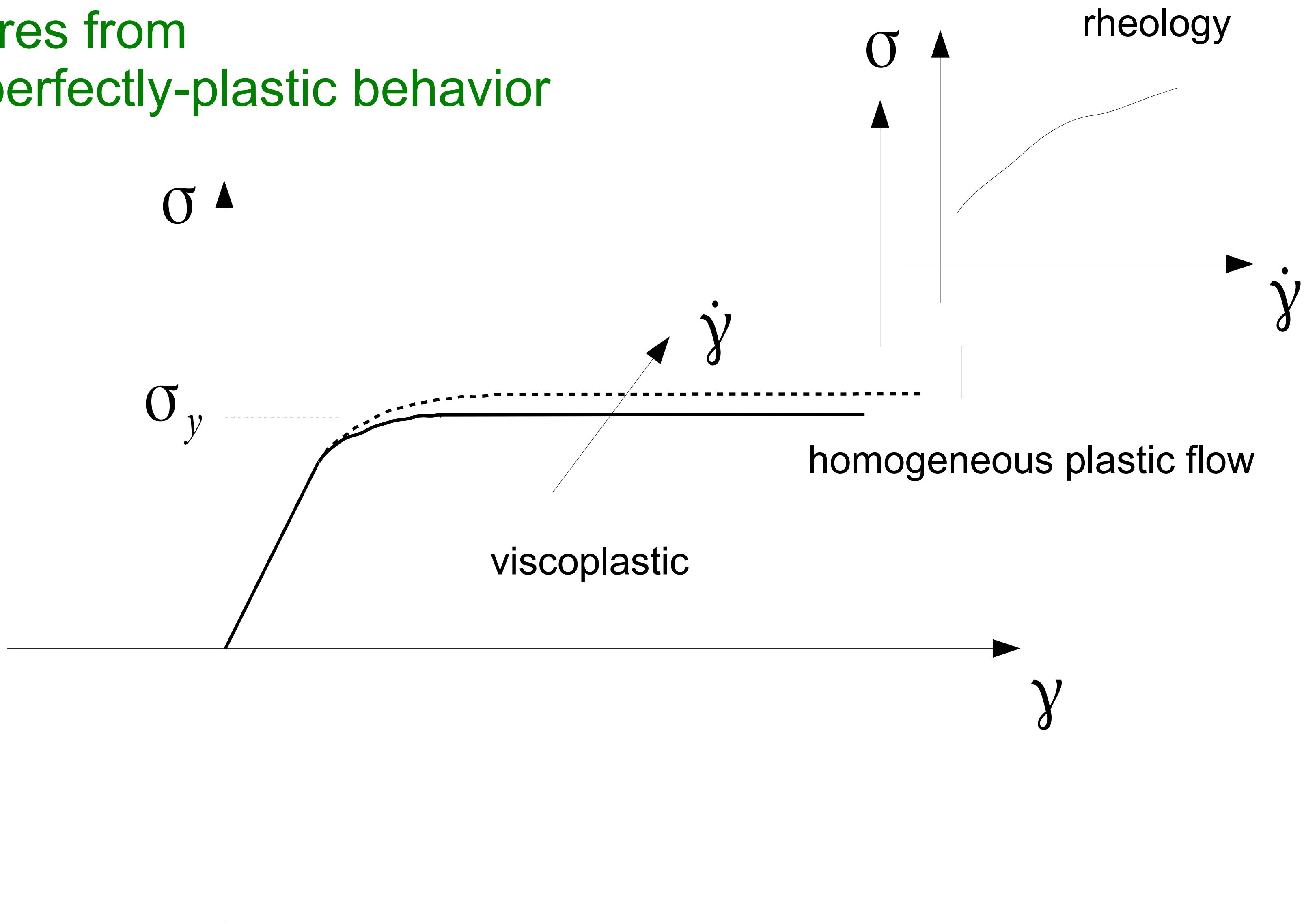
Departures from elastic-perfectly-plastic behavior

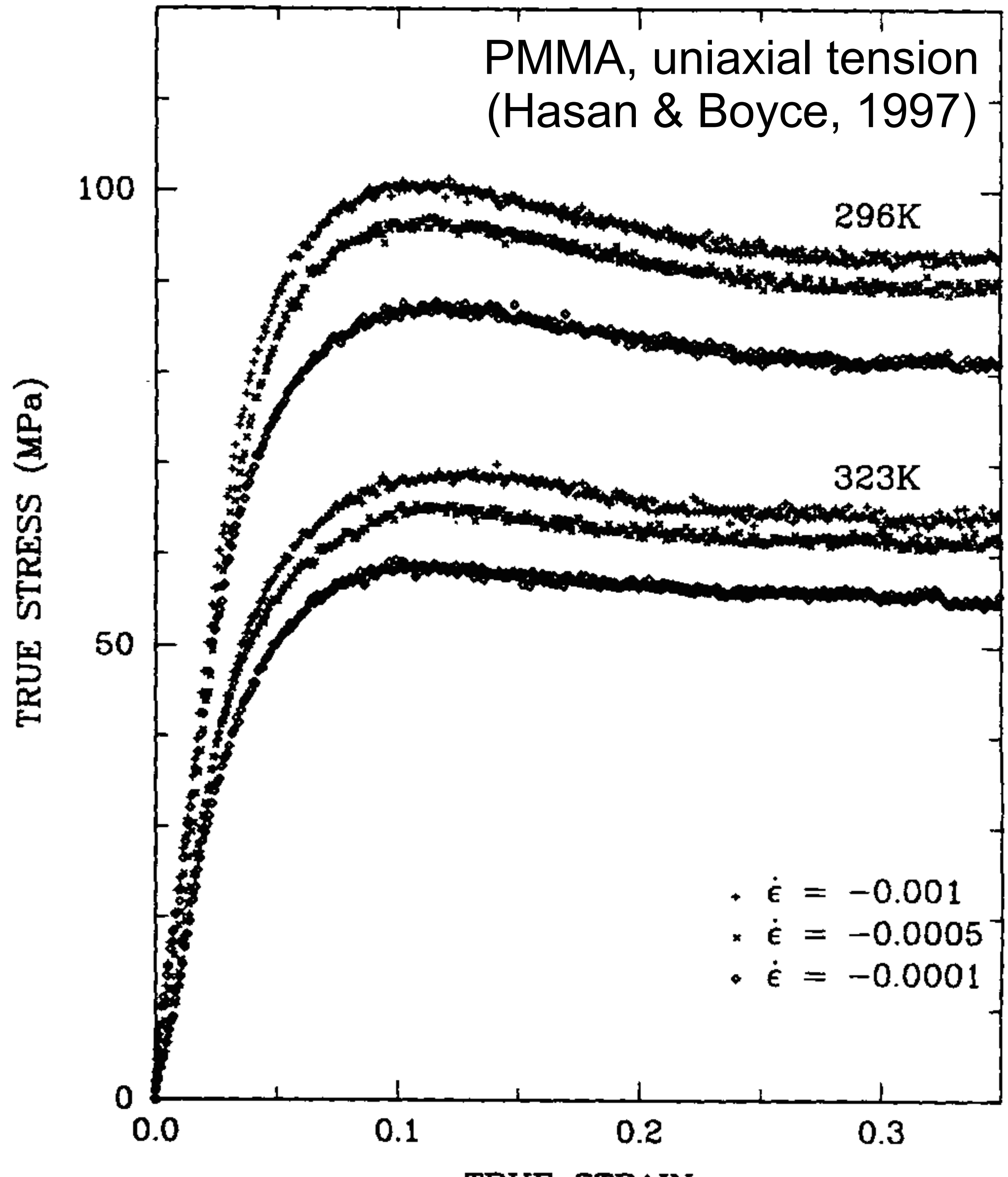


Departures from elastic-perfectly-plastic behavior

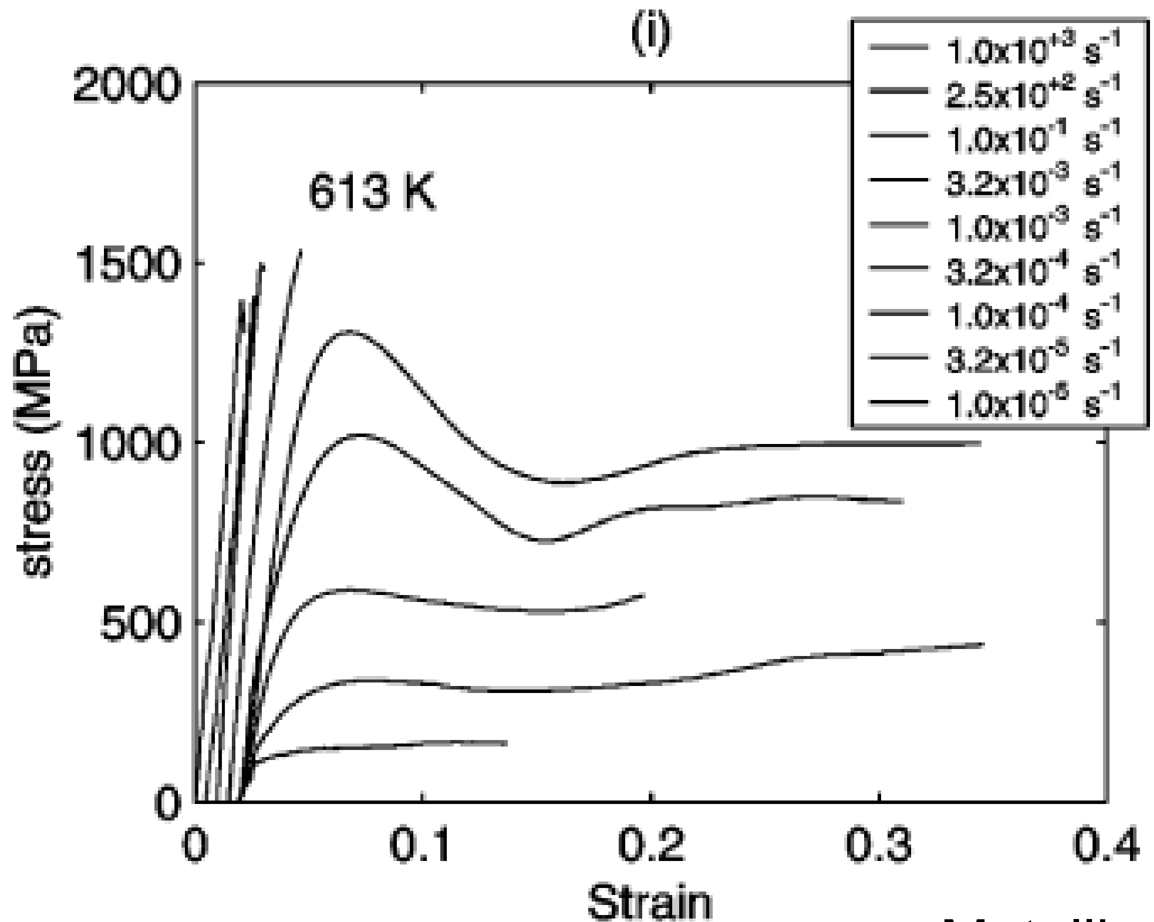


Departures from elastic-perfectly-plastic behavior

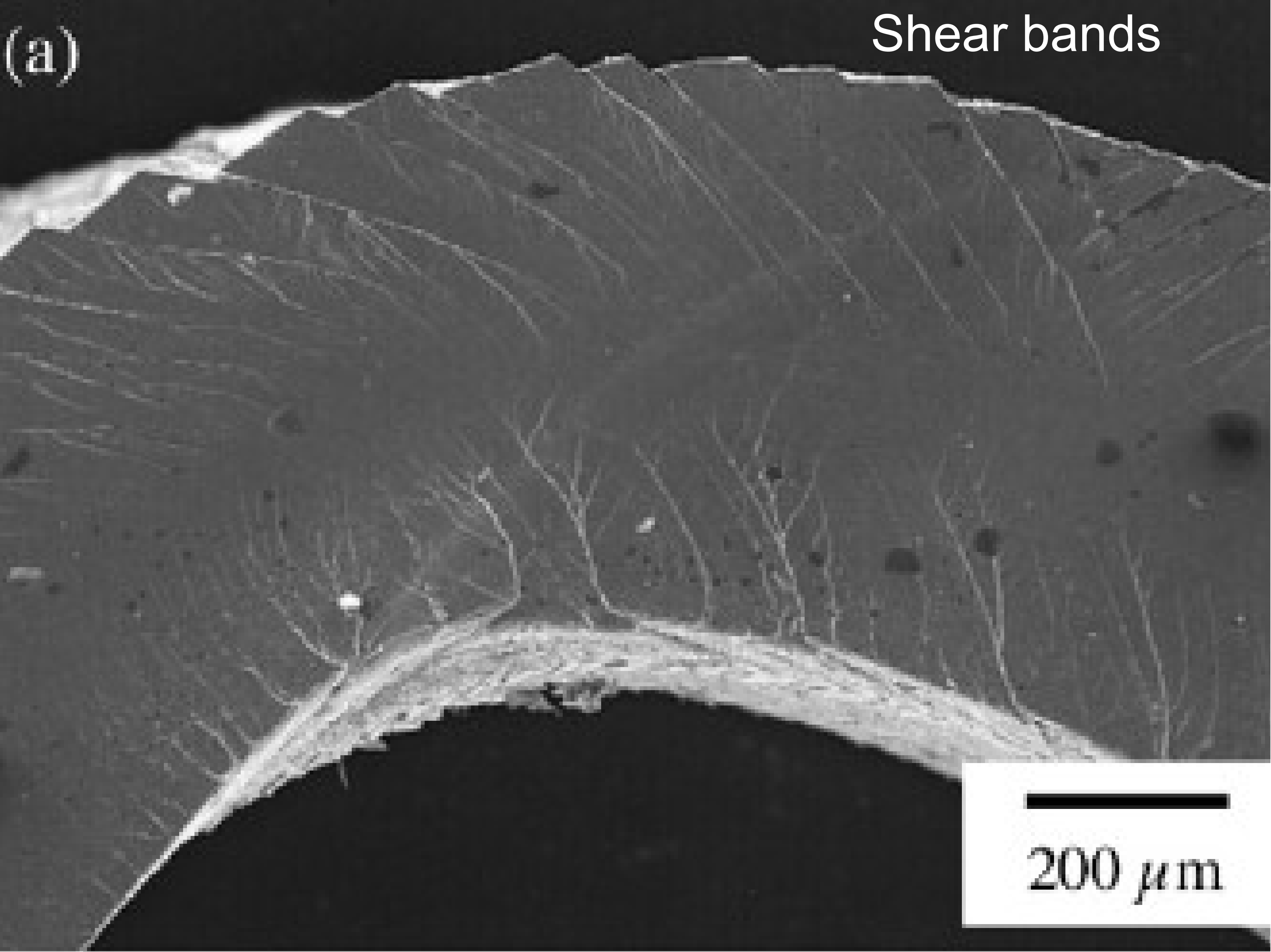



PMMA, uniaxial tension
(Hasan & Boyce, 1997)
TRUE STRESS (MPa)
TRUE STRAIN
0
50
100
0.0
0.1
0.2
0.3
296K
323K
+ $\dot{\epsilon}$ = −0.001
× $\dot{\epsilon}$ = −0.0005
◇ $\dot{\epsilon}$ = −0.0001

C

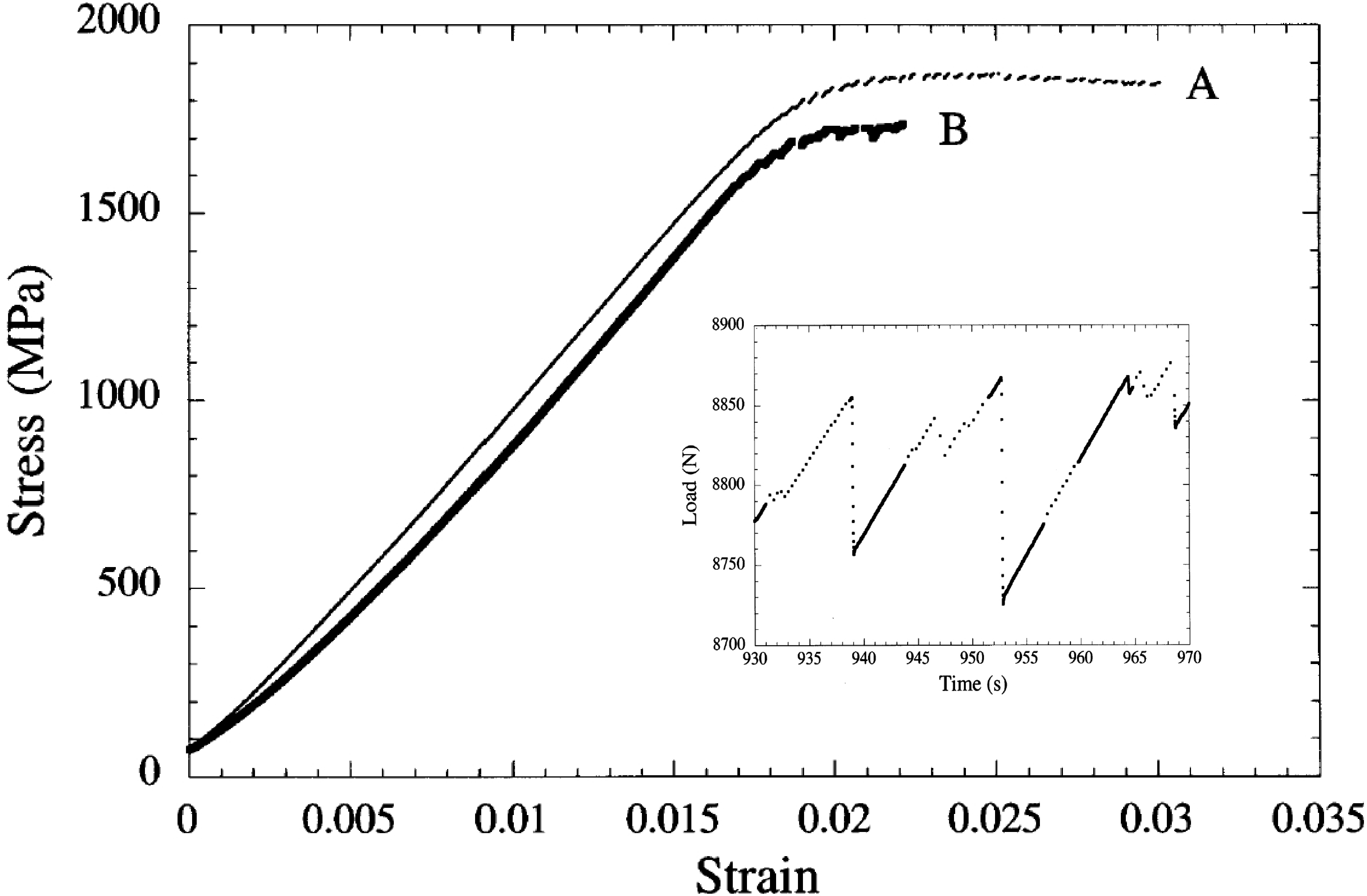


Metallic glass
(Johnson, Caltech)

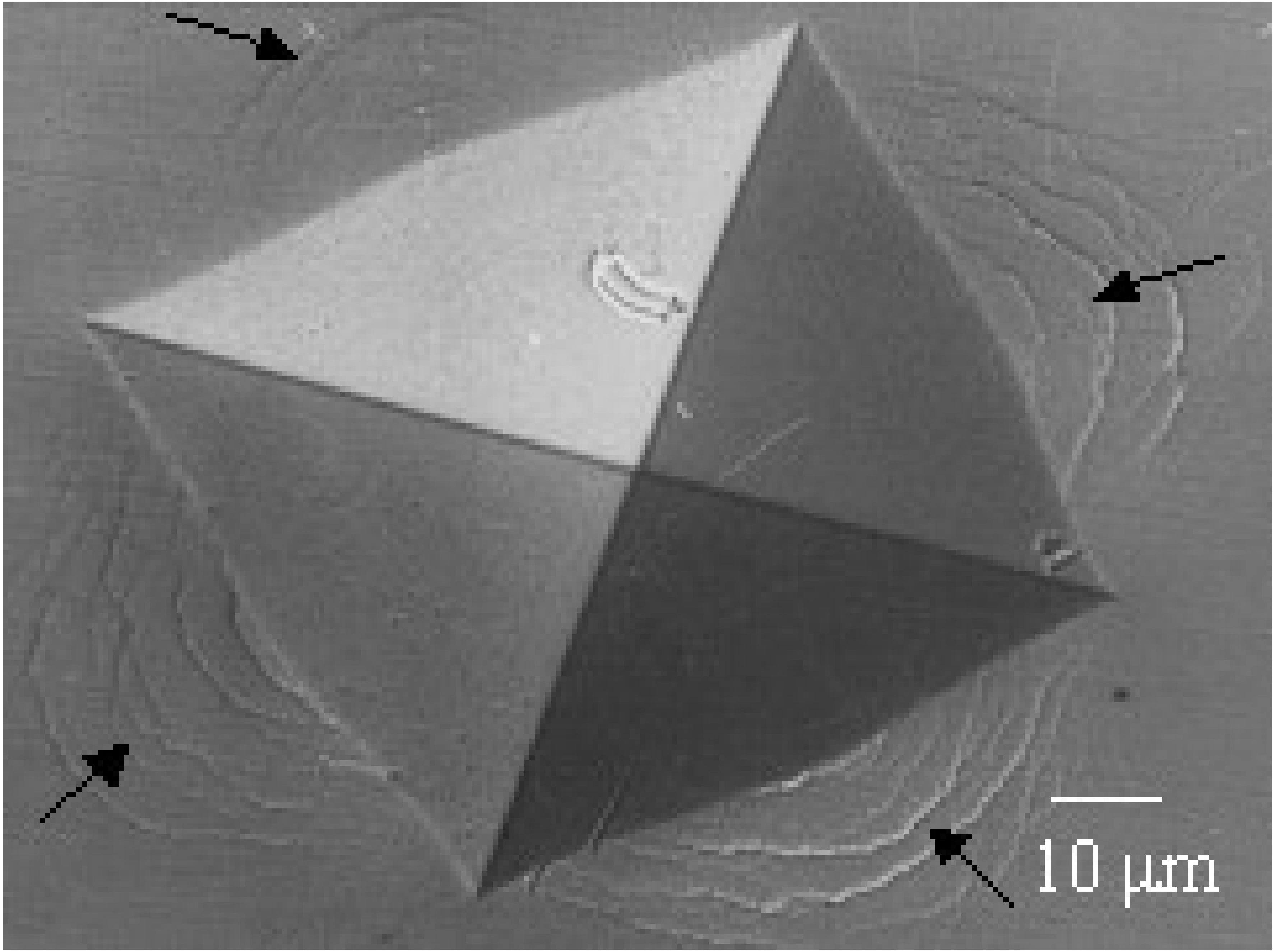

(a)
Shear bands
200 μm

Heating?

Fig. 5. Scanning electron micrograph of the fracture surface of a $Pd_{40}Ni_{40}P_{20}$ sample failed in uniaxial compression.

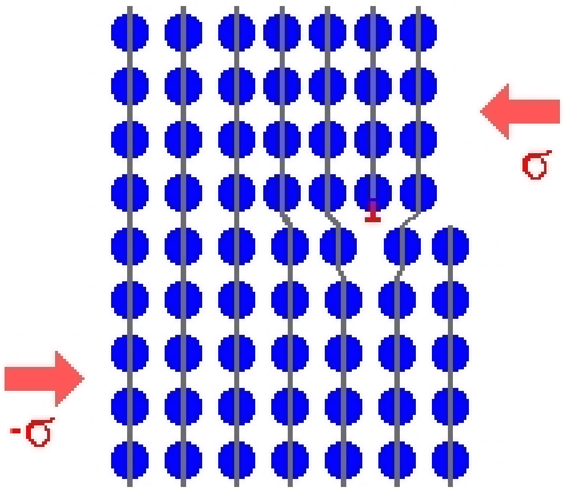


Stress (MPa)
2000
1500
1000
500
0
Strain
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035
A
B
Load (N)
8900
8850
8800
8750
8700
Time (s)
930
935
940
945
950
955
960
965
970


10 µm

In crystals

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



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

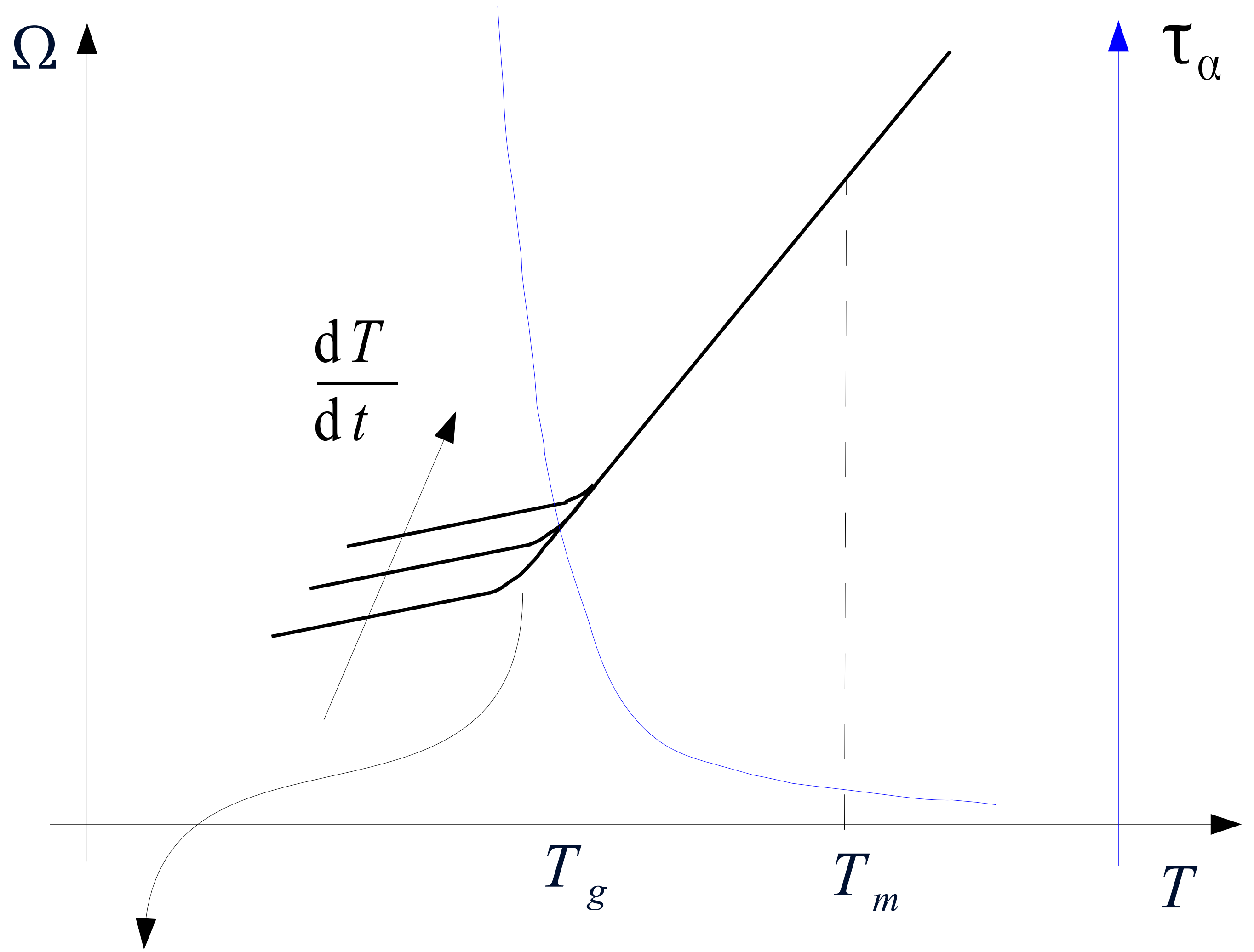
Dislocation dynamics in computer codes since the 1980's

In disordered materials

No topological order => defects?

?

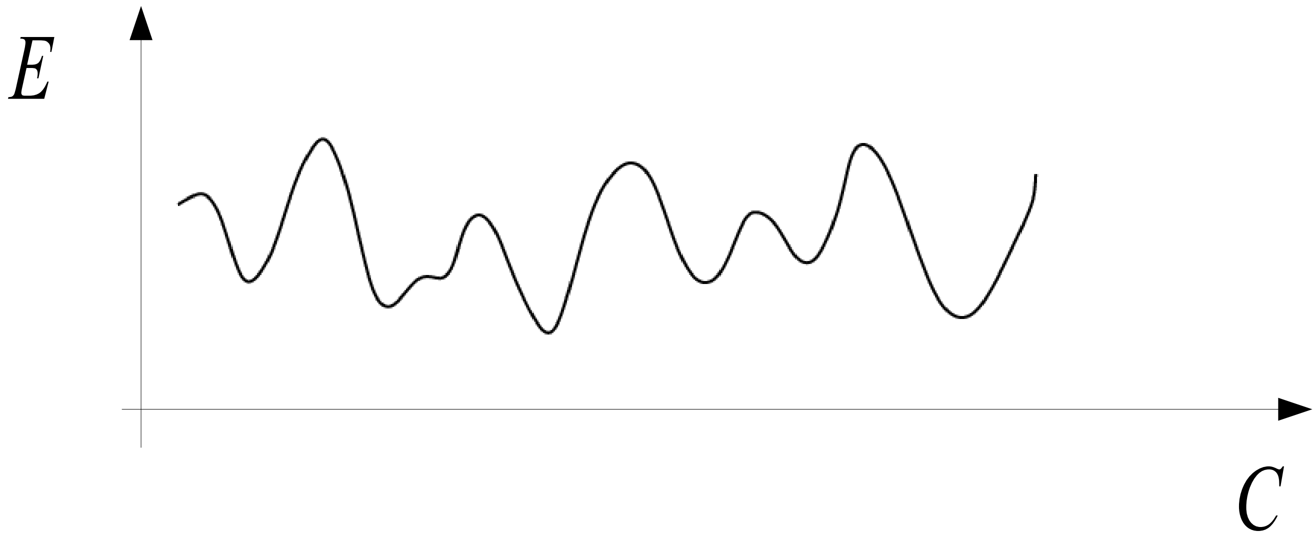
The glass transition



slow down of relaxation dynamics

The potential energy landscape picture

Goldstein (1969)
Stillinger & Weber (1982)



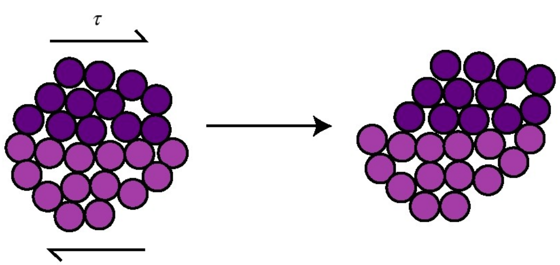
high T: relaxation = hopping among local minima (inherent states)

low T: glass = the system is trapped in IS

What are the elementary mechanisms of deformation in amorphous solids?

Argon (1979):

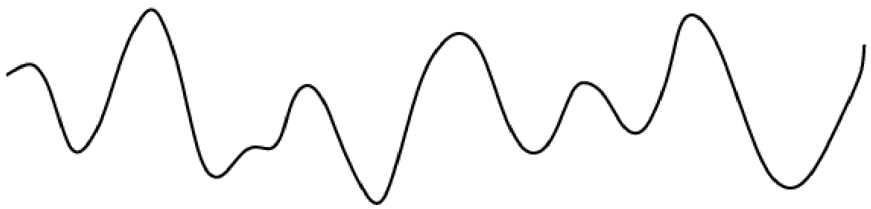
local shear transformations



= flips

In real space

stress-induced
hopping among inherent states



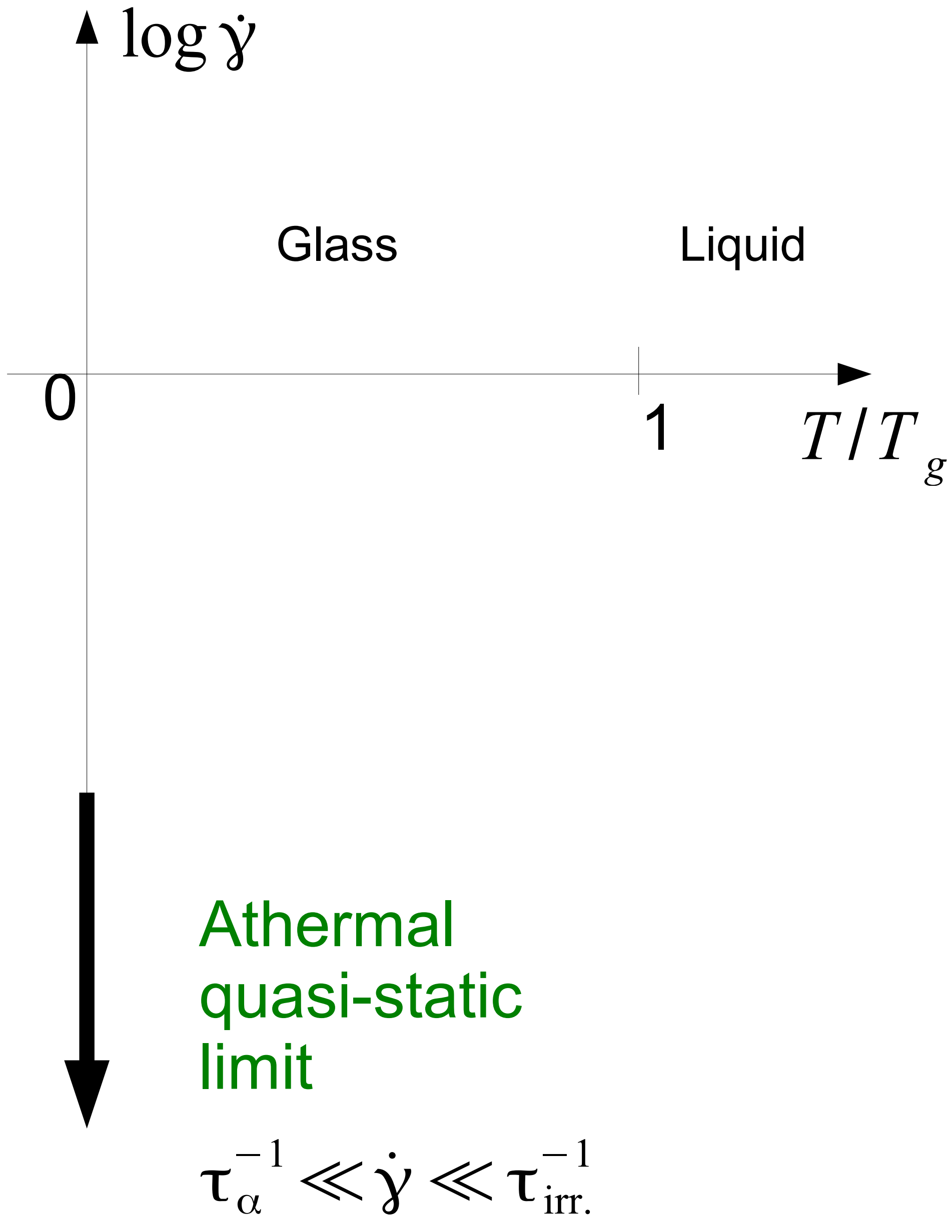
In PEL

When a glass is sheared...

<u>Low temperature:</u> $T < T_g$

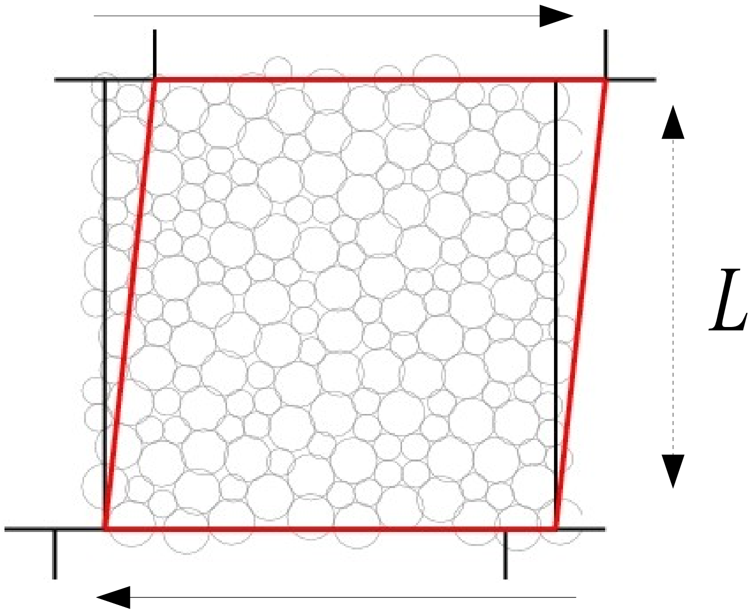
$$\tau_\alpha \gg 1/\dot{\gamma}$$

Neglect any thermally activated process



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

The system resides at all times in
local energy minima



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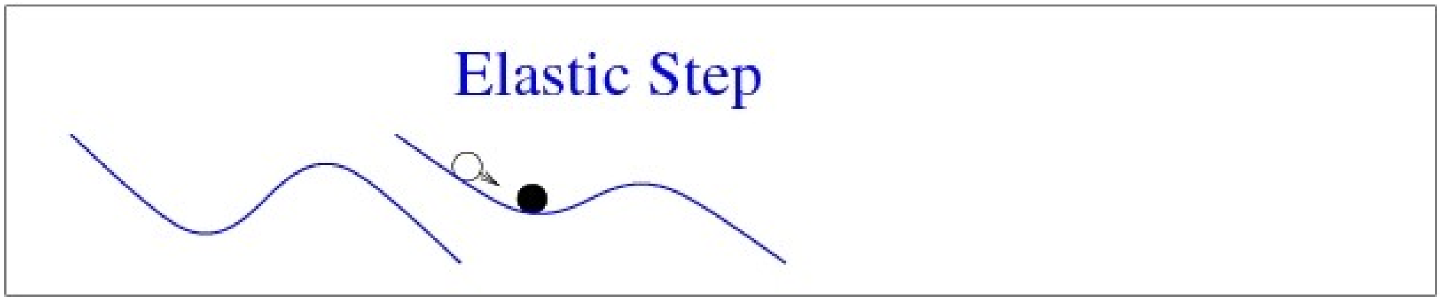
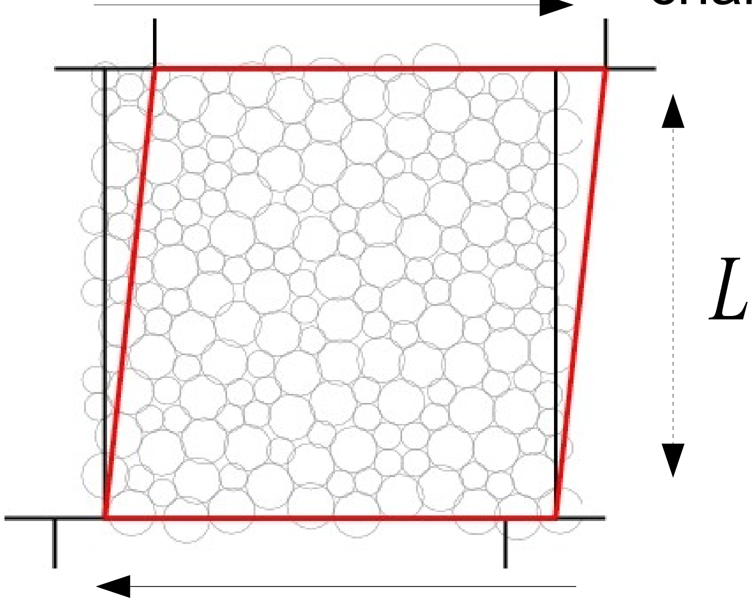


The system resides at all times in local energy minima

It track reversibly strain-induced changes in minima



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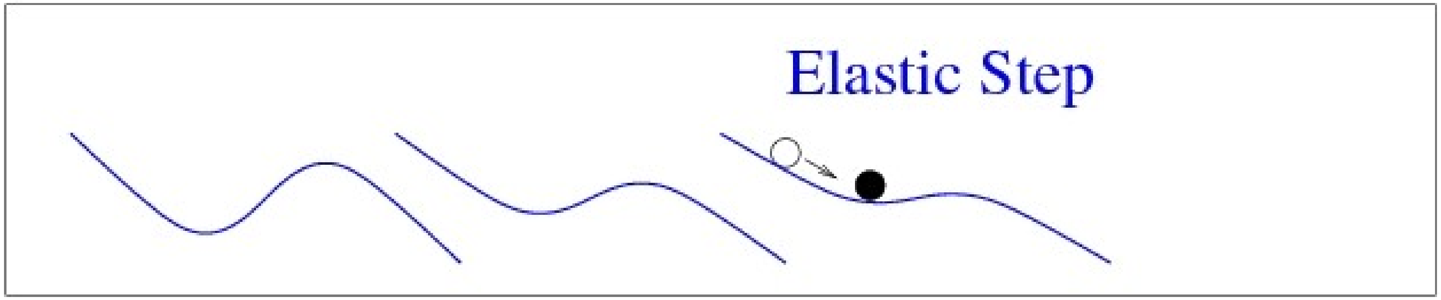

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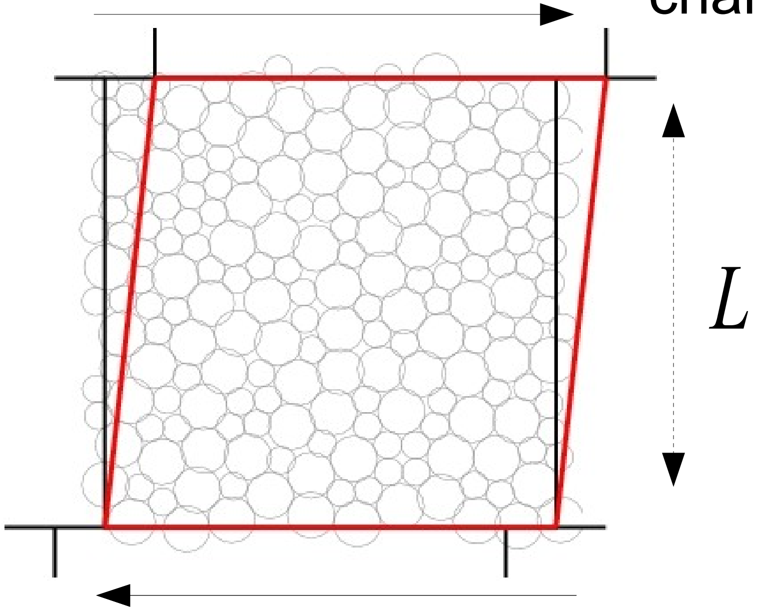
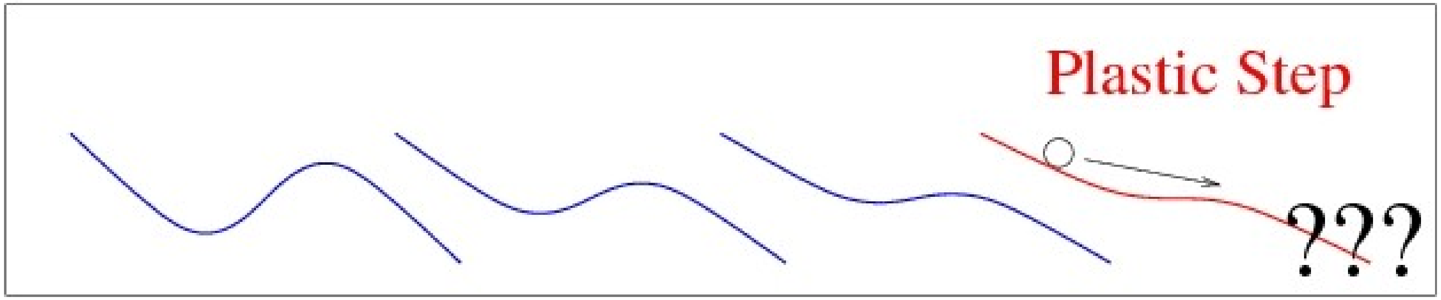


Plasticity in a low-T (finite-sized) glass:



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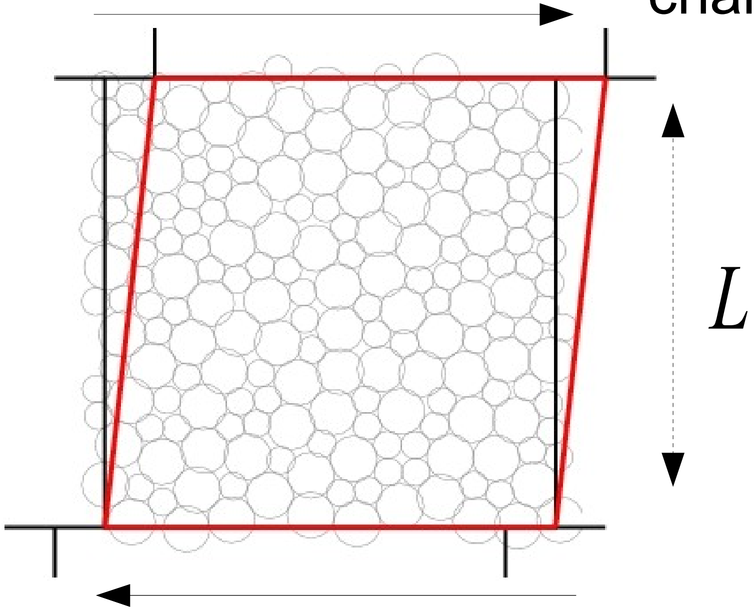


Occasionally the occupied minimum becomes unstable:

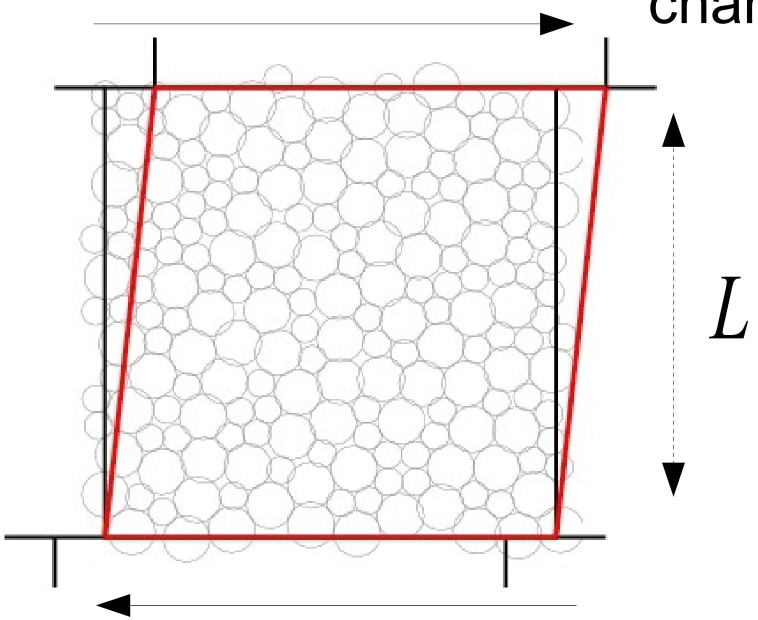
A plastic event then occurs leading to a new local minimum

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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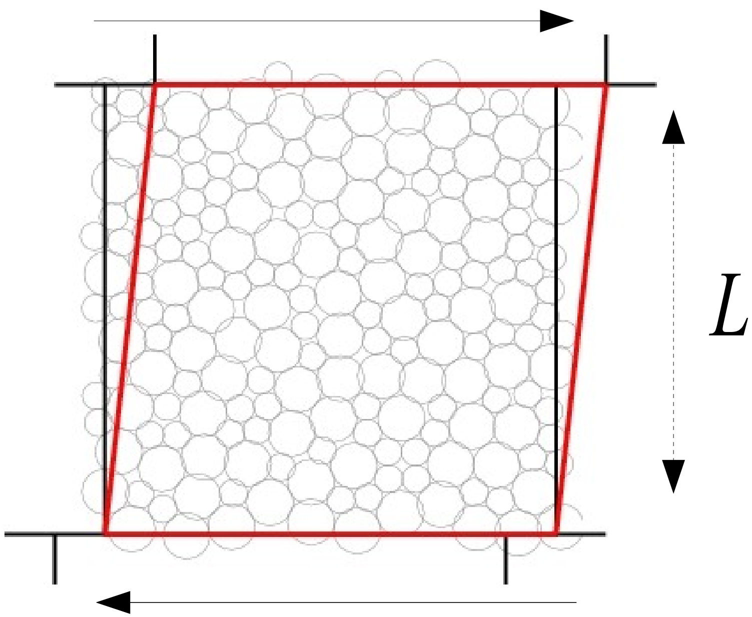
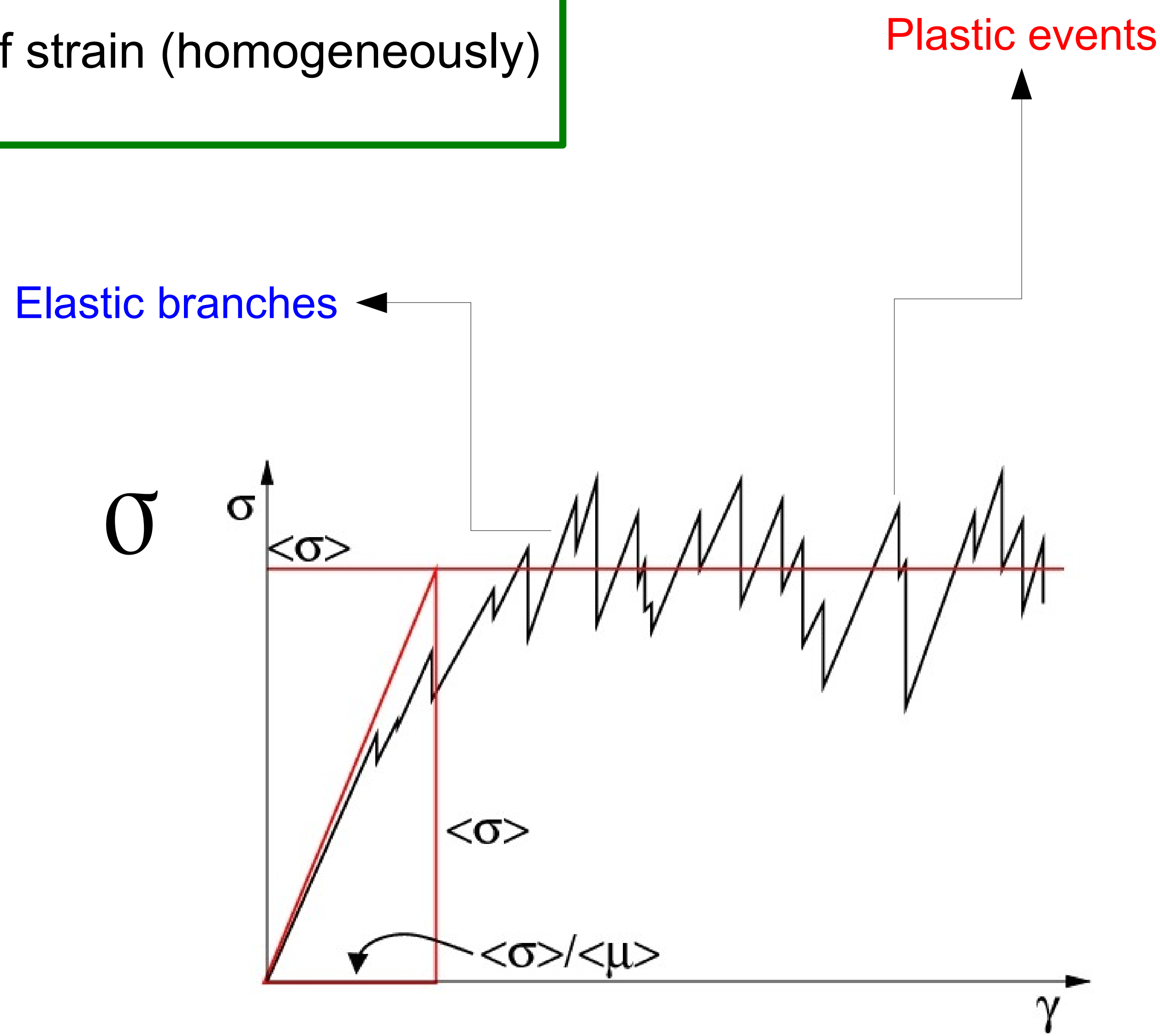
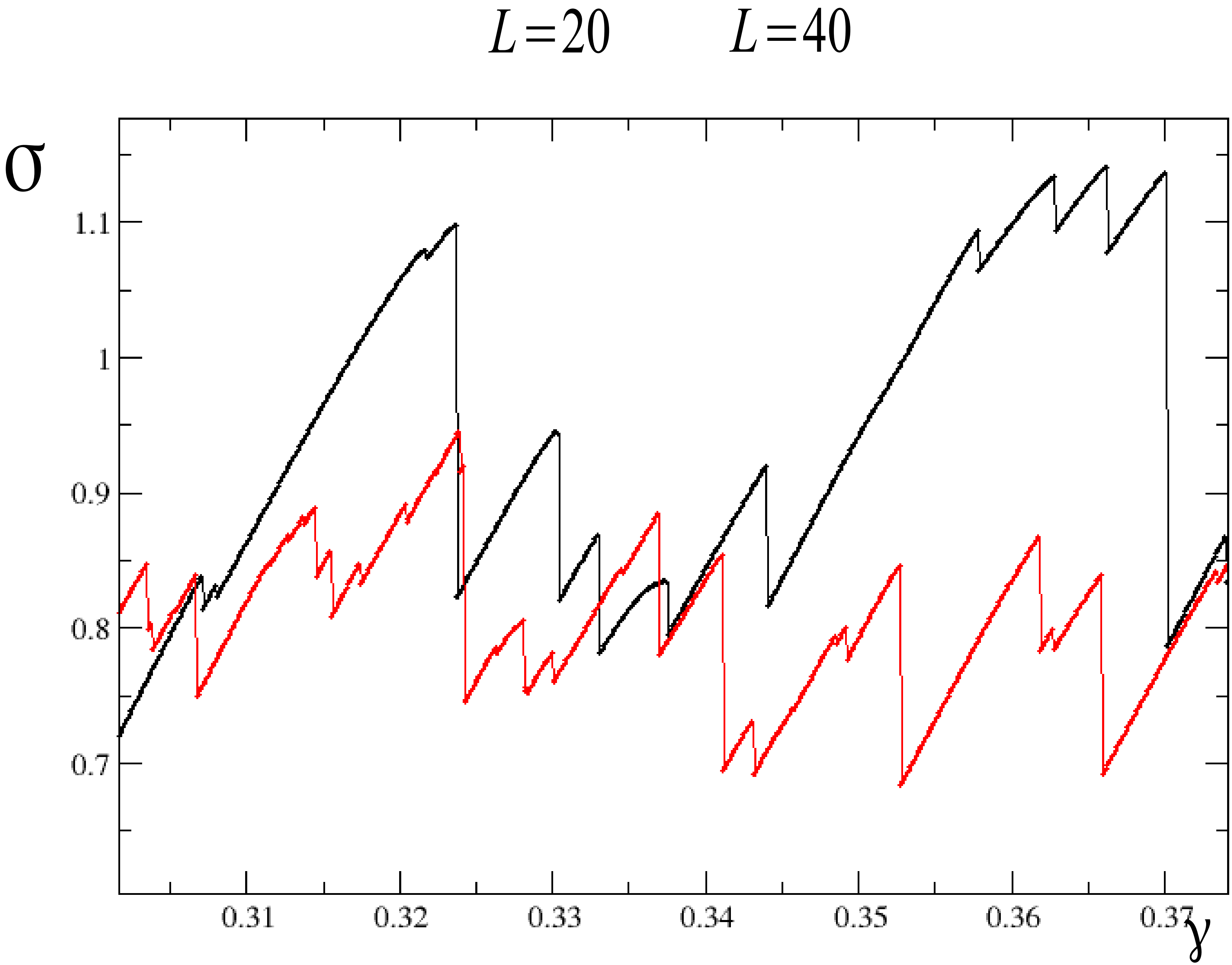
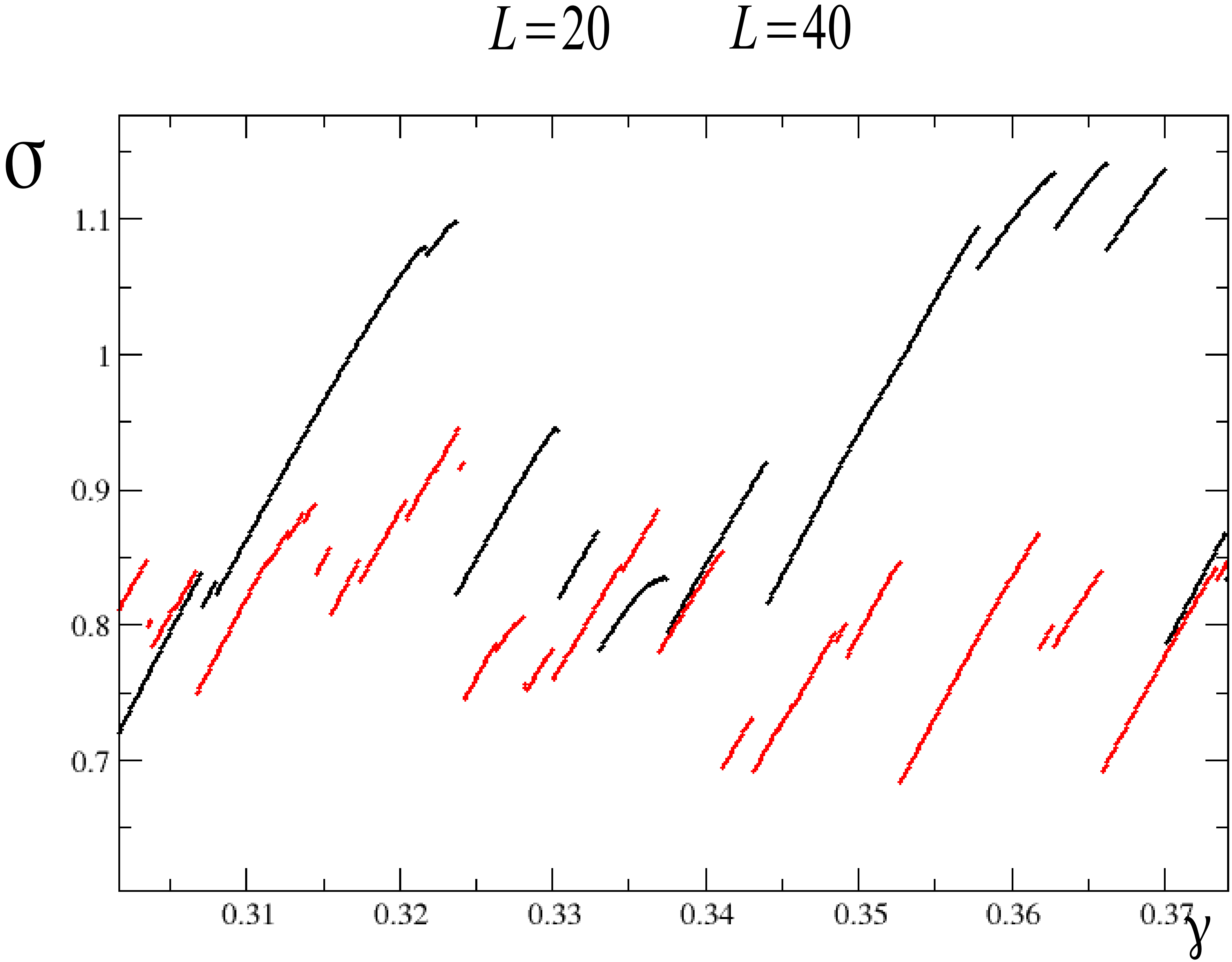






L=20
L=40
σ
1.1
1
0.9
0.8
0.7
0.31
0.32
0.33
0.34
0.35
0.36
0.37
γ



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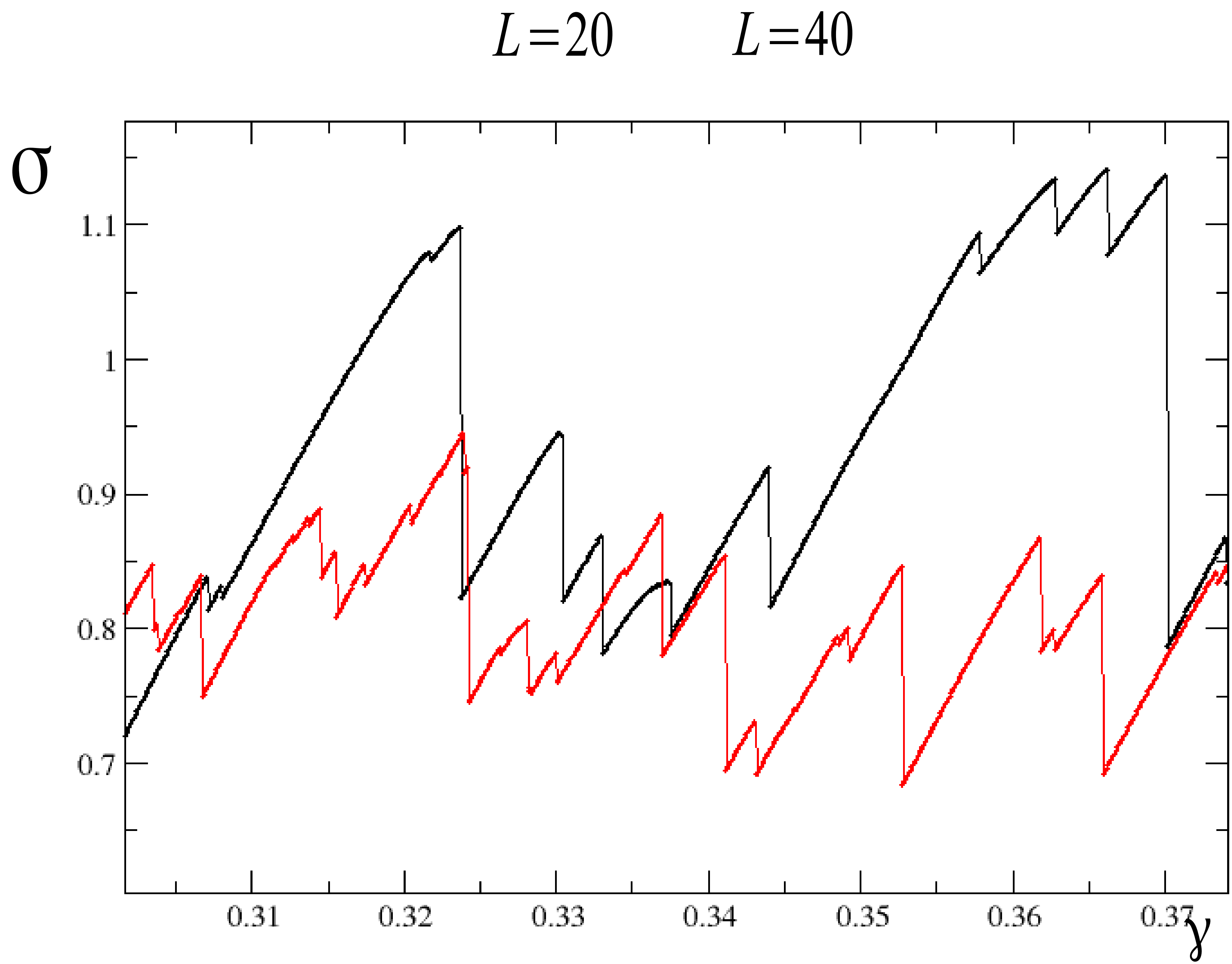
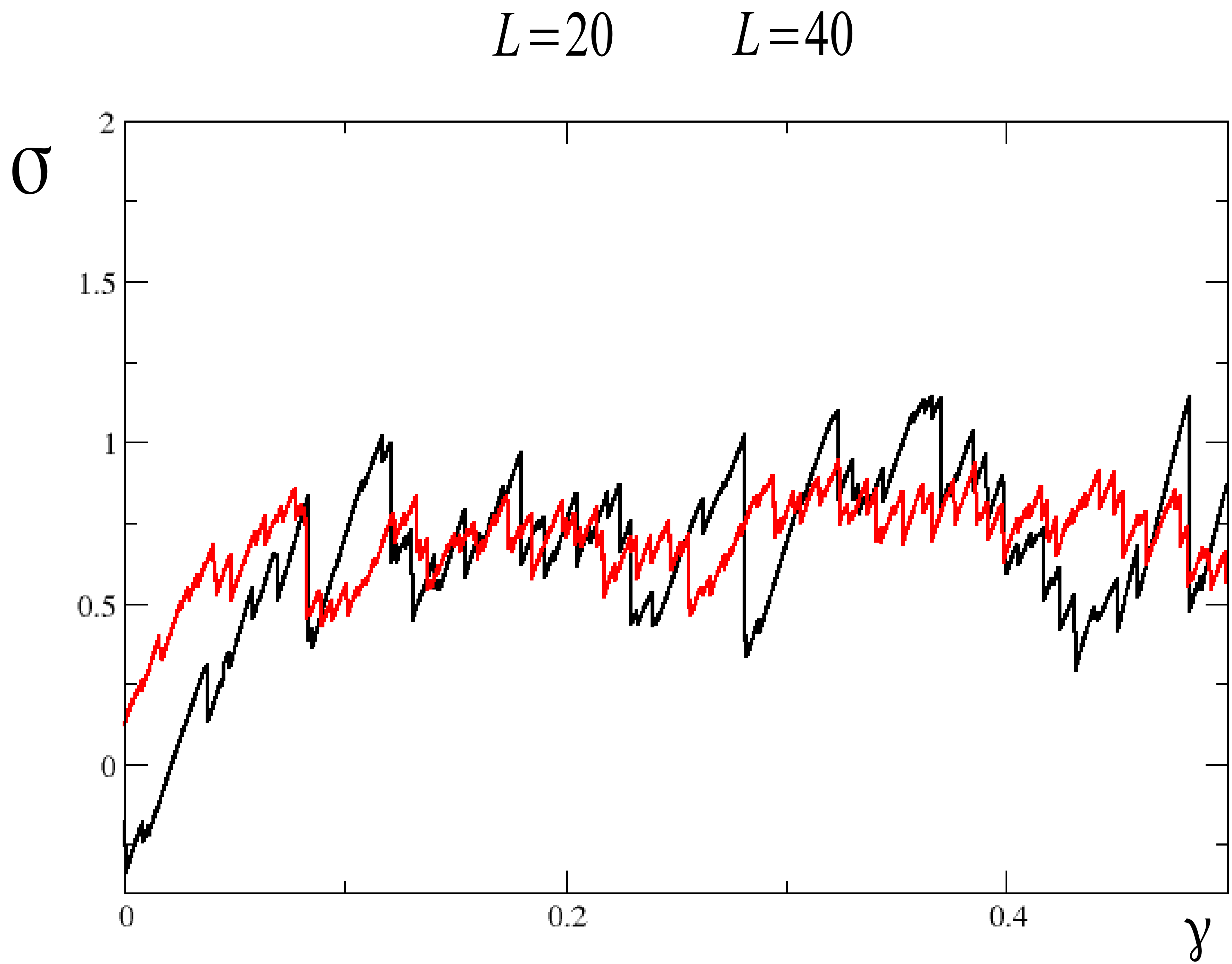
0.35
0.36
0.37
γ

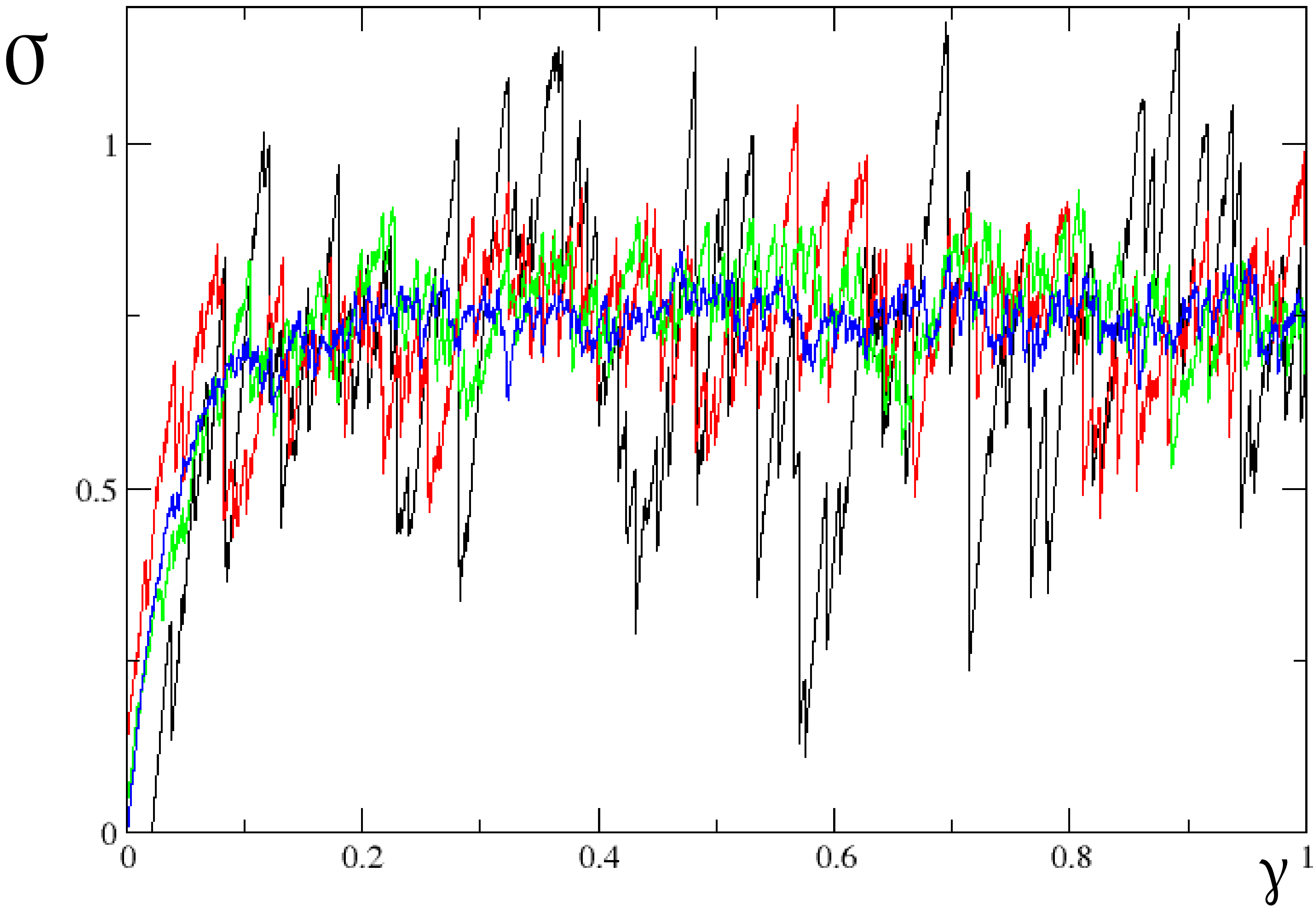


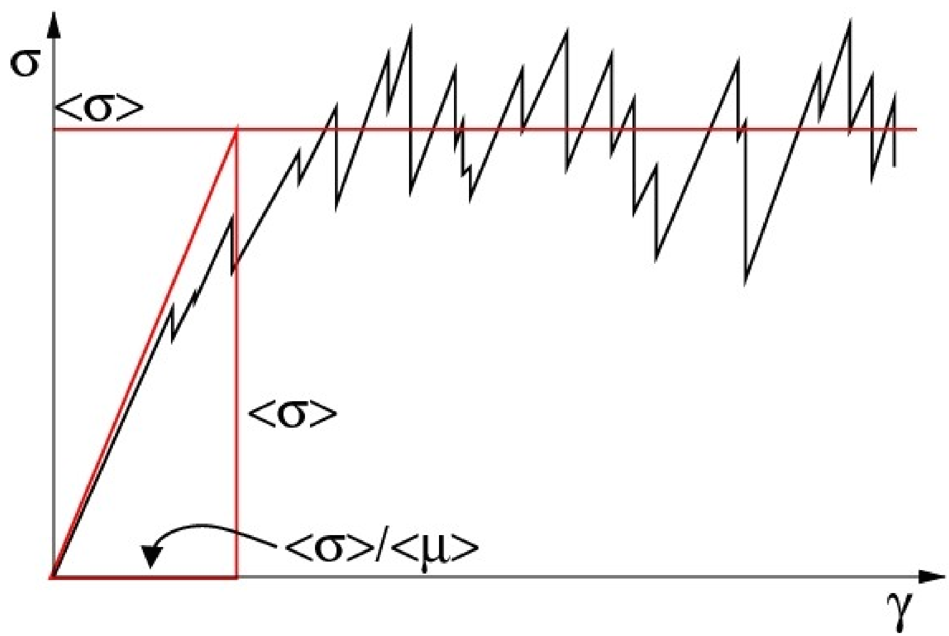
L=20 L=40
σ
1.1
1
0.9
0.8
0.7
0.31
0.32
0.33
0.34
0.35
0.36
0.37
γ



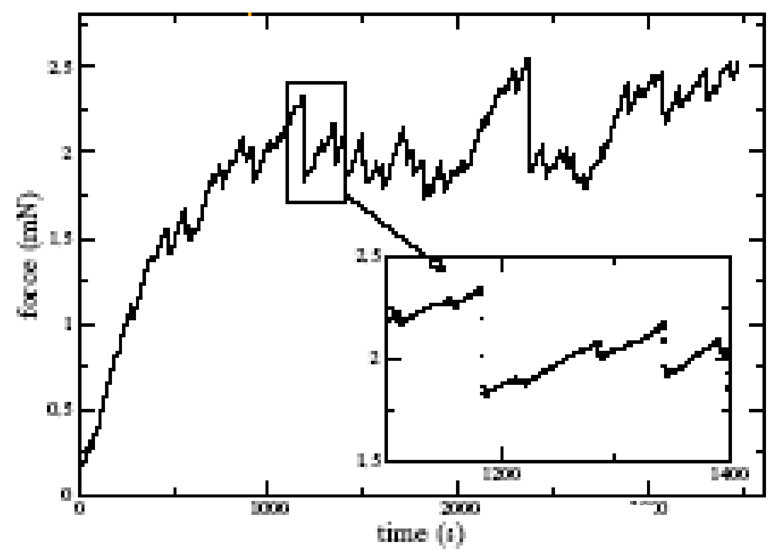
L = 20
L = 40
σ
2
1.5
1
0.5
0
0
0.2
0.4
γ

$L = 20,40,80,160$

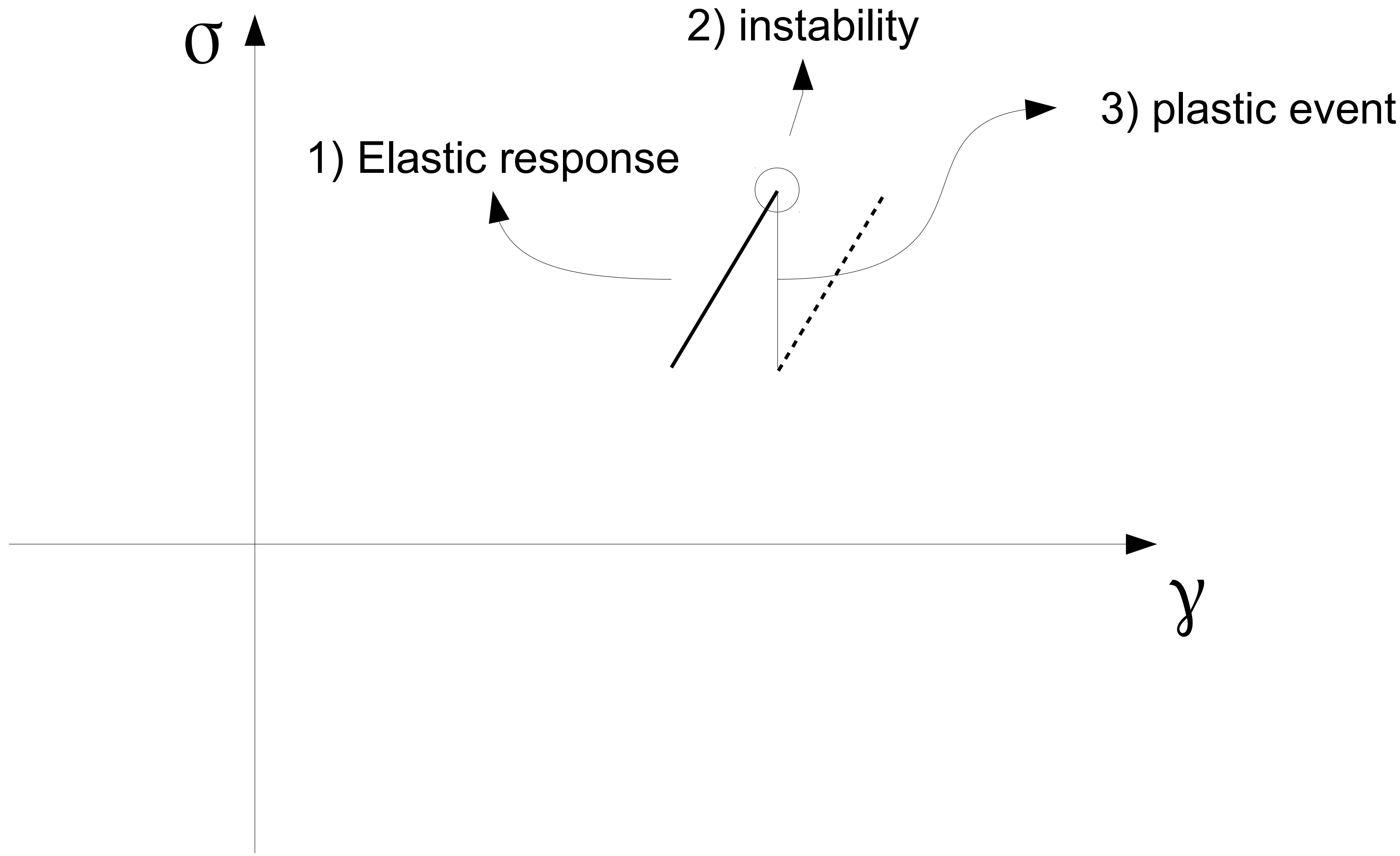




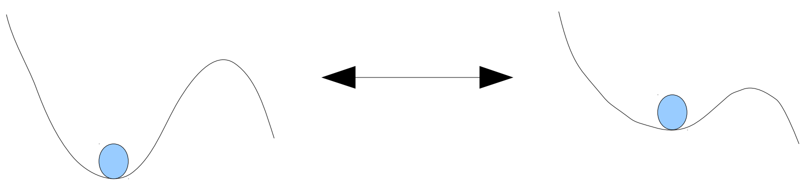
I. Cantat, O. Pitois, Phys. Fluids (2006)



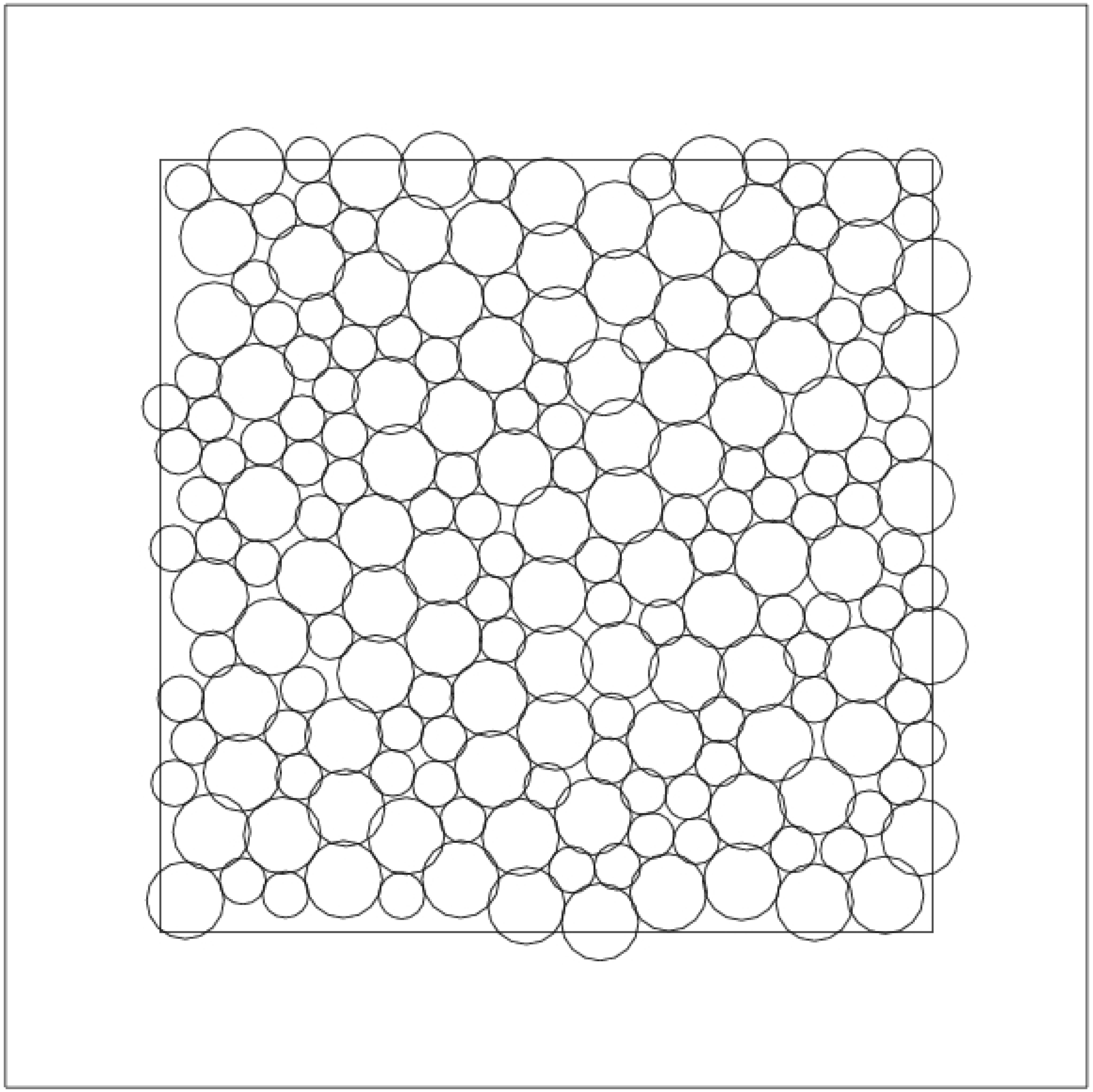
Life and death,... and birth of an elastic branch



1) Elastic response



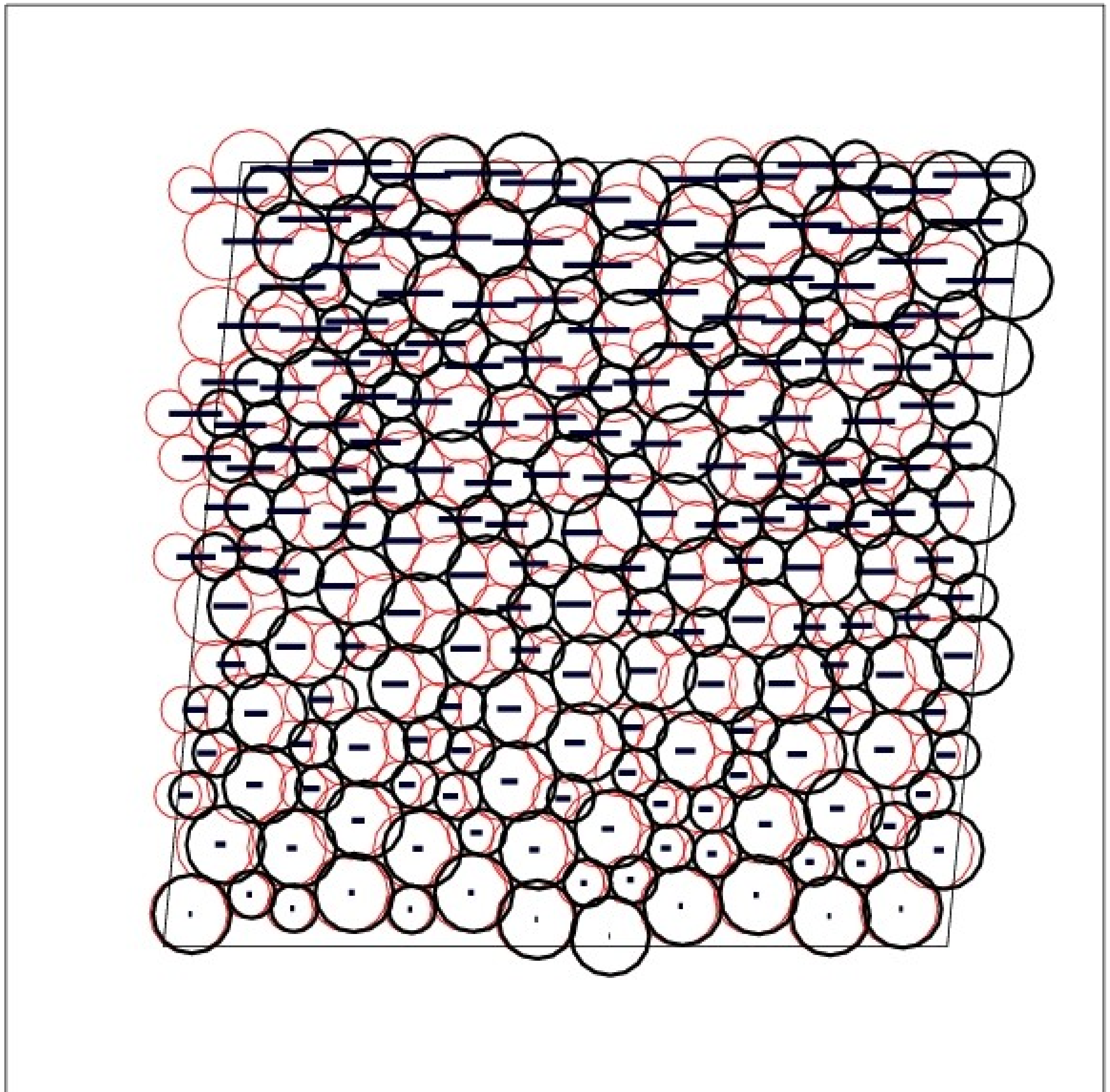
Subject a T=0 amorphous system to homogeneous deformation



γ_0

$\underline{r}_i(\gamma_0)$

Subject a T=0 amorphous system to homogeneous deformation

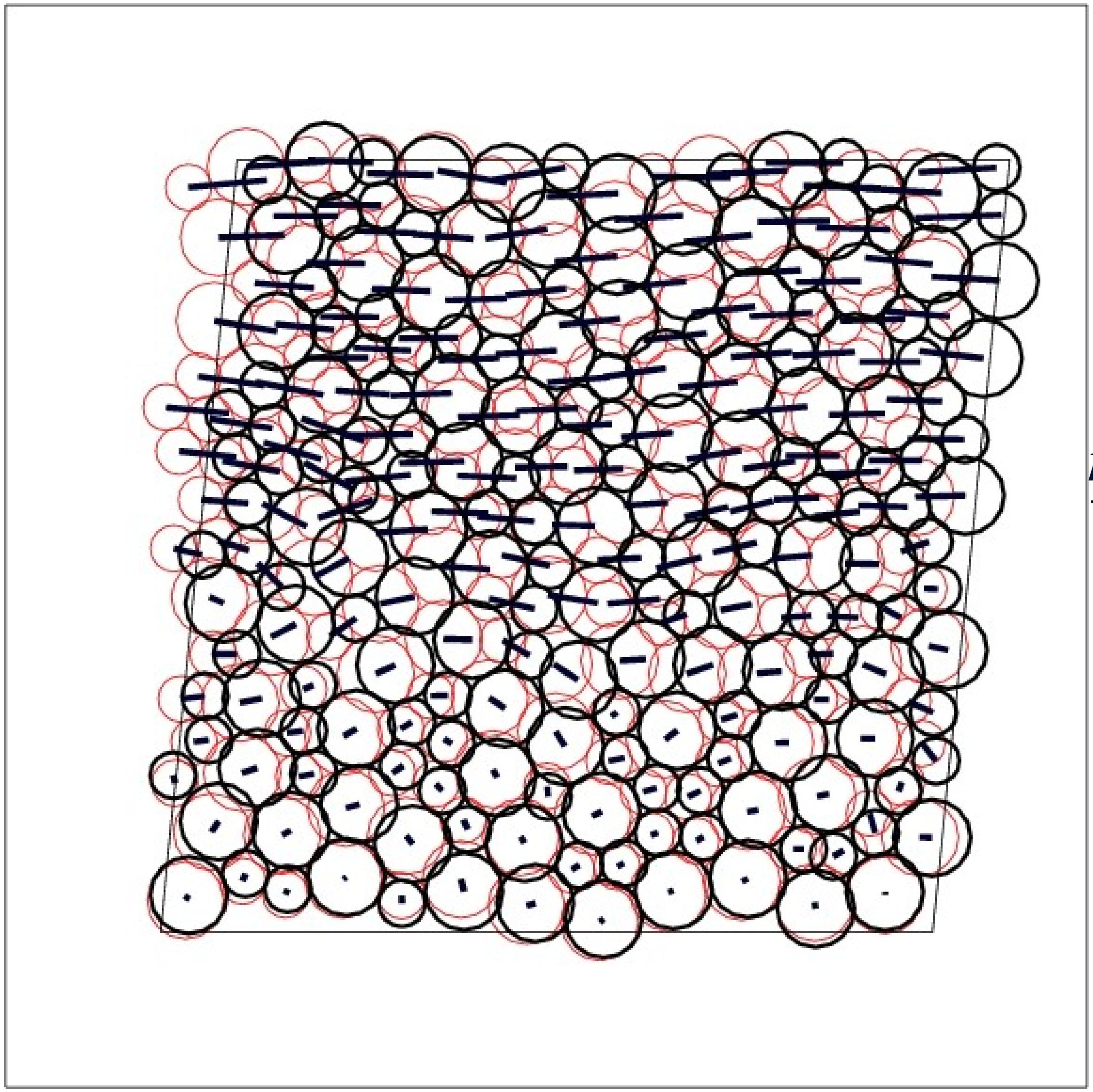


γ_1

$\underline{\underline{F}}.\underline{r}_i(\gamma_0)$

Subject a T=0 amorphous system to homogeneous deformation

Non-affine displacements

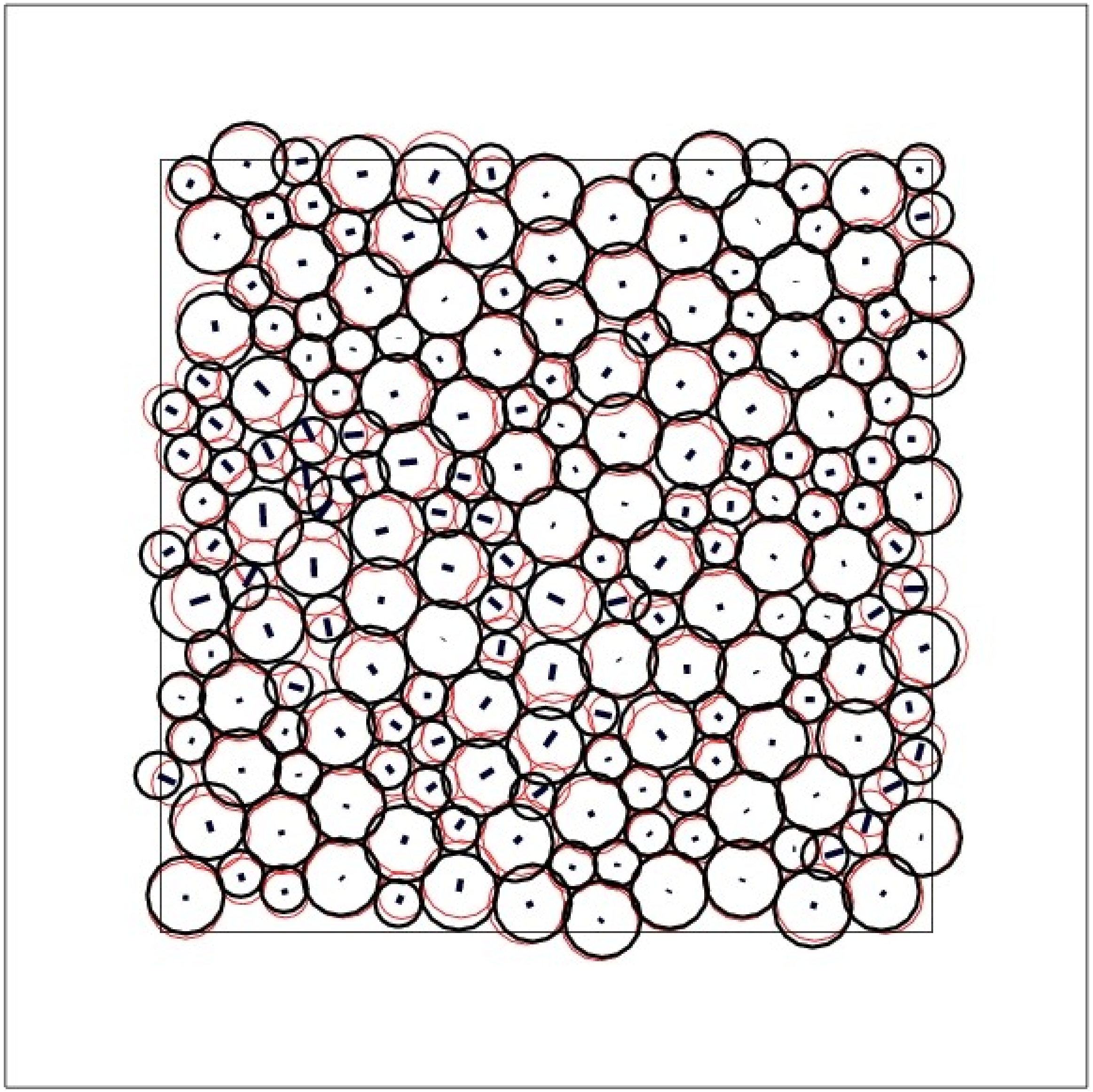


γ_1

$$\underline{r_i}(\gamma_1) \neq \underline{\underline{F}}.\underline{r_i}(\gamma_0)$$

Subject a T=0 amorphous system to homogeneous deformation

Non-affine displacements

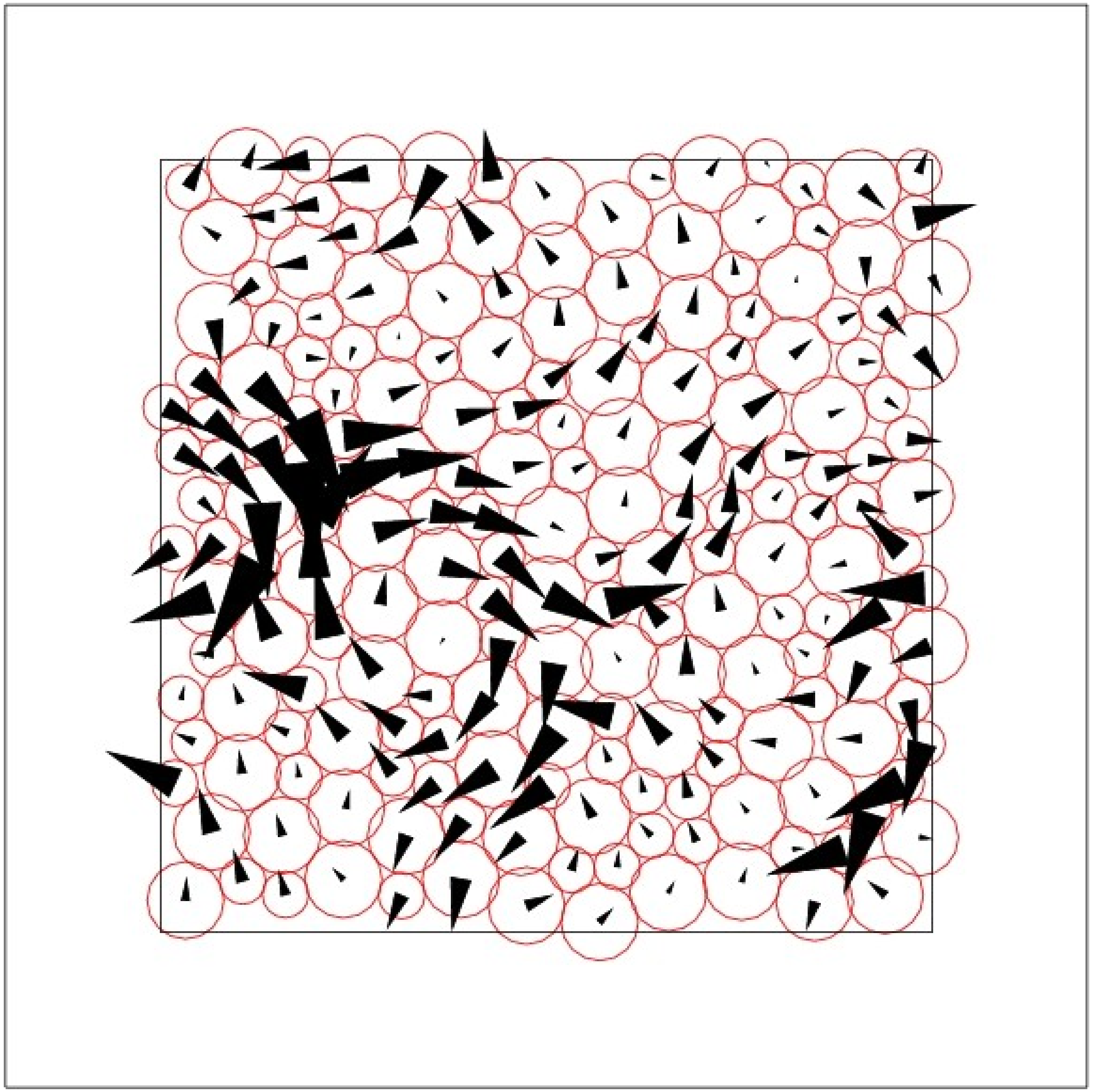


γ_1

$\underline{\underline{F}}^{-1} \cdot \underline{r}_i(\gamma_1)$

Subject a T=0 amorphous system to homogeneous deformation

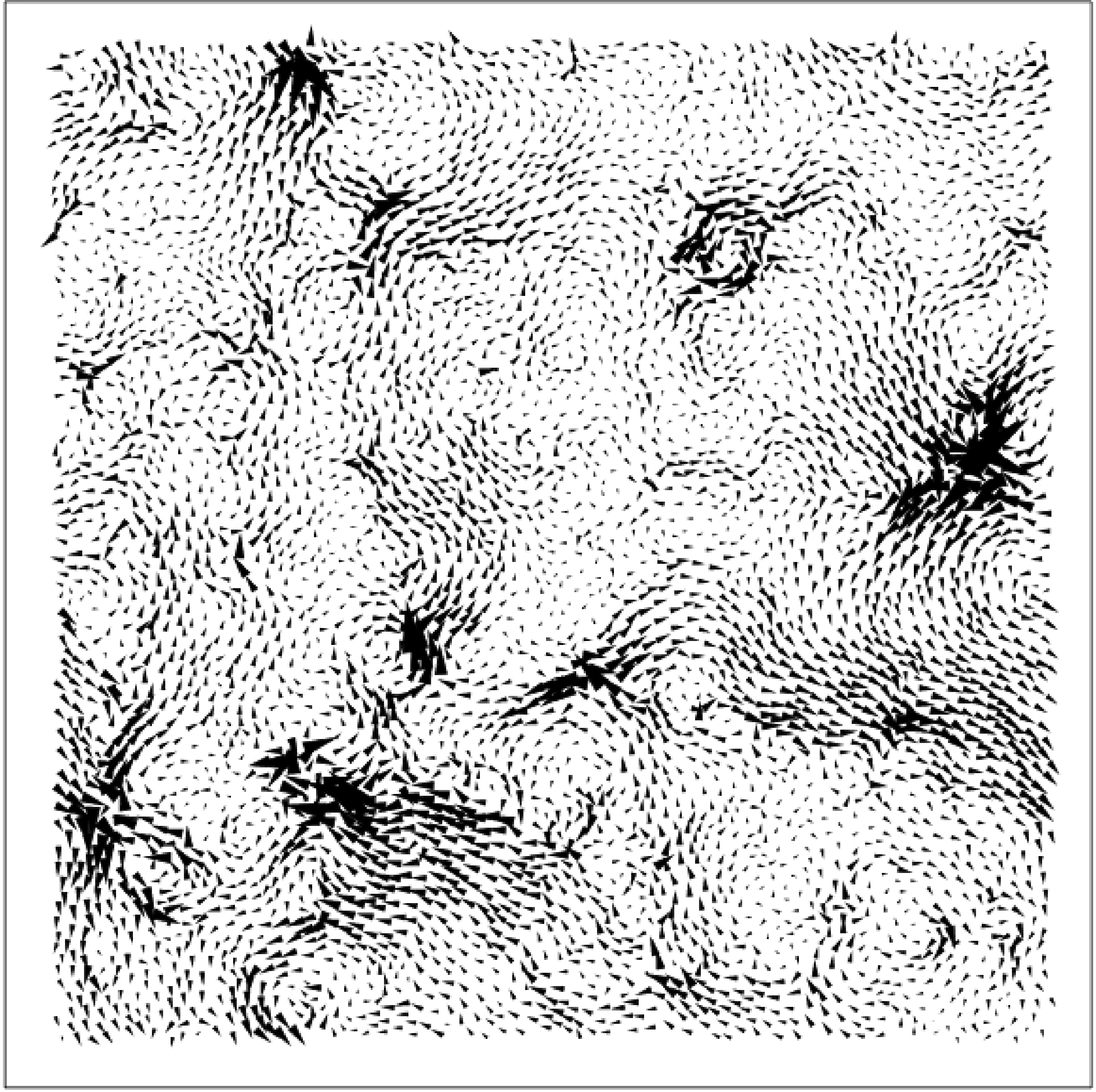
Non-affine displacements



γ_1

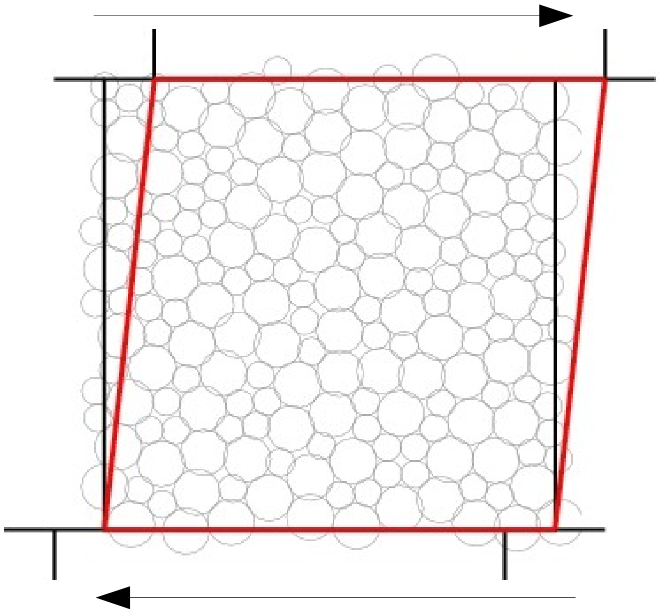
$\underline{\underline{F}}^{-1} \cdot \underline{r}_i(\gamma_1)$

Non-affine displacements



How can we predict these non-affine fields?

J. Stat. Phys. **123**, 415 (2006)

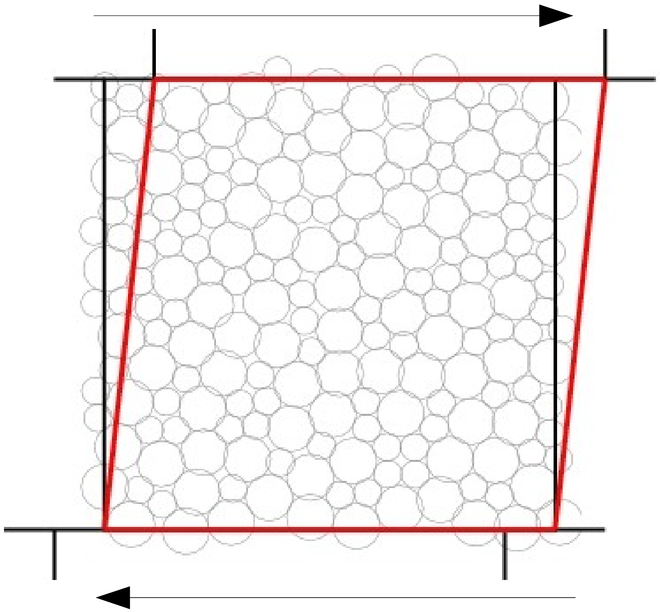


$$U\left(\{\underline{r}_i\};\underline{\underline{F}}\right)$$

Given any reference configuration, $\{\underline{r}_i = \underline{\underline{F}}\,.\,\underline{\underline{r}}_i^0 + \underline{u}_i\}$

$$U\left(\{\underline{u}_i\};\underline{\underline{F}}\right)$$

How can we predict these non-affine fields?



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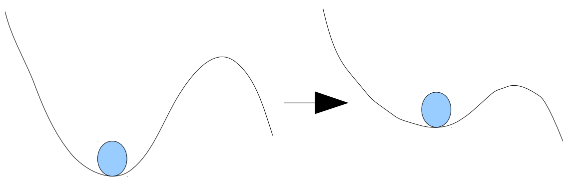
$$U\left(\{\underline{u}_i\};\underline{\underline{F}}\right)$$



$$\left.\frac{\mathrm{d}\,\underline{u}_i}{\mathrm{d}\,F_{\alpha\beta}}\right|_{\underline{F}_i=0}$$

Mechanical equilibrium

It's an implicit problem!

How can we predict these non-affine fields?

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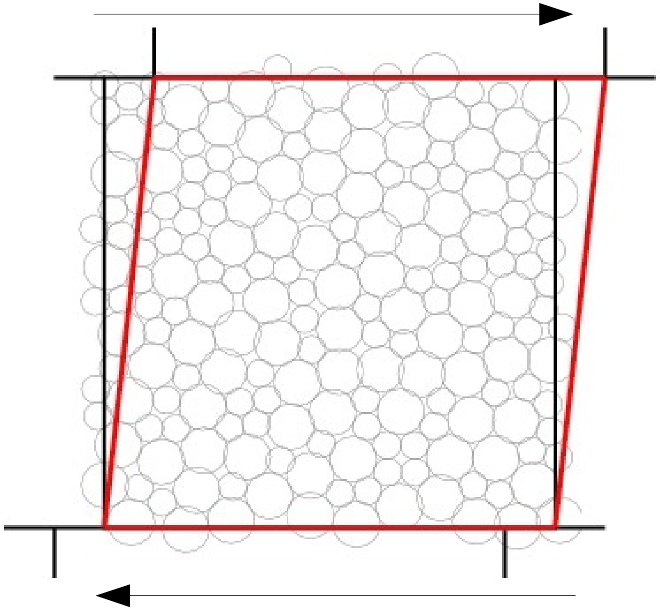
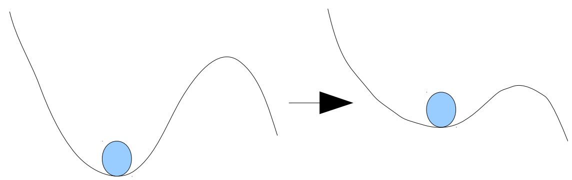


$$U\left(\{\underline{r}_i\};\underline{\underline{F}}\right)$$

Given any reference configuration, $\{\underline{r}_i = \underline{\underline{F}}.\underline{r}_i^0 + \underline{u}_i\}$

$$U\left(\{\underline{u}_i\};\underline{\underline{F}}\right)$$



$$\left.\frac{\mathrm{d}\,\underline{u}_i}{\mathrm{d}\,F_{\alpha\beta}}\right|_{\underline{F}_i=0}$$

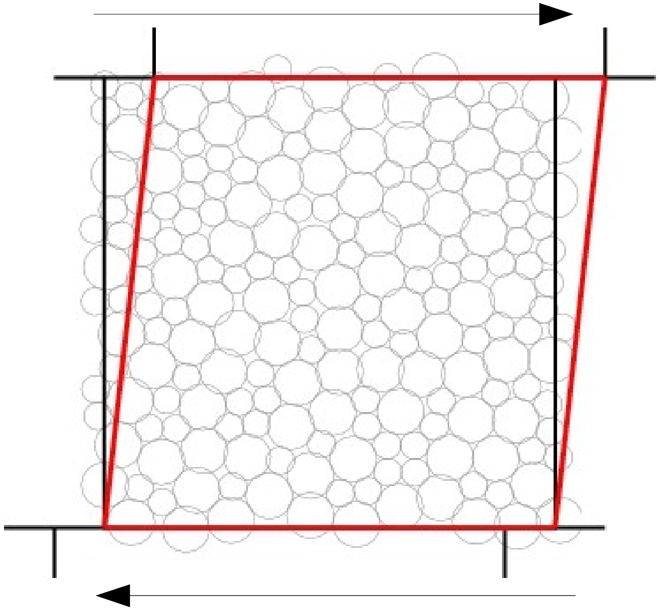
Mechanical equilibrium

It's an implicit problem!

$$\frac{\partial U}{\partial \underline{u}_i} = \frac{\partial U}{\partial \underline{r}_i} = 0$$

How can we predict these non-affine fields?

J. Stat. Phys. **123**, 415 (2006)



$$U\left(\{\underline{r}_i\};\underline{\underline{F}}\right)$$

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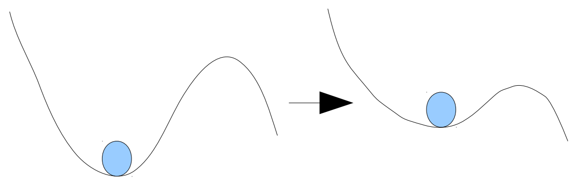

$$\left.\frac{\mathrm{d}\,\underline{u}_i}{\mathrm{d}\,F_{\alpha\beta}}\right|_{\underline{F}_i=0}$$

Mechanical equilibrium

It's an implicit problem!

$$\frac{\partial U}{\partial \underline{u}_i}=0$$

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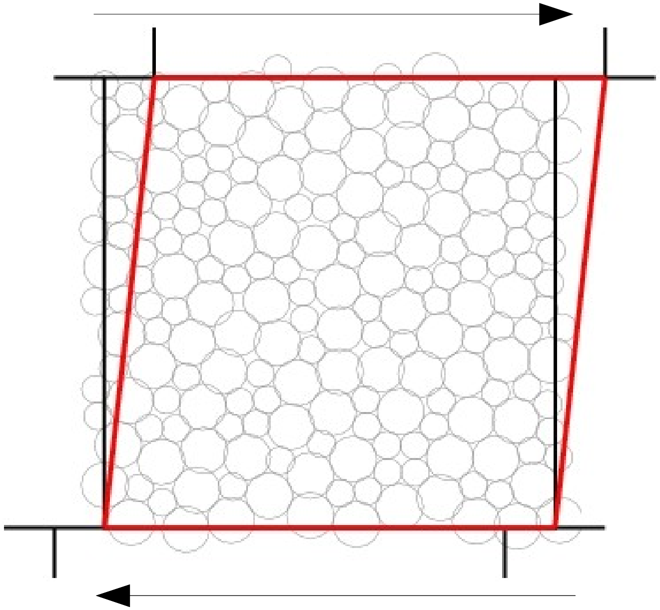
How can we predict these non-affine fields?

J. Stat. Phys. **123**, 415 (2006)



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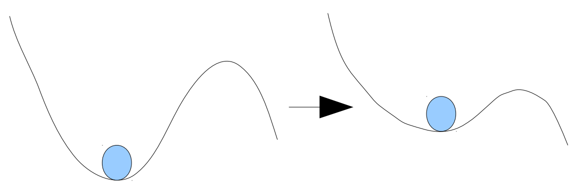

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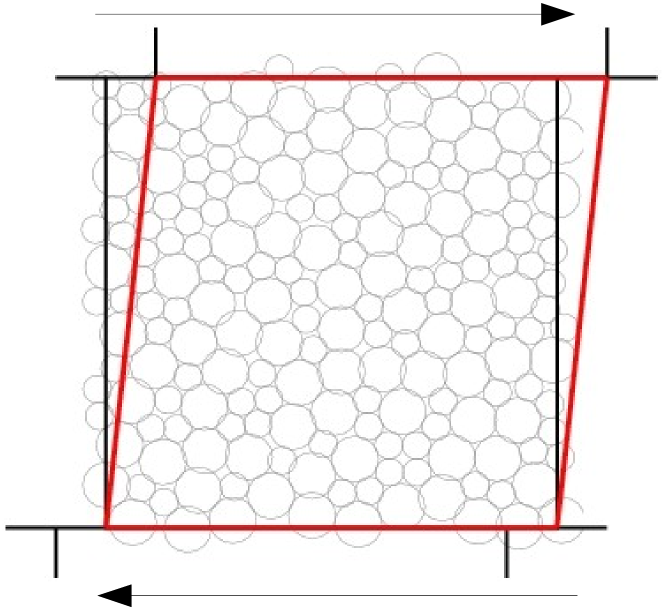
J. Stat. Phys. **123**, 415 (2006)



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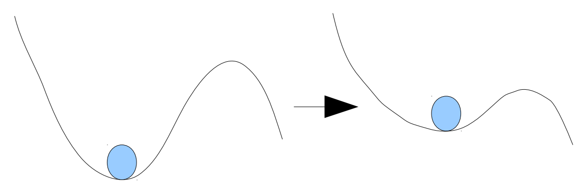

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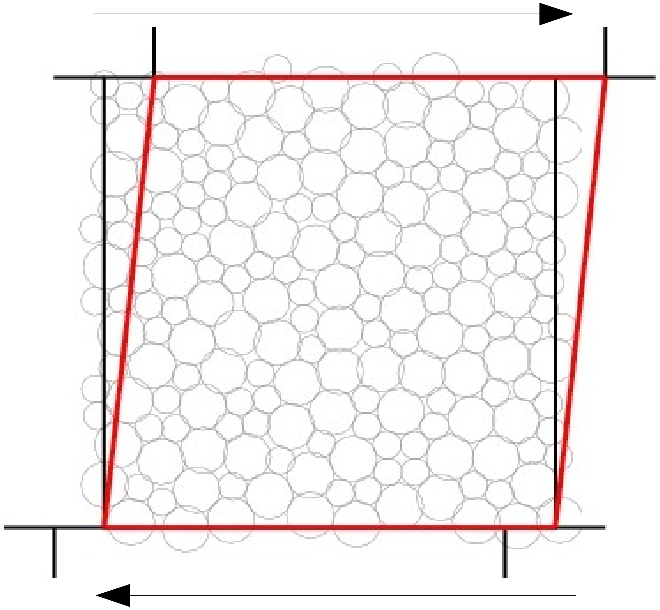

J. Stat. Phys. **123**, 415 (2006)

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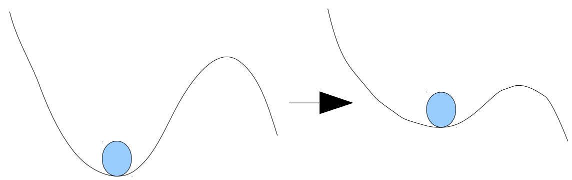

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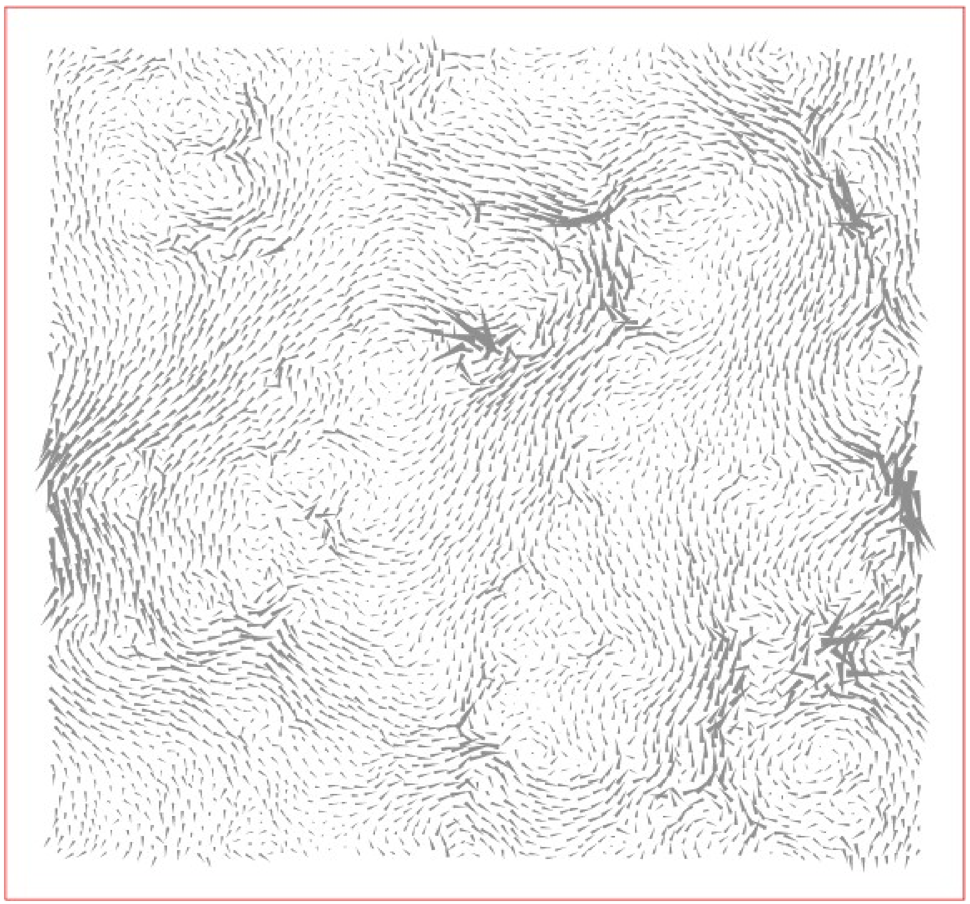
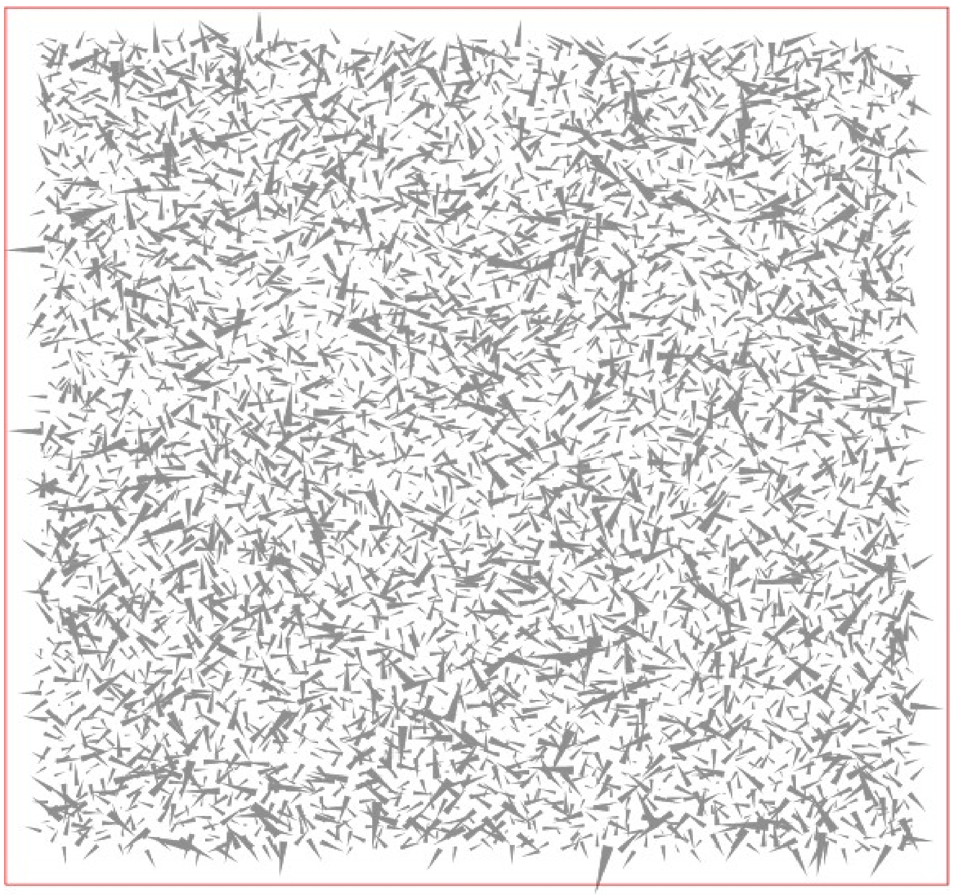
$$=\boldsymbol{H}_{ij} \qquad \equiv -\boldsymbol{\Xi}_{\alpha\beta,i}=\frac{\partial\,\underline{F}_i}{\partial\,F_{\alpha\beta}}$$

$$\boldsymbol{H}_{ij}\cdot\frac{\mathrm{d}\,u_j}{\mathrm{d}\,F_{\alpha\beta}}=\boldsymbol{\Xi}_{\alpha\beta,i}$$

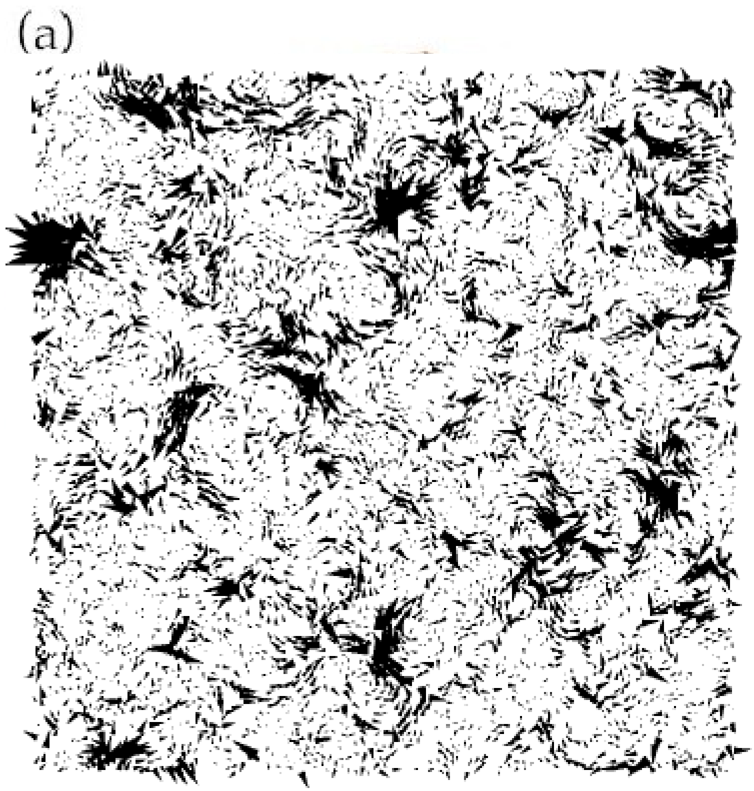
Analytical expression for elastic moduli

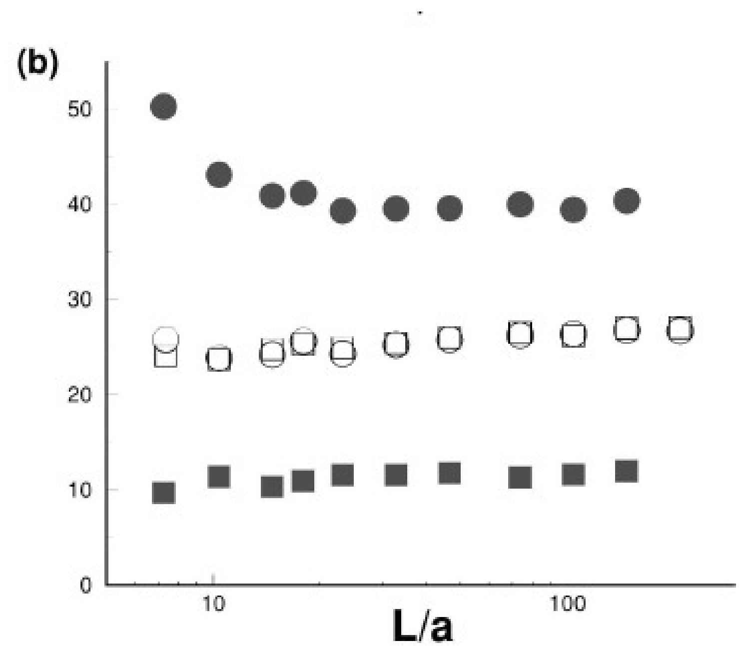
$$\frac{\mathrm{d}u}{\mathrm{d}\gamma} = H^{-1}.\Xi \qquad H_{ij} = \frac{\partial^2 U}{\partial r_i \partial r_j} \qquad \Xi_j = -\frac{\partial^2 U}{\partial \gamma \partial r_j} = \frac{\partial F_j}{\partial \gamma}$$





Size-dependence of Lamé constants

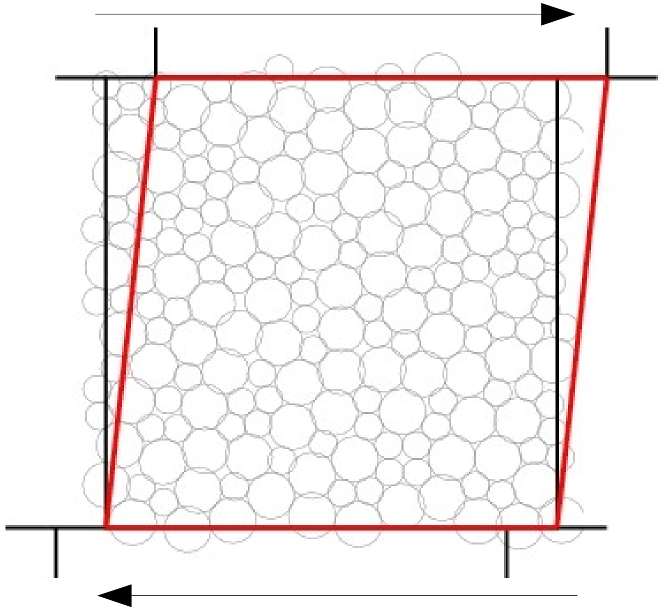




Tanguy *et al*, PRB **66**, 174205 (2002)

How can we compute elastic moduli?

J. Stat. Phys. **123**, 415 (2006)



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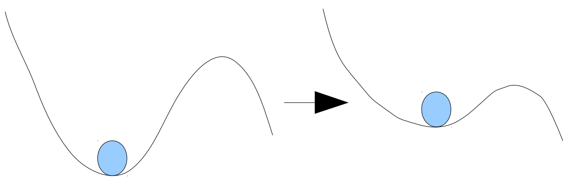


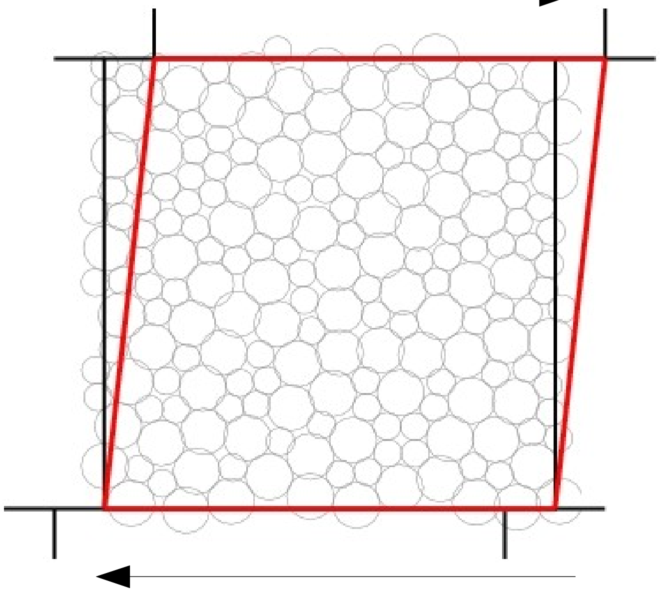
$$\left.\frac{\mathrm{d}\,\underline{u}_i}{\mathrm{d}\,F_{\alpha\beta}}\right|_{\underline{F}_i=0}$$

Mechanical equilibrium

It's an implicit problem!

How can we compute elastic moduli?

J. Stat. Phys. **123**, 415 (2006)



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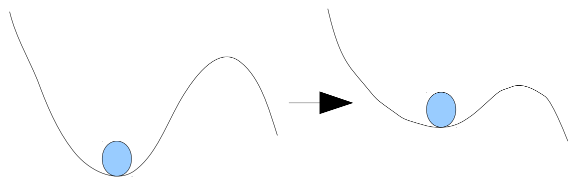

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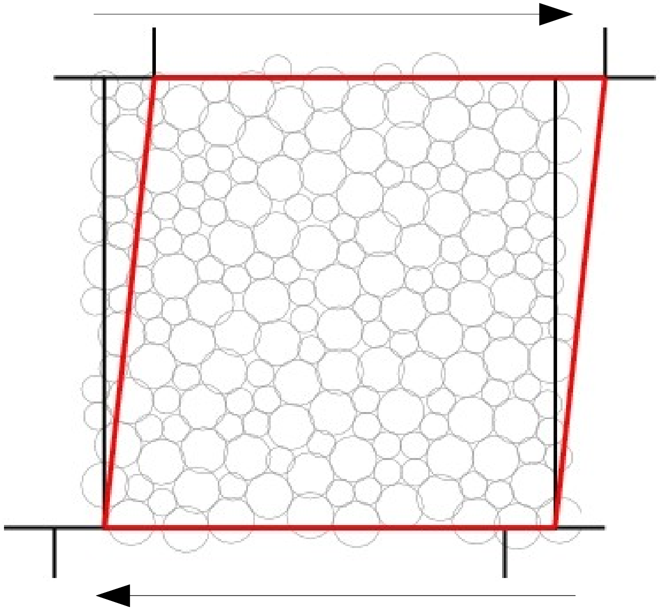
How can we compute elastic moduli?

J. Stat. Phys. **123**, 415 (2006)



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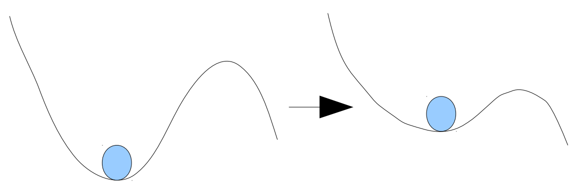

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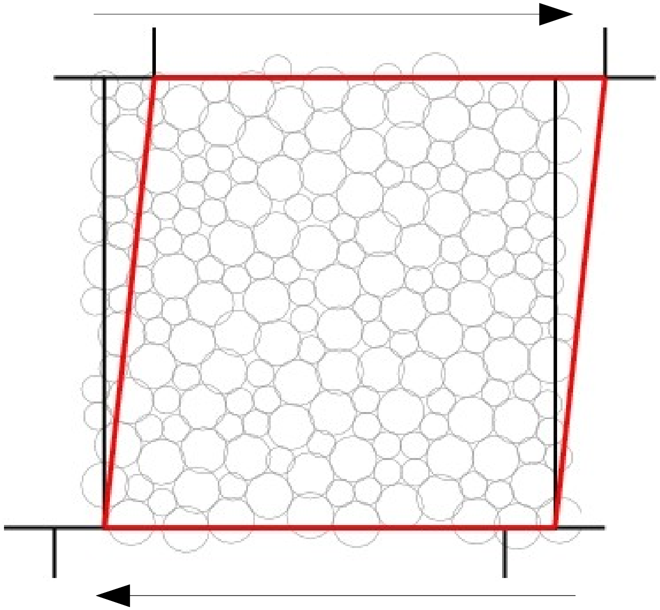
How can we compute elastic moduli?

J. Stat. Phys. **123**, 415 (2006)



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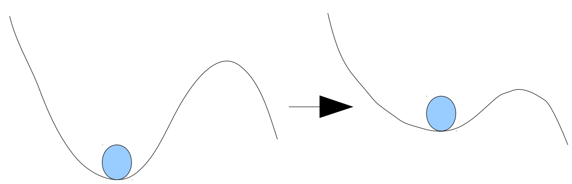

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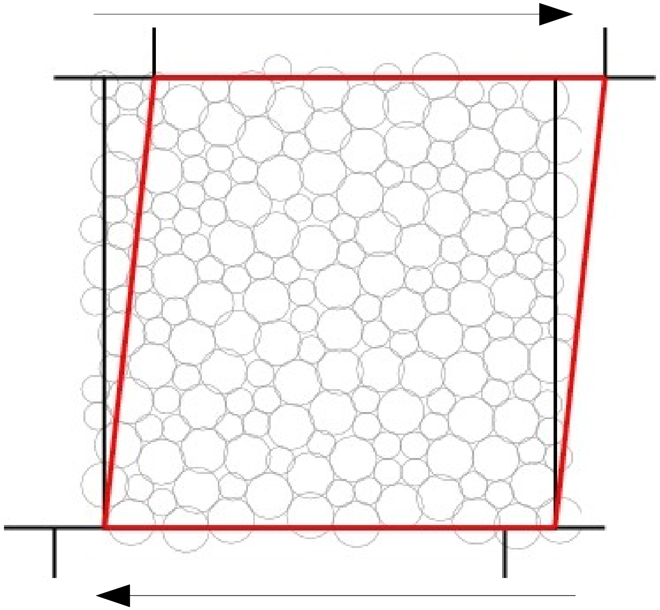

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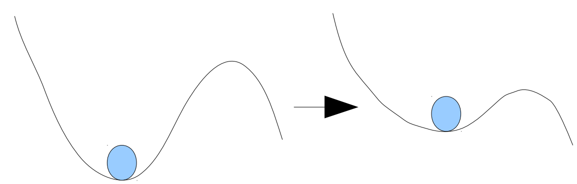

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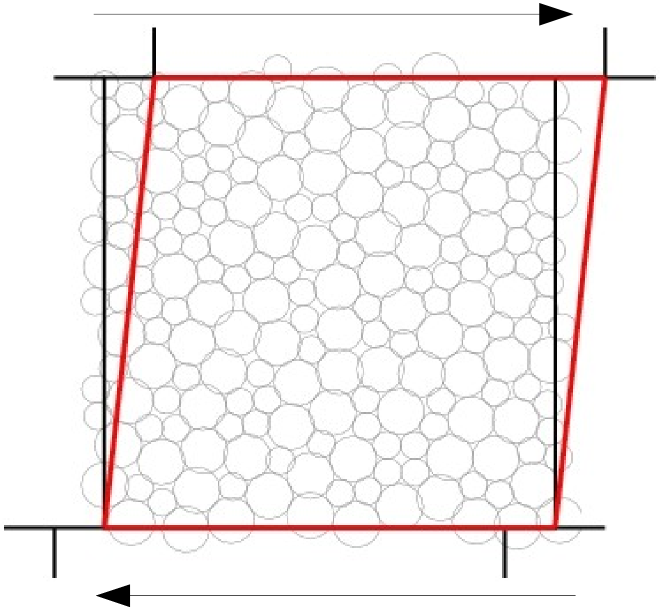
How can we compute elastic moduli?

J. Stat. Phys. **123**, 415 (2006)



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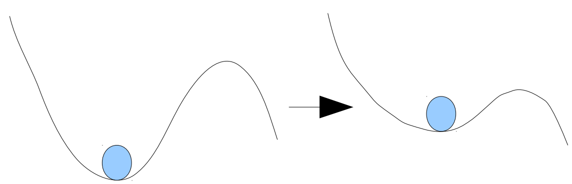

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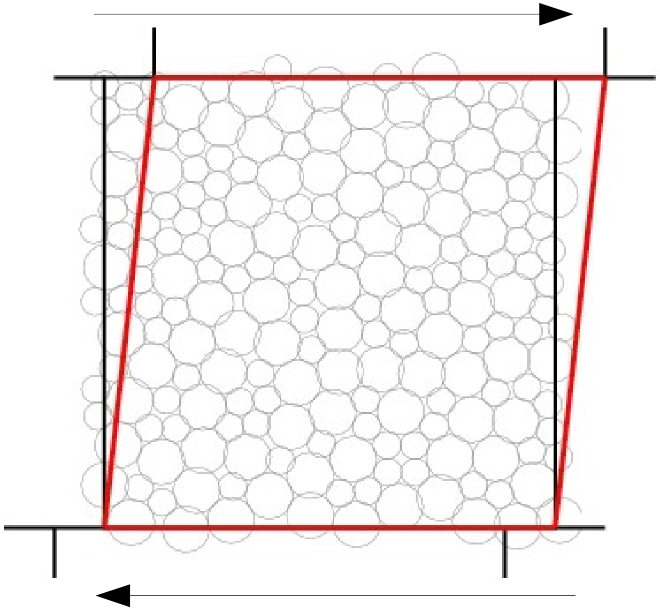
How can we compute elastic moduli?

J. Stat. Phys. **123**, 415 (2006)



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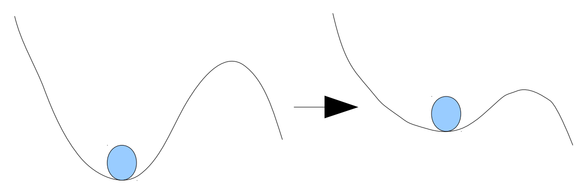

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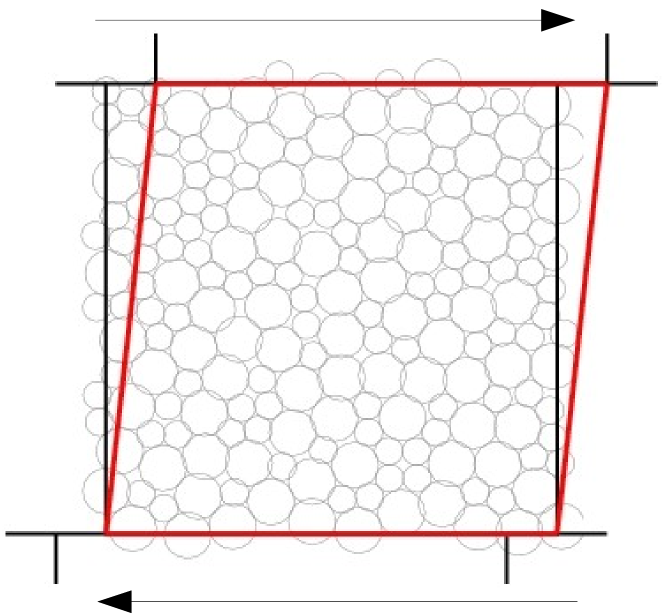
J. Stat. Phys. **123**, 415 (2006)



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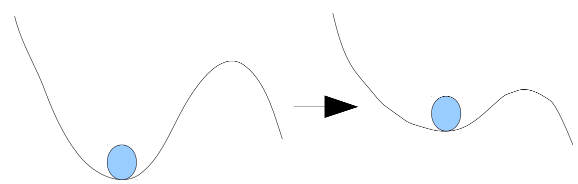

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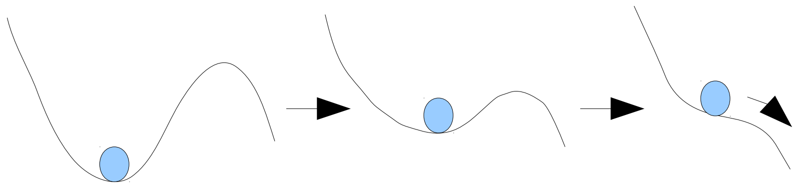
2) Instability



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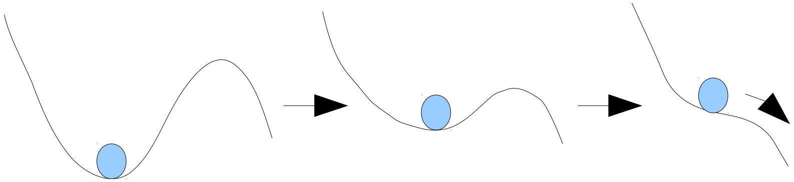


At instability: one eigenmode has 0 eigenvalue

Numerics: instability occurs via the vanishing of a single eigenvalue
= saddle-node bifurcation

Exercise

$$U(x;\gamma) = -\frac{1}{3}x^3 - \gamma x$$

Draw U for: $\gamma < 0$

$\gamma > 0$

When relevant determine local maxima & minima of U

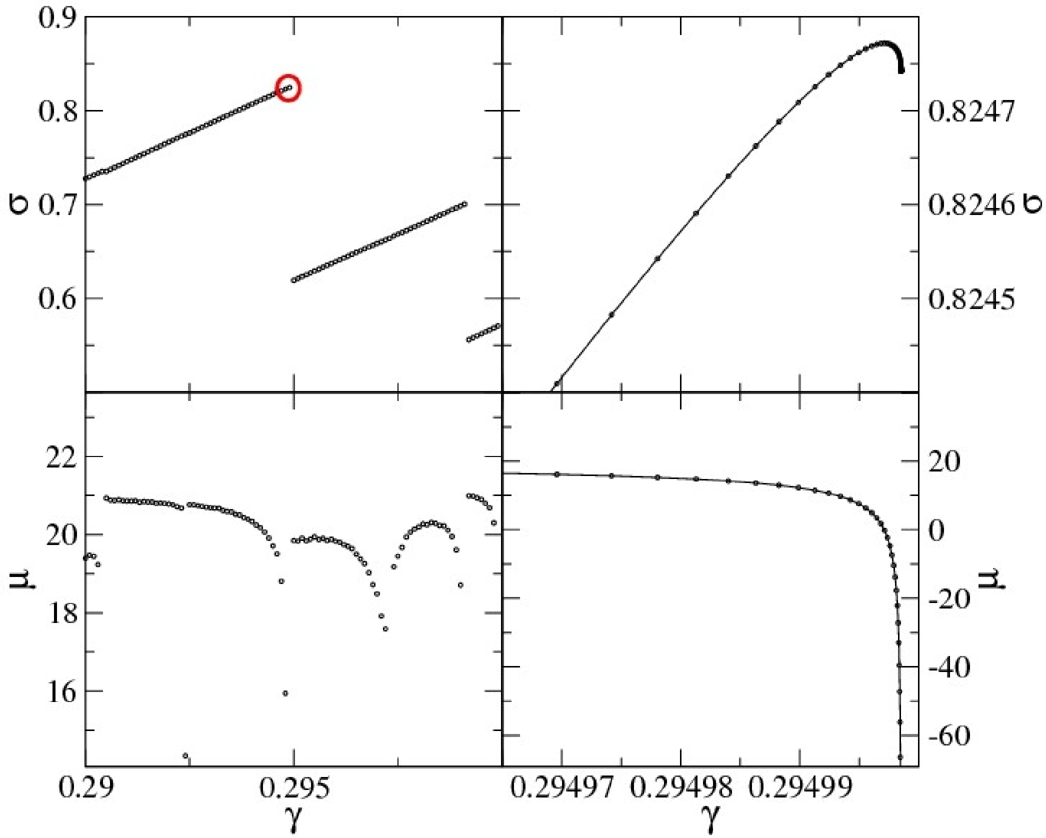
Explain what happens when γ increases from < 0 values

At the minimum, determine U' and U''

What would be the energy barrier limiting
activation from the local minimum?

Plasticity in governed by saddle-node bifurcations

The onset of a plastic event is controlled by the vanishing of a single eigenvalue



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

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

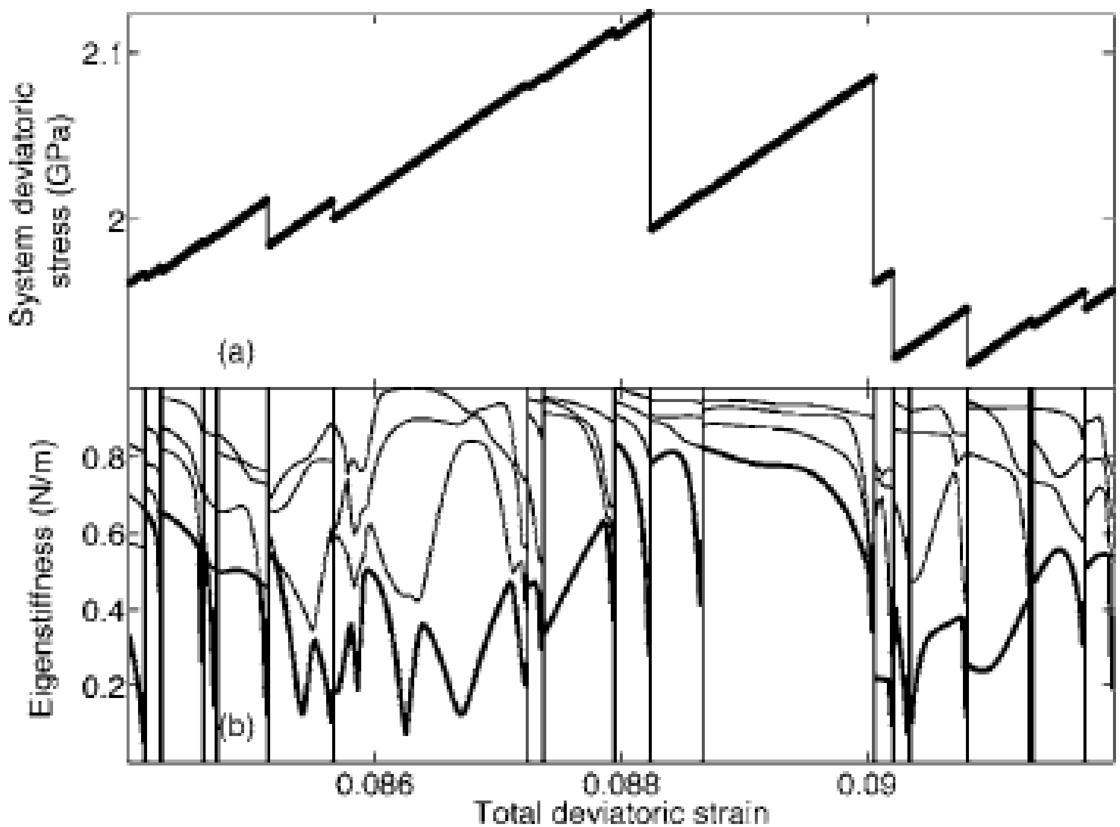
$$\mu \sim -A/\sqrt{\gamma_c - \gamma}$$

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

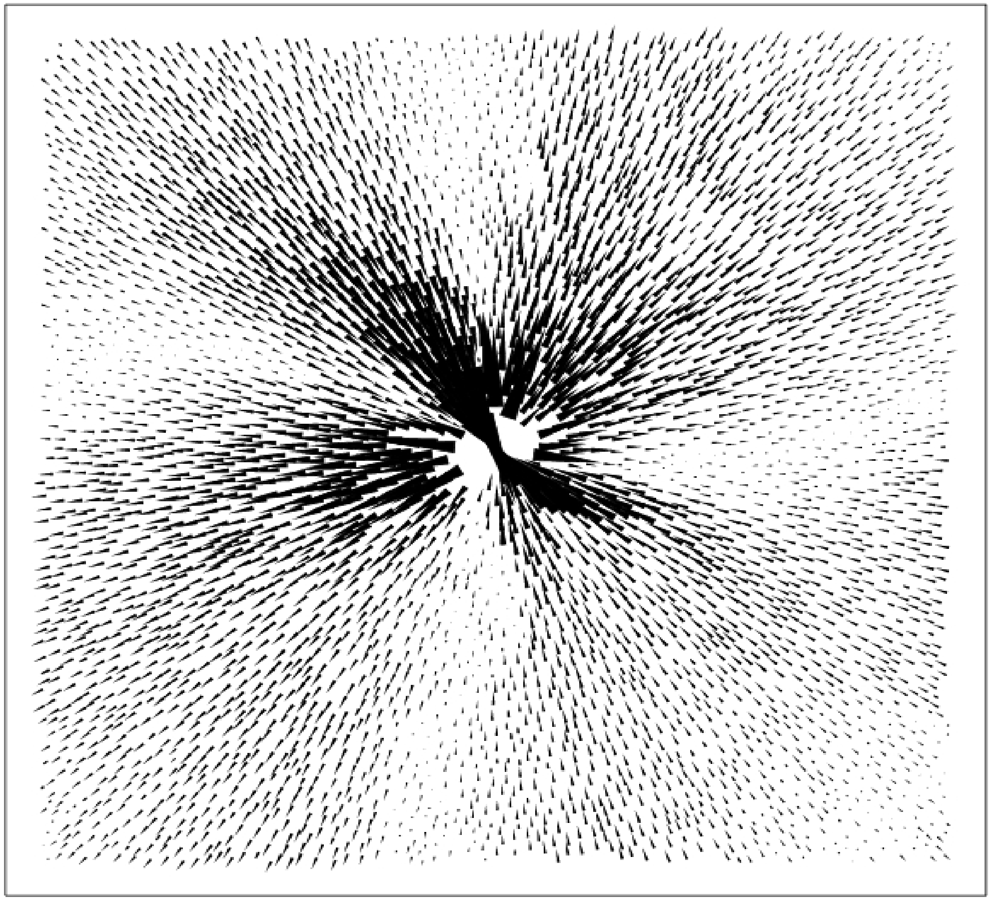
$$\frac{dr}{d\gamma} \rightarrow \infty$$

Dynamics of eigenvalues

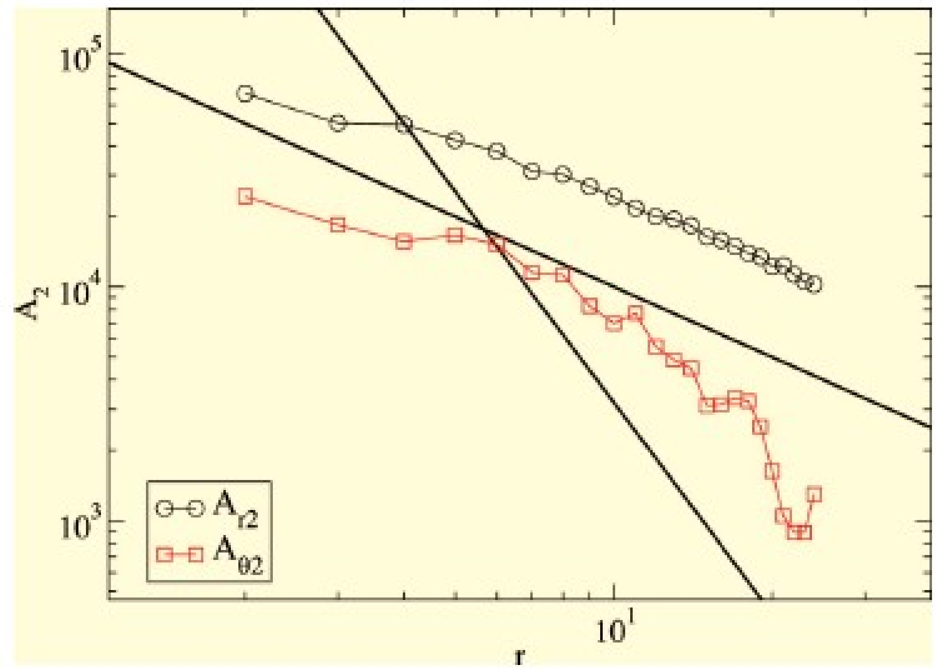
Demkowicz and Argon, PRB 72, 255206 (2005)



Zero-modes present slow decay ~ Eshelby fields



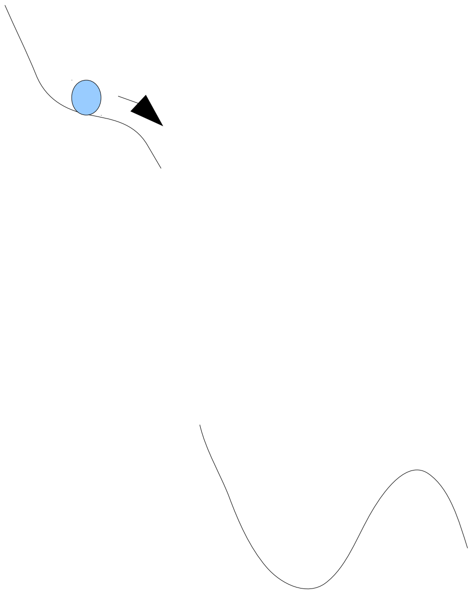
PRE 74, 016118 (2006)



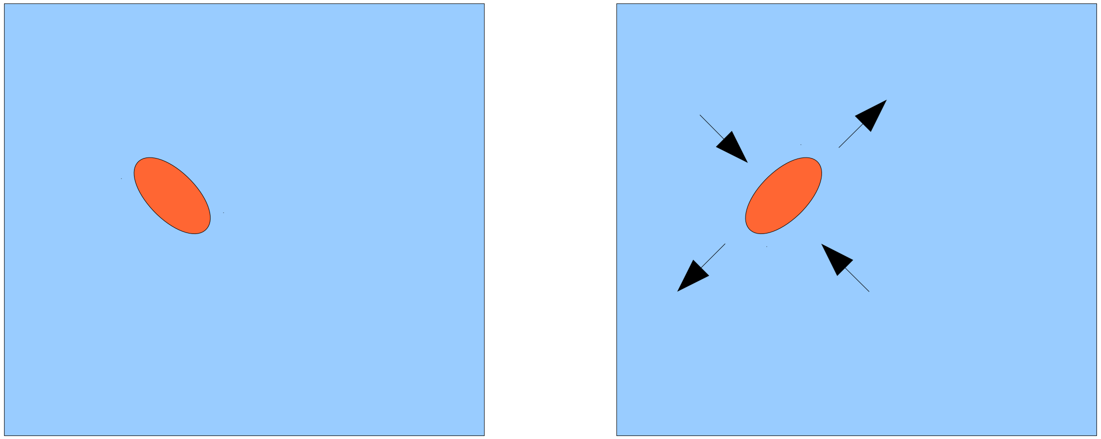
$$\vec{u} = \frac{2 a^2 \Delta \epsilon_0}{\pi} \frac{x\, y}{r^4} \vec{r}$$

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

3) Plastic event



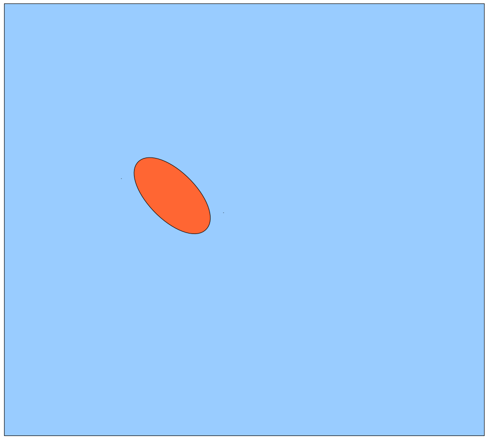
The Eshelby problem

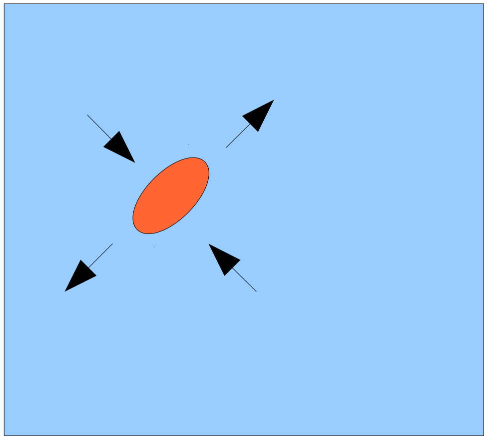


Eshelby (1957): the effect of the transformation can be modeled by forces lying at the boundary

A transforming zone is embedded in an elastic medium

The Eshelby problem

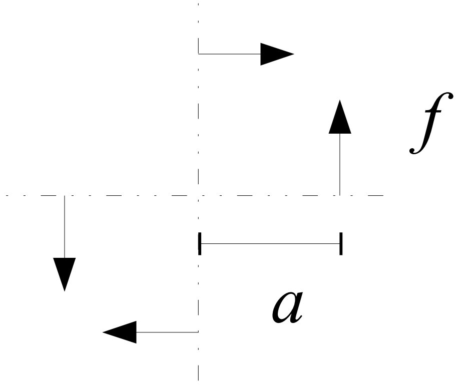




Eshelby (1957): the effect of the transformation can be modeled by forces lying at the boundary

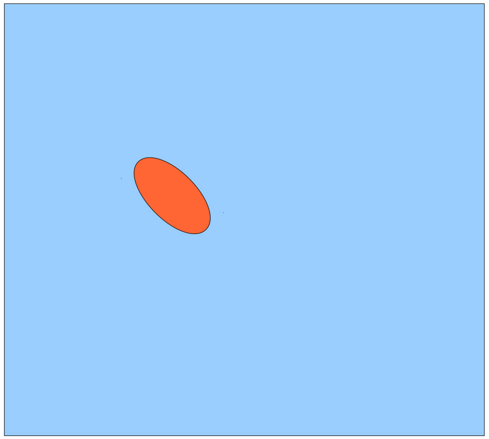
Picard *et al*, EPJE, **15**, 371 (2004)

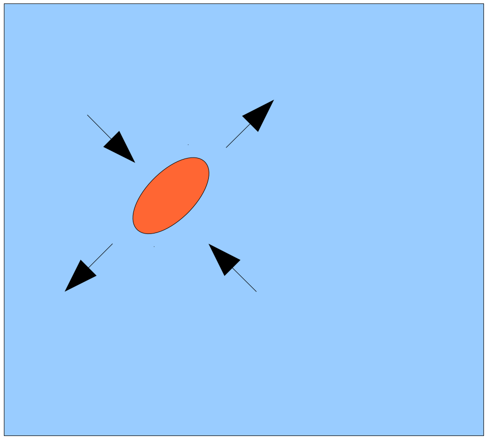
$$\begin{cases} \mu \Delta \vec{u} - \nabla p = \sum_i \vec{f}_i \delta(\vec{r} - \vec{r}_i) \\ \nabla . \vec{u} = 0 \end{cases}$$



Dipolar strength: $f\, a = \mu\, a^2 \Delta \epsilon_0$

The Eshelby problem





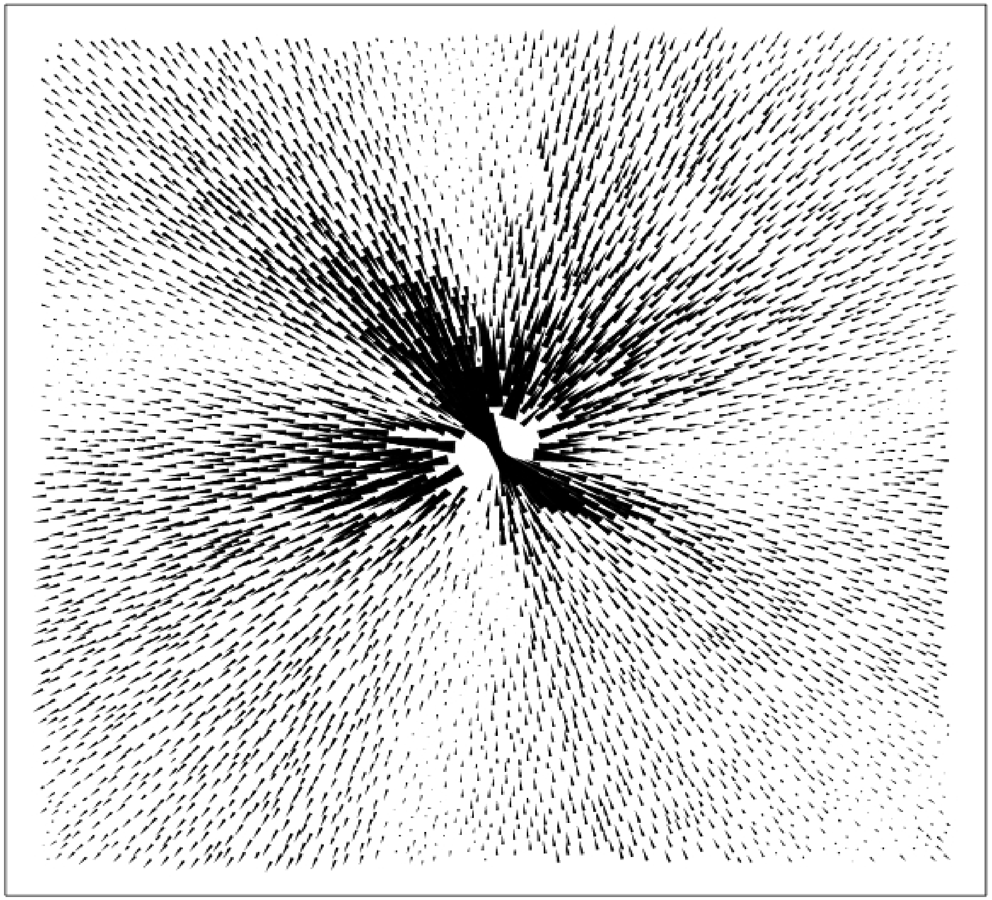
Eshelby (1957): the effect of the transformation can be modeled by forces lying at the boundary

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

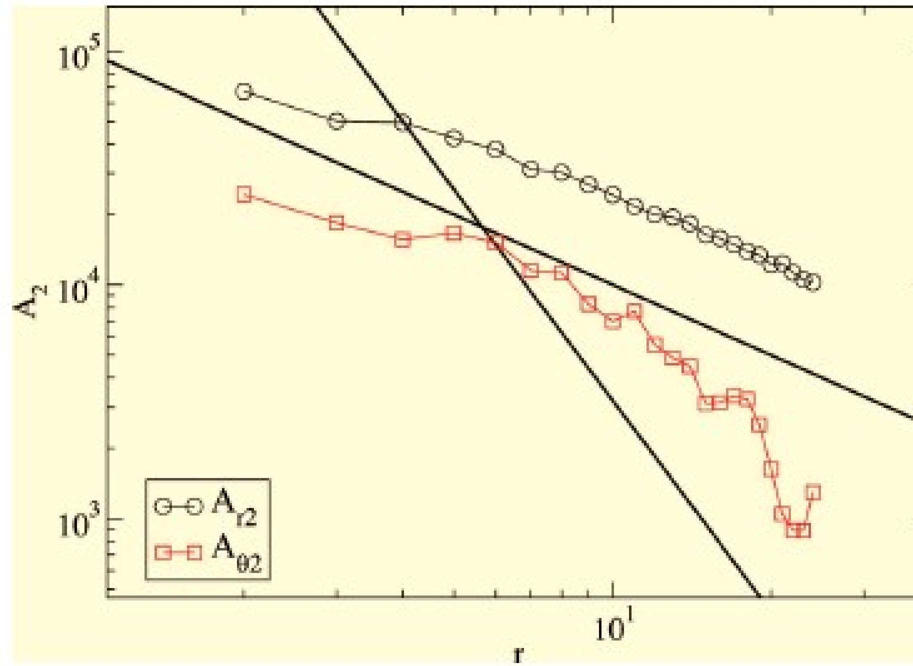
$$\sigma_{xy} = \frac{2\mu\, a^2 \Delta \epsilon_0}{\pi} \frac{\cos(4\theta)}{r^2}$$

A transforming zone is embedded in an elastic medium

Zero-modes present slow decay ~ Eshelby fields

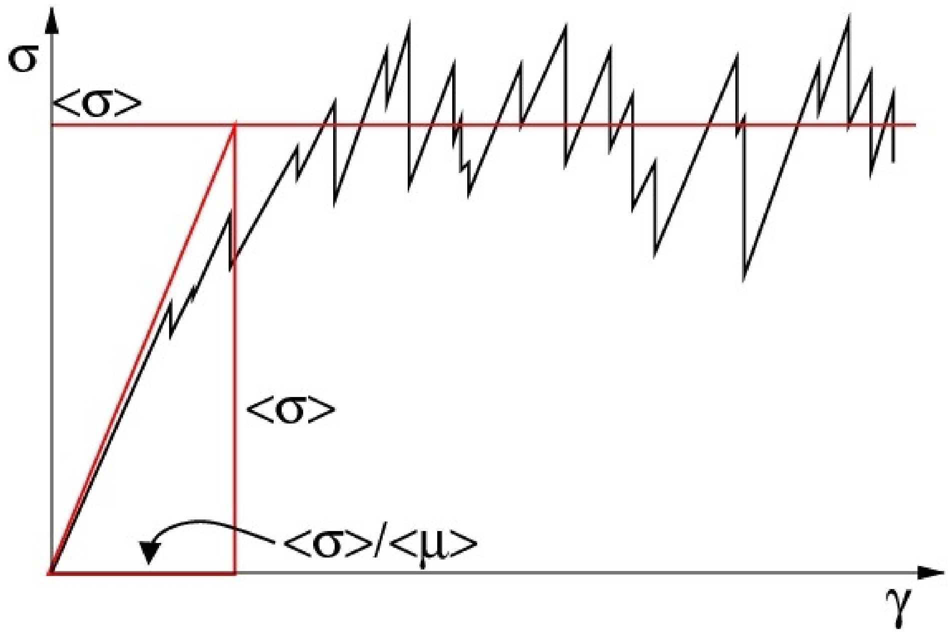


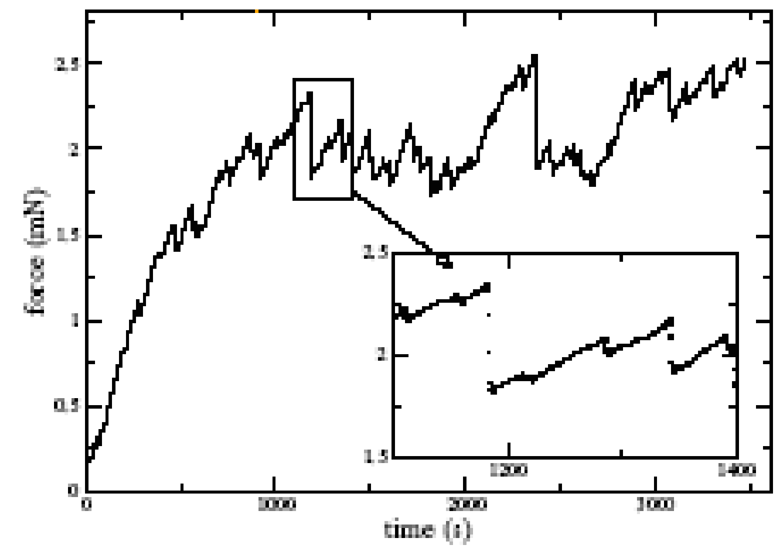
PRE 74, 016118 (2006)



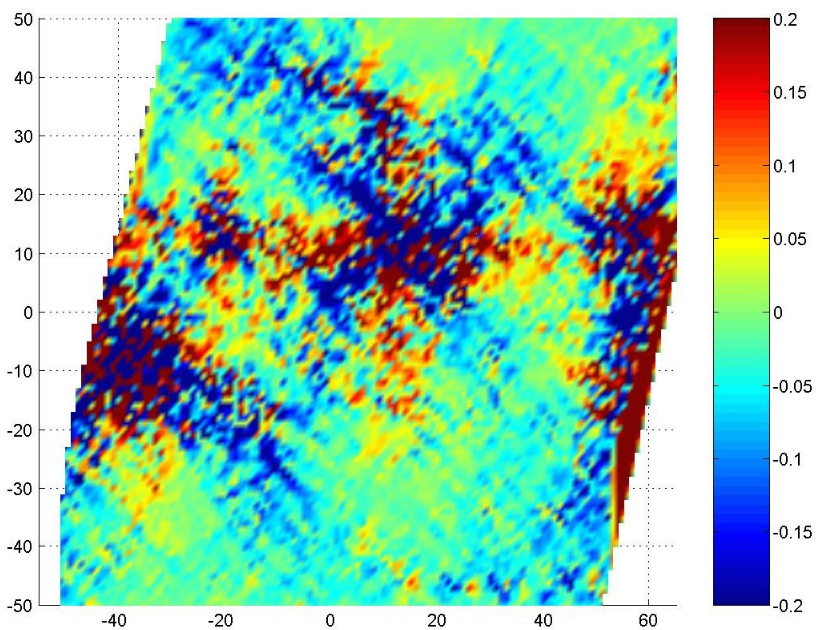
$$\vec{u} = \frac{2 a^2 \Delta \epsilon_0}{\pi} \frac{x\, y}{r^4} \vec{r}$$

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

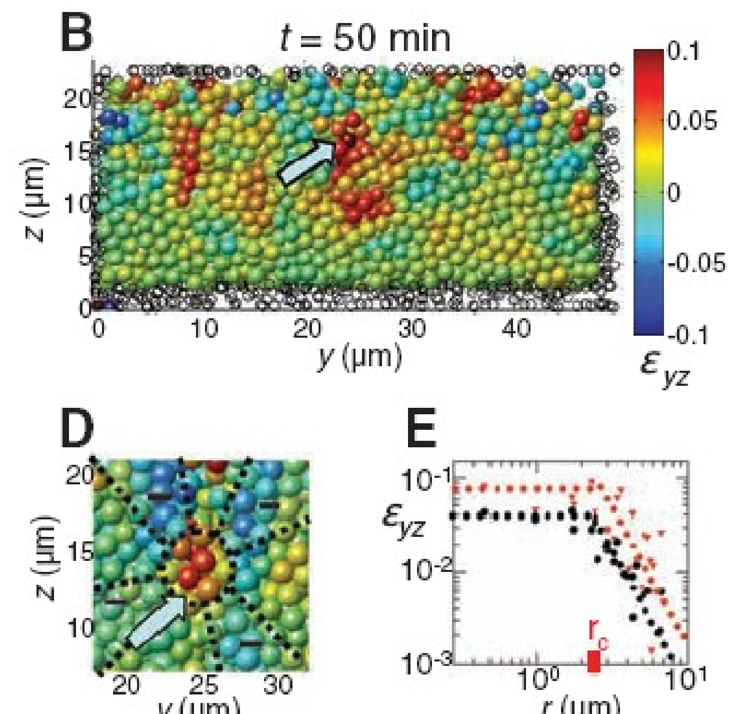




I. Cantat, O. Pitois, Phys. Fluids (2006)

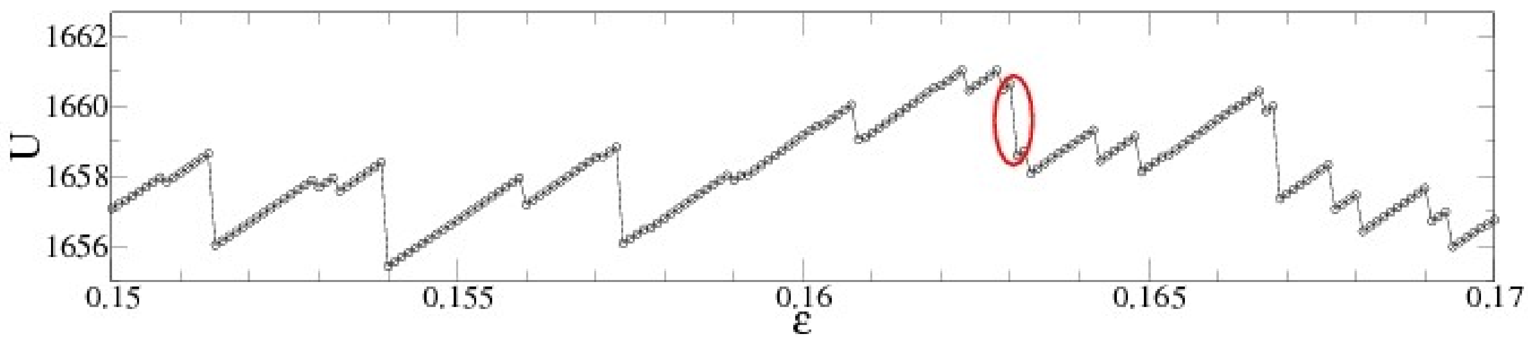


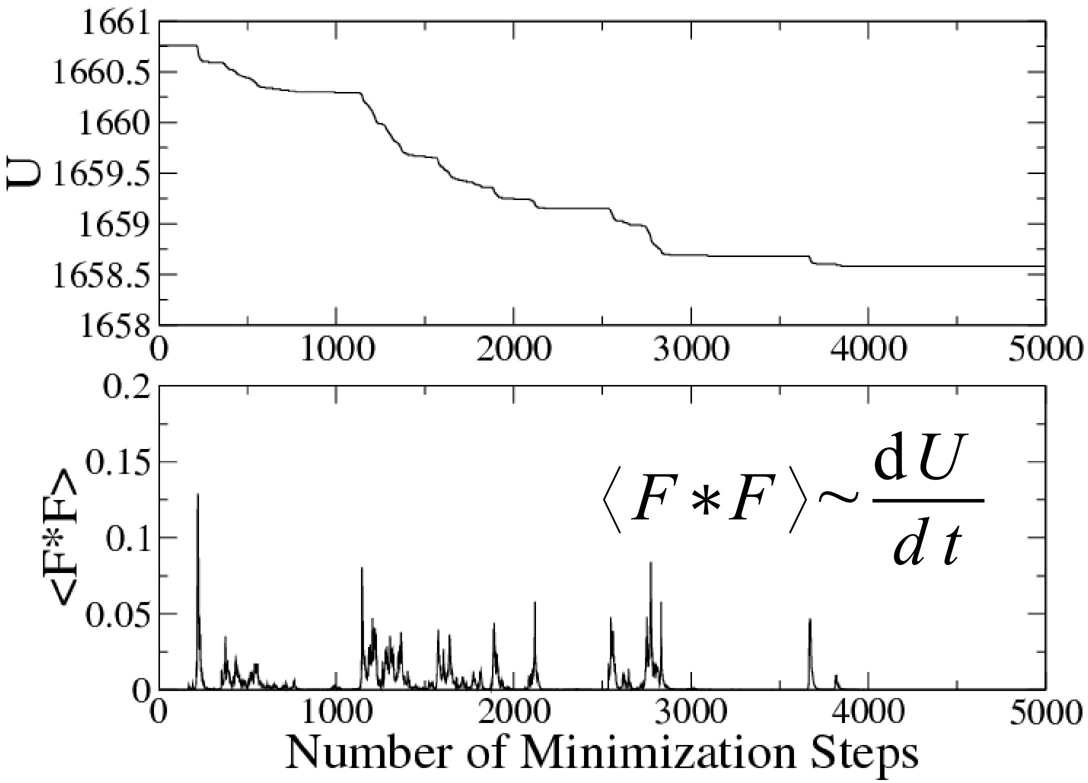
Tanguy *et al* PRE (2006)



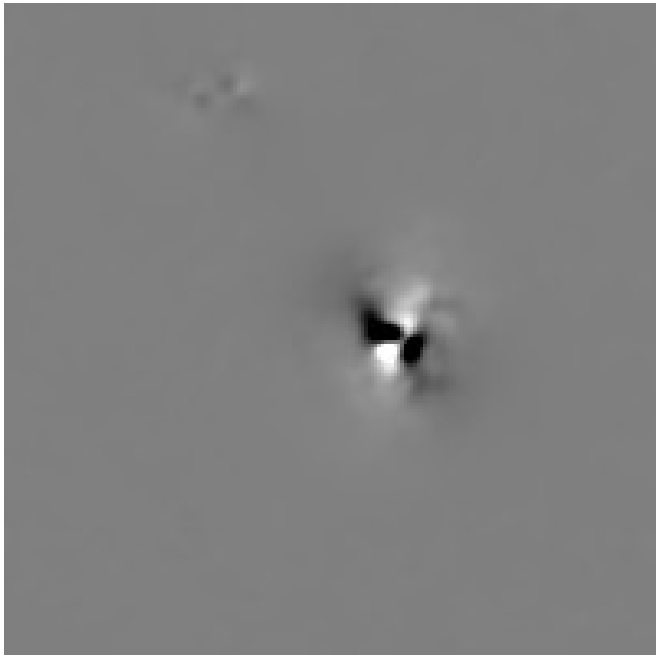
Schall, Spaepen & Weitz (2007)

Focus on steady state

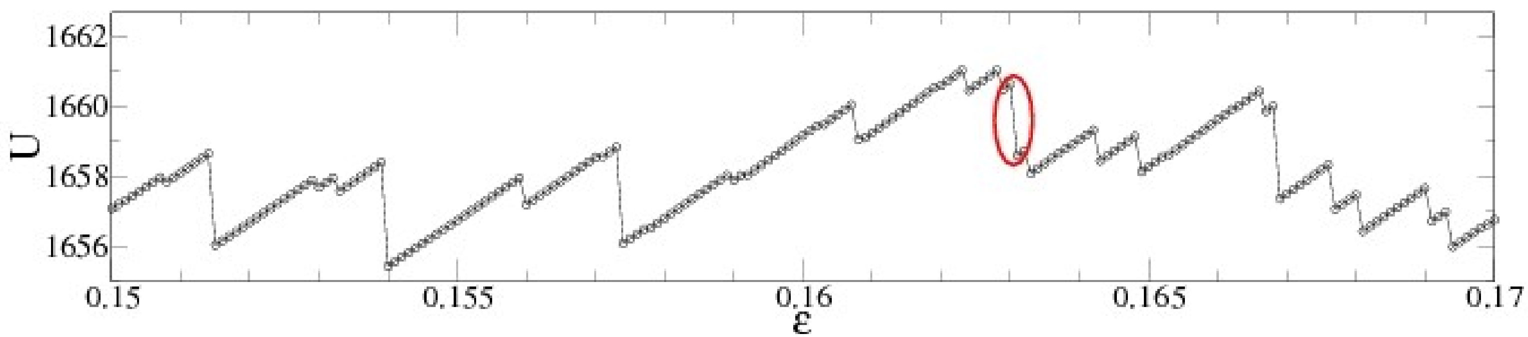


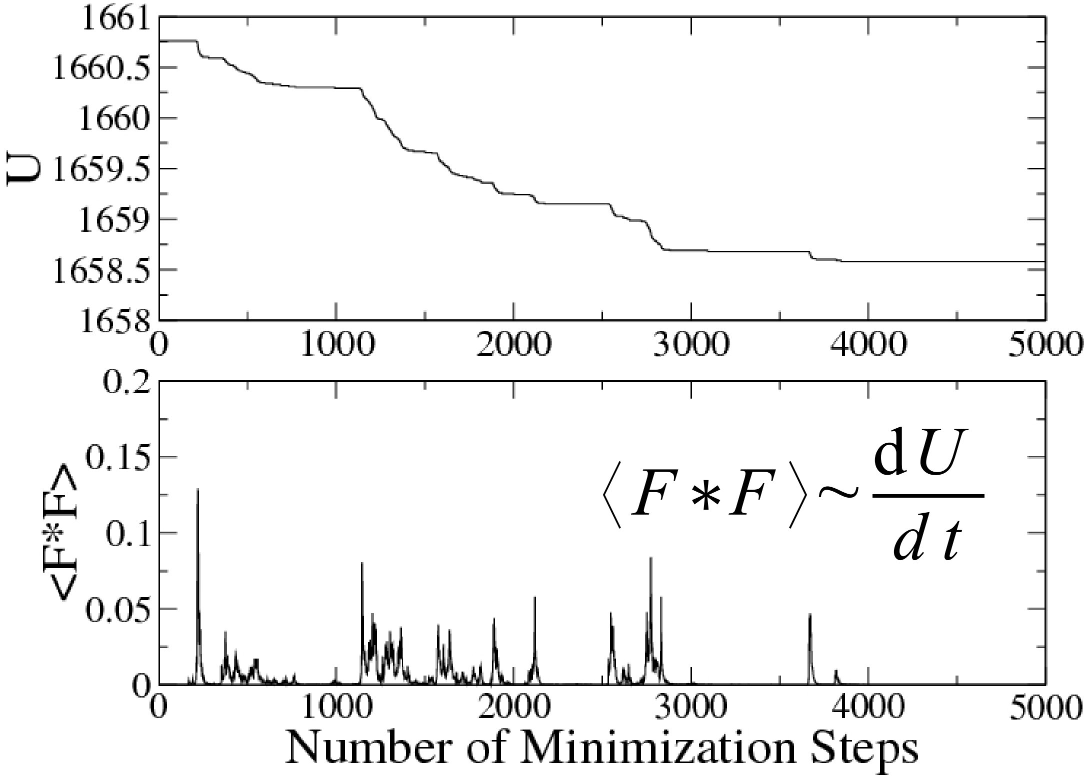


$$\langle F * F \rangle \sim \frac{\mathrm{d}U}{dt}$$



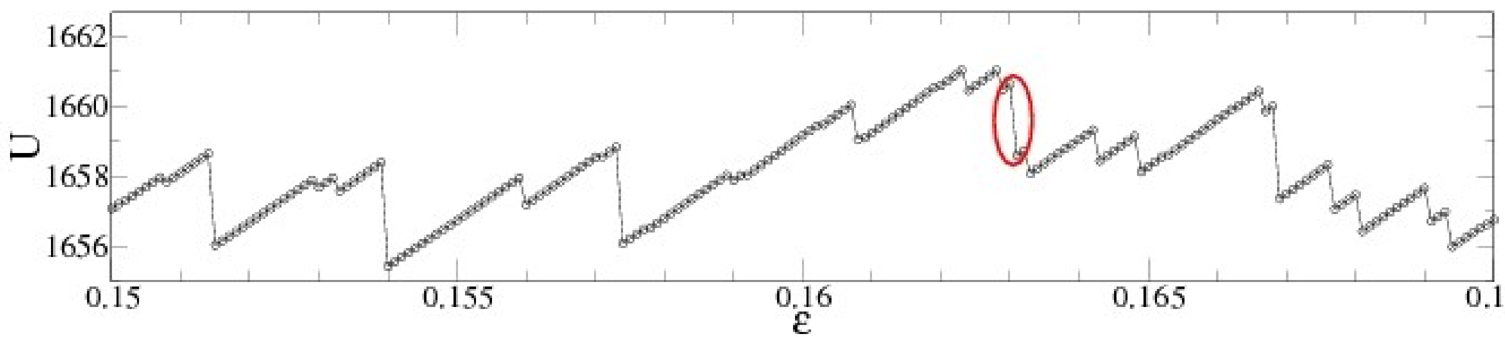
Focus on steady state

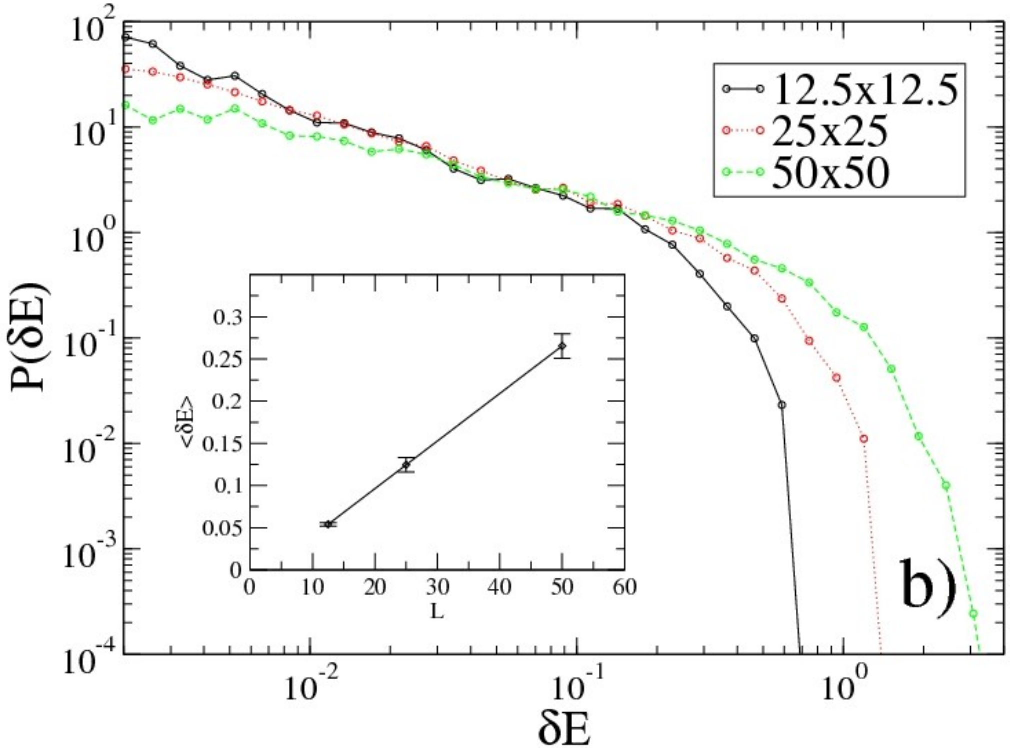




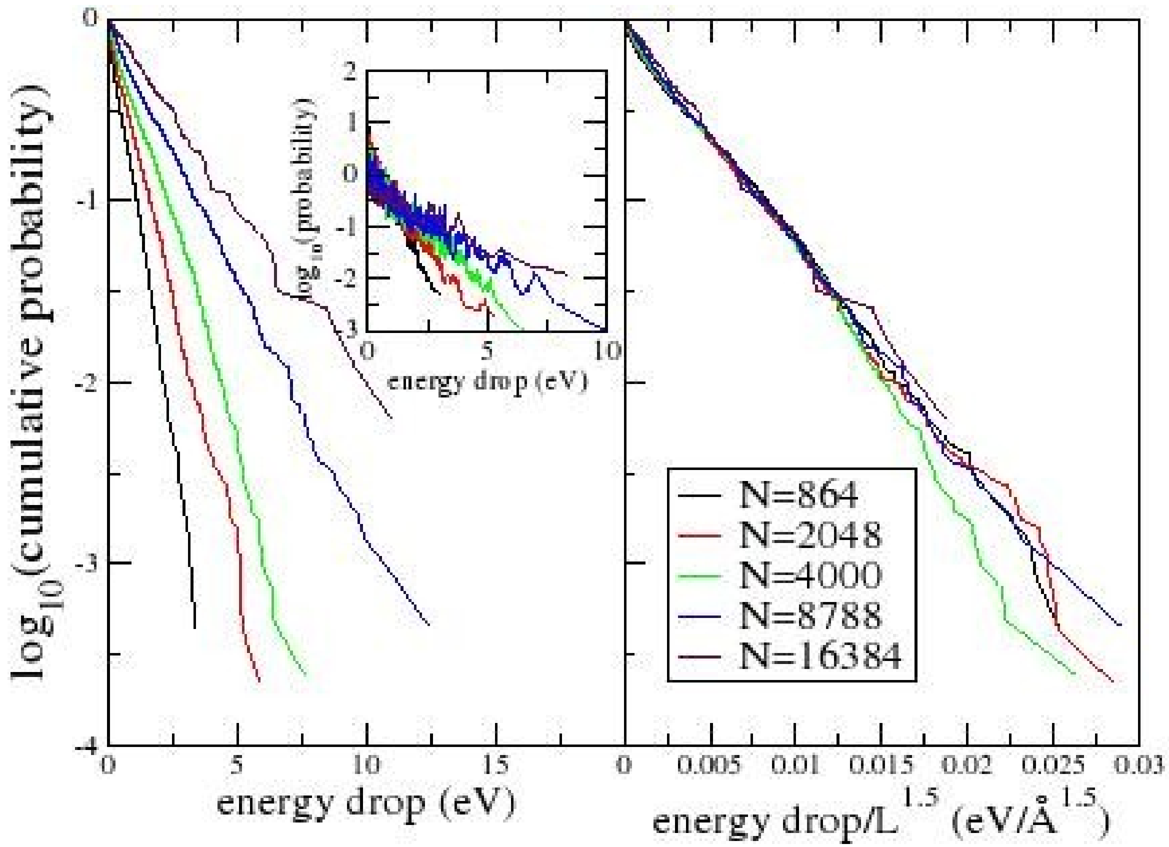
$$\langle F * F \rangle \sim \frac{dU}{dt}$$

Focus on steady state





3D simulations: $Mg_{0.85}Cu_{0.15}$



Average event sizes

<u>In 2D</u>

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

$$\Delta E \sim L$$

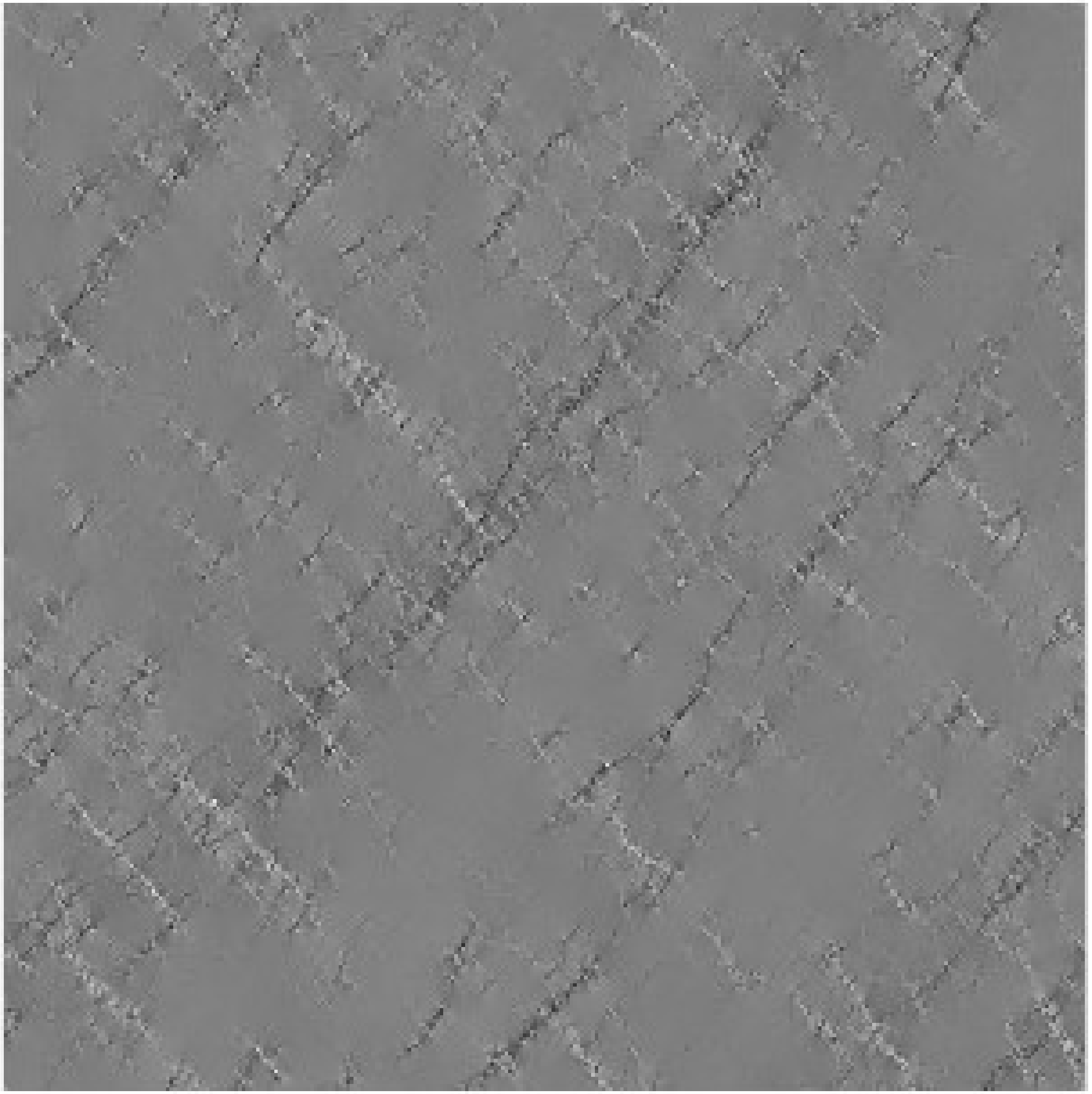
E. Lerner and I. Procaccia,
PRE 79, 066109 (2009)

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

<u>In 3D</u>

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

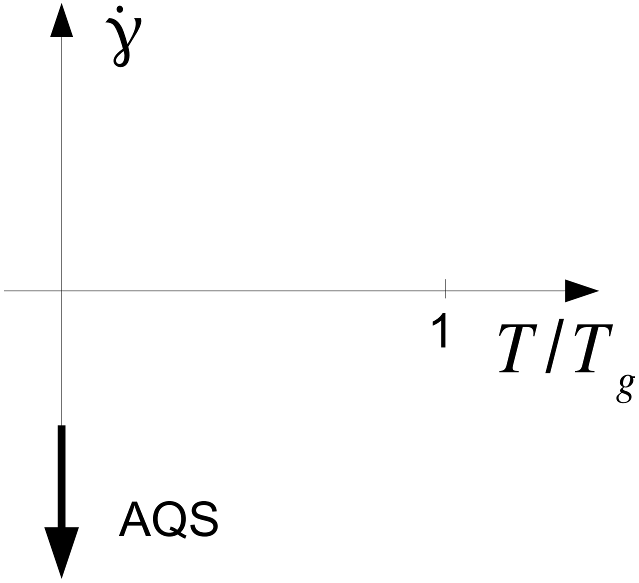
$$\Delta E \sim L^{1.4}$$



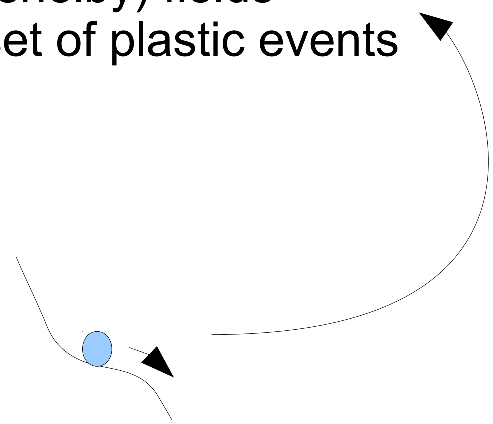
$$\omega = \partial_y u_x - \partial_x u_y$$

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

Partial conclusion

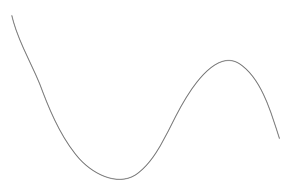


Elementary quadrupolar (Eshelby) fields
can be observed at the onset of plastic events



Plastic events are avalanches
- power law distribution
- size of largest events ~ L

Yet, it is difficult to isolate
zone flips during avalanches



What causes avalanche behavior?

Origin of avalanche behavior

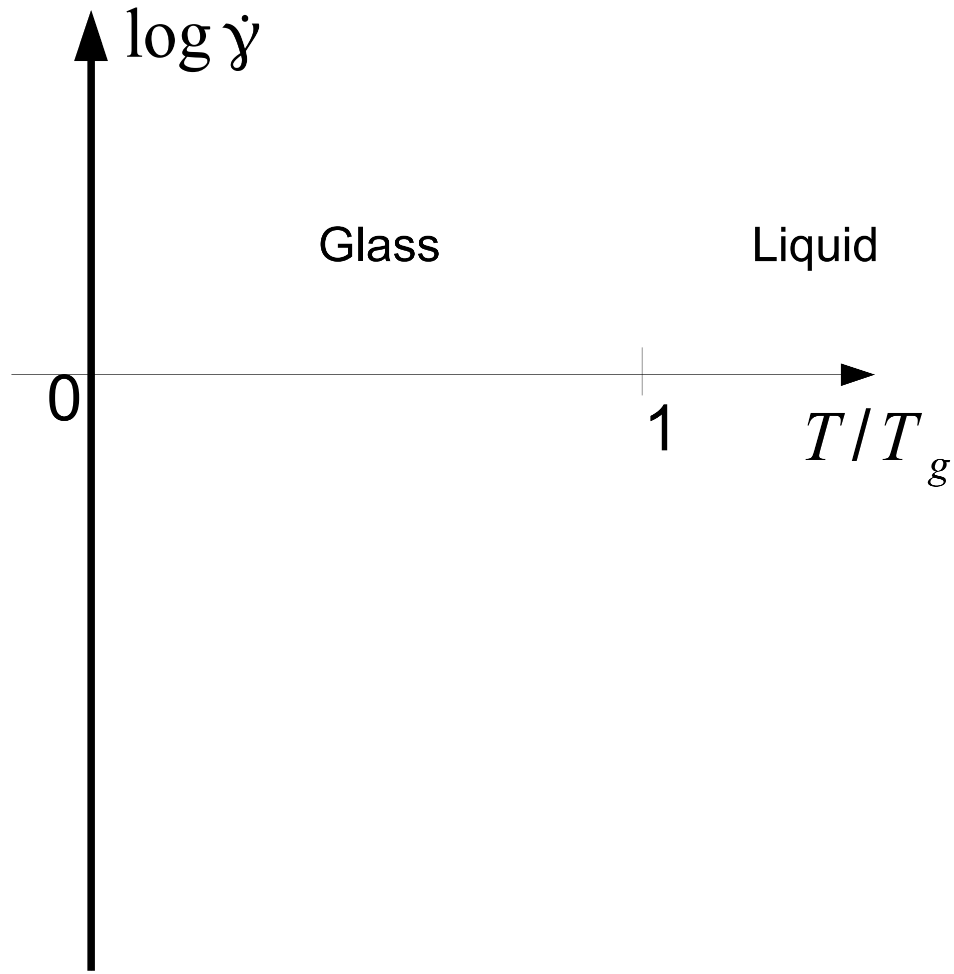
Advection by external drive in elastic regime:

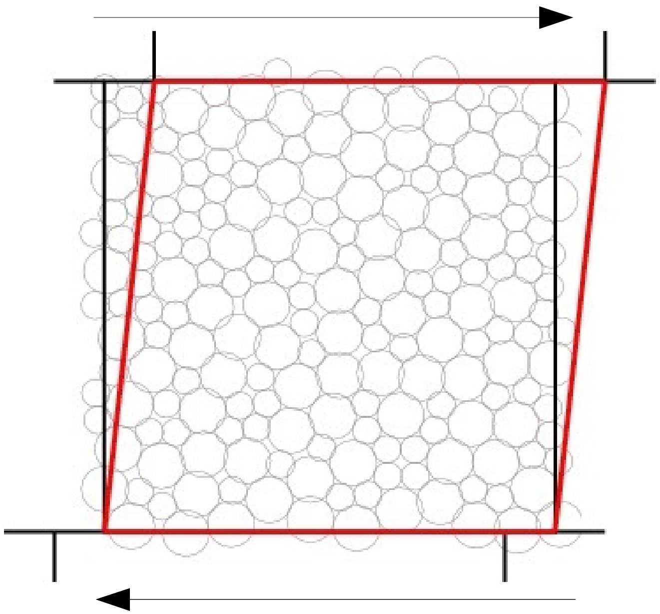
- progressive softening
- brings weak zones near threshold

Zone flips produce long-ranged Eshelby fields

- modify the internal strain of neighboring already weak zones
- which hence may trigger their flipping
  = secondary events
- chain rule.... avalanche behavior

Athermal deformation





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

Binary Lennard-Jones

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

- Standard MD simulation
- Damping forces

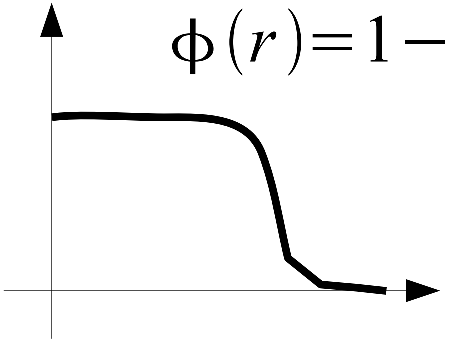
$$f_{ij} = \frac{m}{\tau} \phi(r)(\vec{v}_j - \vec{v}_i)$$

<u>This form of dissipation guarantees that:</u>

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

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

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



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

Non-affine velocity

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

$L = 160$

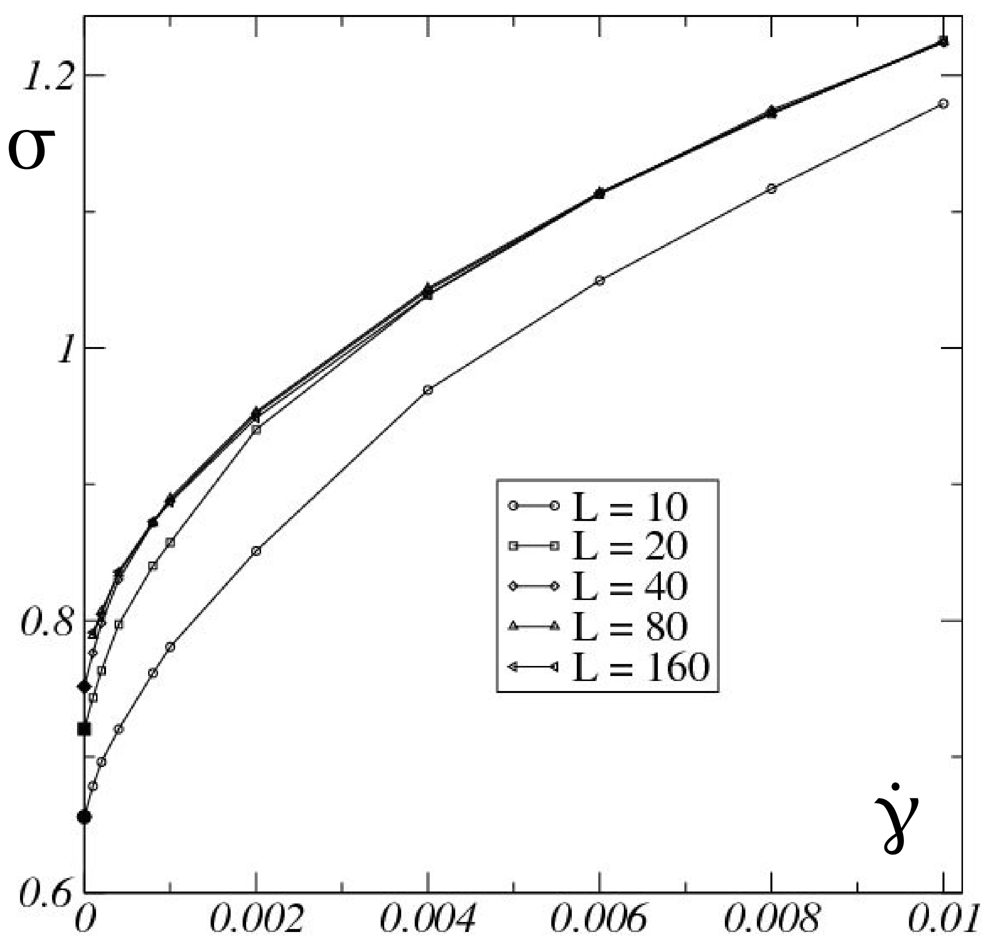
$\dot{\gamma} = 5.10^{-5}$

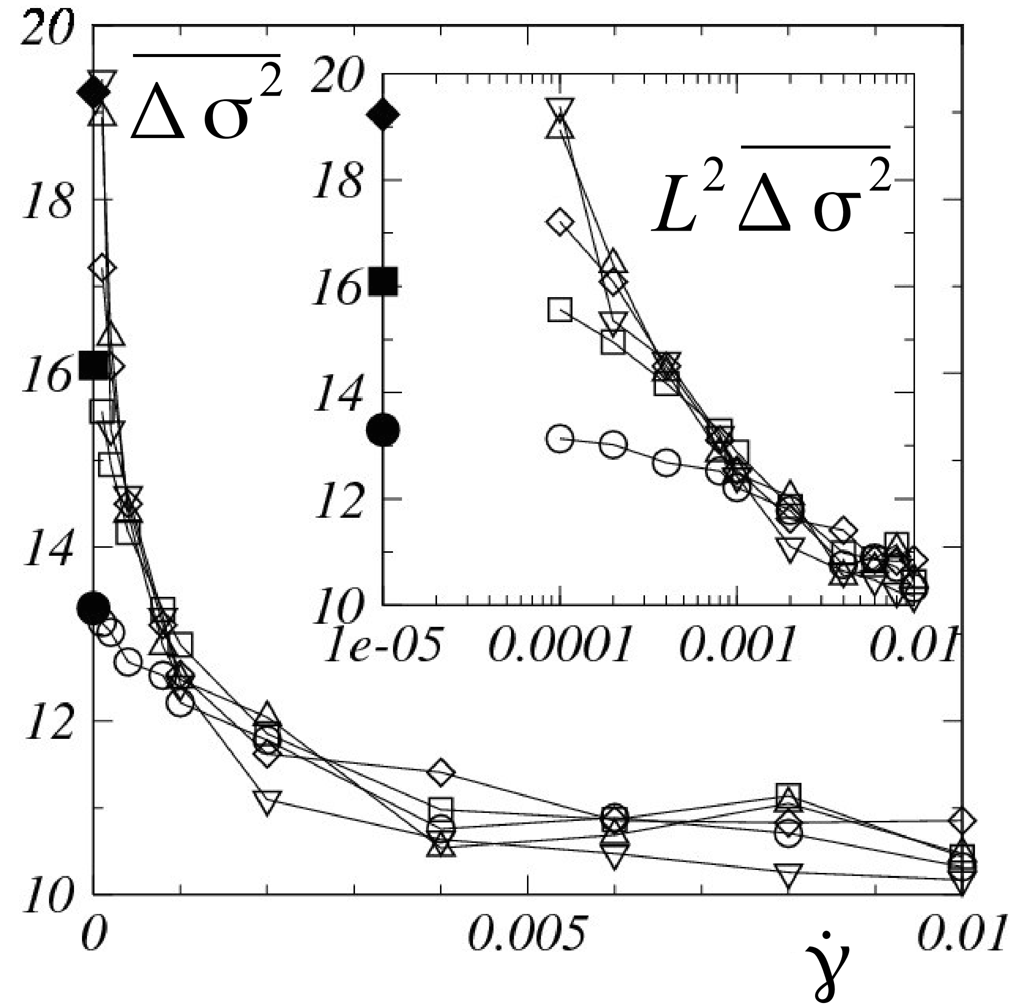
PRL 103, 065501 (2009)

$T < 10^{-4}$

Stress and stress fluctuations

PRL 103, 065501 (2009)





Herschel-Bulkley rheology

$$\sigma = \sigma_y + A\sqrt{\dot{\gamma}}$$

The stress fluctuations:

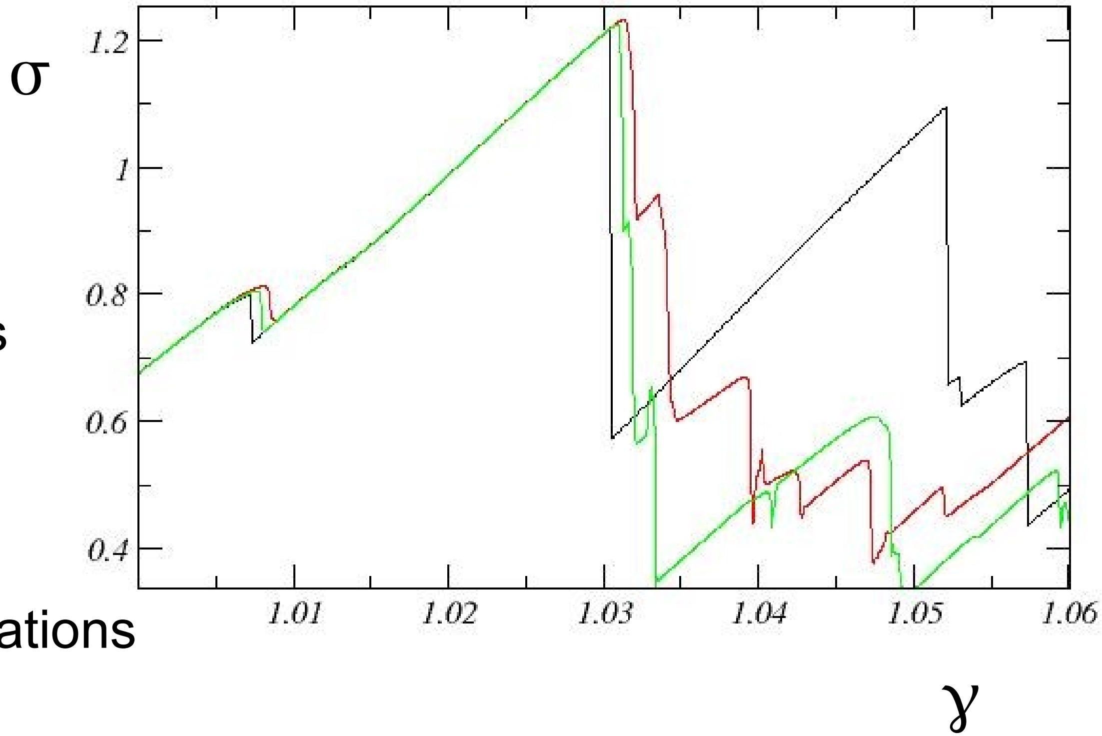
- converge to QS values when $\dot{\gamma} \to 0$
- present normal statistics when $\dot{\gamma} > 10^{-3}$

The strain field

From the dynamics of non-affine velocity field, we see that:
- flips generate quadrupolar displacement fields ~ shear transformations
- acoustic propagation of long range signals

so, the AQS picture seems to remain valid

yet:
- are flips correlated?
- are there avalanches?



<u>In the AQS limit:</u>

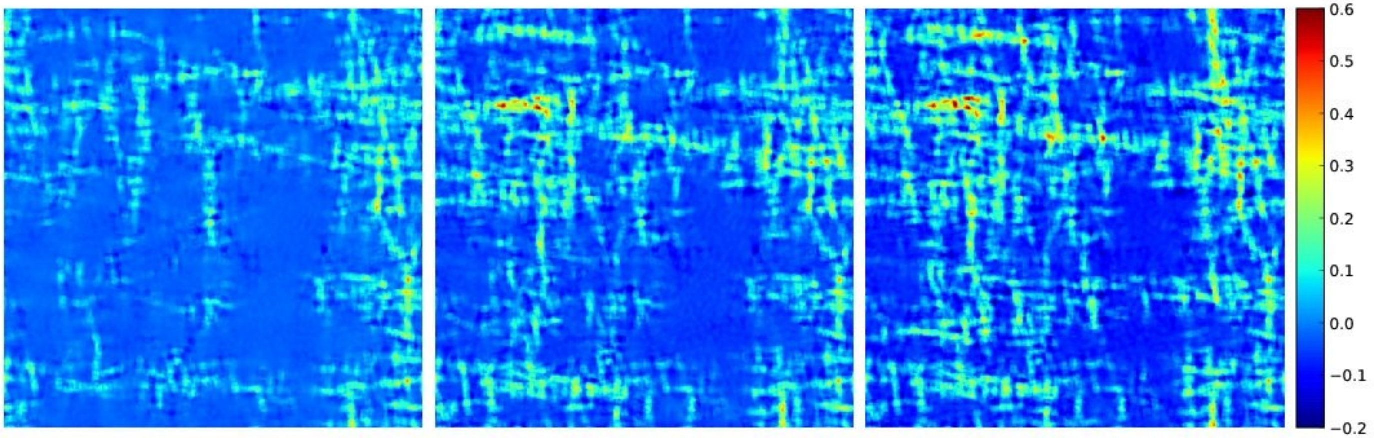
Plastic events = discontinuous drops
= avalanches

<u>At finite strain-rates:</u>

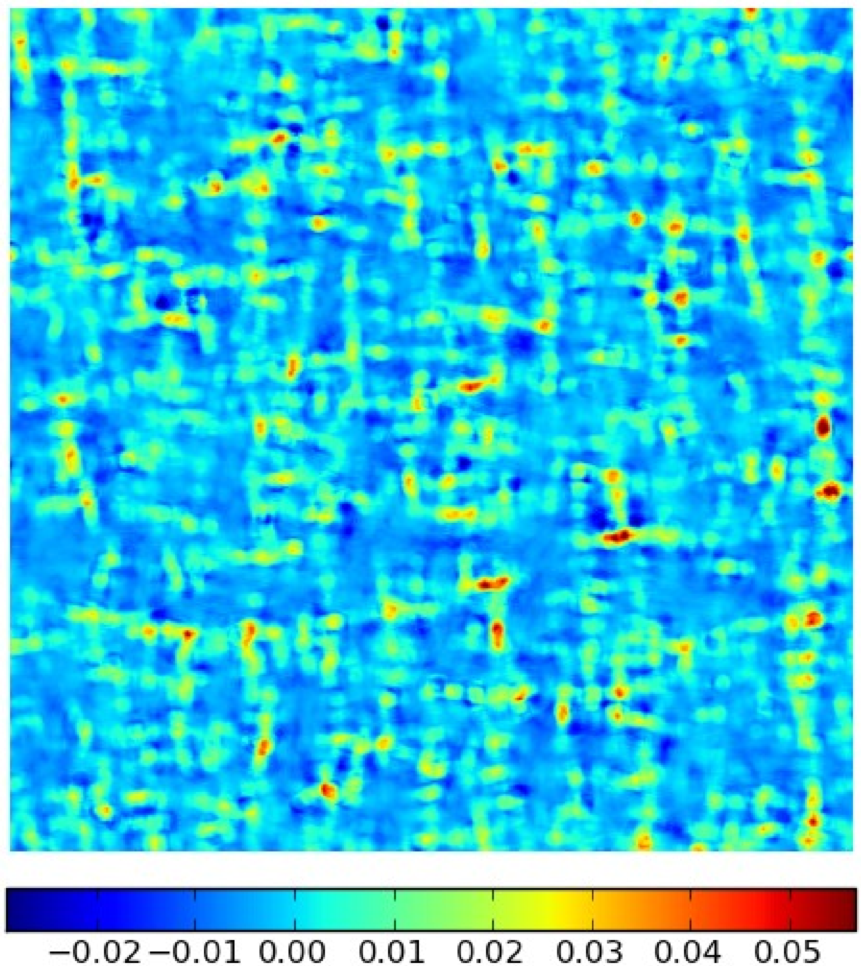
Flips and avalanches have finite durations

Deformation maps

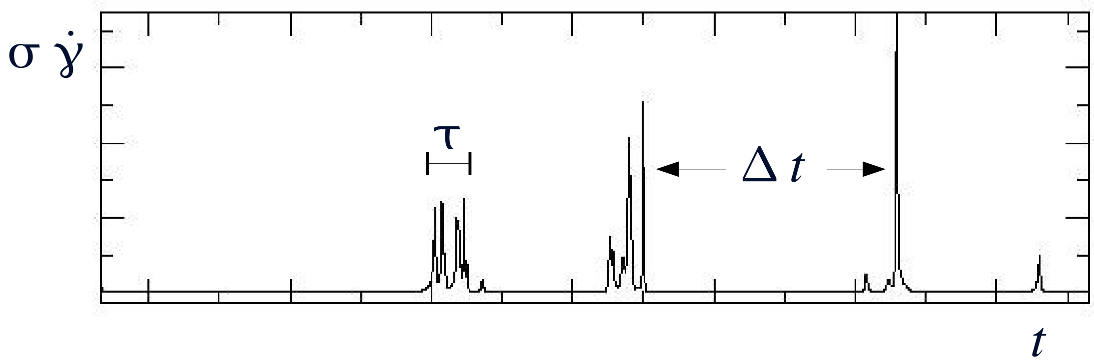
$\epsilon_{xy}(\vec{r})$



$\gamma = 1\%$ $\gamma = 5\%$ $\gamma = 20\%$


−0.02 −0.01 0.00 0.01 0.02 0.03 0.04 0.05

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



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

Average interval — event duration

event duration → single flips? / avalanches?

Estimating the flip rate...

Each flips releases on average:

a strain $\Delta \epsilon_0$

in a region of size a^2

In steady state, over a large strain interval:

$N_f(\Delta \gamma)$

Average number of flips?

Each Eshelby flip induces:

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

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

$$\Delta \overline{\sigma_{xy}} = \frac{2 \mu a^2 \Delta \epsilon_0}{L^2}$$

Estimating the flip rate...

Each flips releases on average:

a strain $\Delta \epsilon_0$

in a region of size a^2

In steady state, over a large strain interval:

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

Average number of flips

Each Eshelby flip induces:

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

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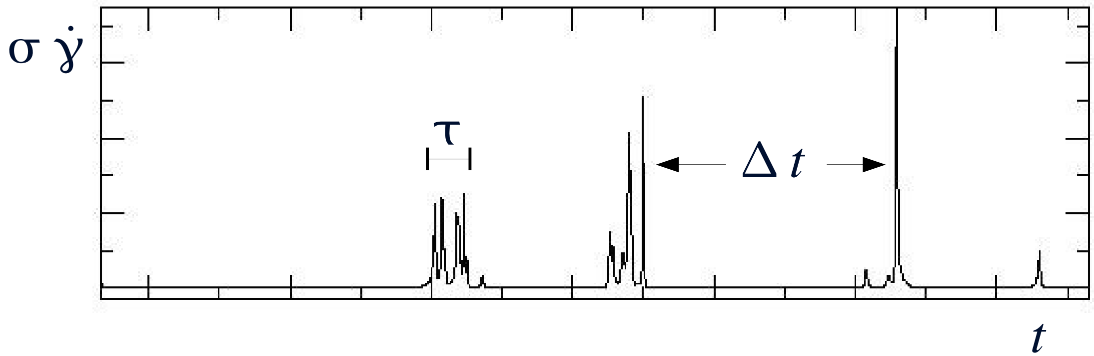
$$\Delta\overline{\sigma_{xy}} = \frac{2\mu a^2\Delta\epsilon_0}{L^2}$$

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

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



$$\dot{\gamma} \ll \dot{\gamma}_c \approx \Delta\epsilon_0\, a\, c_s / L^2$$

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

Average interval

event duration

single flips?

avalanches?

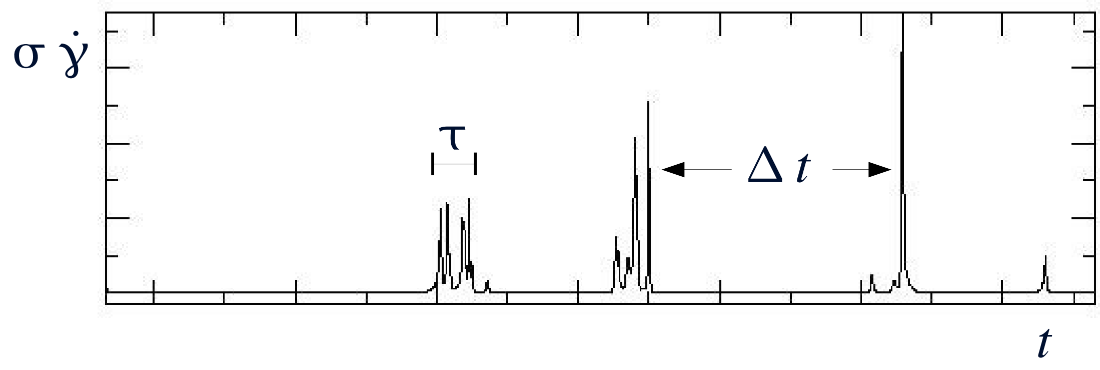
$$\tau_{\rm flip} \sim a/c_s$$

$$\langle \Delta t_{\rm flip} \rangle = \frac{a^2}{L^2}\frac{\Delta\epsilon_0}{\dot{\gamma}}$$

Atomic glass:

$a \sim 1\,\mathrm{nm} \quad L \sim 1\,\mathrm{mm} \;\rightarrow\; \dot{\gamma}_c \sim 4.10^{-2}\,\mathrm{s}^{-1}$

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



$$\dot{\gamma} \ll \dot{\gamma}_c \approx \Delta \epsilon_0 \, a \, c_s / L^2$$

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

Average interval

event duration

- single flips?
- avalanches?

$$\tau_{flip} \sim a/c_s$$

$$\langle \Delta t_{flip} \rangle = \frac{a^2}{L^2} \frac{\Delta \epsilon_0}{\dot{\gamma}}$$

$$\dot{\gamma} \ll \dot{\gamma}_c a/L$$

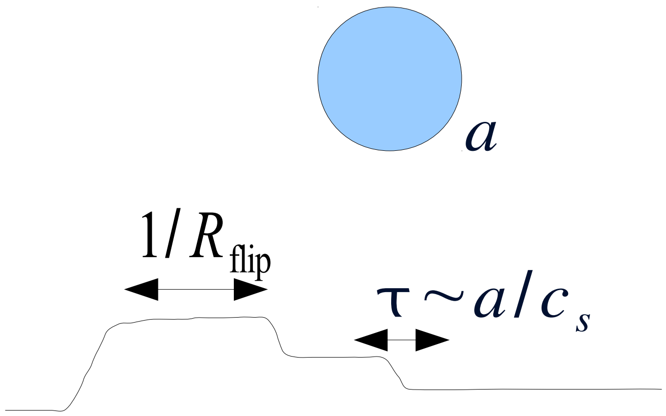
Atomic glass:

$a \sim 1\,\mathrm{nm} \quad L \sim 1\,\mathrm{mm} \rightarrow \quad \dot{\gamma}_c \sim 4.10^{-2}\,\mathrm{s}^{-1}$

What is the noise received by a weak zone?

System size: L

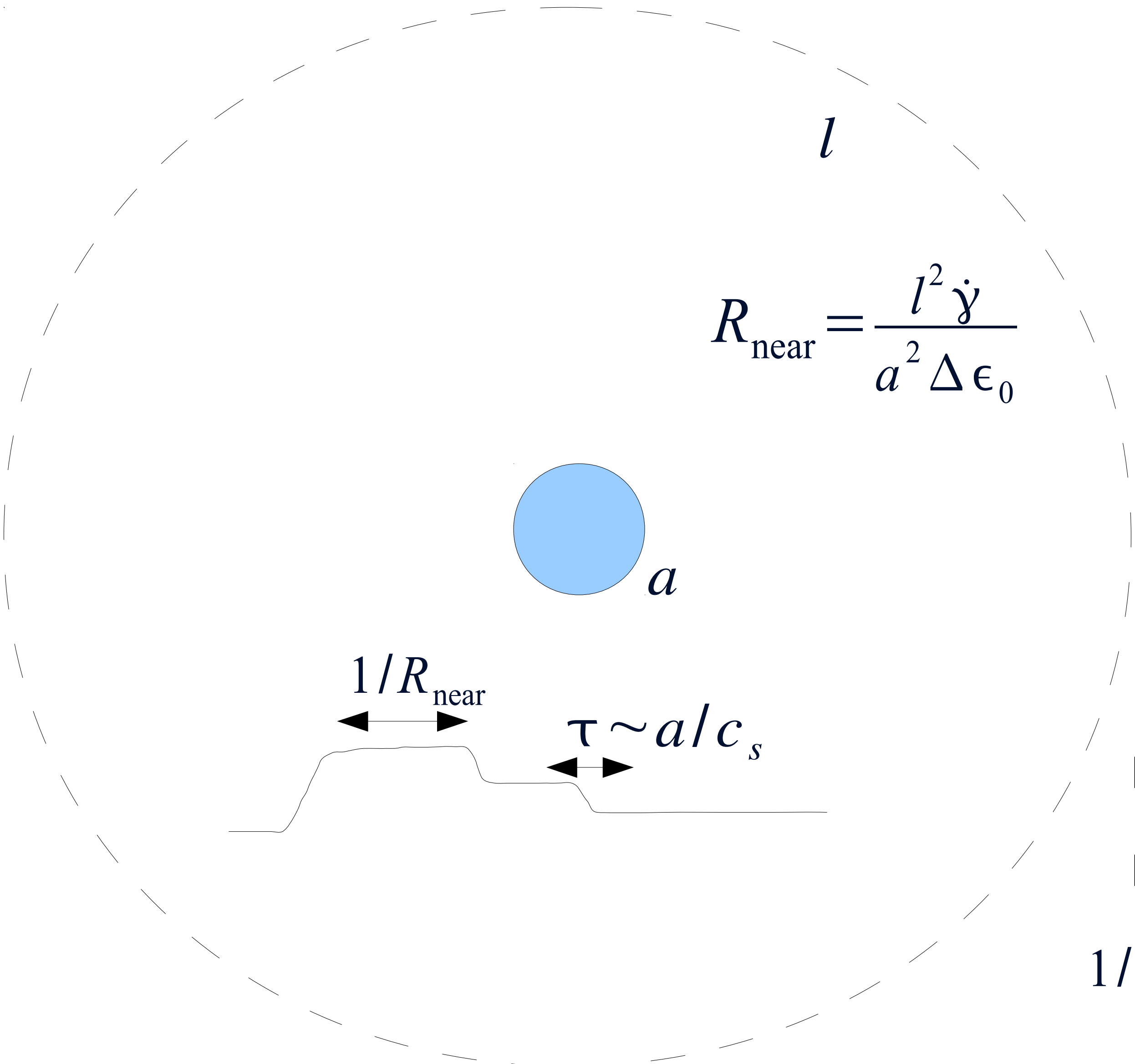
Total flip rate: $R_{\text{flip}} = \dfrac{L^2 \dot{\gamma}}{a^2 \Delta \epsilon_0}$



Previous estimate provides condition when signals
originating from the whole system
overlap

yet, are all signals equal?

What is the noise received by a weak zone?



System size: L

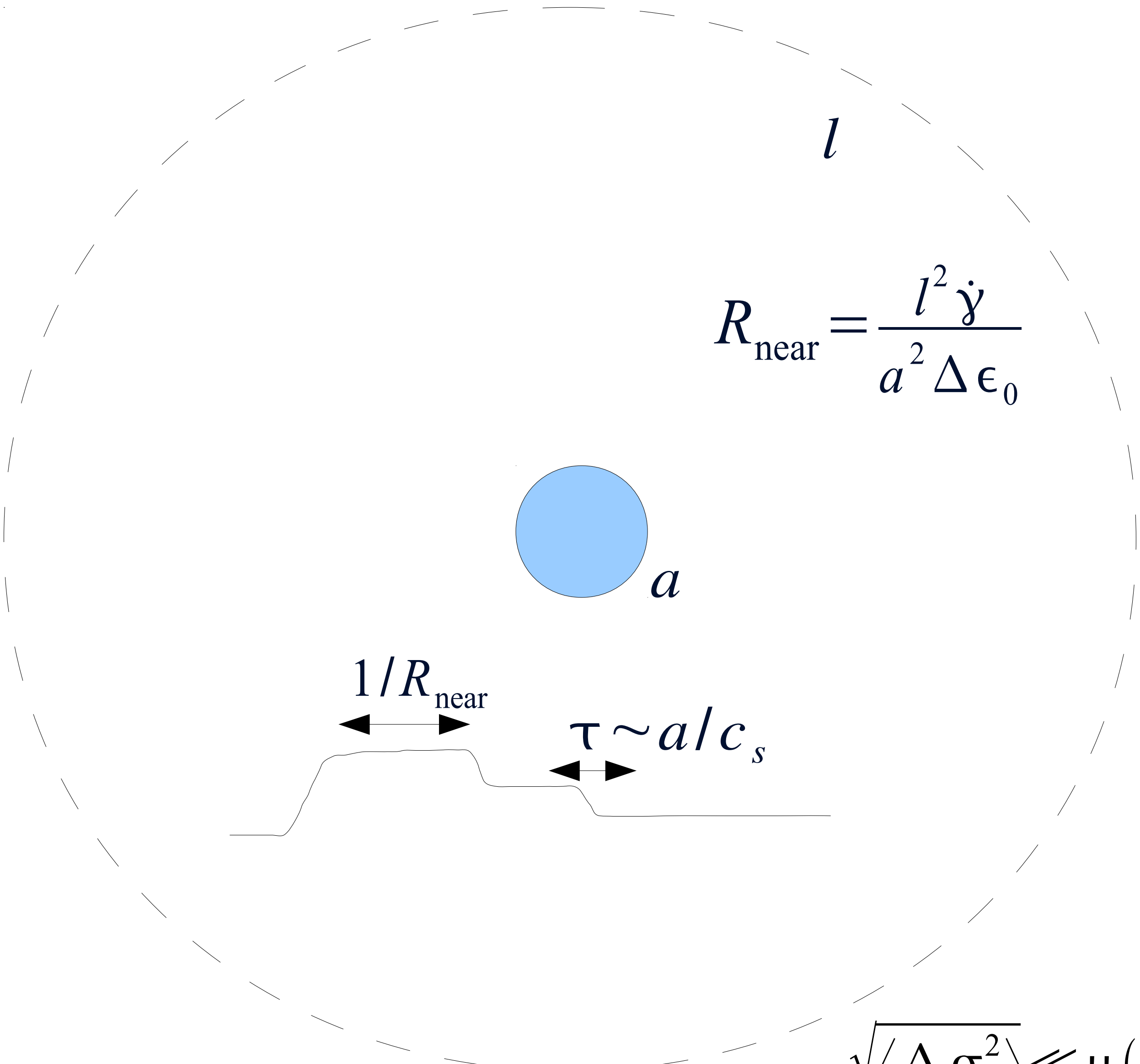
Total flip rate: $R_{\text{flip}} = \frac{L^2 \dot{\gamma}}{a^2 \Delta \epsilon_0}$

Now isolate a nearby region of size l

Near field signals are separated iff:

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

What is the noise received by a weak zone?



$$R_{\text{near}} = \frac{l^2 \dot{\gamma}}{a^2 \Delta \epsilon_0}$$

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

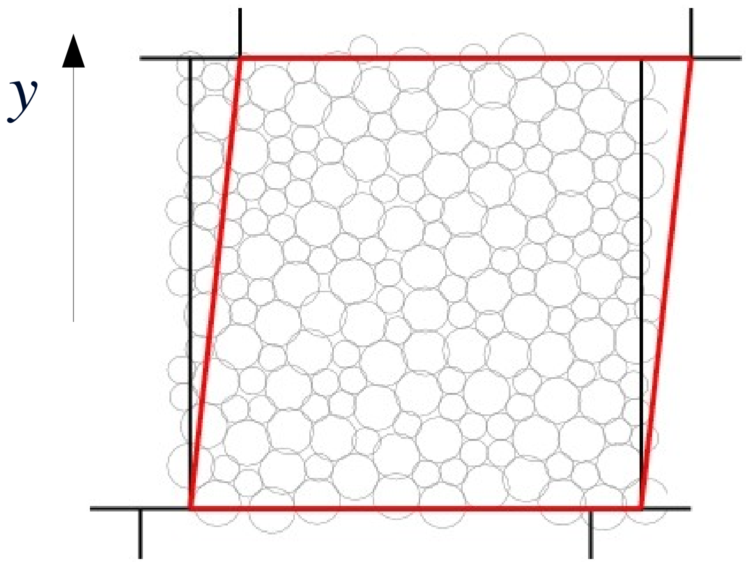
Local stress diffuses by:

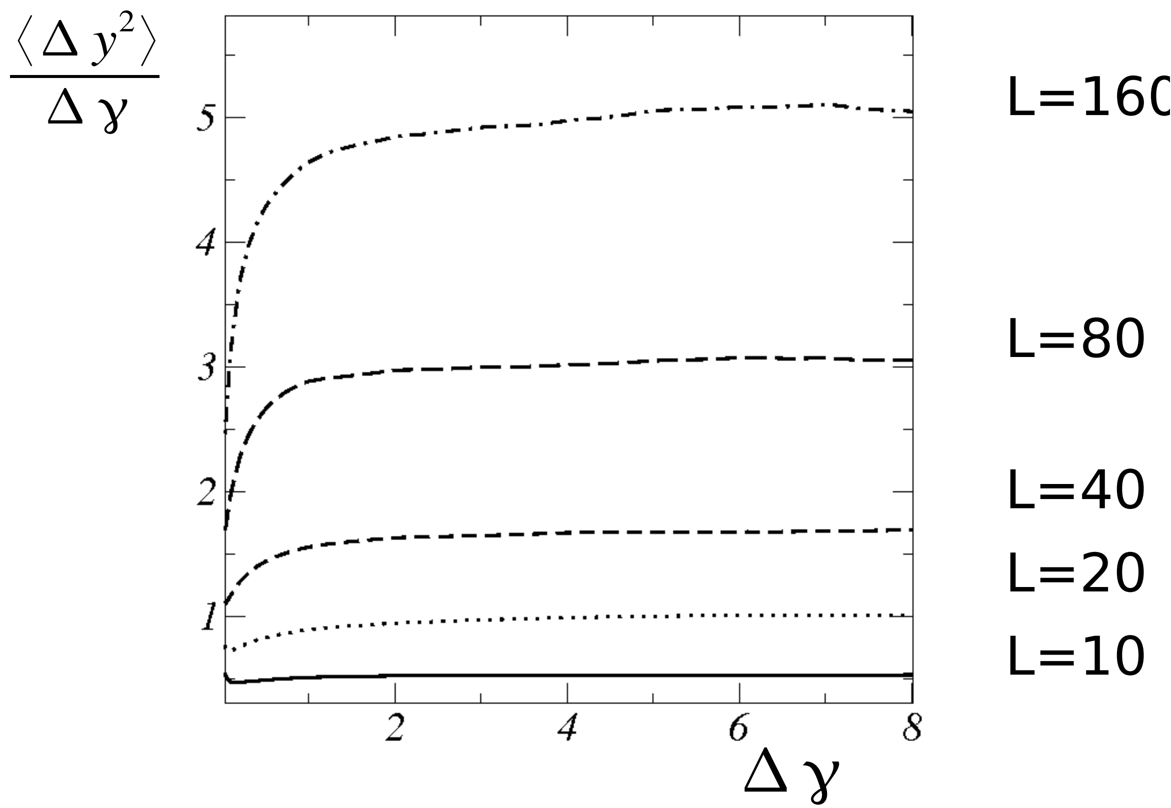
$$\langle \Delta \sigma^2 \rangle \sim \dot{\gamma} \tau (\mu^2 a^2 \Delta \epsilon_0 / l^2)$$

$$\sqrt{\langle \Delta \sigma^2 \rangle} \ll \mu (a^2 \Delta \epsilon_0 / l^2) \Leftrightarrow l \ll \sqrt{a^2 \Delta \epsilon_0 / \dot{\gamma} \tau_{\text{flip}}}$$

How to characterize avalanches?

Transverse diffusion coefficient





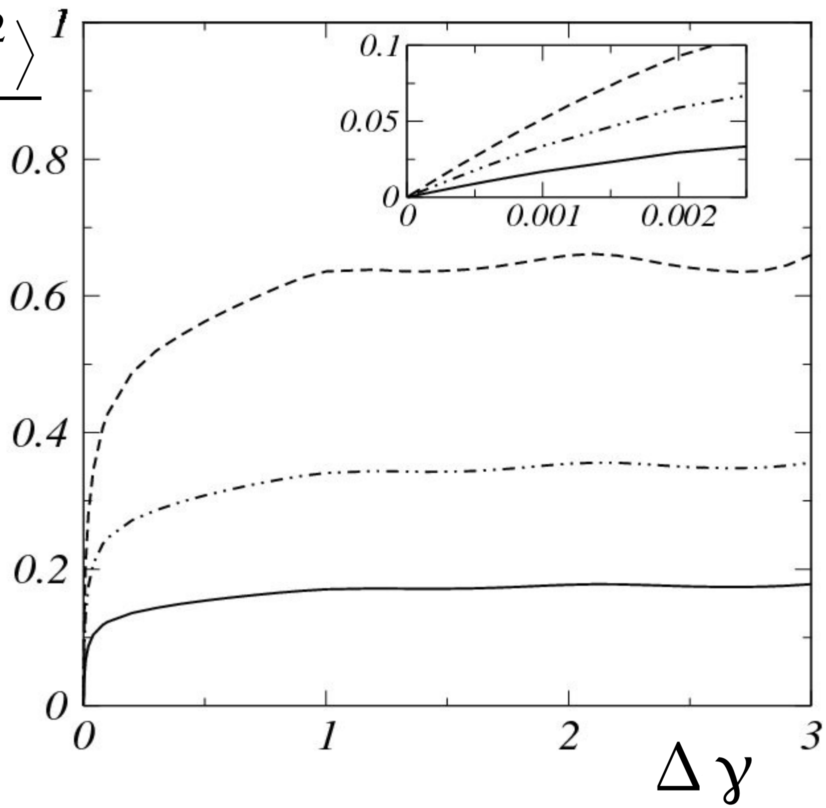
$$\frac{\langle \Delta y^2 \rangle}{\Delta \gamma} \longrightarrow \widehat{D} = D / \dot{\gamma}$$

with L

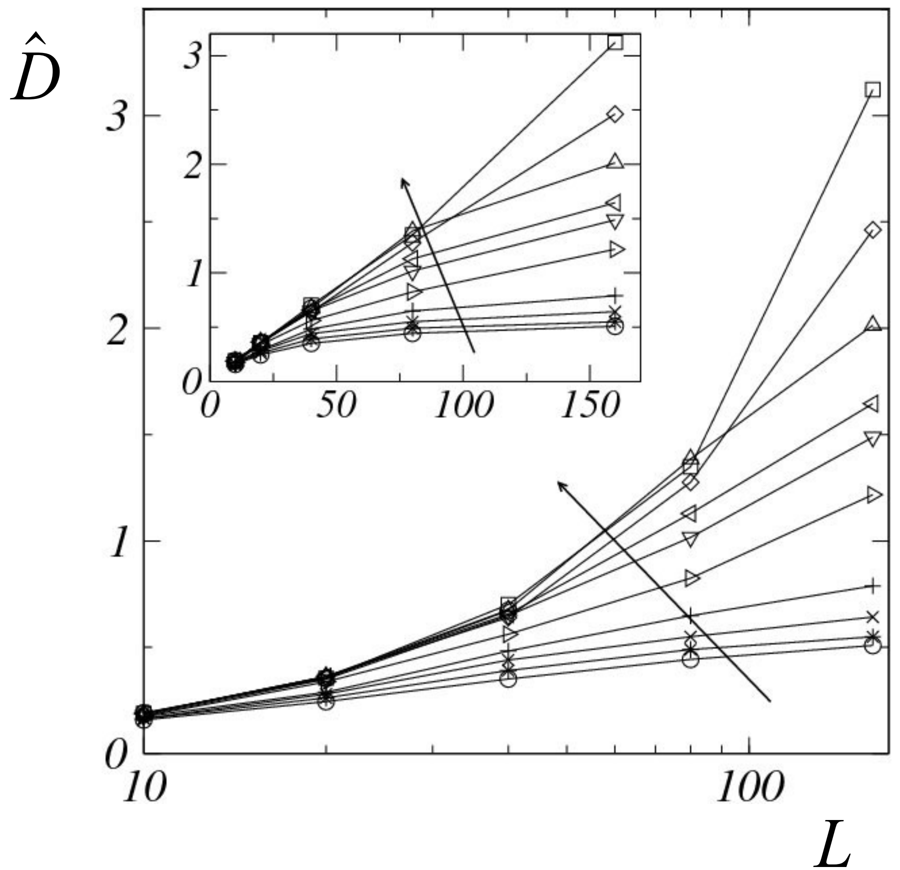
Transverse diffusion at finite strain rate

Track the transverse motion of particles:

$$\frac{\langle \Delta y^2 \rangle}{\Delta \gamma}$$



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



$$\hat{D}(\dot{\gamma}, L) \sim \ln L \qquad (\dot{\gamma} = 10^{-2})$$
$$\sim L \qquad (\dot{\gamma} = 10^{-4})$$

JACKS School, Bengalore 2012

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>

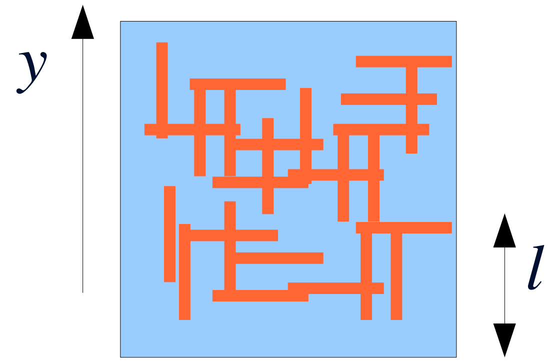
$$N_f(\Delta\gamma) = \frac{L^2 \Delta\gamma}{a^2 \Delta\epsilon_0}$$

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

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

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

<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)

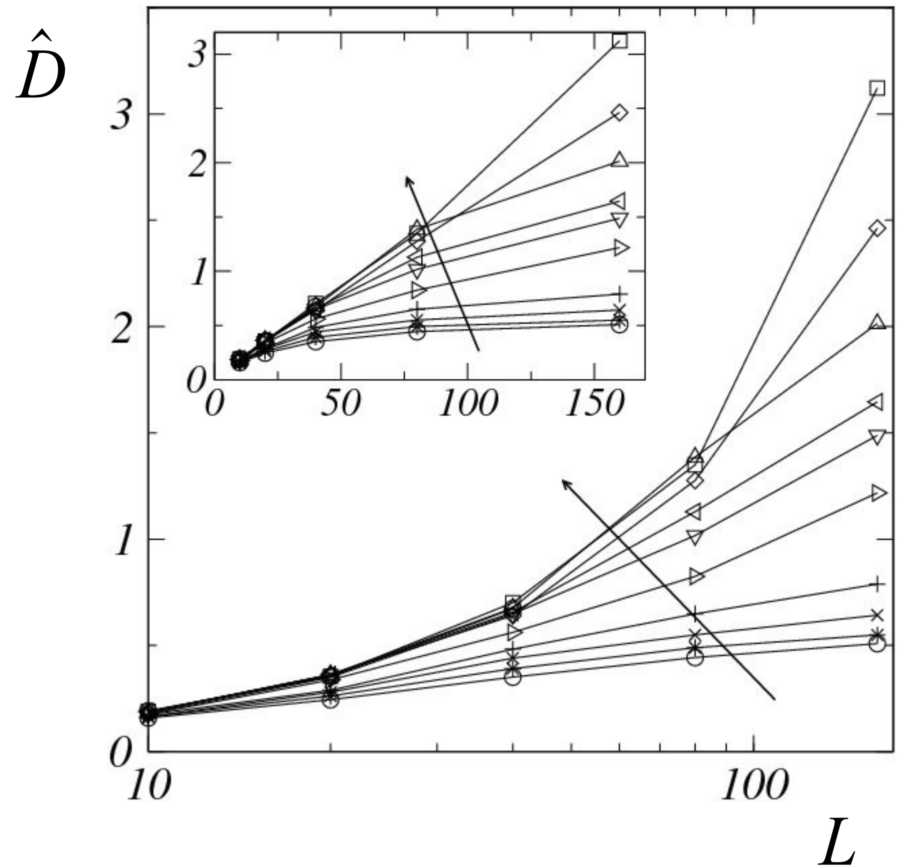
Athermal, finite strain rate: transverse diffusion

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

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

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

QS regime



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

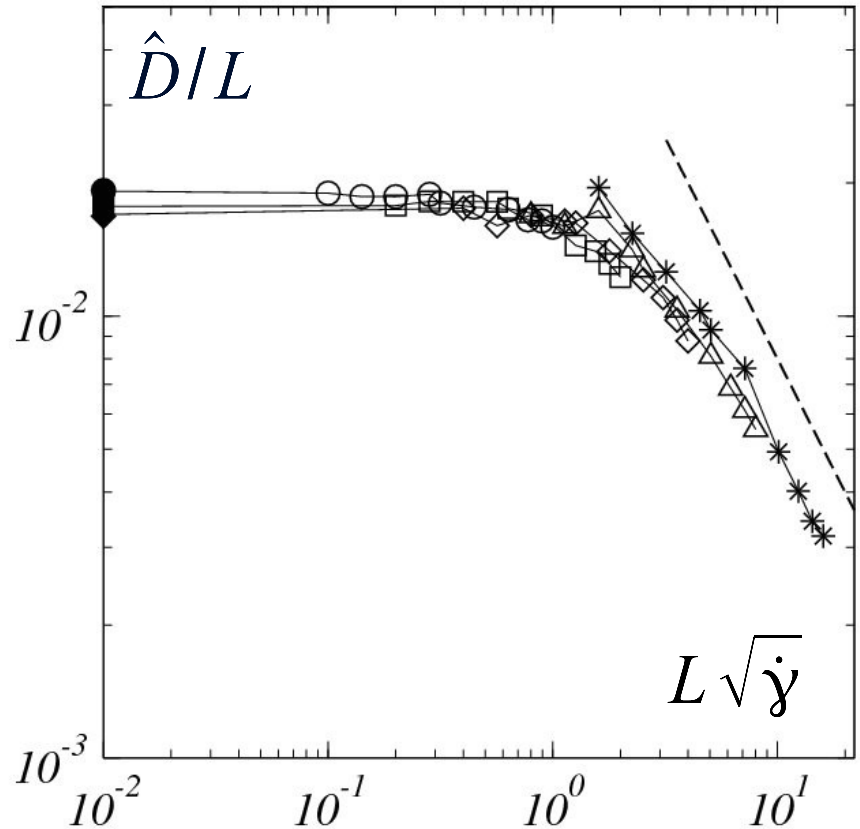
Athermal, finite strain rate: transverse diffusion

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

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

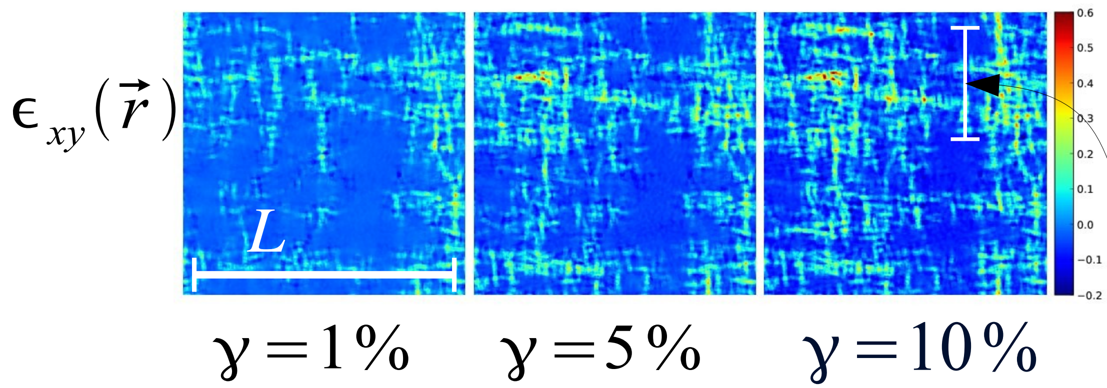
$\dot{\gamma} \to 0 \Rightarrow l \sim L \qquad \hat{D} \sim L$

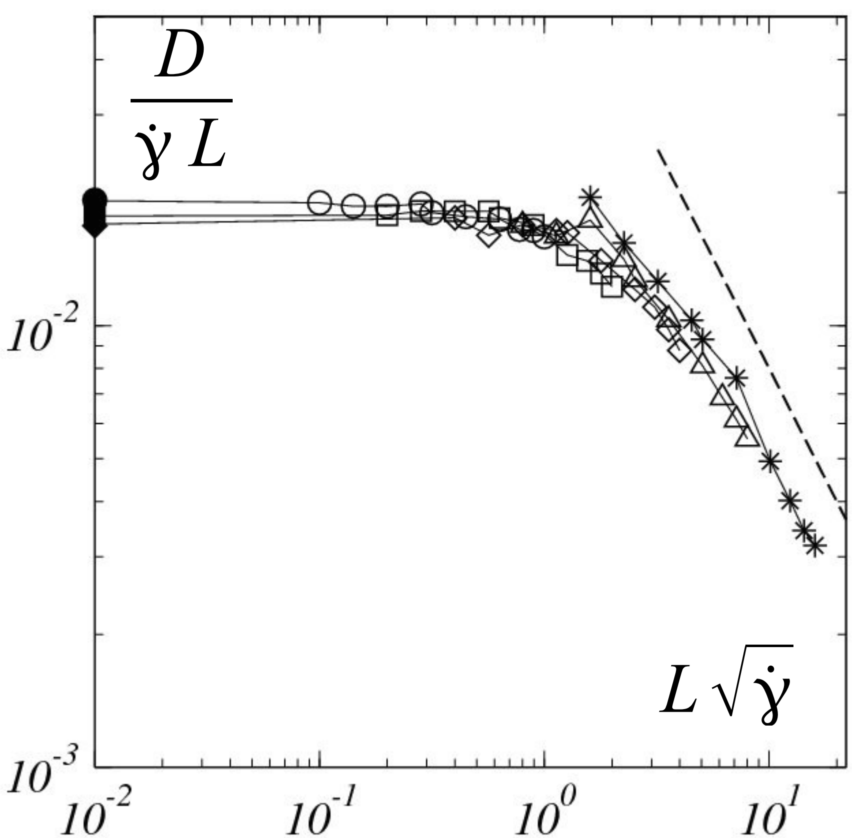
QS regime

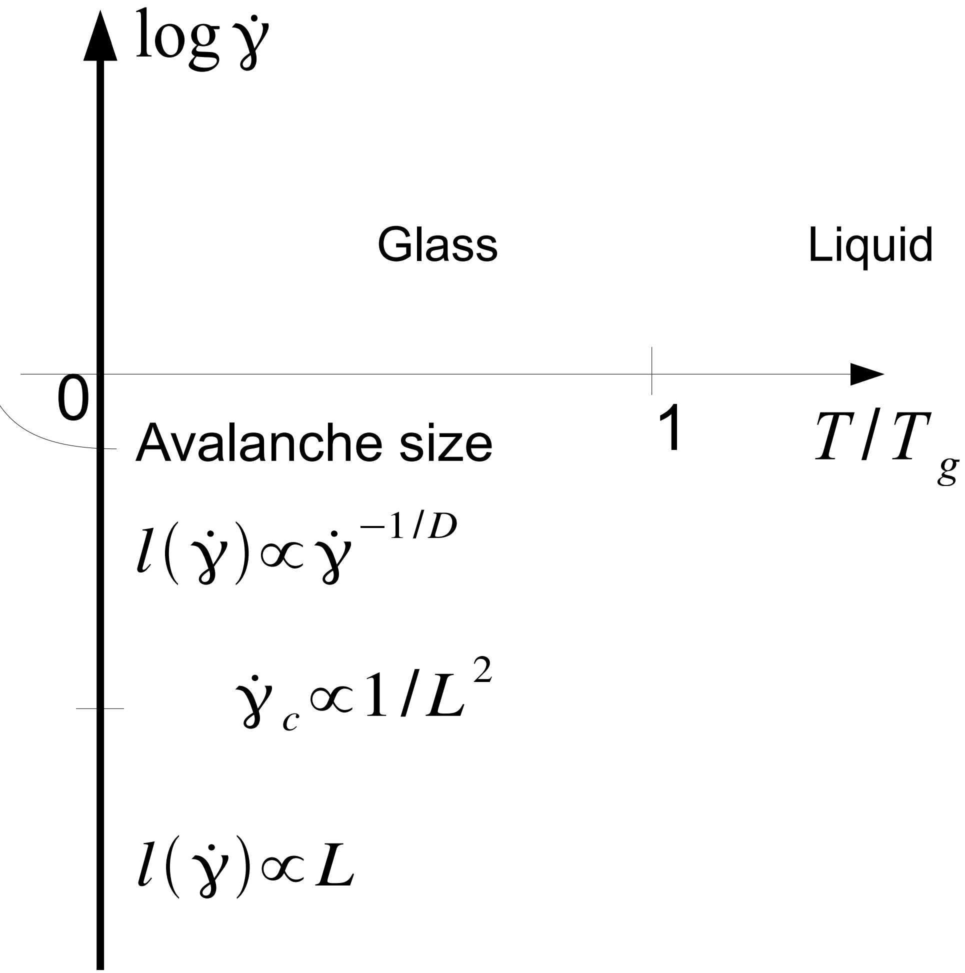


Using $l(\dot{\gamma}) \propto 1/\sqrt{\dot{\gamma}} \Rightarrow \hat{D}/L = f(L\sqrt{\dot{\gamma}})$

Athermal, finite-strain rate







Inferences

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

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

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

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

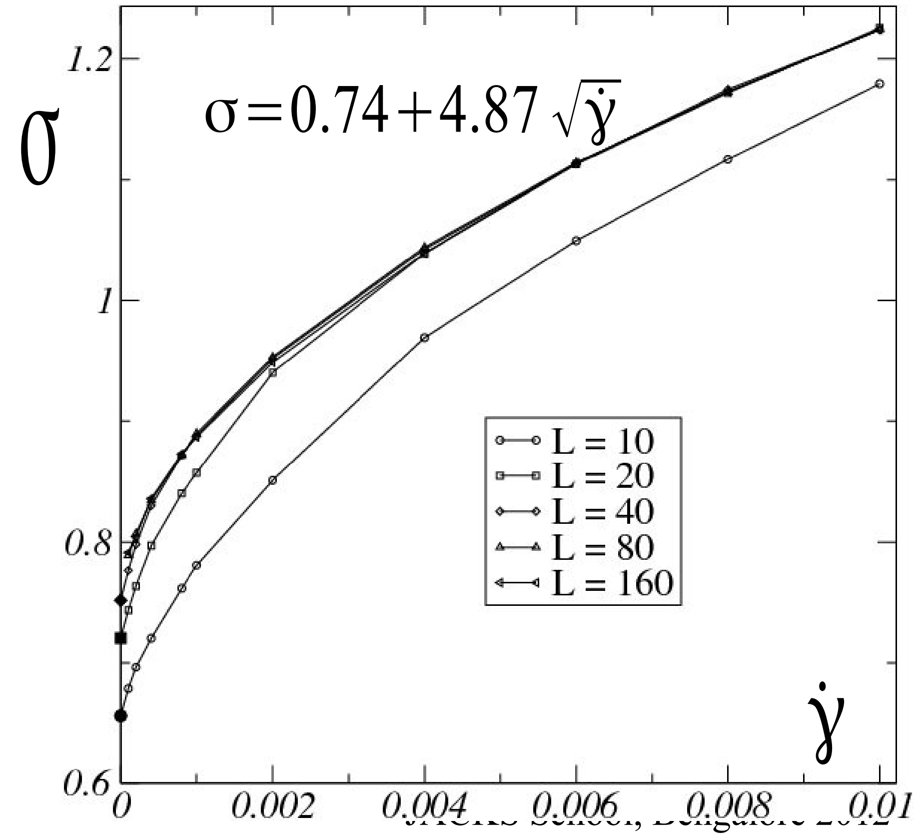
guess: $\sigma - \sigma_y \approx \mu\dot\gamma\,\tau_{\rm av}$

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

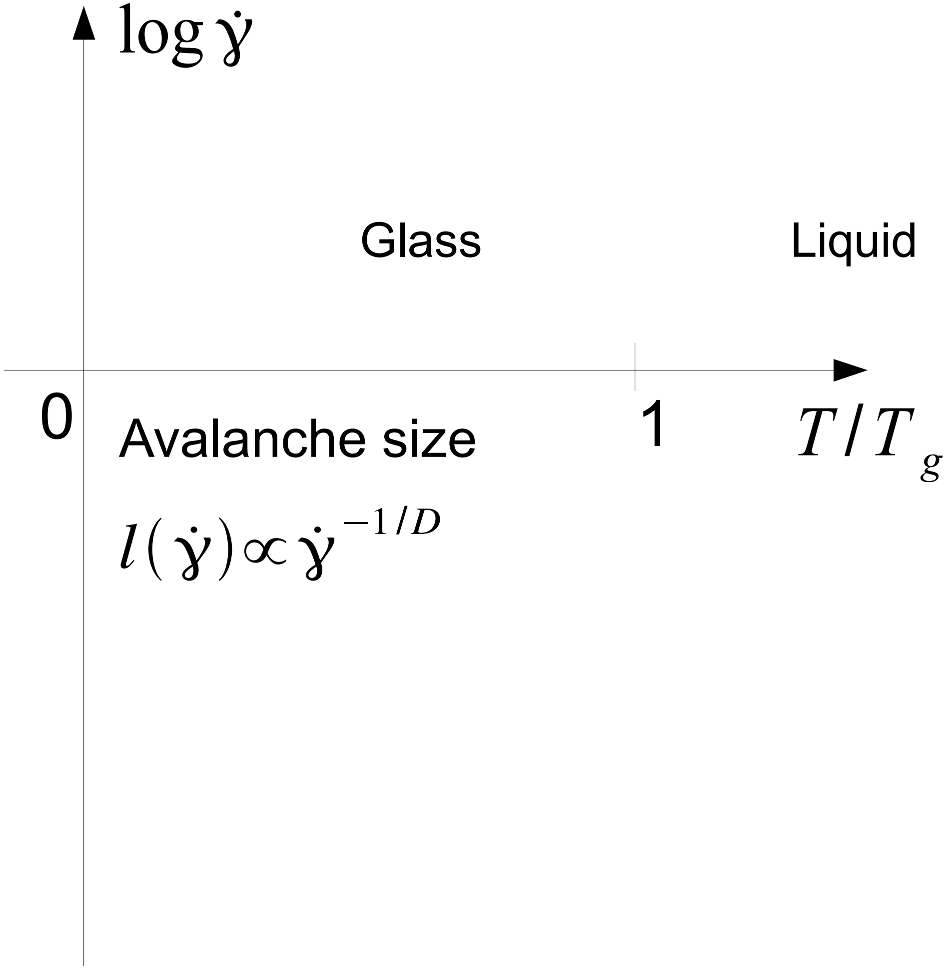
$\Rightarrow$

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

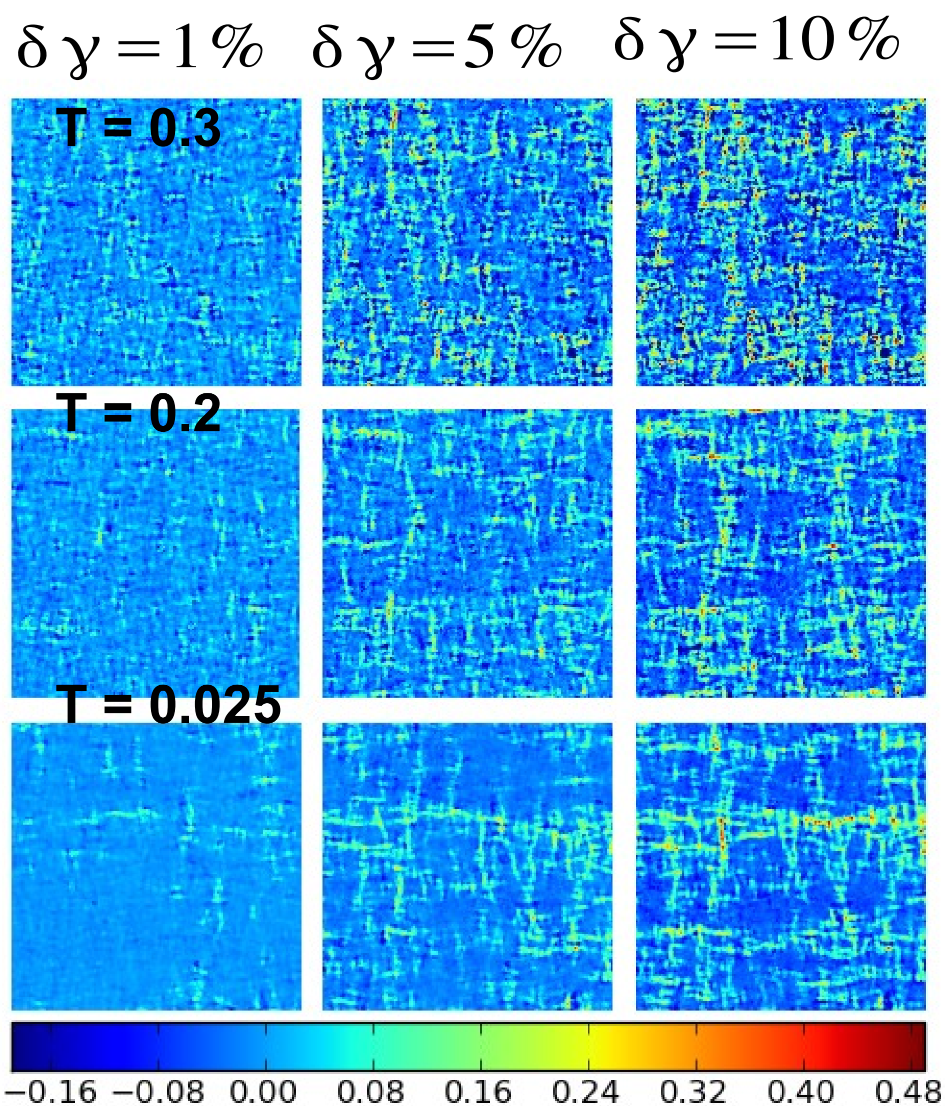
$$C = \frac{\mu}{2c_s} a^2 \frac{\Delta\epsilon_0}{\tau} \approx 6.5$$

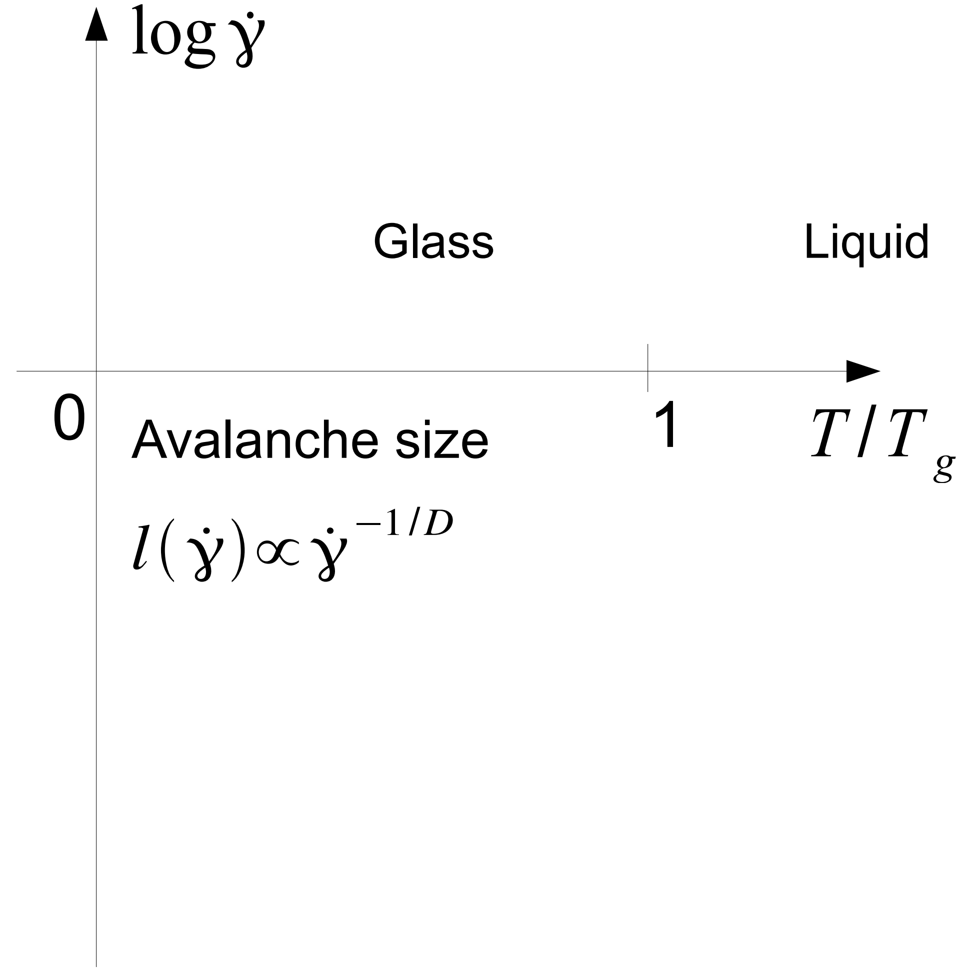


At finite temperature



At finite temperature



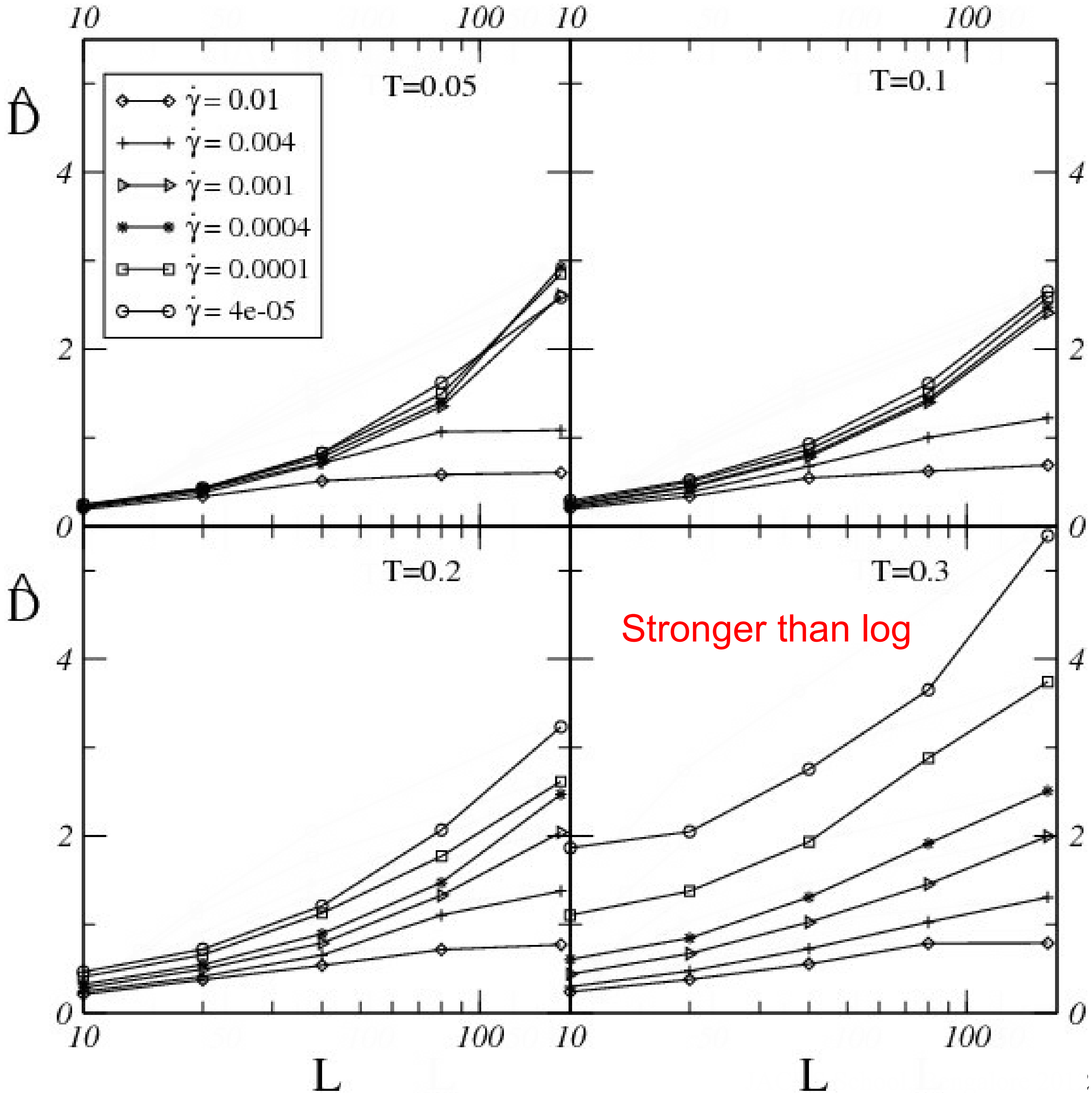


Chattoraj *et al* PRL 105, 266001 (2010)

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

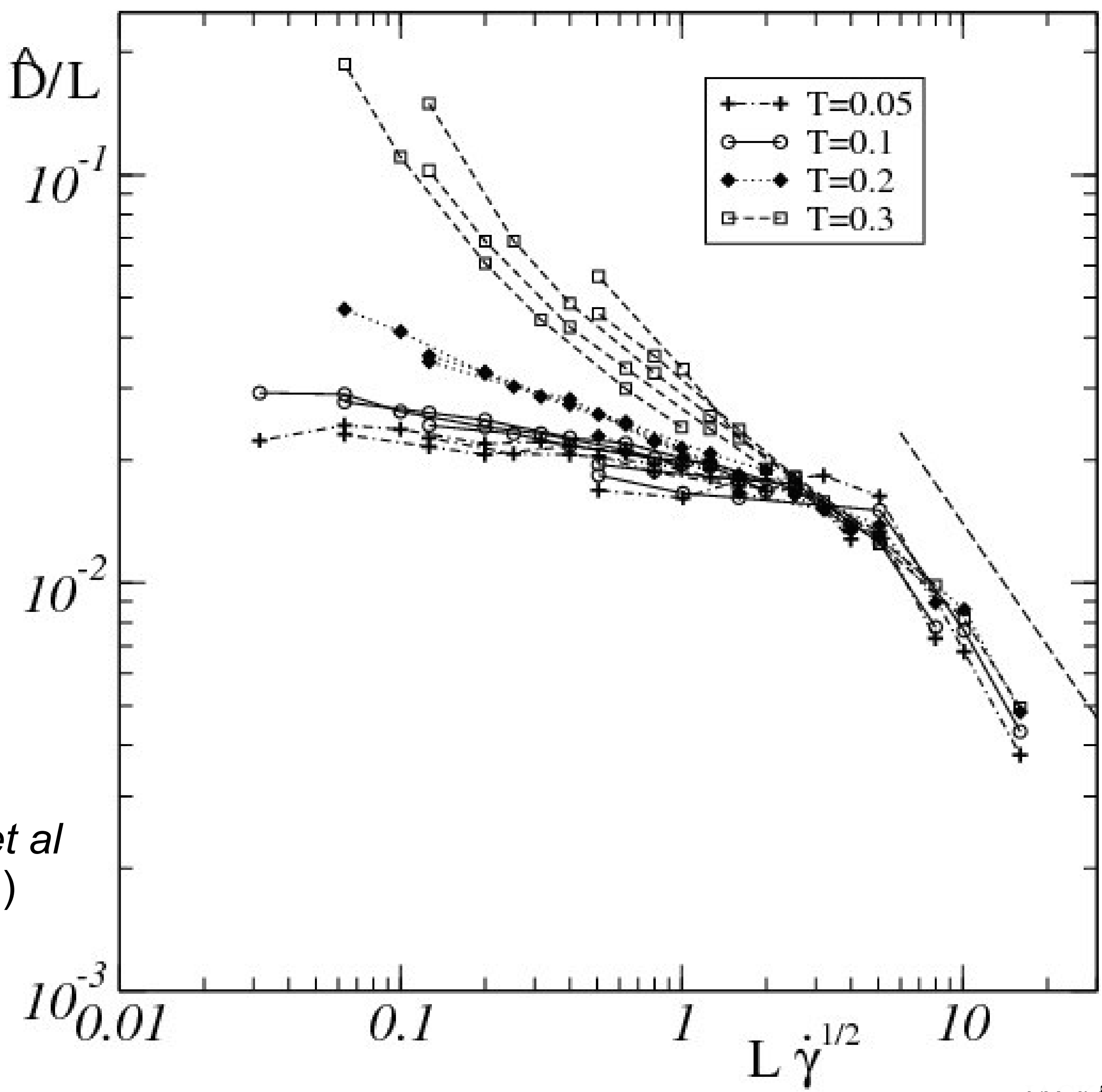
- Standard MD simulation
- Velocity rescaling

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



Chattoraj *et al* PRE (2011)

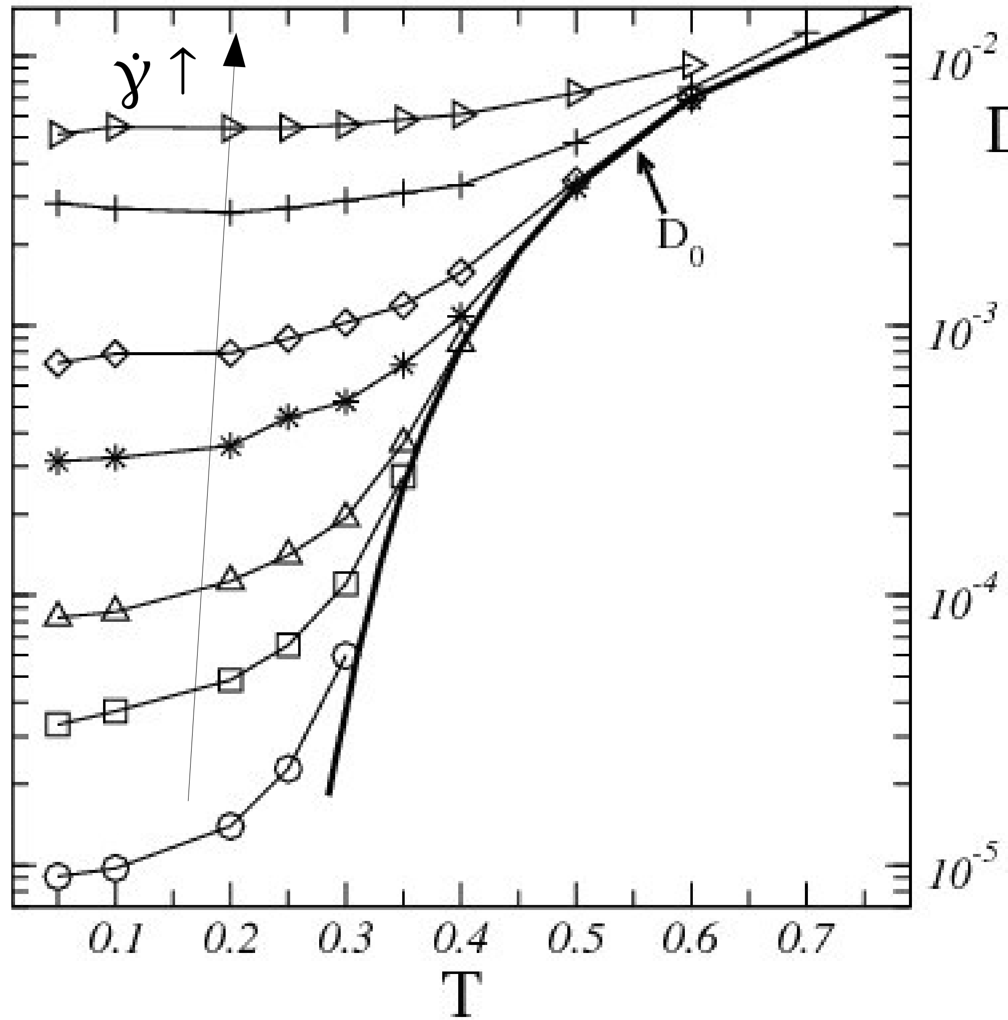
At finite T



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

Chattoraj *et al*
PRE (2011)

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

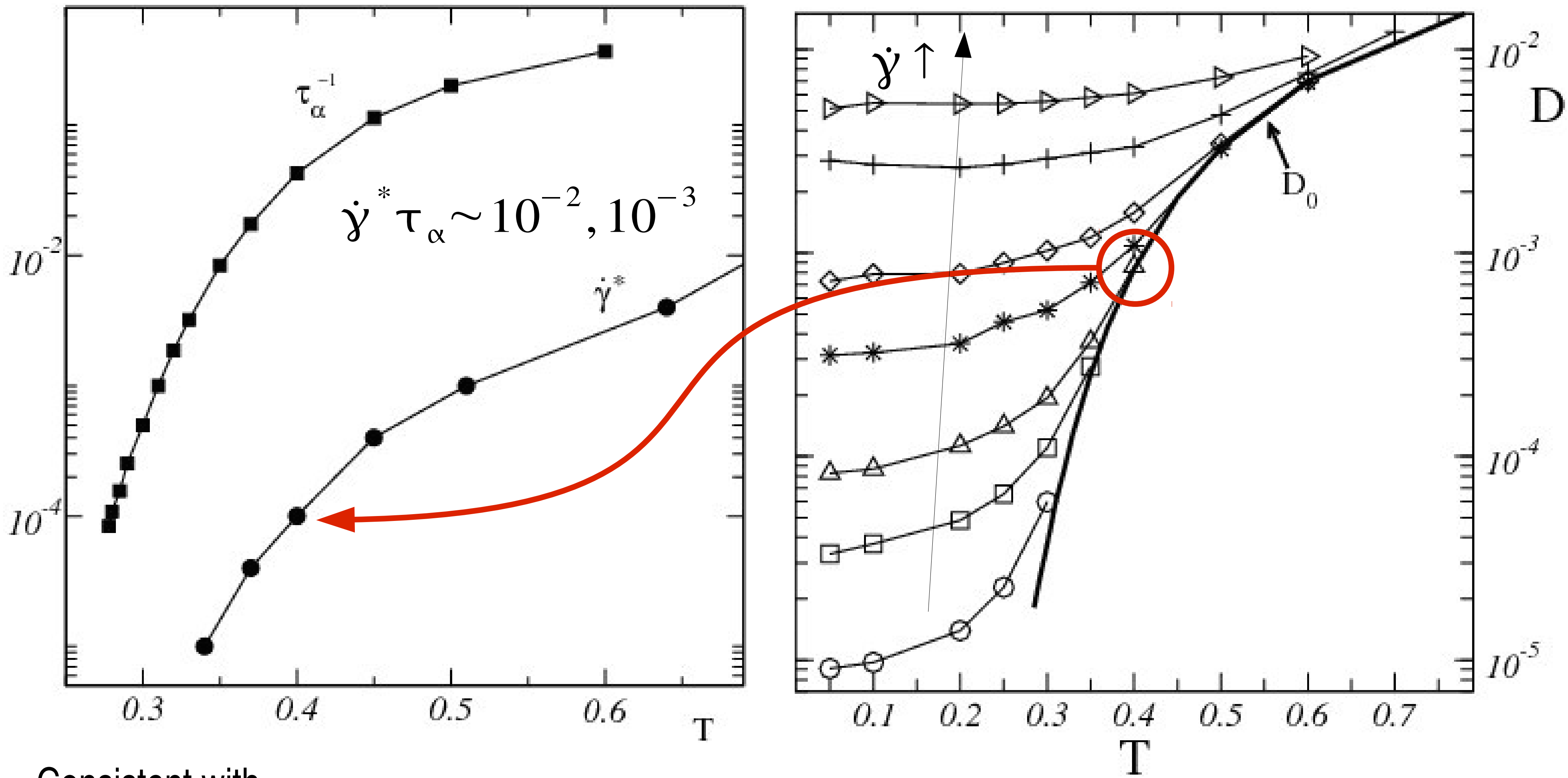


<u>Finite T, finite strain-rate simulations:</u> $T \neq 0 \quad \dot{\gamma} \neq 0$

- Standard MD simulation
- Velocity rescaling

Chattoraj *et al*, *PRE 2011*

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

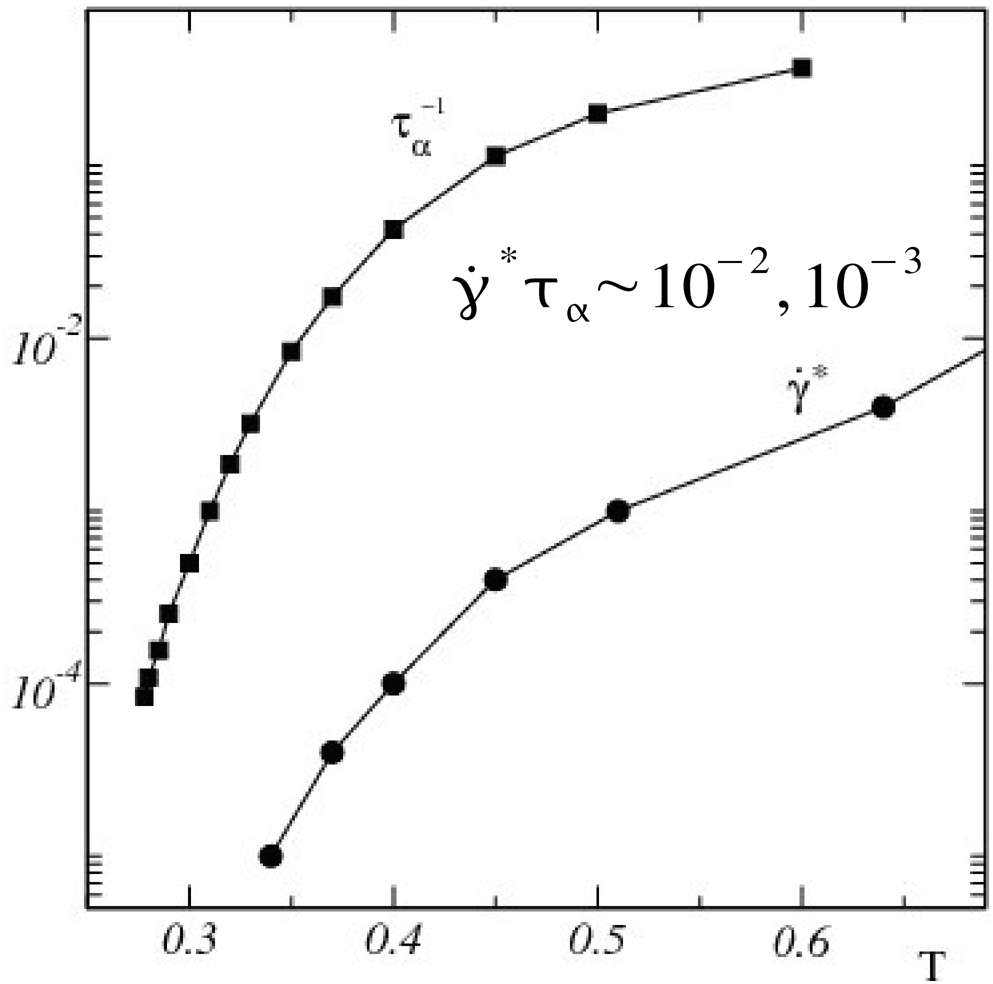


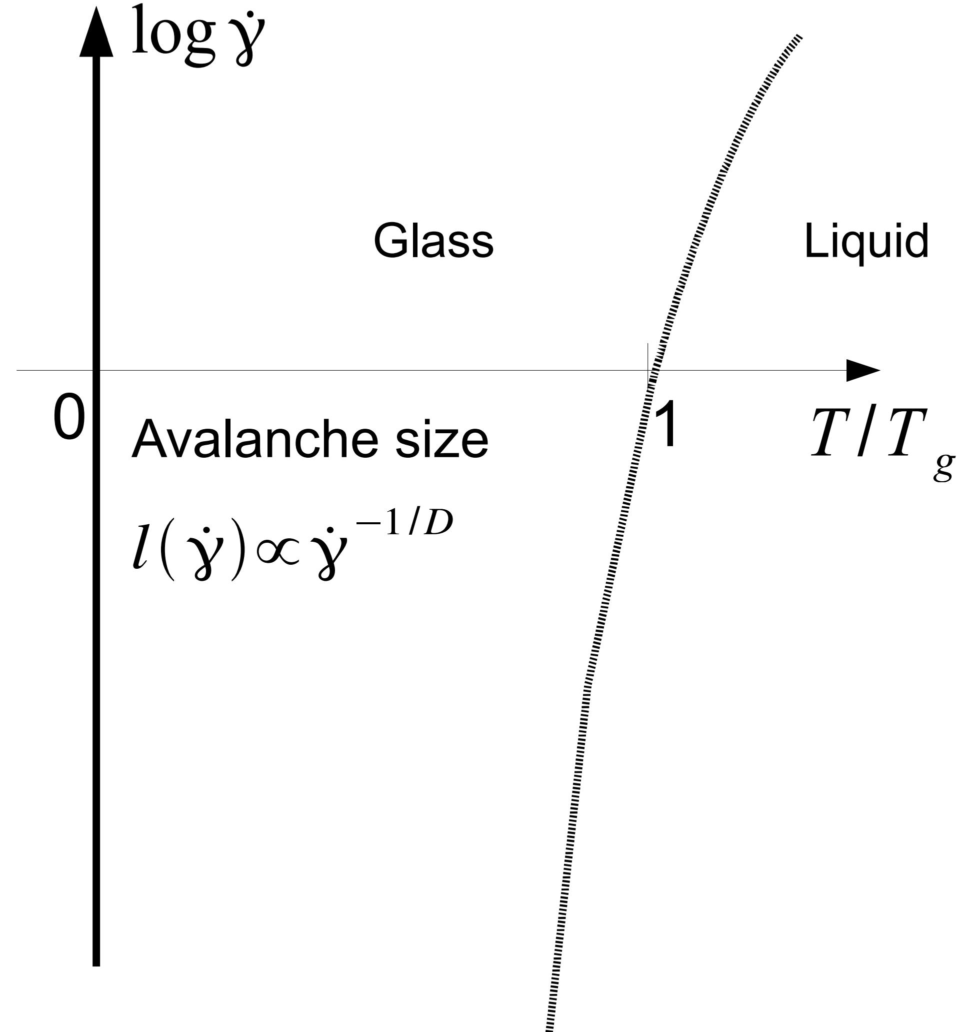
Consistent with Furukawa et al, PRL (2009)

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

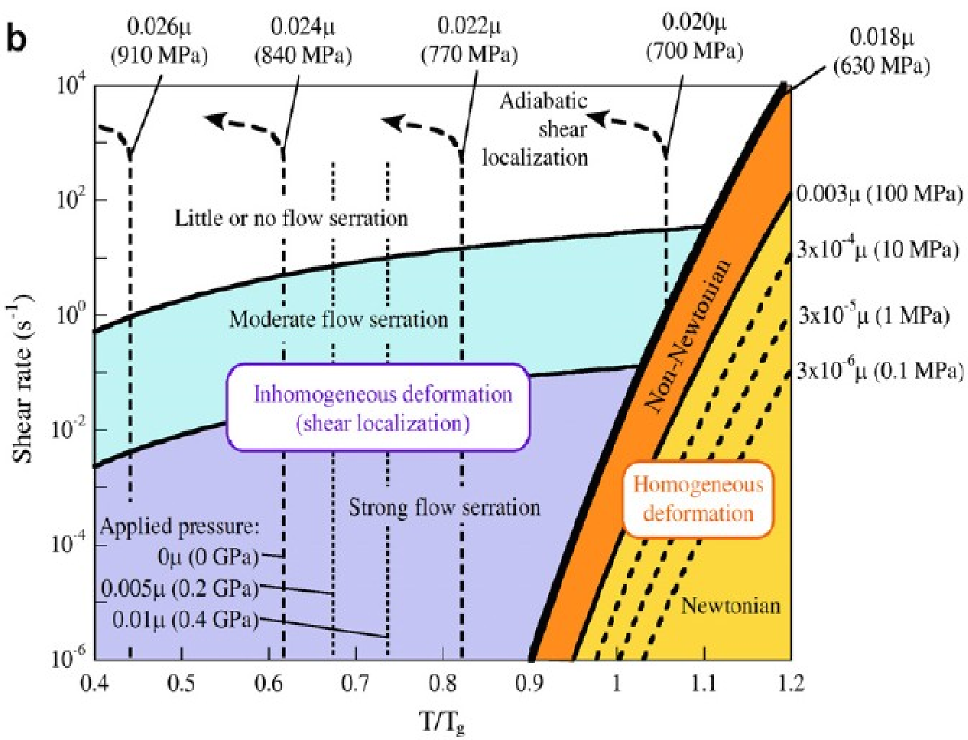
- Standard MD simulation
- Velocity rescaling

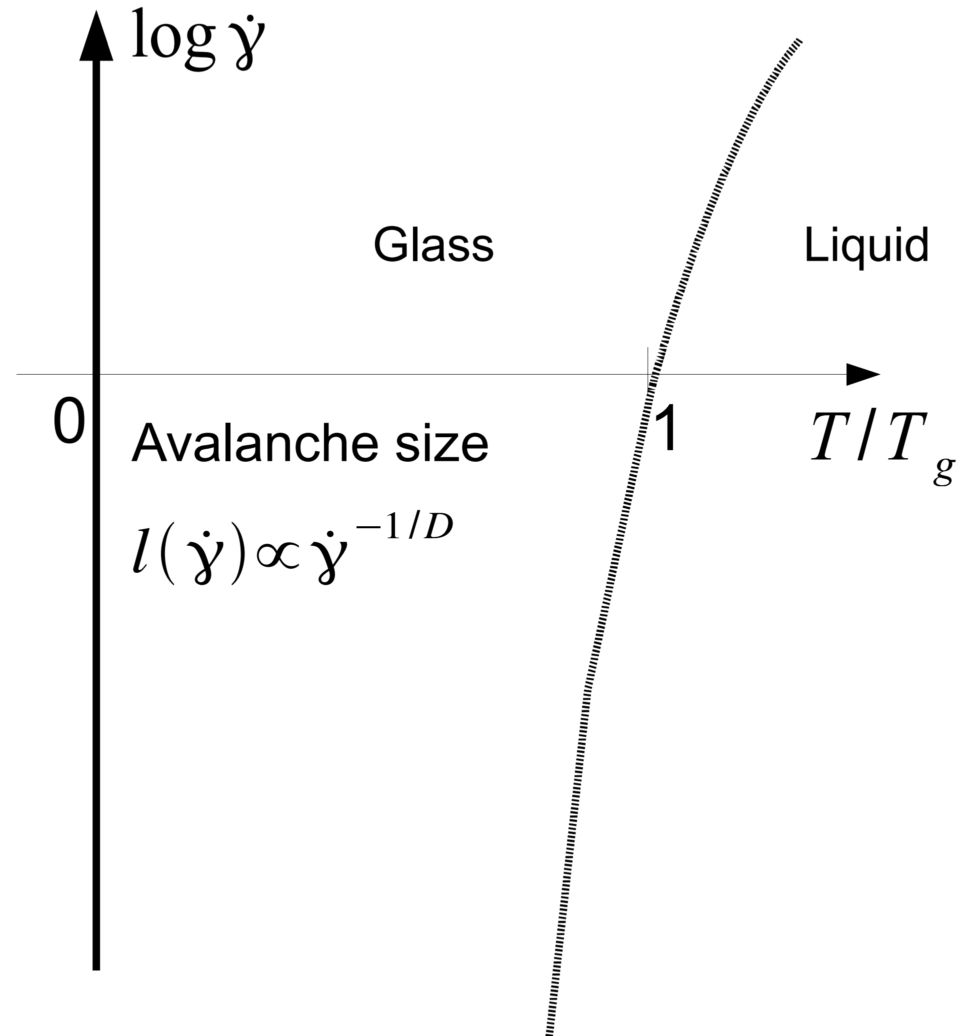
Chattoraj *et al*, *PRE 2011*


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
0
1
T/T_g
Avalanche size
$l(\dot{\gamma}) \propto \dot{\gamma}^{-1/D}$

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





Partial conclusion: elements of a phenomenology

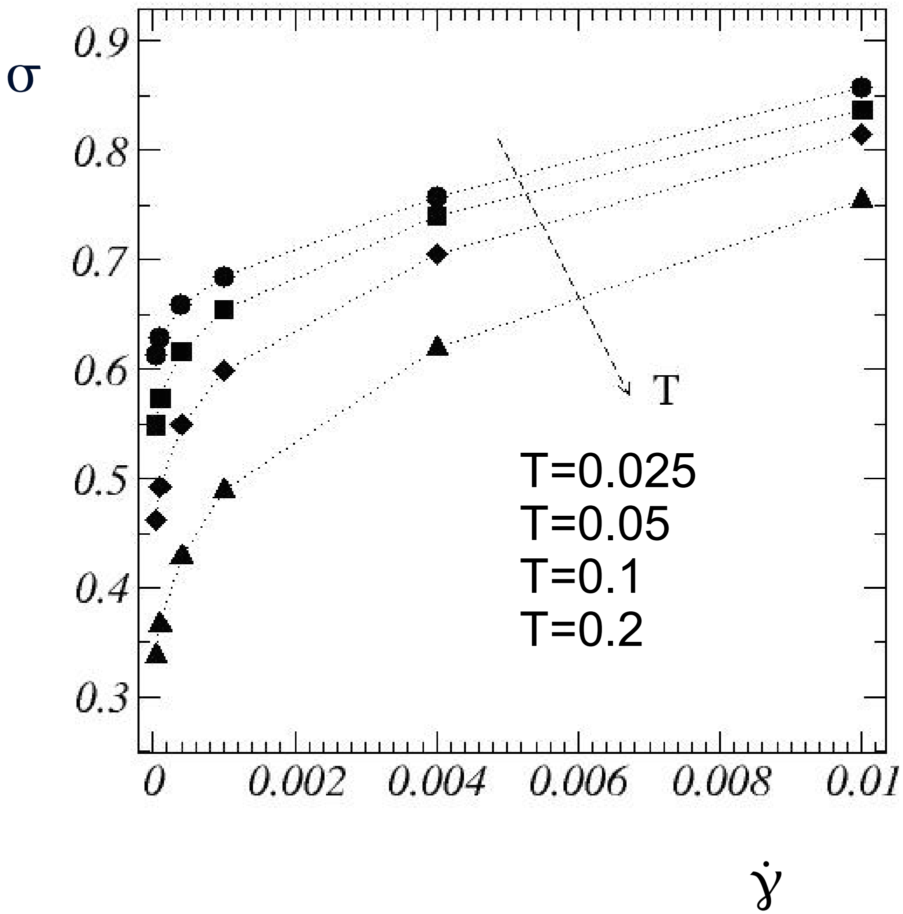
- AQS simulations support the following phenomenology:
  - Plasticity results from local shear transformations (as Argon proposed)
  - Zones are progressively convected towards instability
  - Each flip produces an Eshelby-like field likely to trigger secondary flips

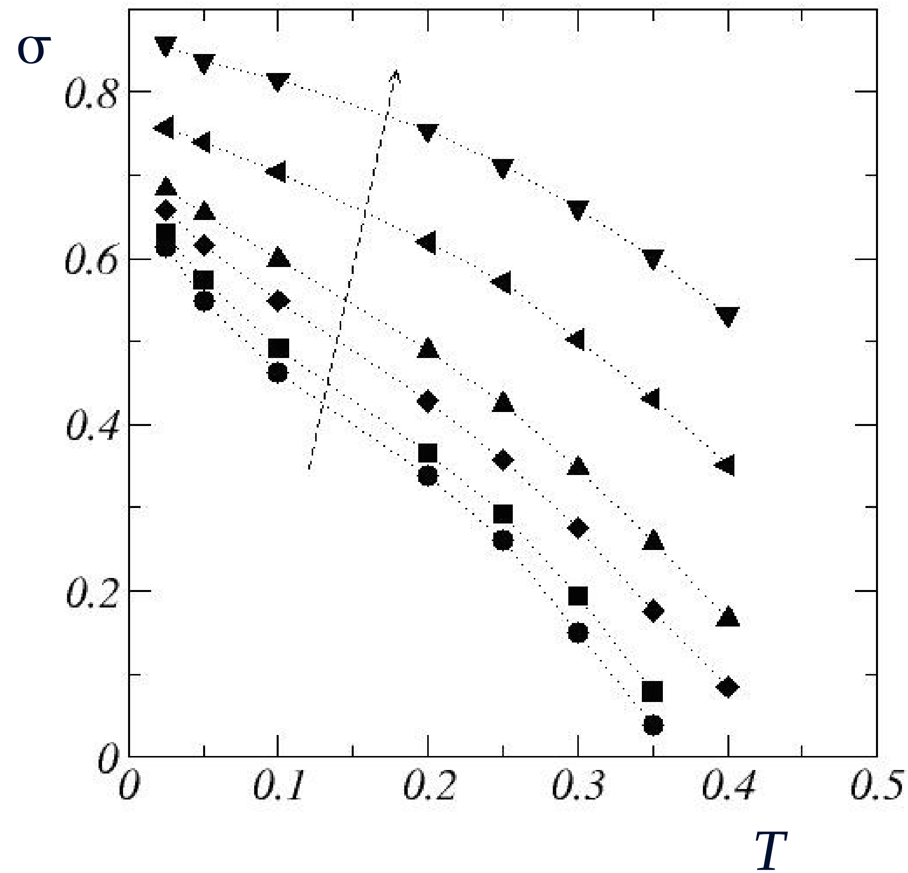
  This shows up as system-spanning avalanches

- 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 hese changes govern stress/strain-rate relation

- At finite T < Tg:
  - Avalanches continue to be present and are only progressively blurred when approaching Tg

Stress data

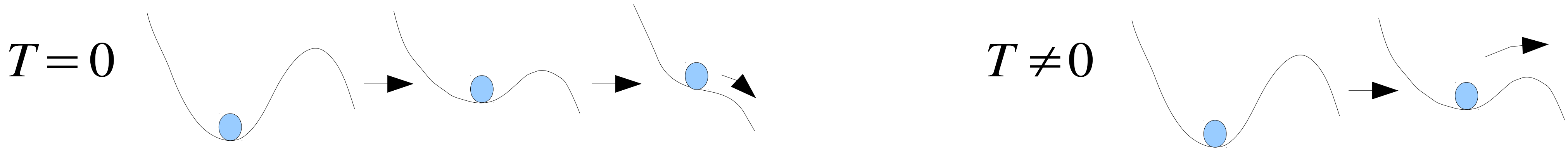


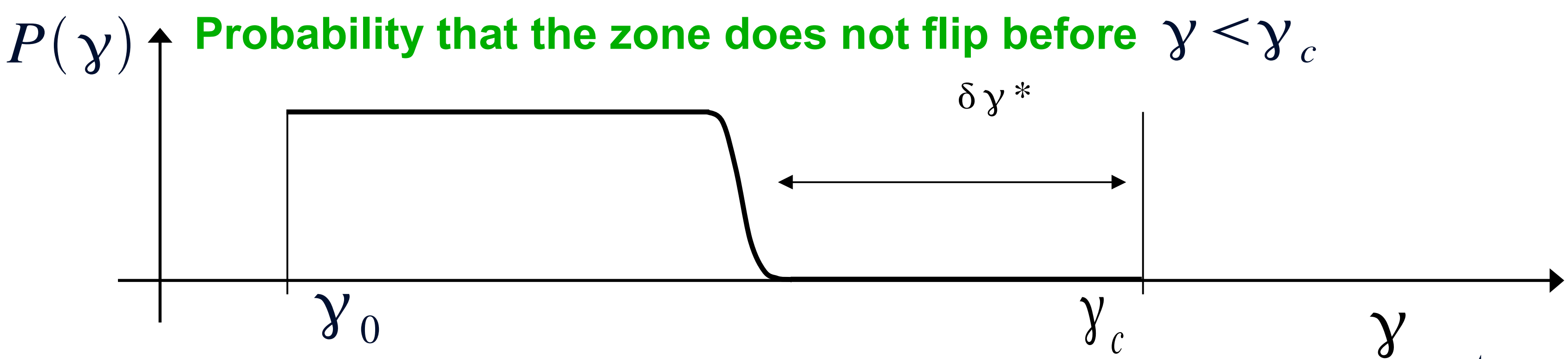


$\sigma(\dot{\gamma})$

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

Activation and driven zones





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

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

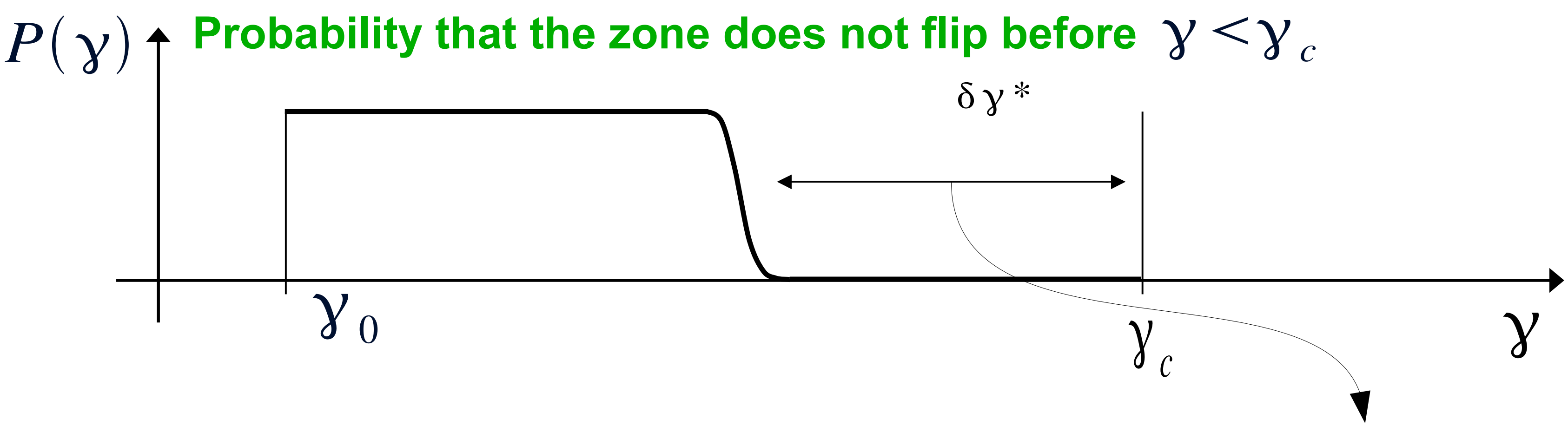
$$\Rightarrow P(\gamma;\gamma_0) = \exp\left(-\frac{1}{\dot{\gamma}}\int_{\gamma_0}^{\gamma} R(\gamma')\,d\gamma'\right)$$

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

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

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

Chattoraj et al, PRL 105, 26601 (2010)

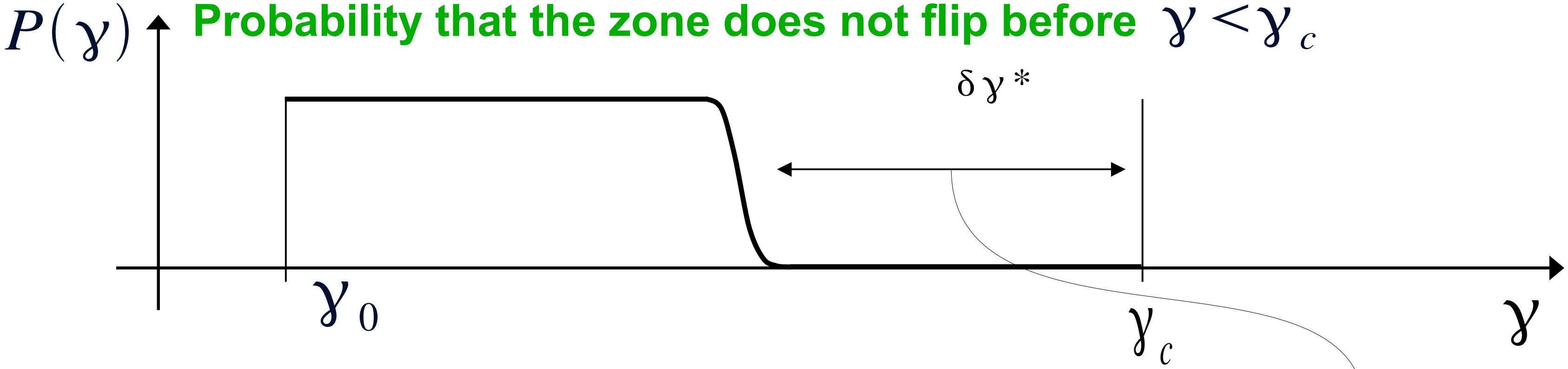


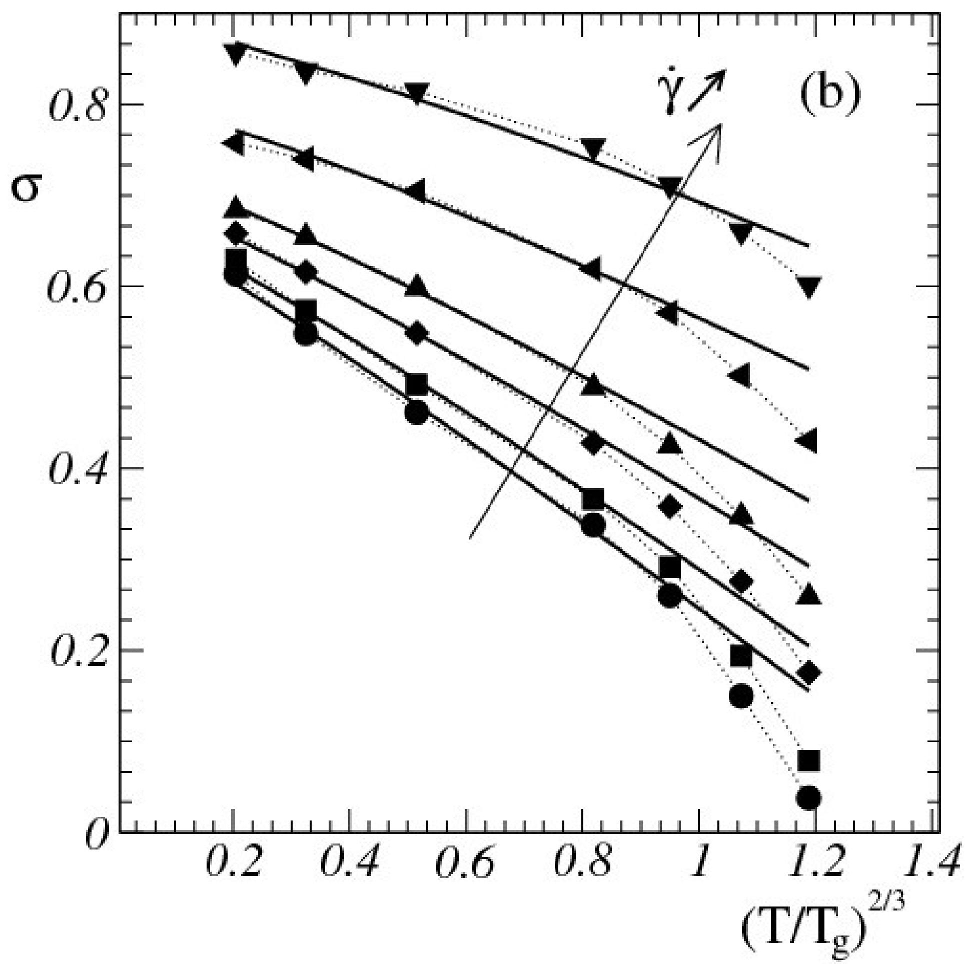
$$\delta\gamma^* \sim \left[\frac{T}{B} \ln\left(\frac{2}{3} \frac{\nu}{\dot{\gamma}} \left(\frac{T}{B} \right)^{5/6} \right) \right]^{2/3}$$

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

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

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

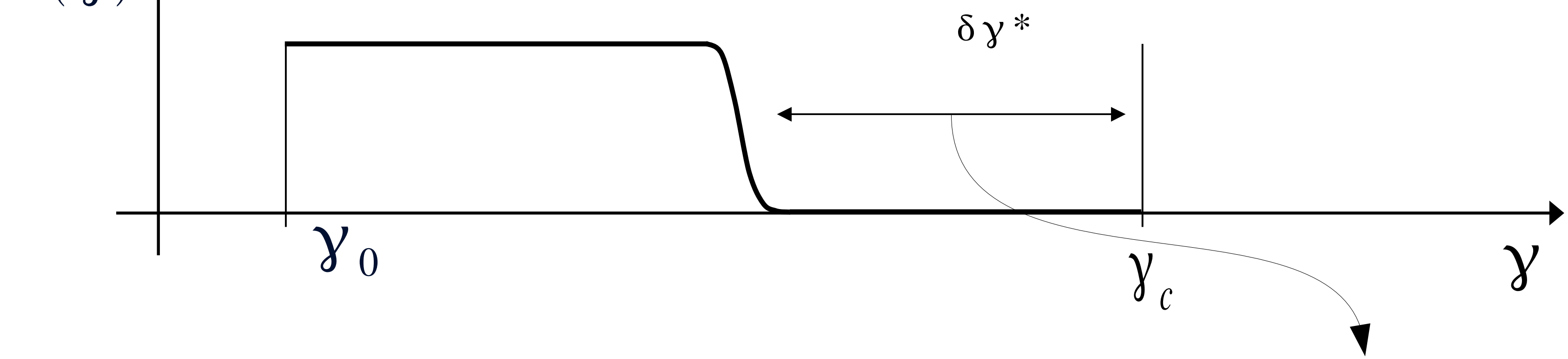




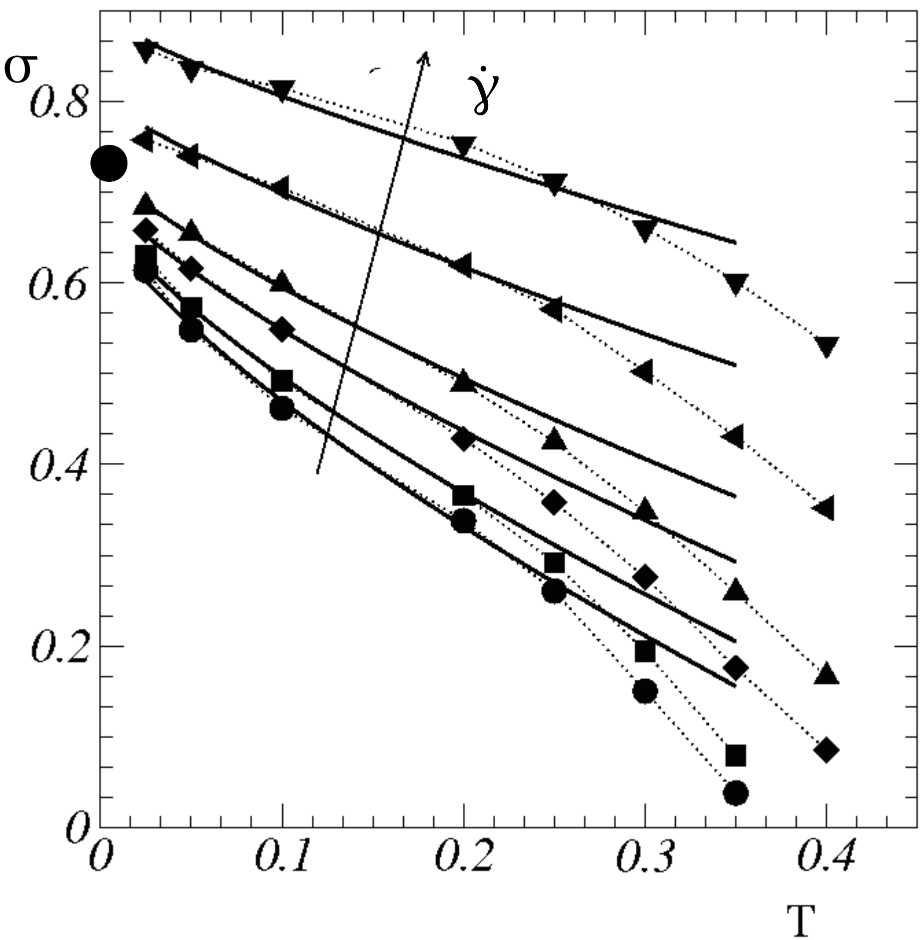
$$\delta\gamma^* \sim \left[\frac{T}{B}\ln\left(\frac{2}{3}\frac{\nu}{\dot{\gamma}}\left(\frac{T}{B}\right)^{5/6}\right)\right]^{2/3}$$

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

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

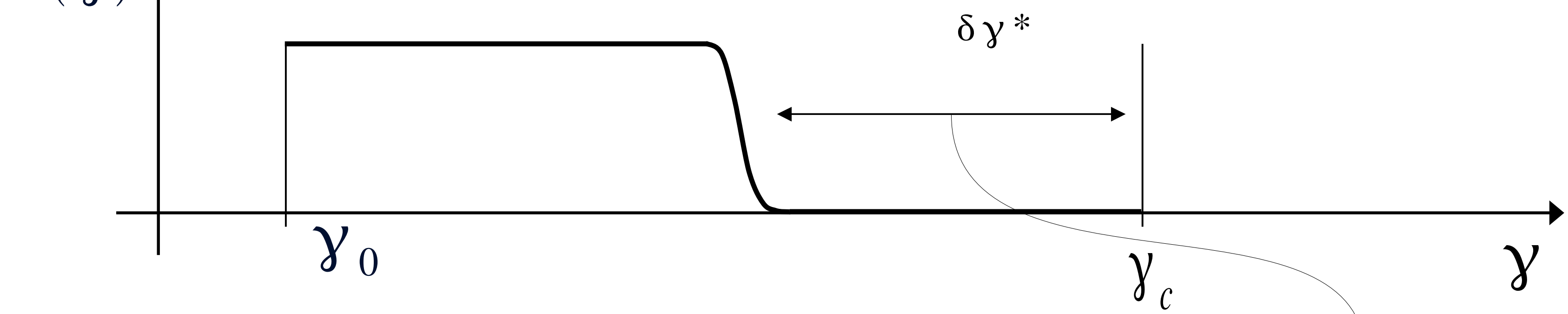


$$\delta\gamma^* \sim \left[\frac{T}{B} \ln\left(\frac{2}{3} \frac{\nu}{\dot{\gamma}} \left(\frac{T}{B} \right)^{5/6} \right) \right]^{2/3}$$

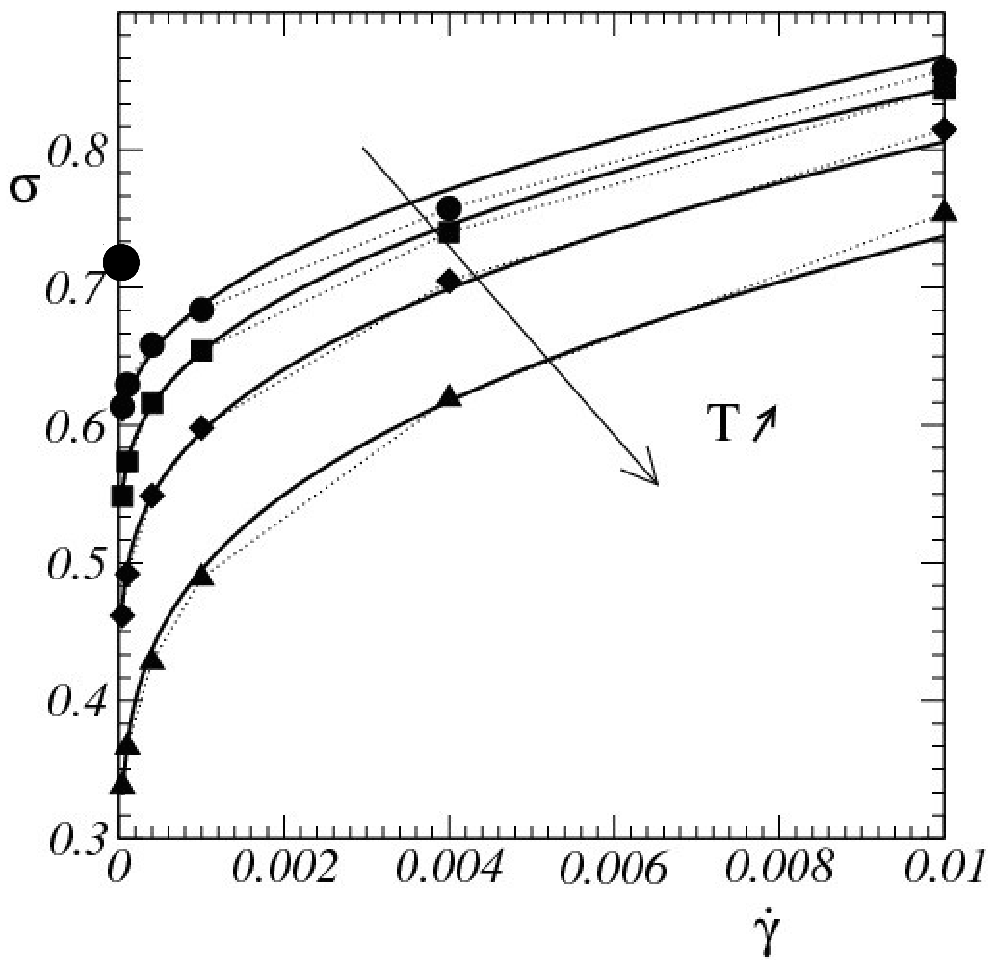


$$\sigma(\dot{\gamma}; T) = \sigma(\dot{\gamma}; T=0) - 2\mu\,\overline{\delta\gamma^*}$$

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



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

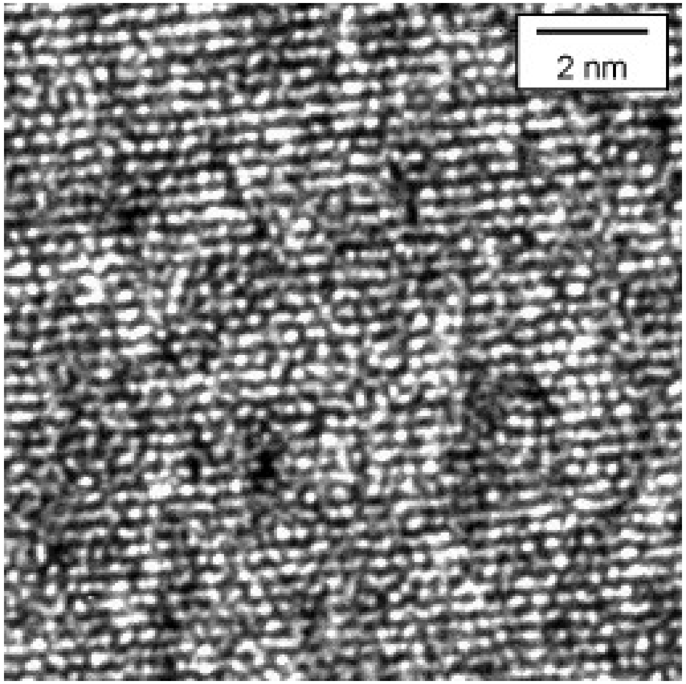


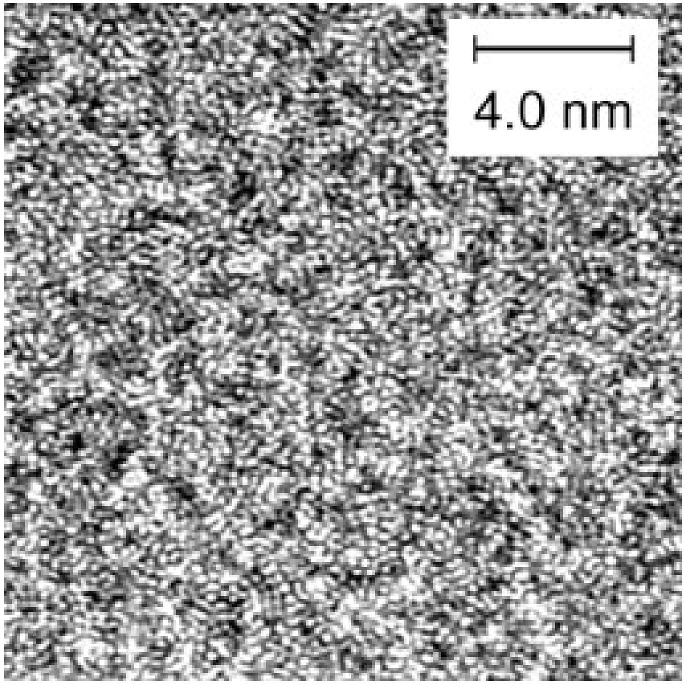
$$\sigma(\dot{\gamma};T) = \sigma(\dot{\gamma};T=0) - 2\mu\overline{\delta\gamma^*}$$

Metallic glasses

Zr-Ti-Cu-Ni-Al Alloy

TEM Hufnagel





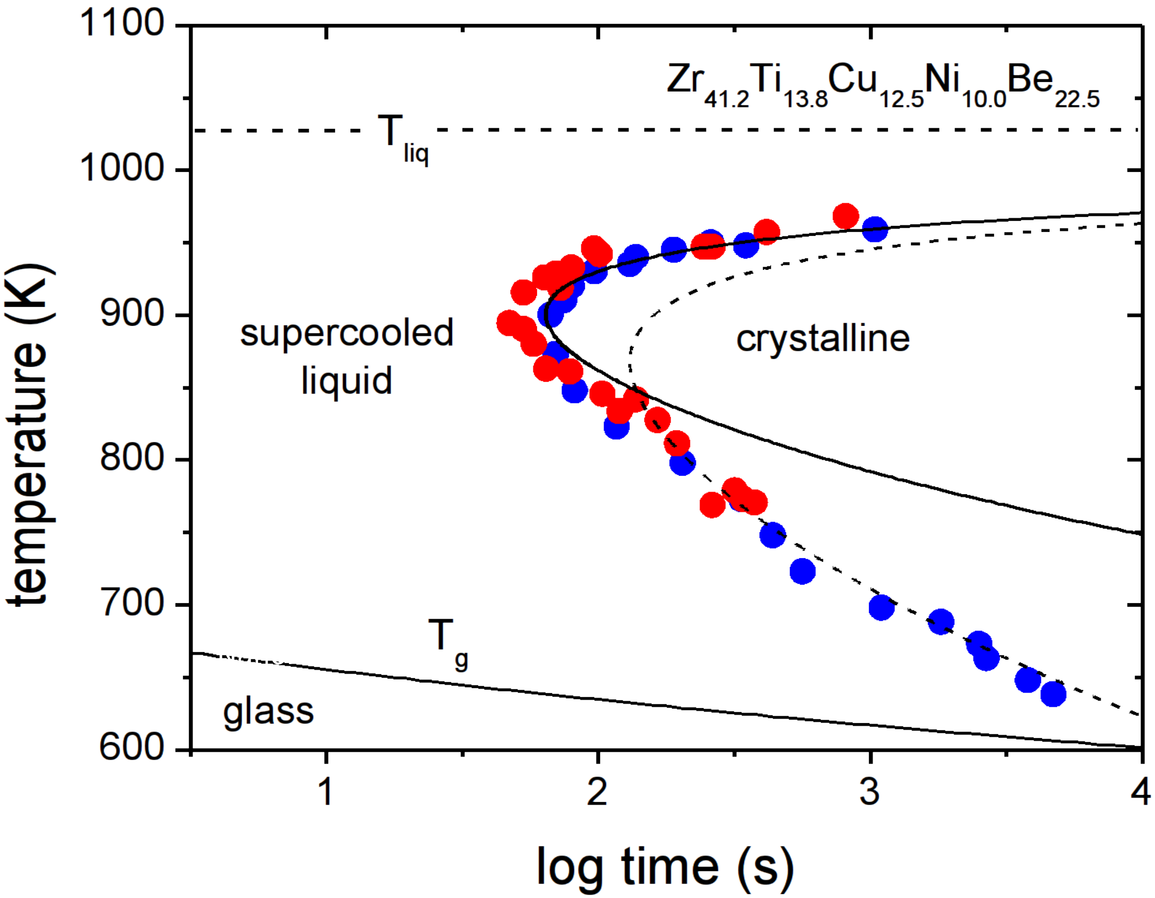
Fabrication: avoiding cristallization

Examples of Critical Cooling Rates (°C/s) for Glass Formation

Material	Homogeneous nucleation	Heterogeneous nucleation contact angle (deg)		
		100	60	40
SiO_2 glass[a]	9×10^{-6}	10^{-5}	8×10^{-3}	2×10^{-1}
GeO_2 glass[a]	3×10^{-3}	3×10^{3}	1	20
$Na_2O{\cdot}2SiO_2$ glass[a]	6×10^{-3}	8×10^{-3}	10	$3 \times 10^{+2}$
Salol	10			
Water	10^{7}			
Ag	10^{10}			
Typical metal[a]	9×10^{8}	9×10^{9}	10^{10}	5×10^{10}

[a] After P. I. K. Onorato and D. R. Uhlmann, J. Non-Cryst. Sol., 22(2), 367–378 (1976).

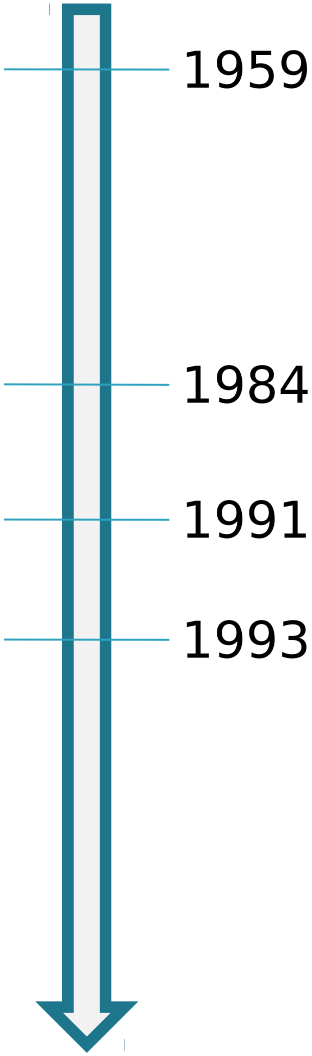
Fabrication: avoiding cristallization



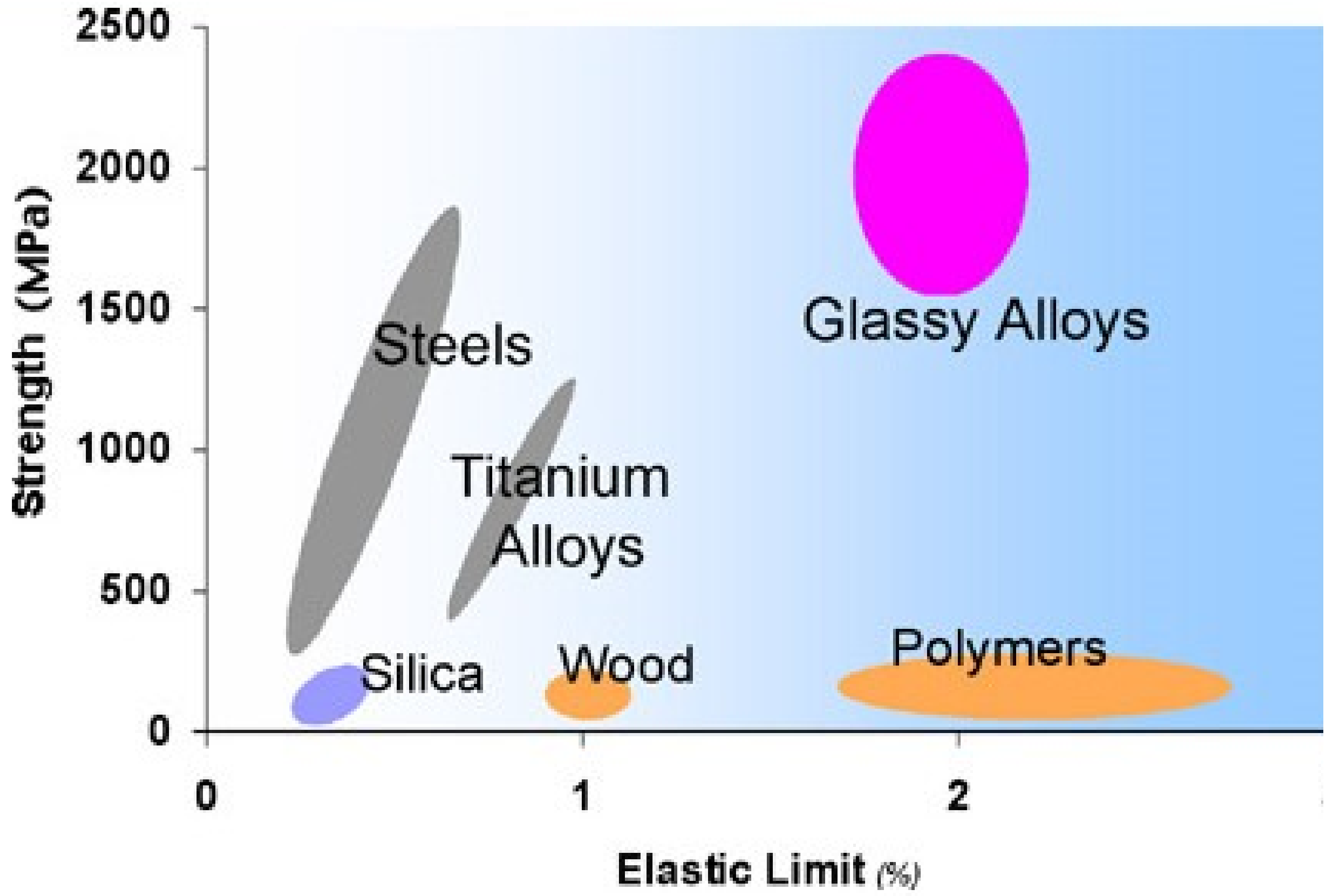
AuSi, NbNi, ZrCu, FeB,...
10^5-10^6 K/s

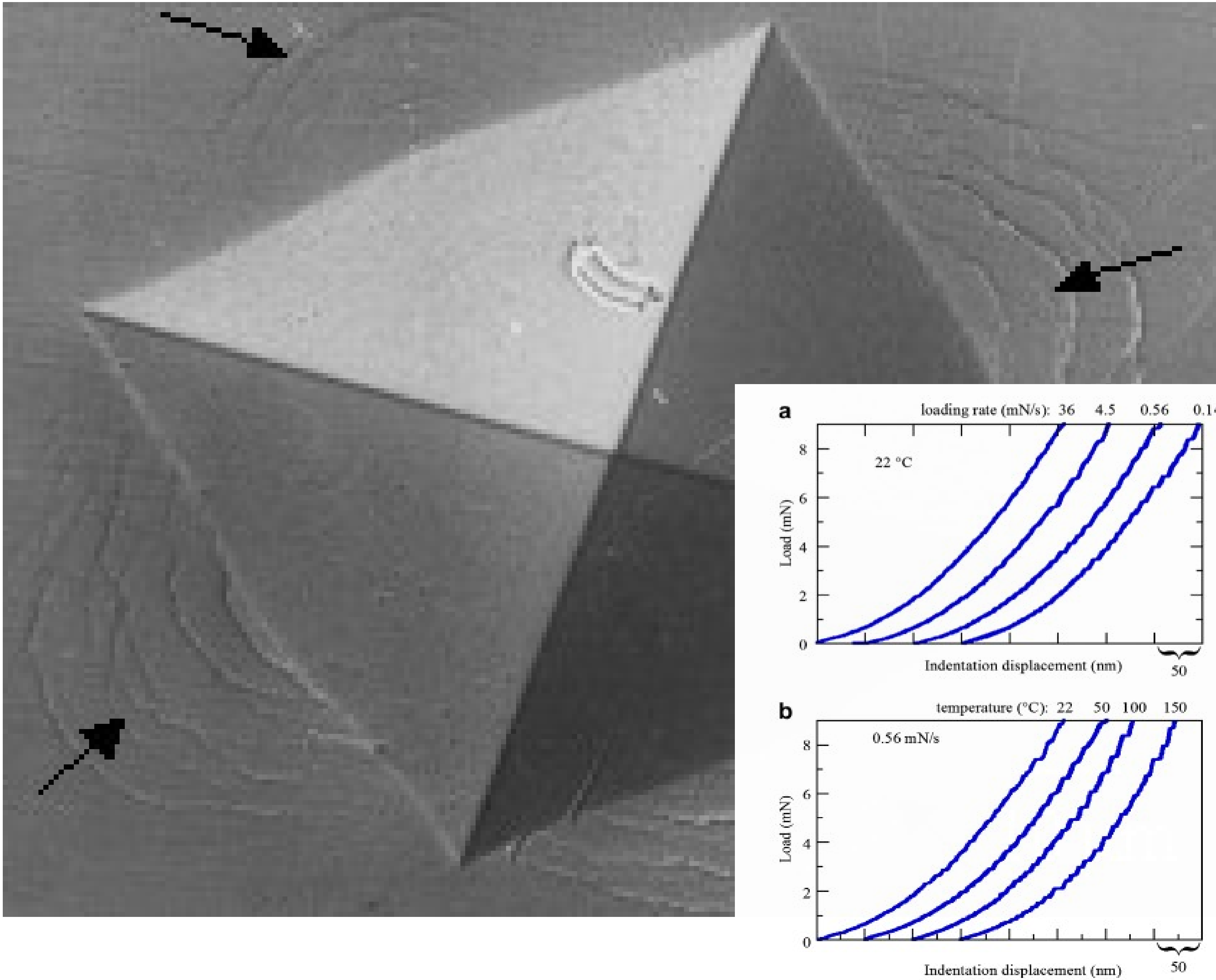
Bulk metallic glasses,
Ni-Pd-P, La-Al-Ni,
Mg-Cu-Y,Zr-Al-Ni-Cu
100 K/s

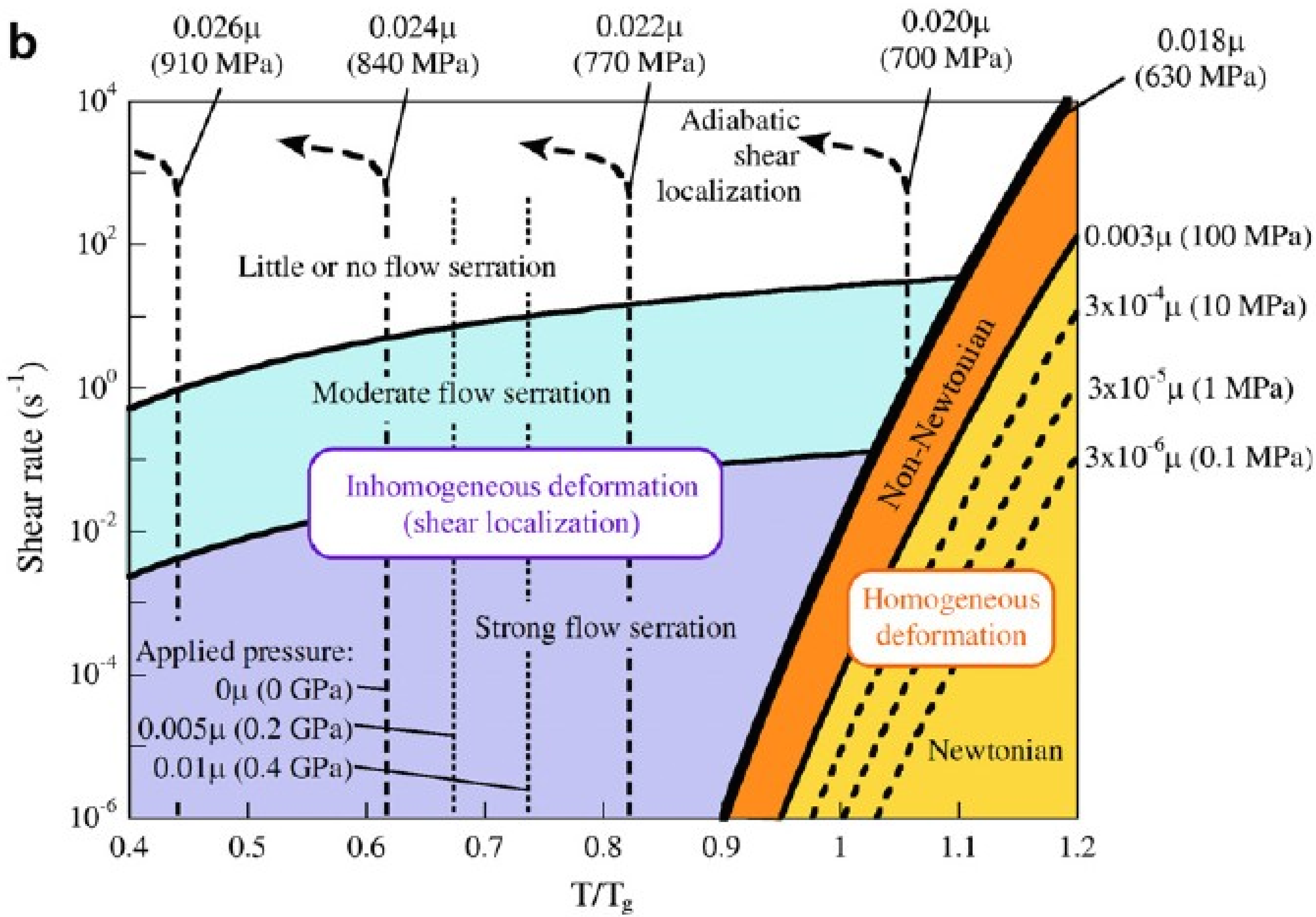
Zr-Ti-Cu-Ni-Be,
Zr-Ti-Al-Cu-Ni,...
1 K/s



Metallic glasses: high strength




a
loading rate (mN/s): 36 4.5 0.56 0.14
22 °C
Load (mN)
0
2
4
6
8
Indentation displacement (nm)
50
b
temperature (°C): 22 50 100 150
0.56 mN/s
Load (mN)
0
2
4
6
8
Indentation displacement (nm)
50



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

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]

Conclusion

Low T

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

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