Plastic deformation of metallic and hard-sphere colloidal glasses

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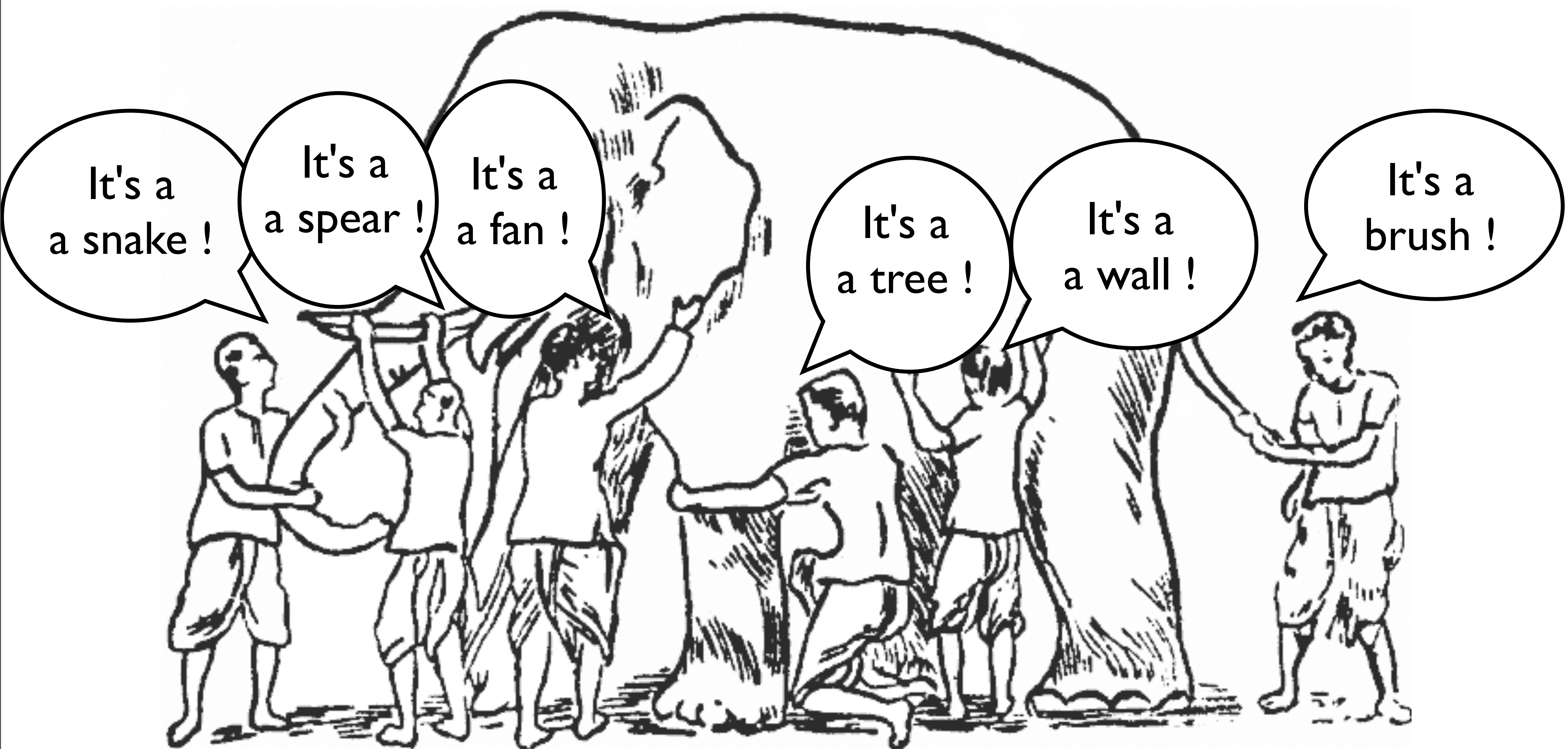
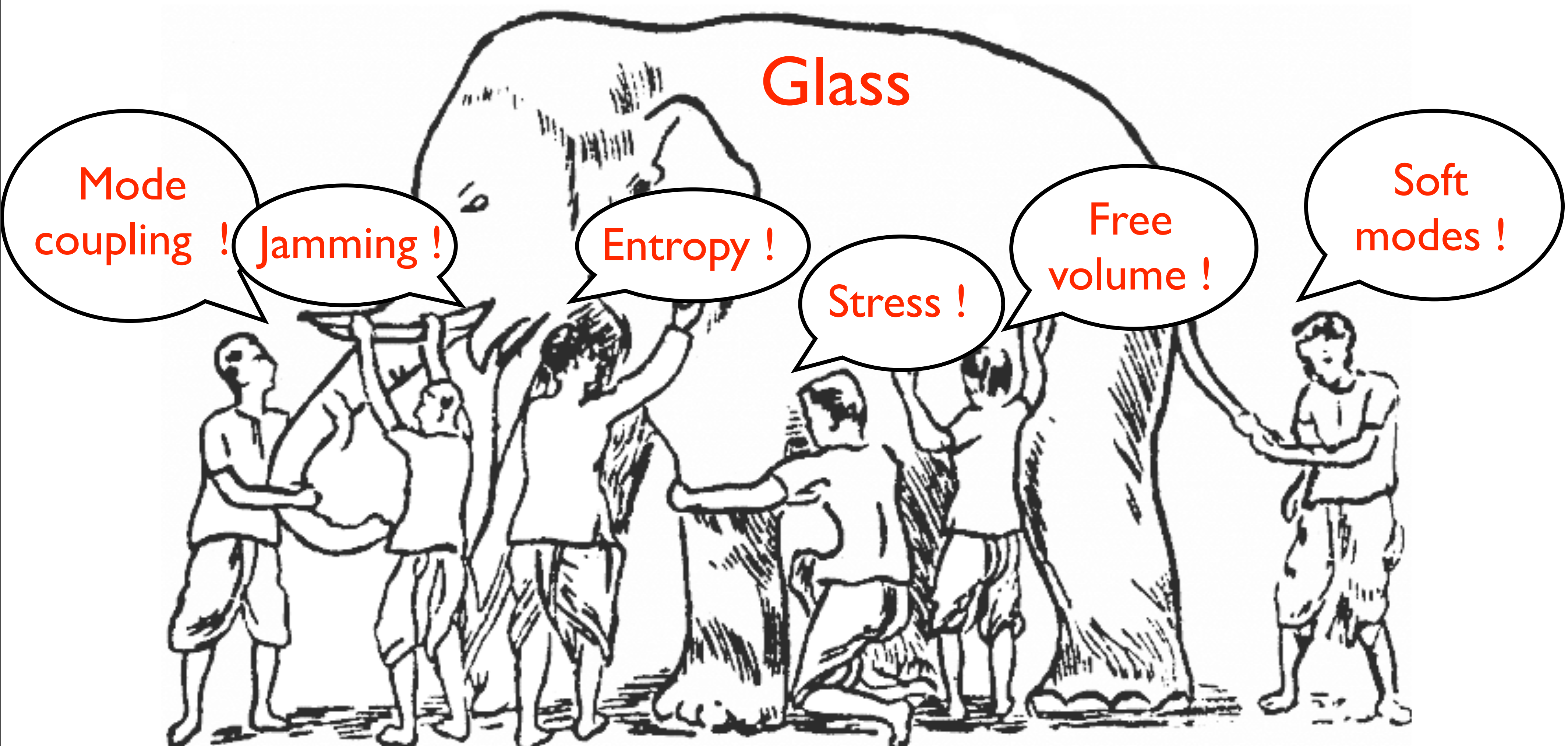
June 24, 2010

The blind men and the elephant



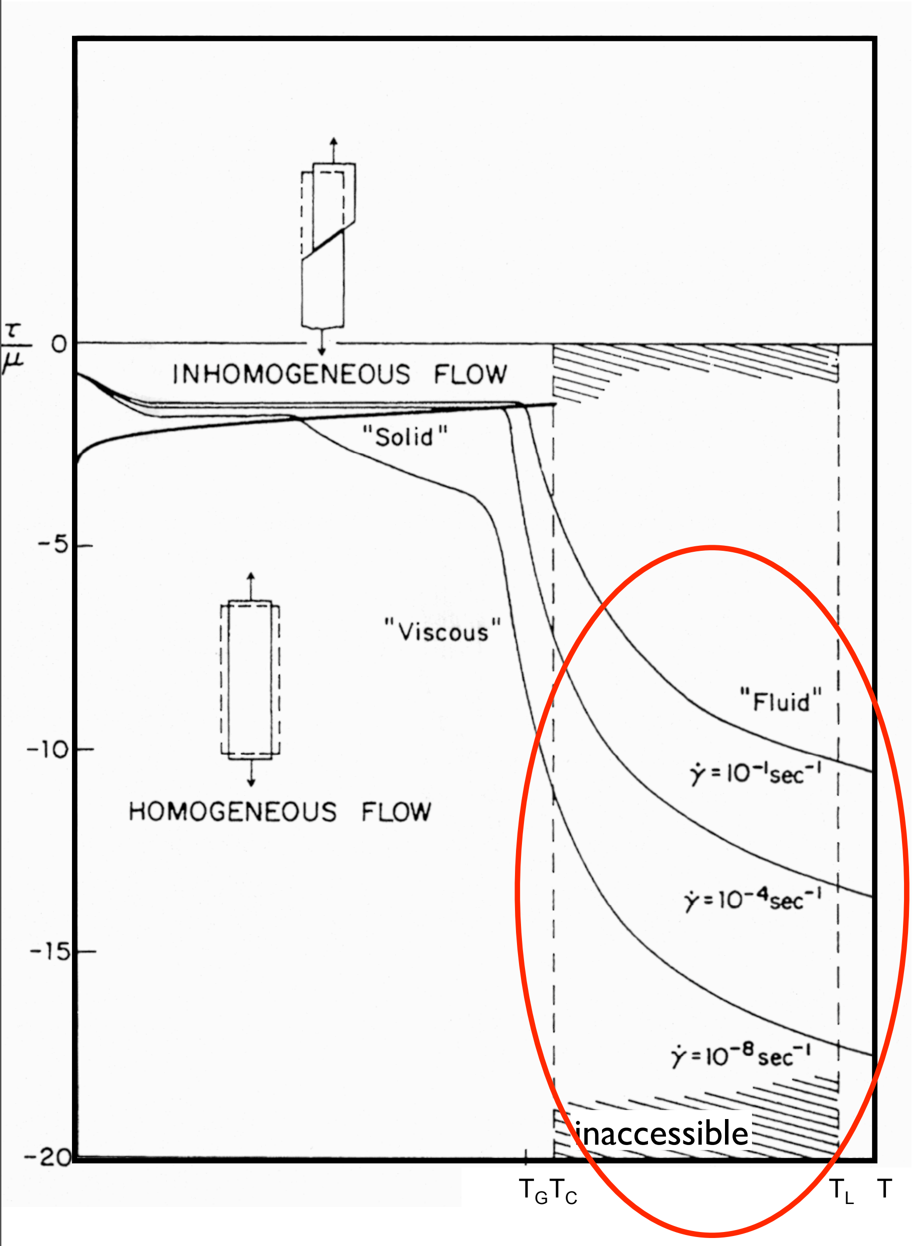
The blind men and the elephant



And so these men of Indostan
Disputed loud and long,
Each in his own opinion
Exceeding stiff and strong.
Though each was partly in the right,
They all were in the wrong.

-- John Godfrey Saxe (1816-1887)

Liquid flow

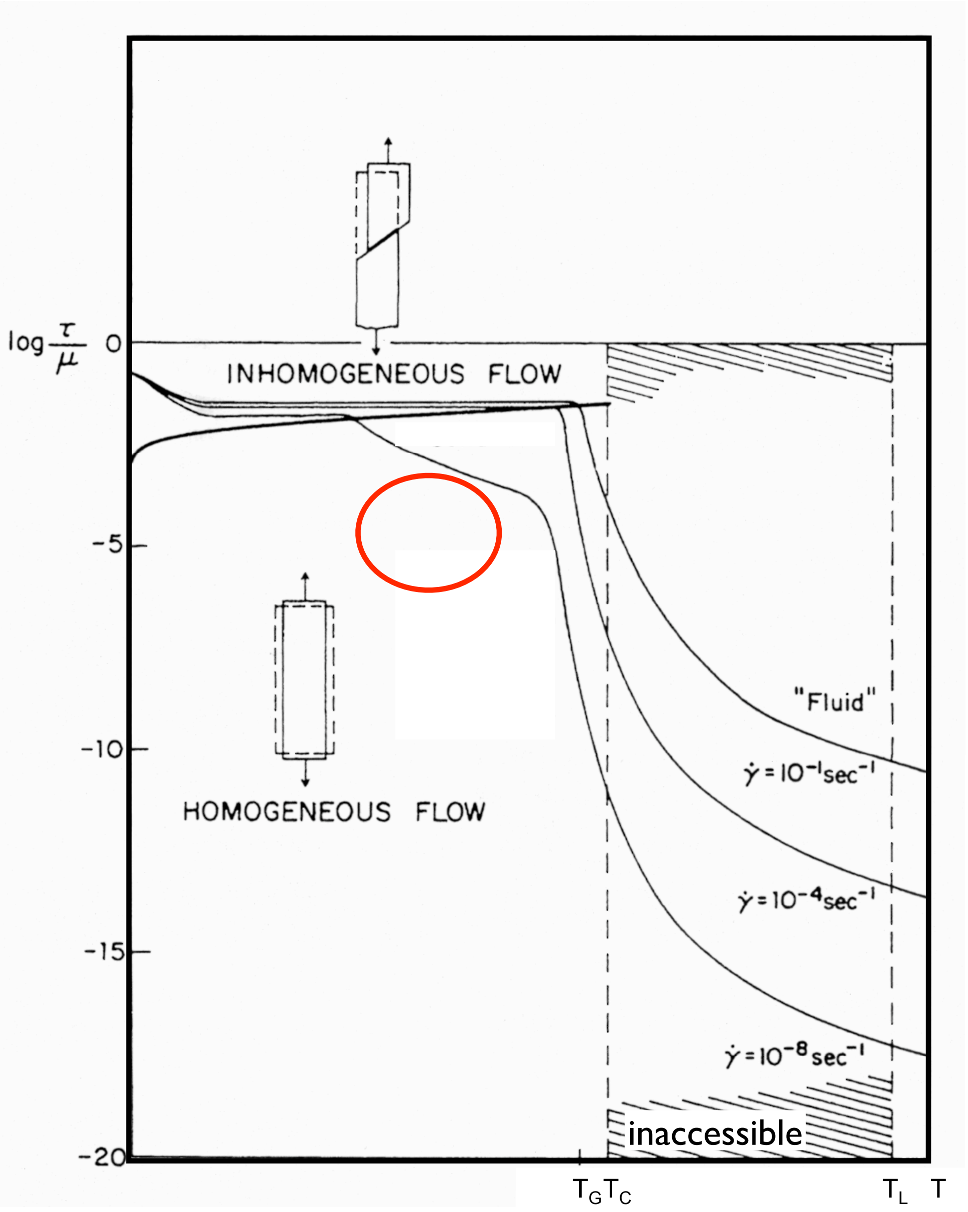


Newtonian viscous:
strain rate ∝ stress

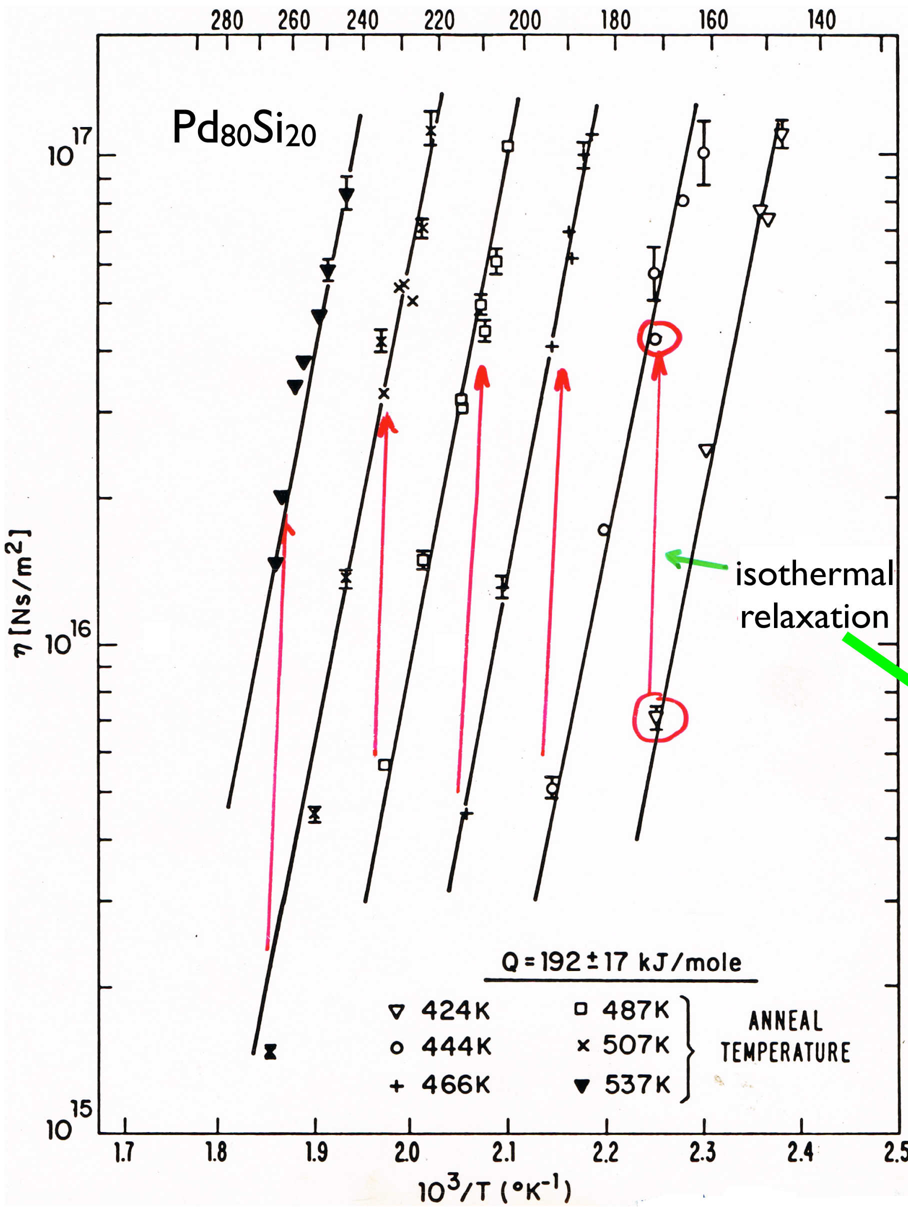
viscosity
Fulcher-Vogel-Tammann form

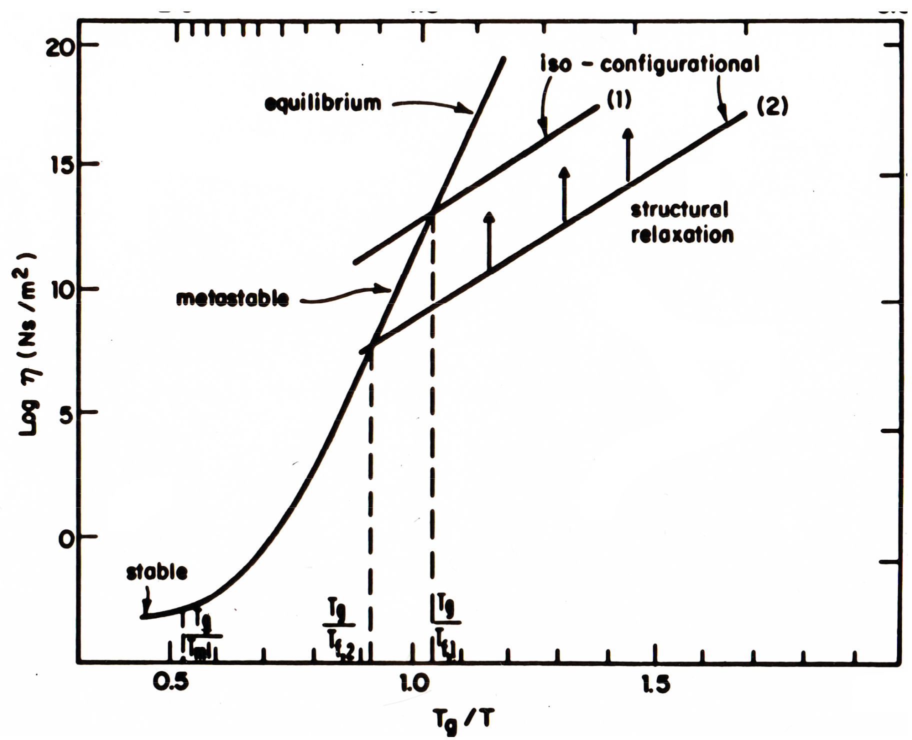
$$\eta = \eta_o \exp\left(\frac{B}{T - T_o}\right)$$

Glass at low stress, far from equilibrium



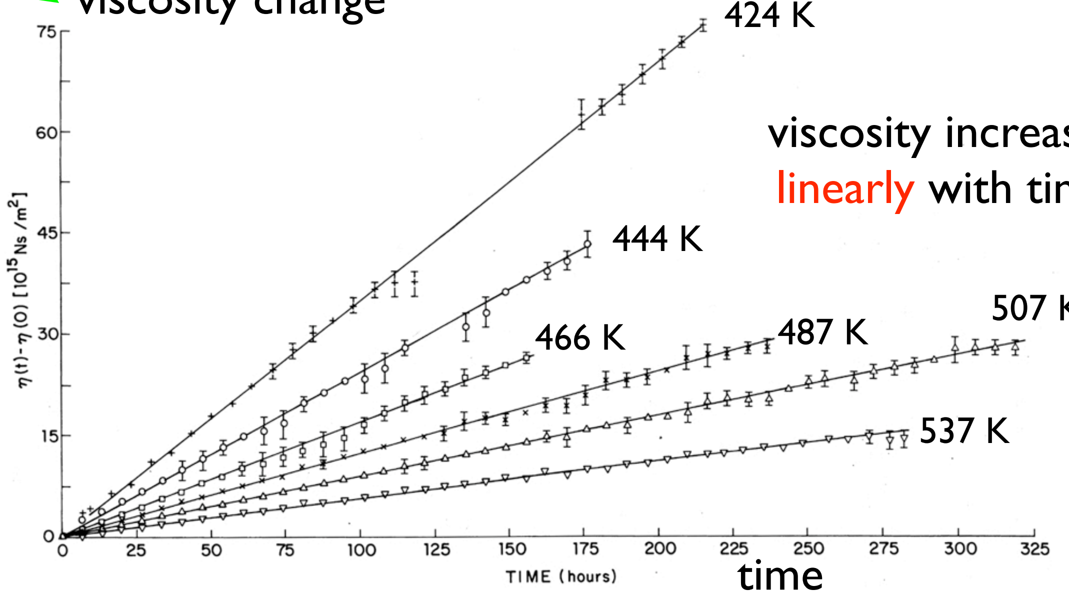
Effects of structural relaxation on viscosity





viscosity change

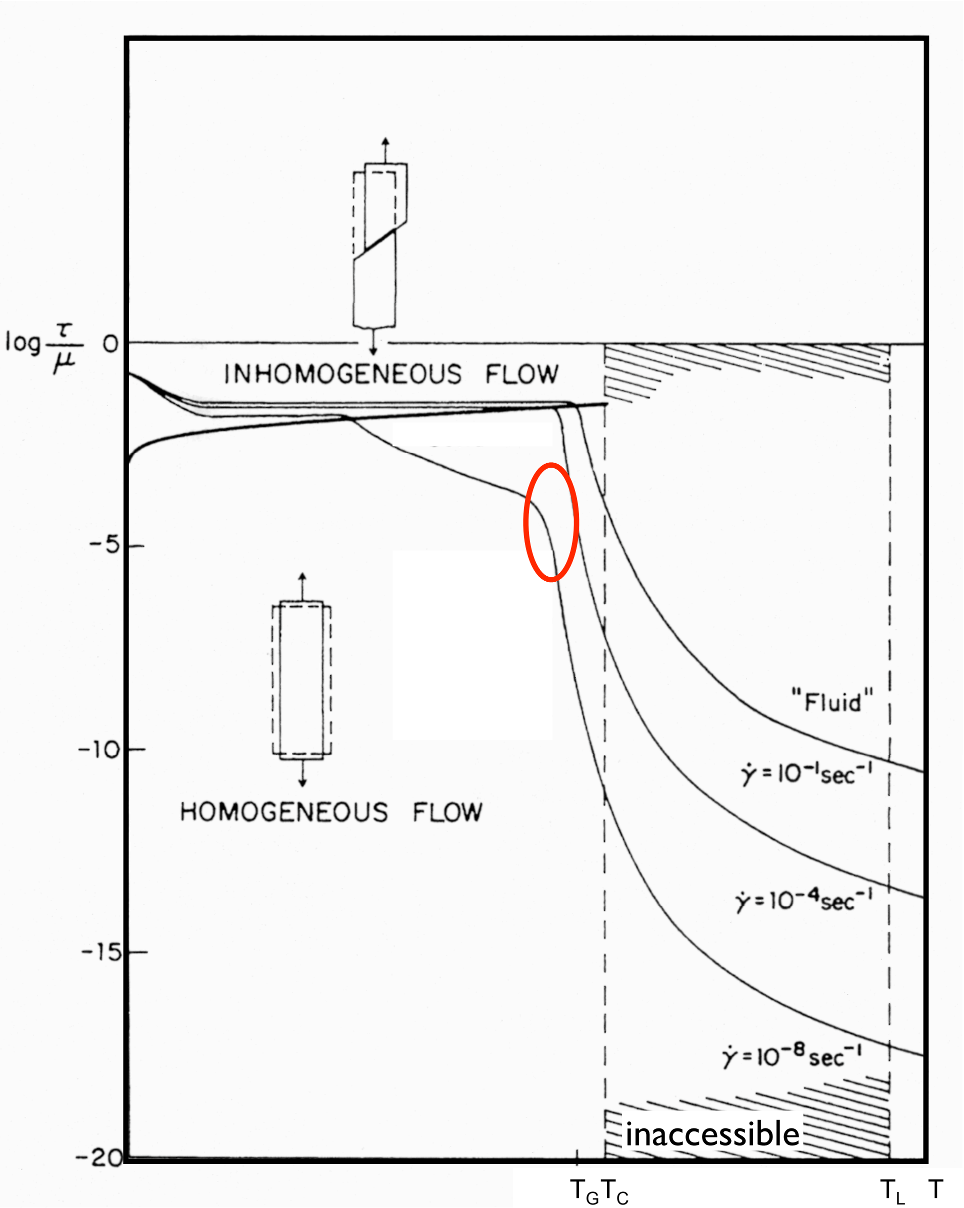
Taub & FS, 1980



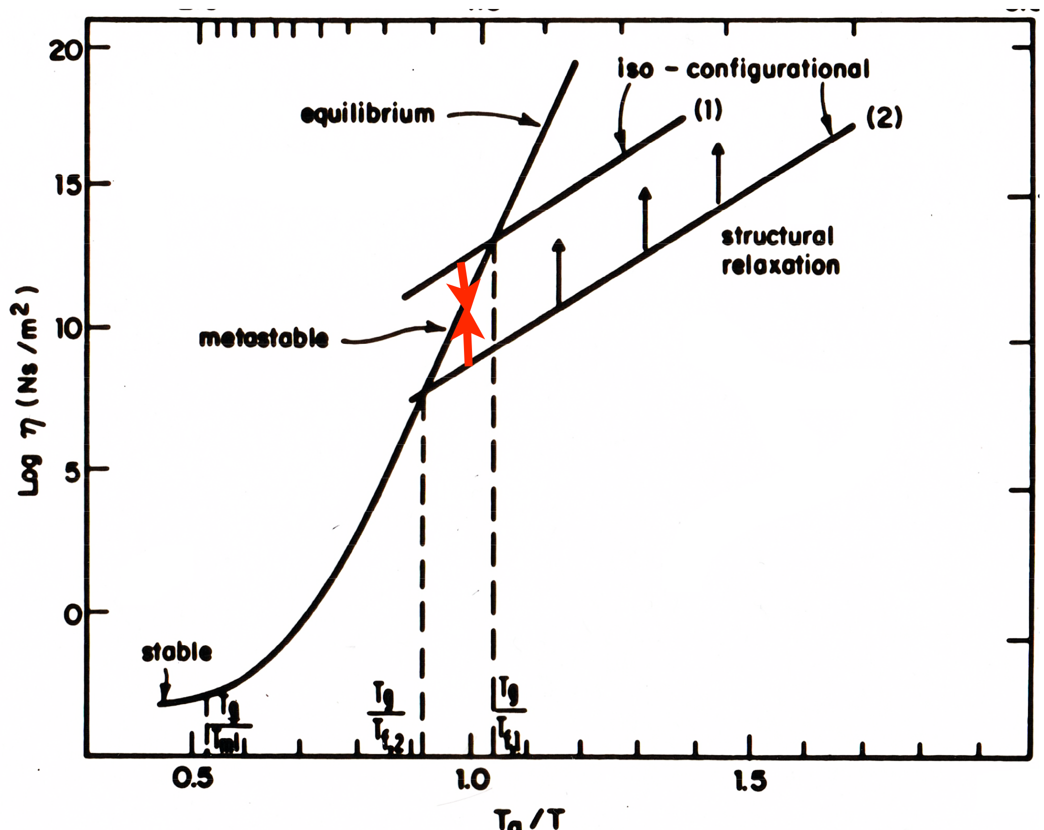
viscosity increases linearly with time

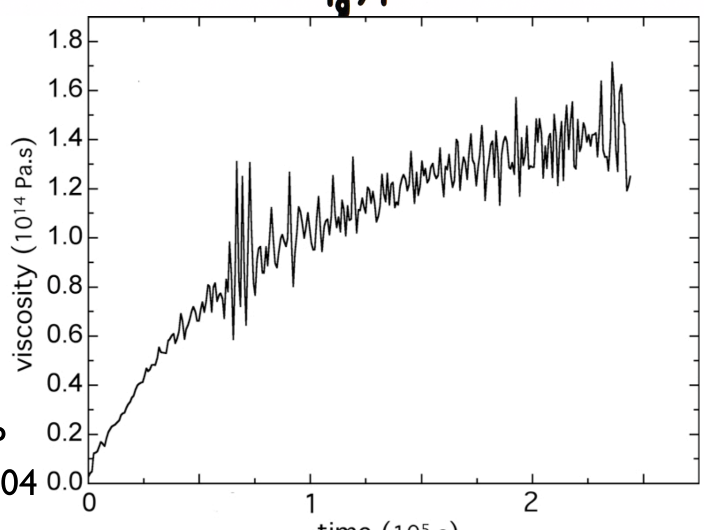
time

Glass at low stress, near equilibrium

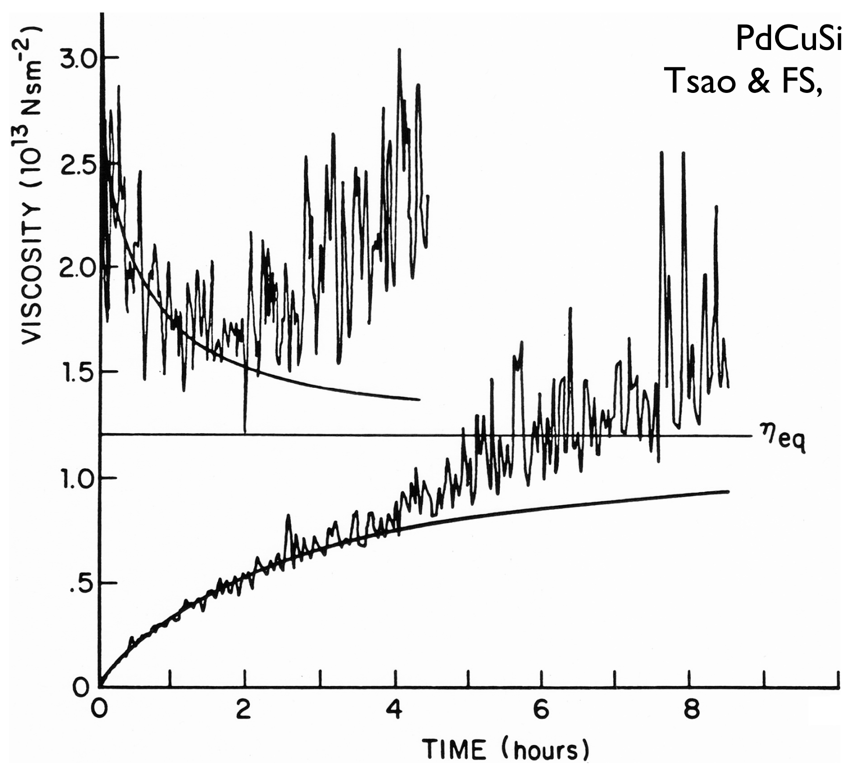


Structural relaxation with saturation



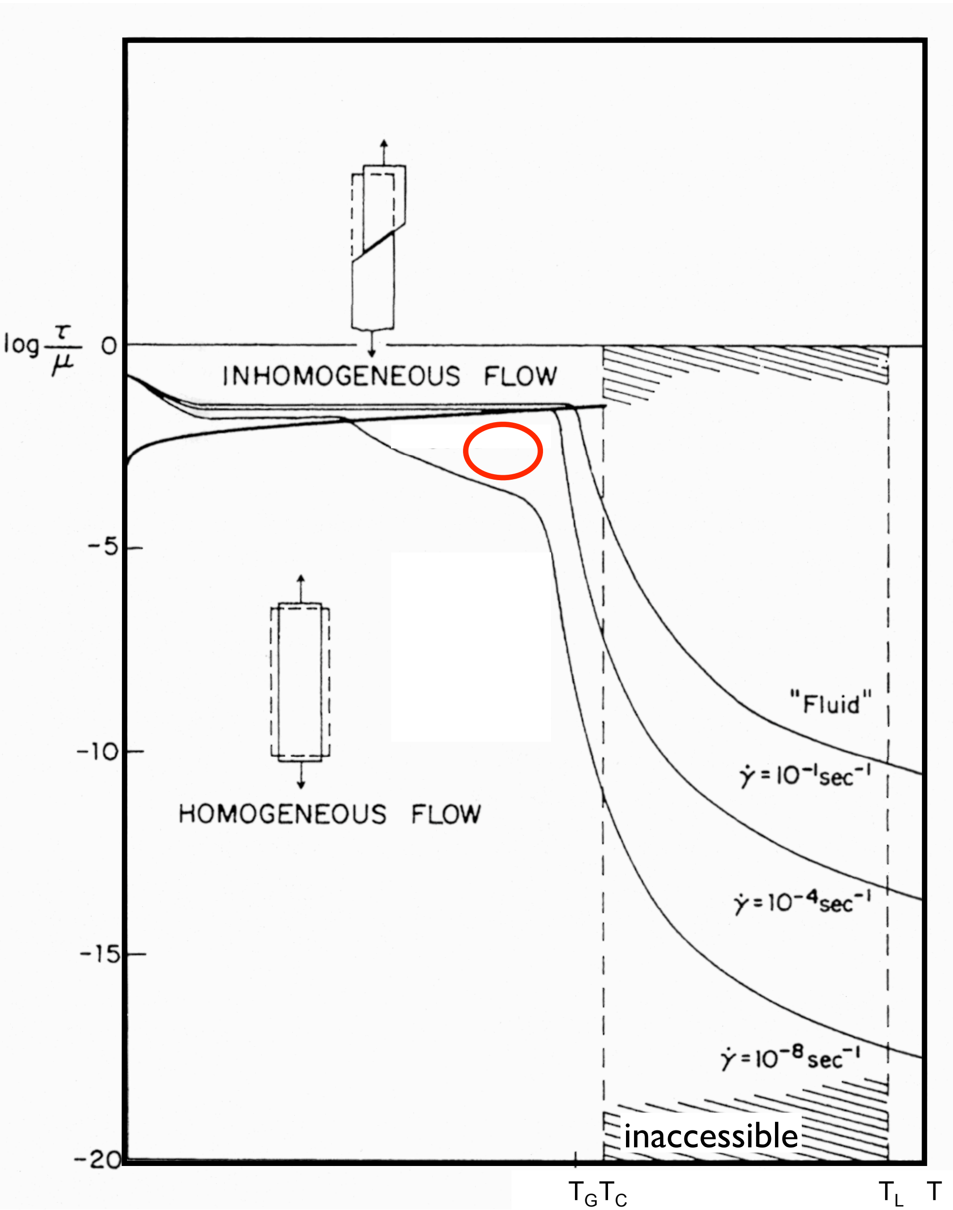


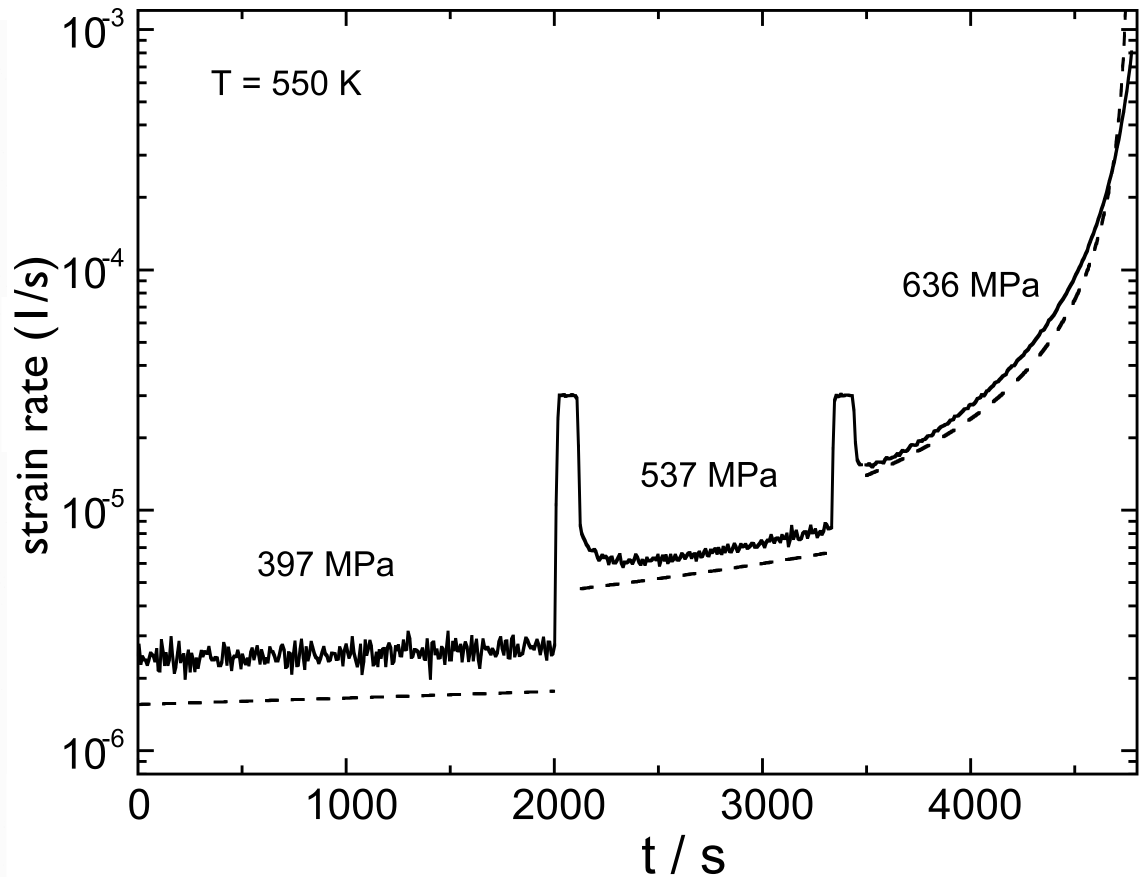
PdNCuiP
Heggen, 2004



PdCuSi
Tsao & FS, 1983

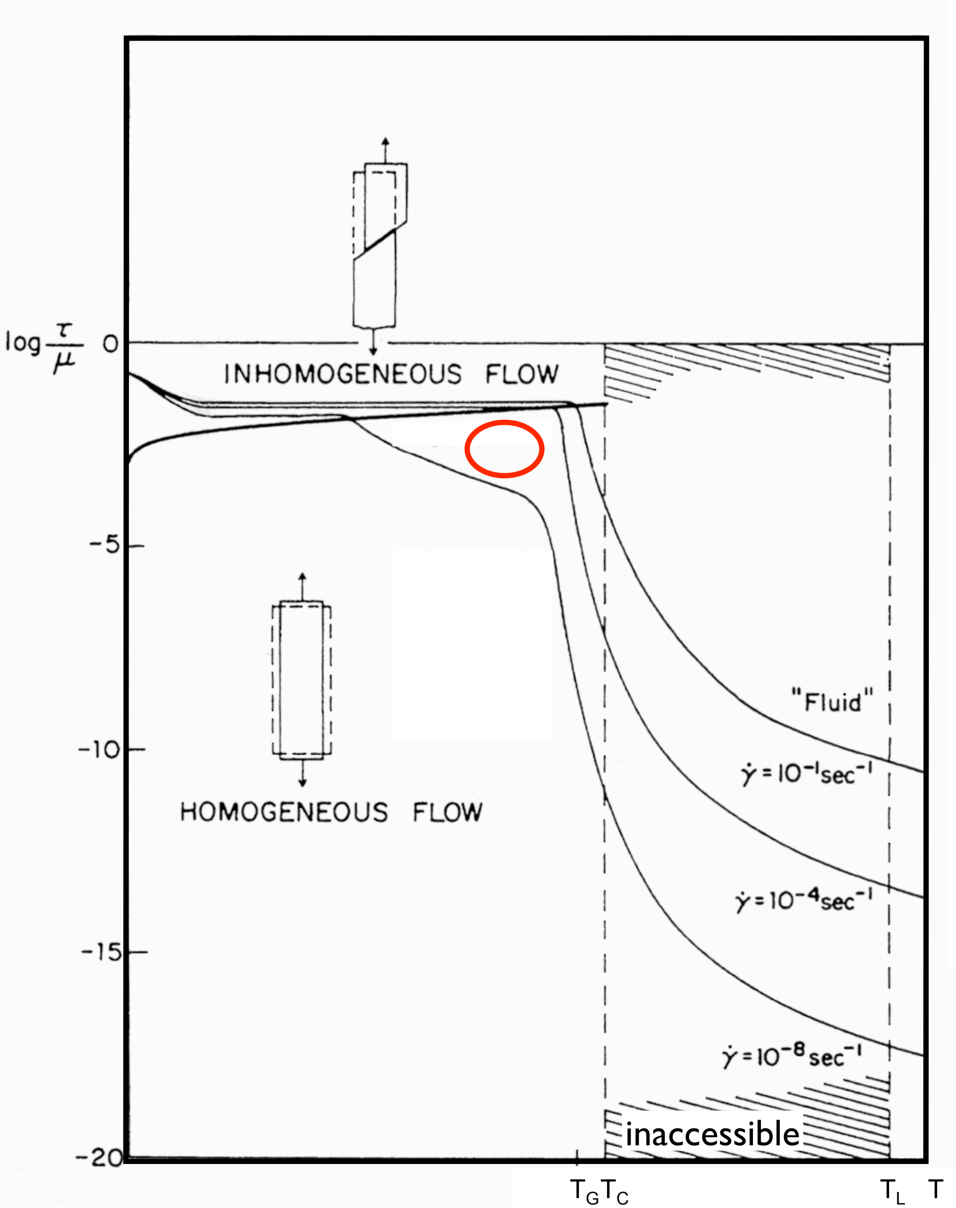
Glass at high stress



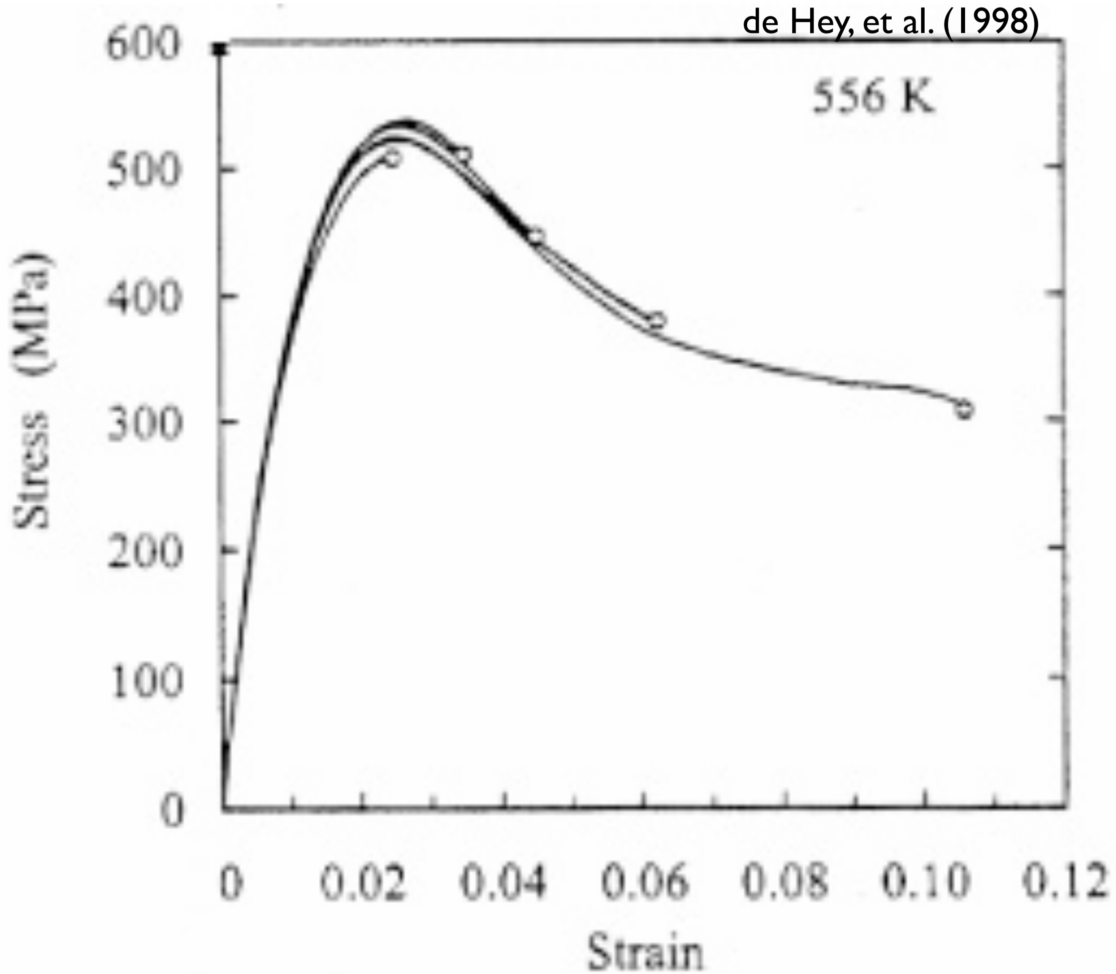


deformation-induced softening

Glass at high stress

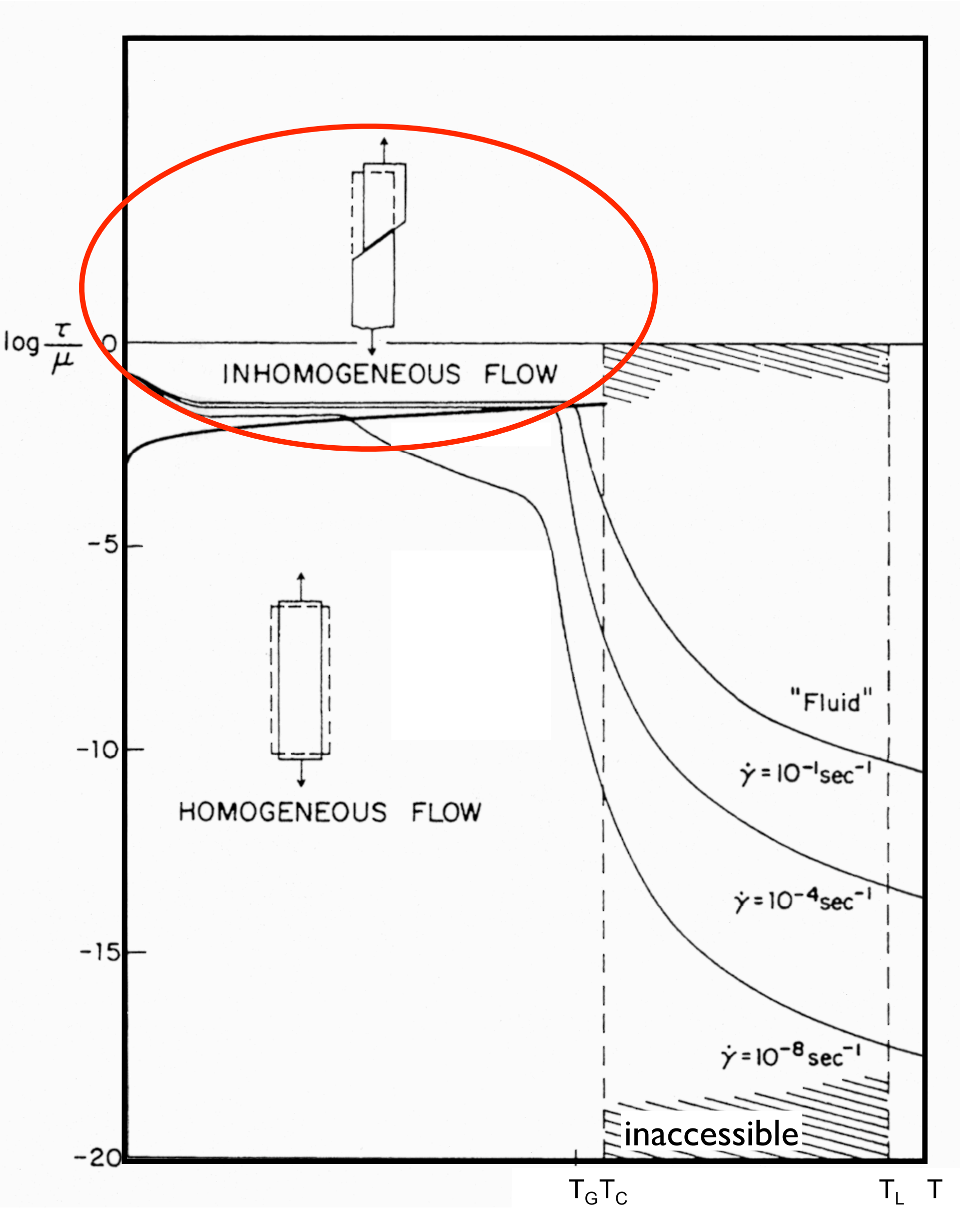


de Hey, et al. (1998)

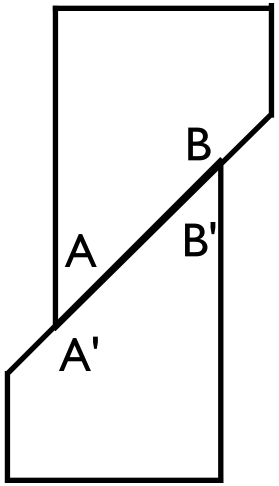


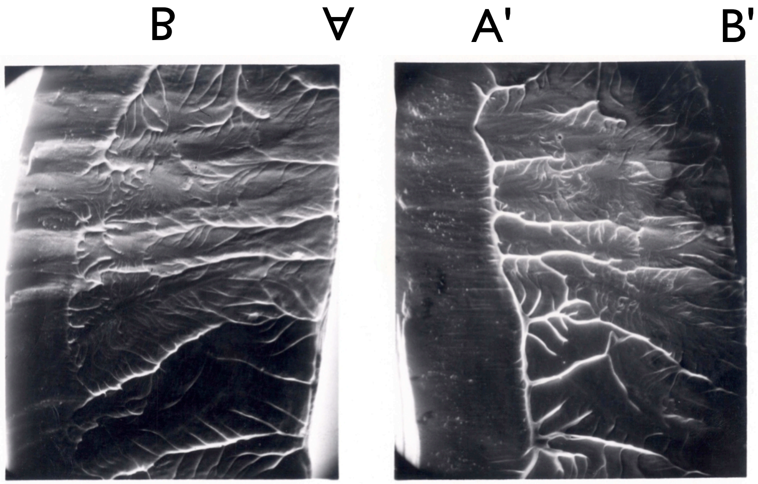
deformation-induced softening

Inhomogeneous flow

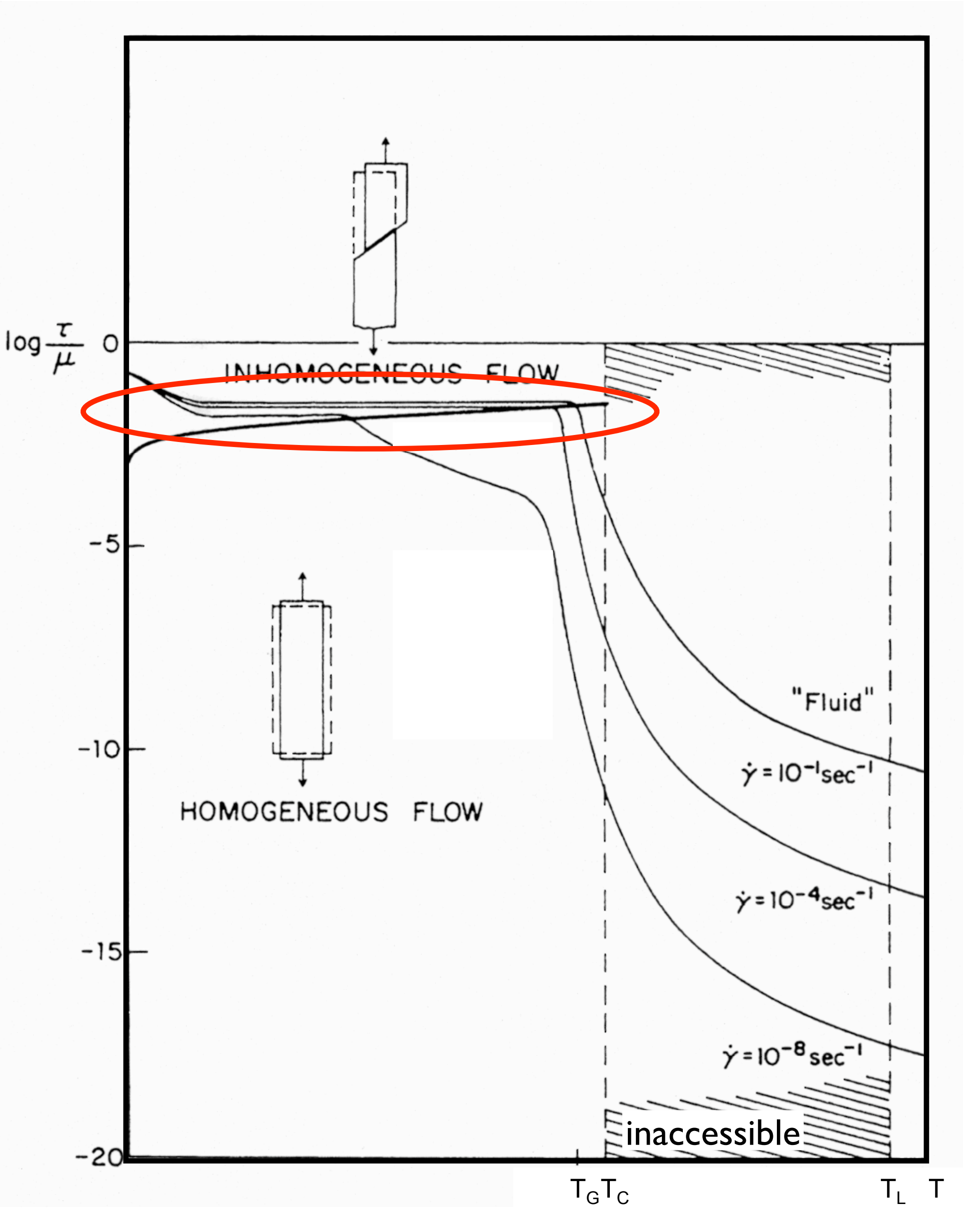


catastrophic
deformation-induced
softening





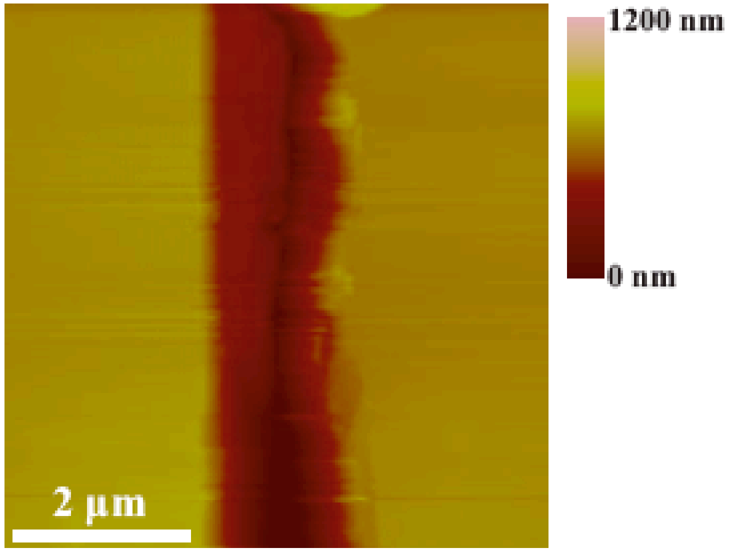
Homogeneous flow in the same regime

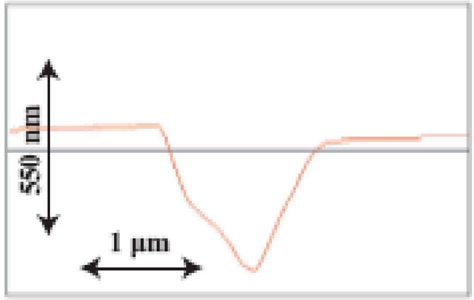


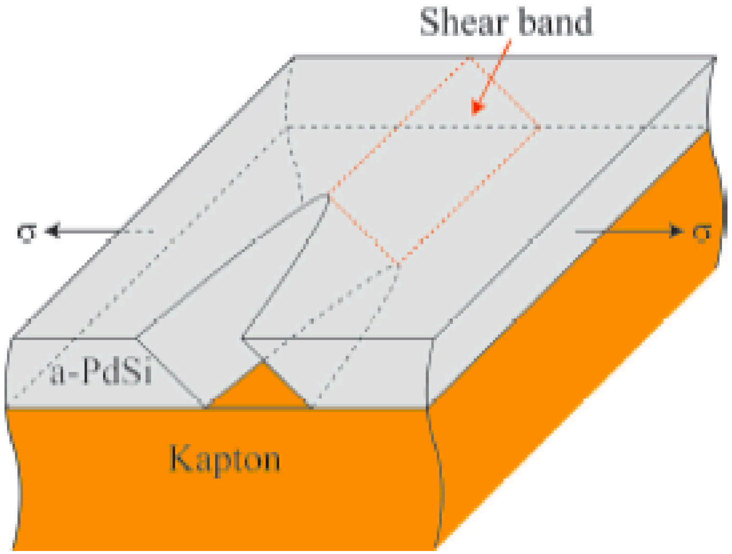
Minimize the effect of the shear bands:

metallic glass film
on compliant substrate
(Kapton)

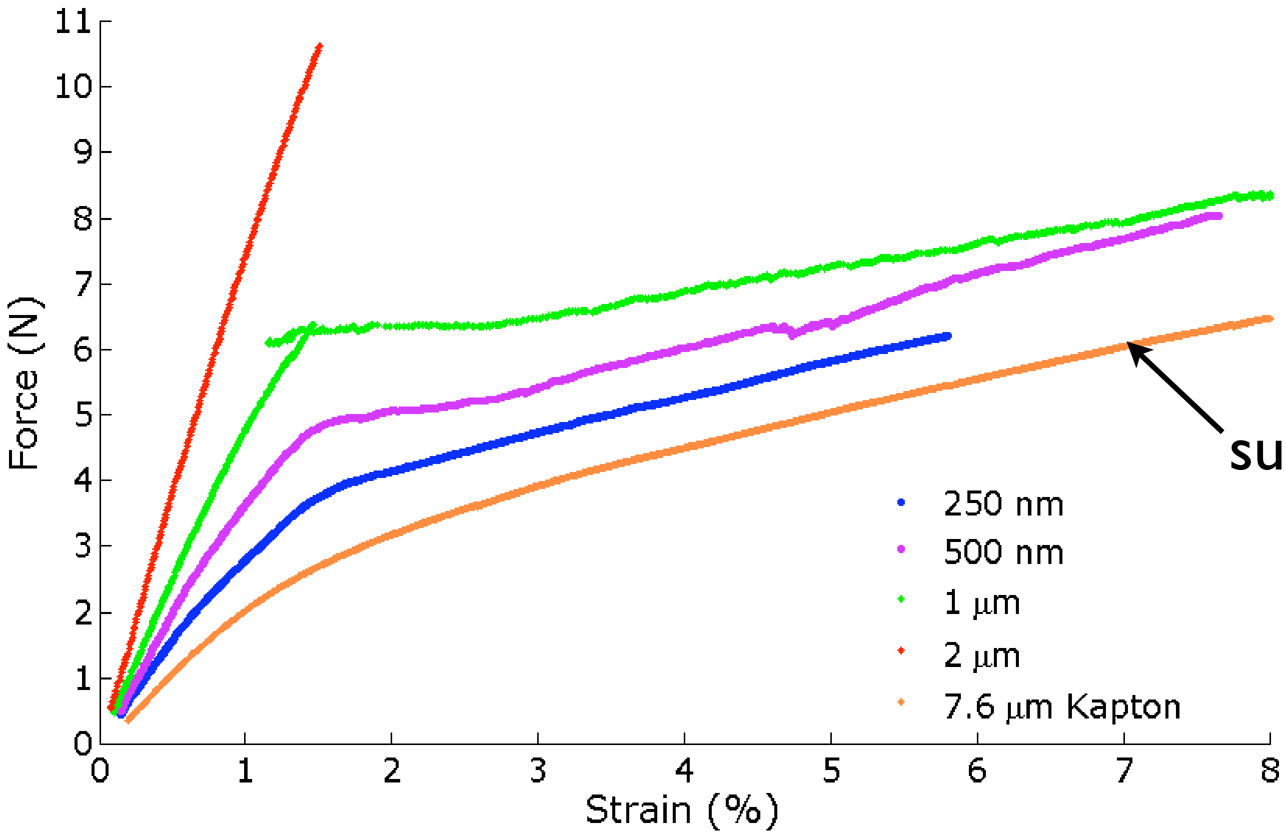
AFM of a crack: shear band profile







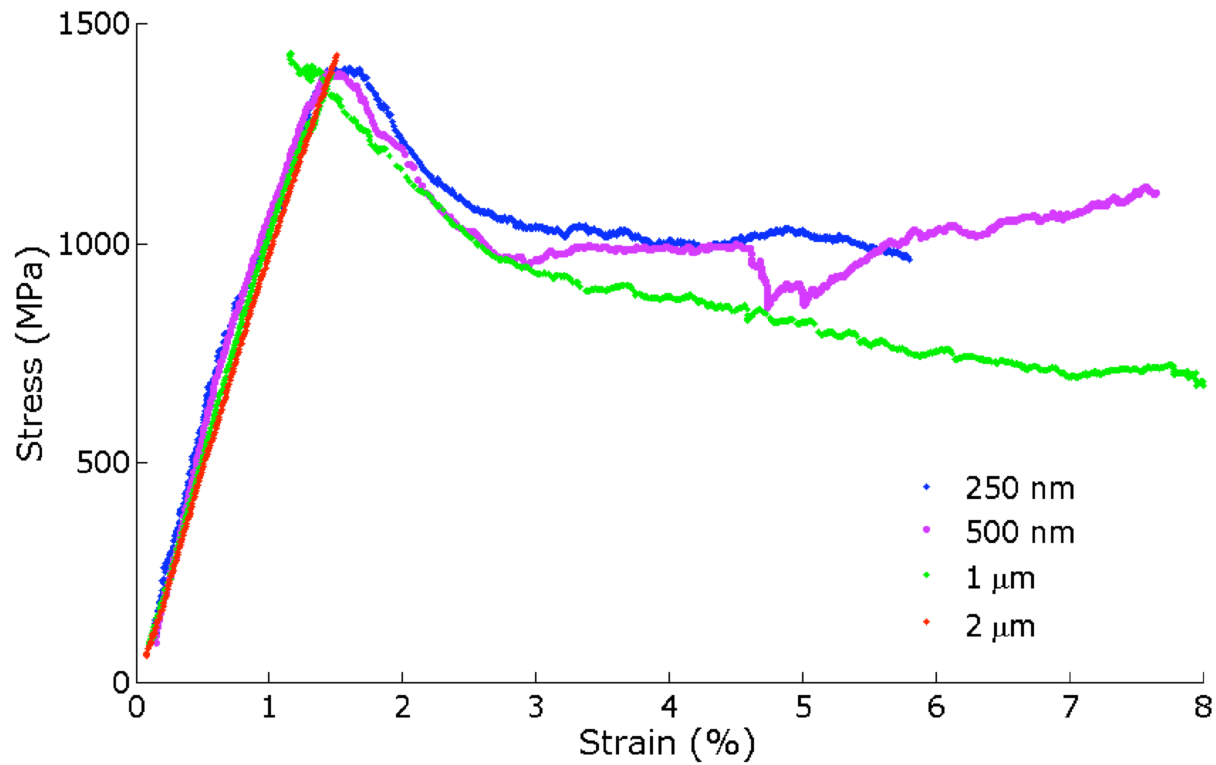
Thin film a-PdSi on kapton



subtract kapton component

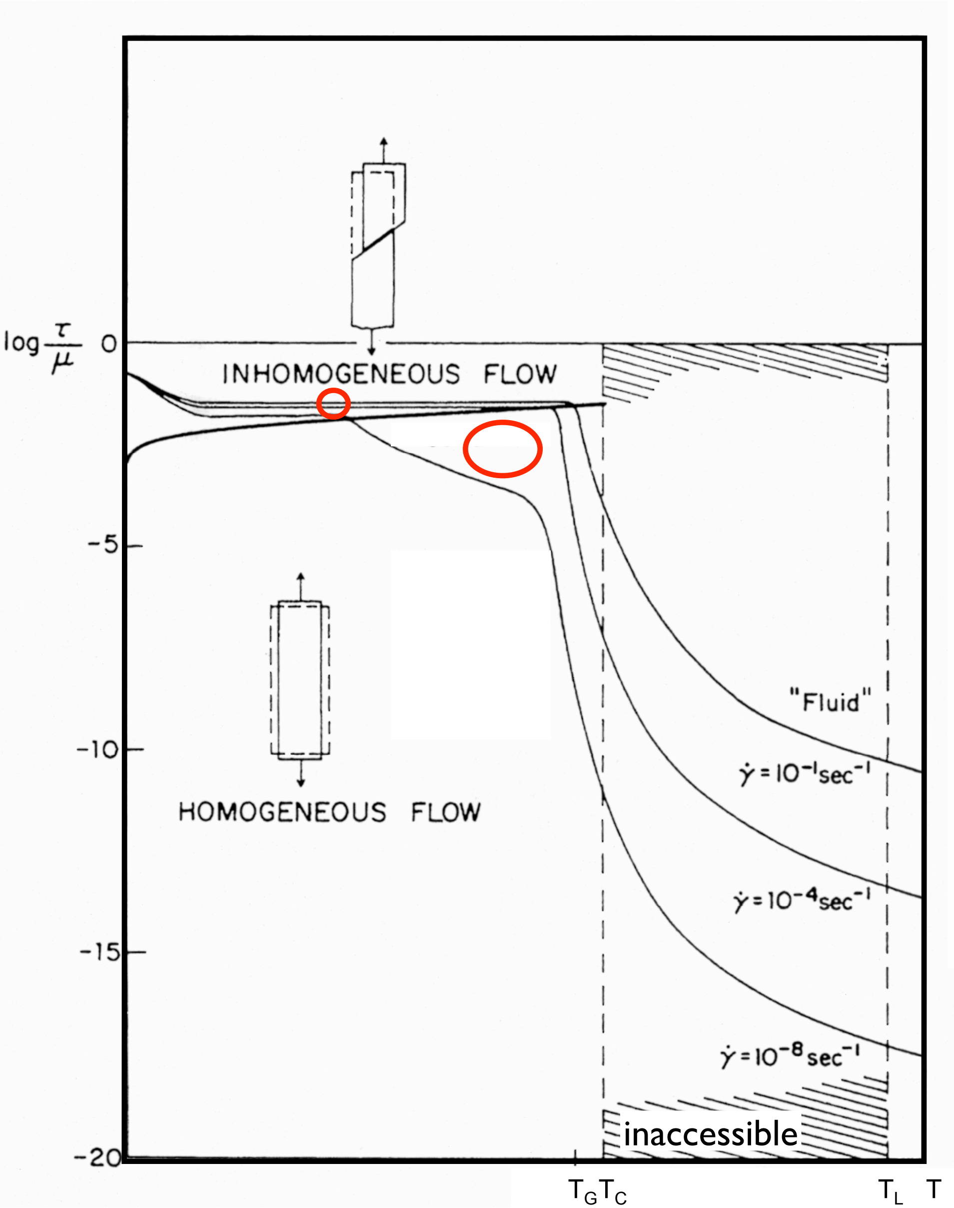
Thin film a-PdSi on kapton

Yield strength: 1.4 ± 0.2 GPa



Young's modulus: 95 ± 6 GPa

Glass at high stress



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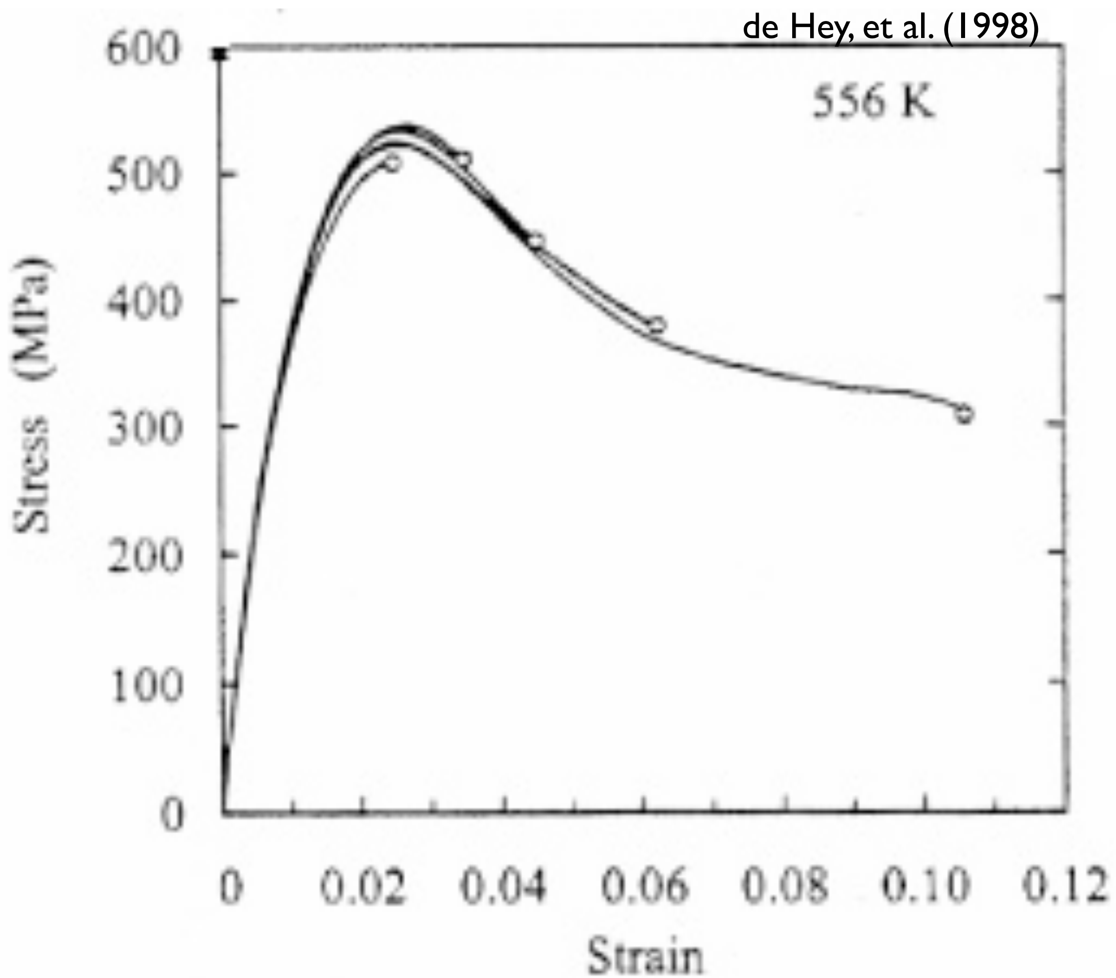
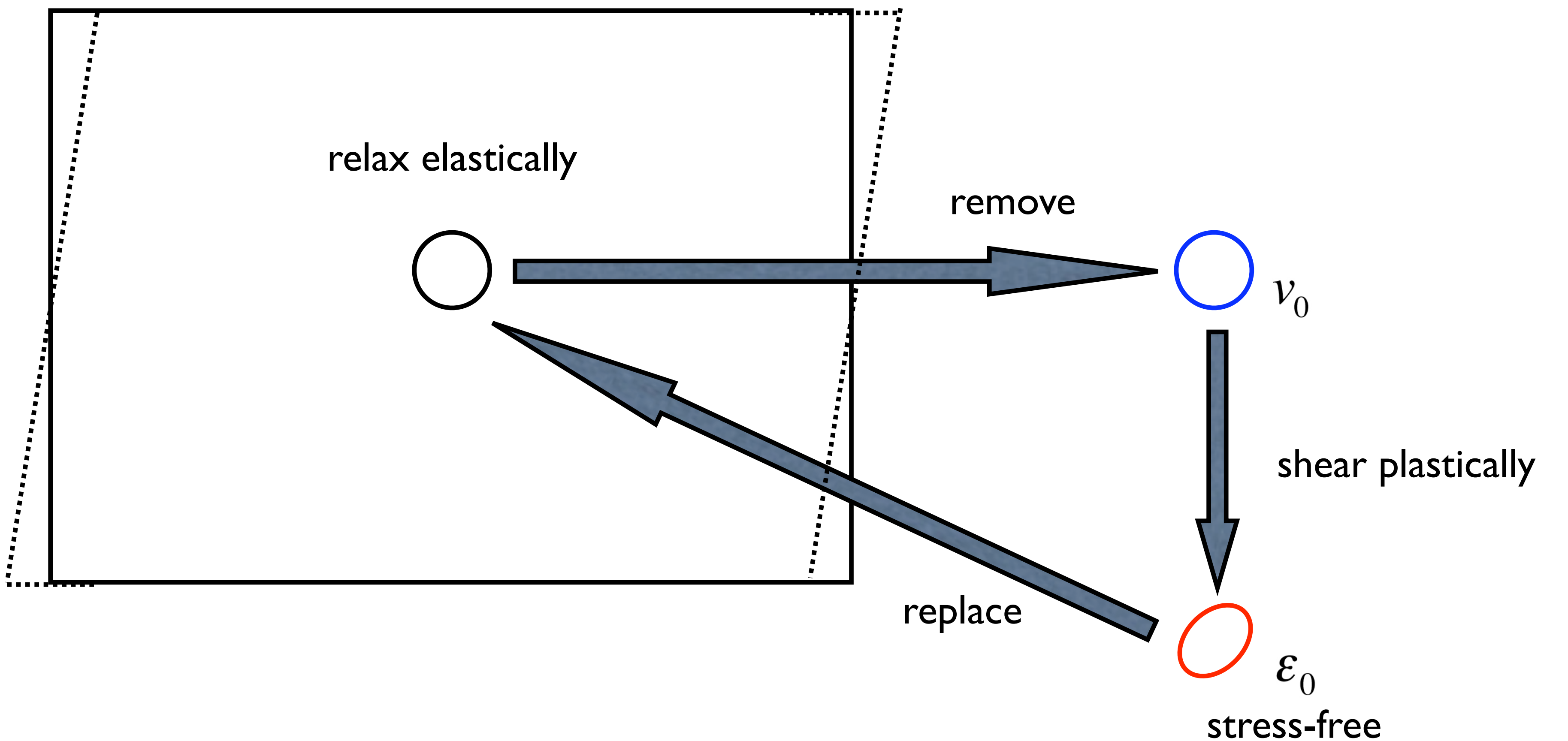


deformation-induced softening

What governs flow on the atomic scale ?

The Eshelby problem

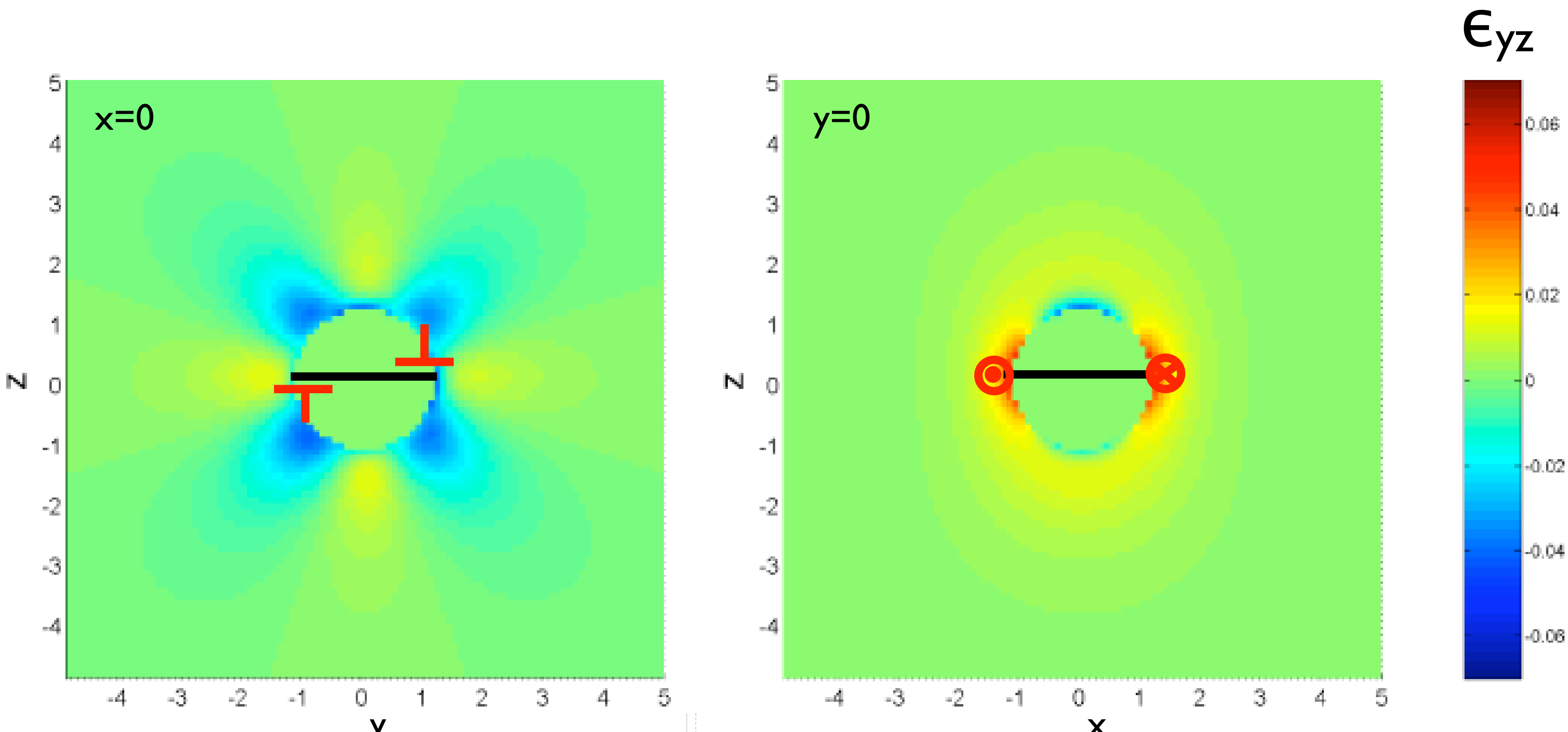
J. D. Eshelby, Proc. Roy. Soc. A 241, 376 (1957)



rearrangement of atoms irreversible

The Eshelby problem

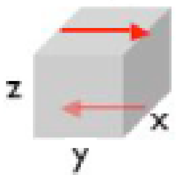
J. D. Eshelby, Proc. Roy. Soc. A 241, 376 (1957)



side view

head-on view

elastic field similar to that of a dislocation loop



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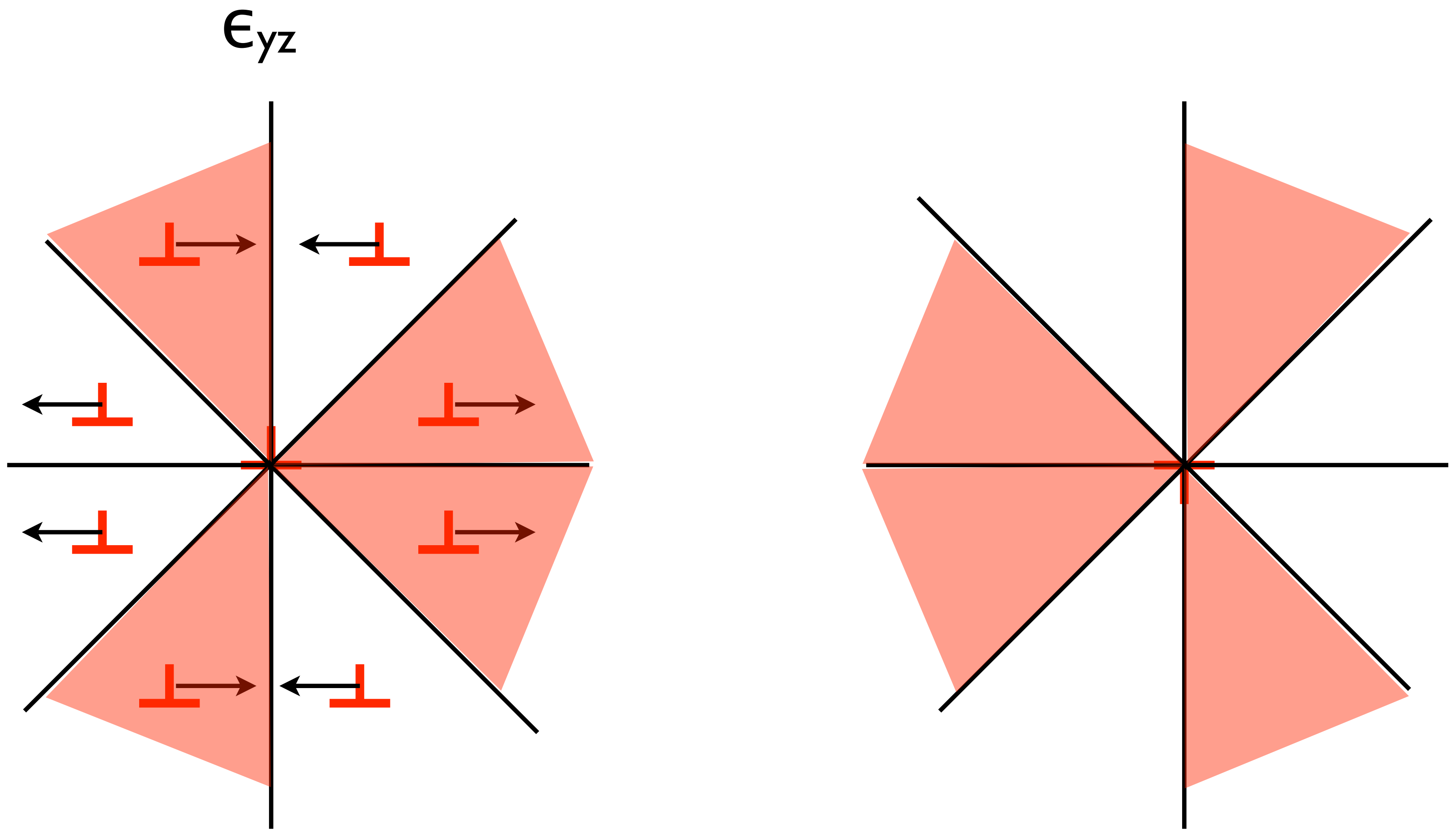

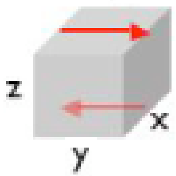

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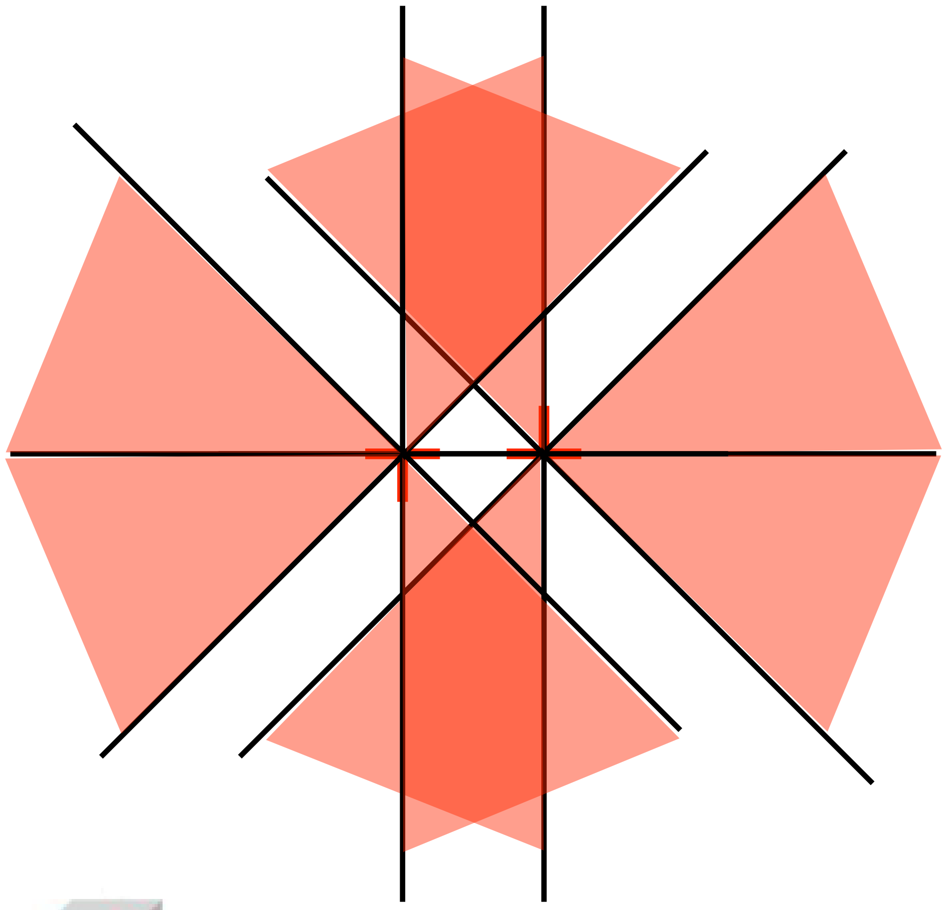

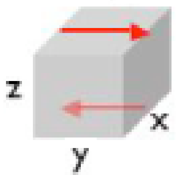

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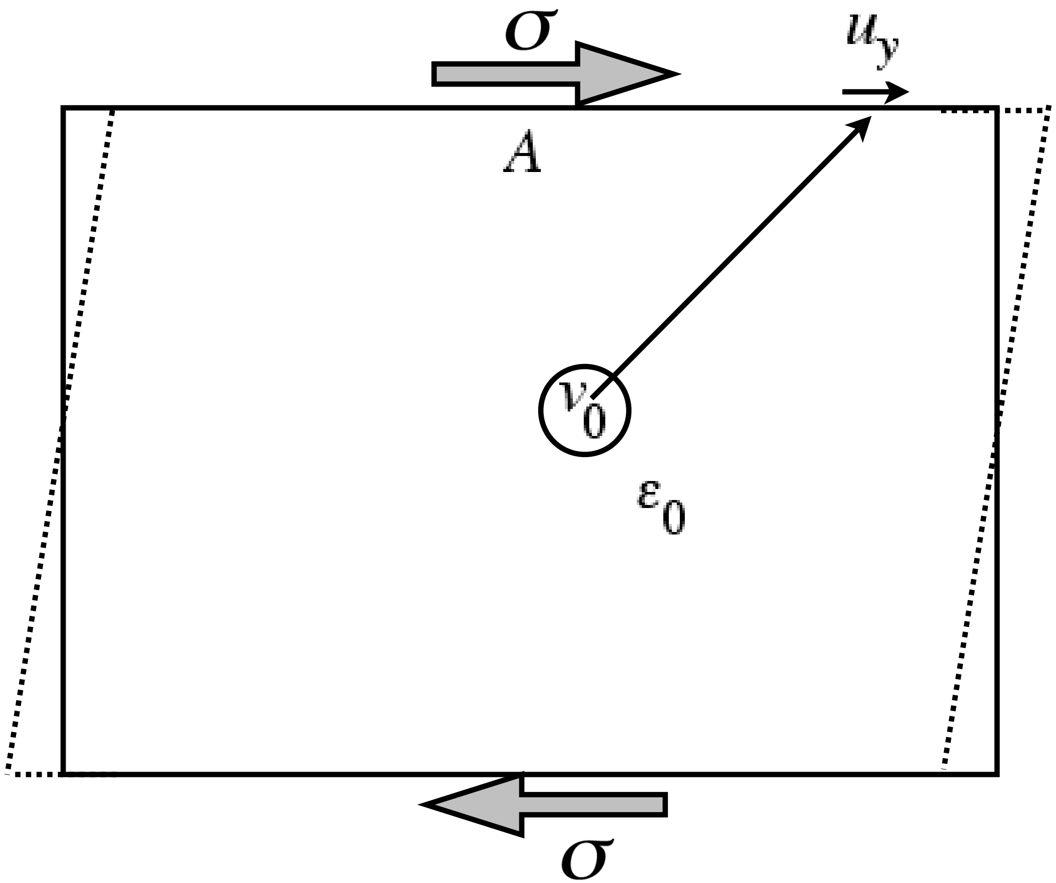


far-field solution

$$u_y = \varepsilon_0 \frac{4-5\nu}{20\pi(1-\nu)} v_0 \left[\frac{5(1-2\nu)}{2(4-5\nu)} \frac{z}{r^3} + 30 \frac{y^2 z}{r^5}\right]$$

$$\varepsilon_{yz} = \frac{1}{2}\left(\frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y}\right) \propto \frac{1}{r^3}$$

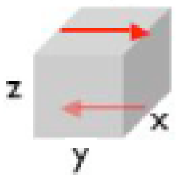
work done by external stress

$$W = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} u_y \, \sigma dx dy = \sigma \varepsilon_0 v_0 = \sigma A < u_y >$$

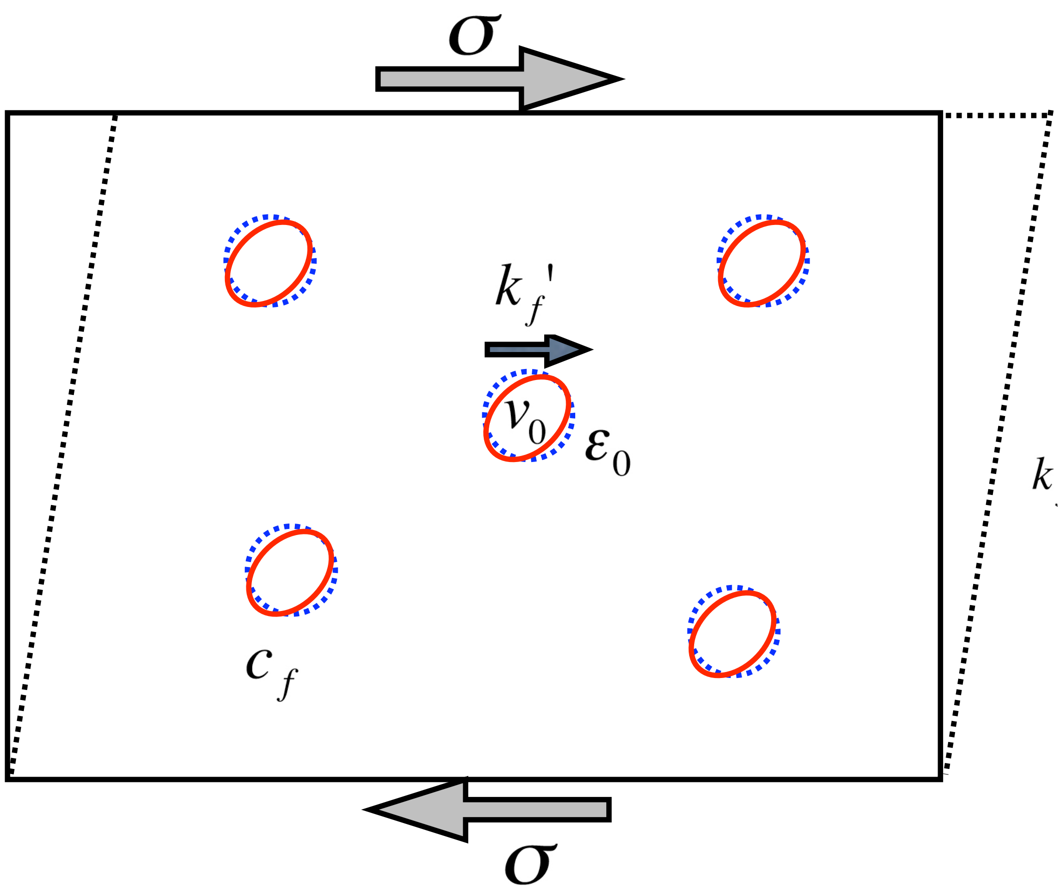
macroscopic strain

$$\varepsilon = \frac{< u_y >}{z} = \frac{\varepsilon_0 v_0}{zA} = \varepsilon_0 \frac{v_0}{V}$$

volume fraction of inclusion



General constitutive flow law



$$\dot{\varepsilon} = \varepsilon_o v_o k_f' \frac{c_f}{\Omega}$$

work upon jump $\sigma\varepsilon_o v_o$

$$k_f' = \nu\left[\exp\left(-\frac{Q-(\sigma\varepsilon_o v_o/2)}{kT}\right) - \exp\left(-\frac{Q+(\sigma\varepsilon_o v_o/2)}{kT}\right)\right]$$

$$k_f' = \nu\exp\left(-\frac{Q}{kT}\right)2\sinh\left(\frac{\sigma\varepsilon_o v_o}{2kT}\right)$$

$$\dot{\varepsilon} = 2c_f k_f \frac{\varepsilon_o v_o}{\Omega}\sinh\left(\frac{\sigma\varepsilon_o v_o}{2kT}\right)$$

low stress $\sinh\left(\frac{\sigma\varepsilon_o v_o}{2kT}\right) \approx \frac{\sigma\varepsilon_o v_o}{2kT}$

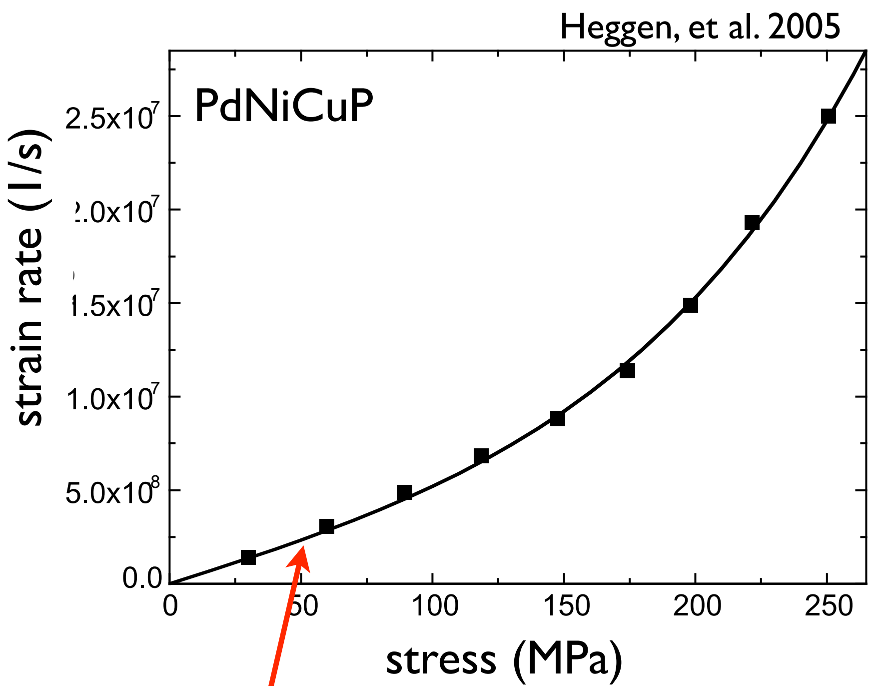
$$\dot{\varepsilon} = \frac{c_f k_f (\varepsilon_o v_o)^2 \sigma}{\Omega kT}$$

Newtonian viscous

$$\eta \equiv \frac{\sigma}{\dot{\varepsilon}} = \frac{\Omega kT}{c_f k_f (\varepsilon_o v_o)^2}$$

viscosity

Test of the constitutive law



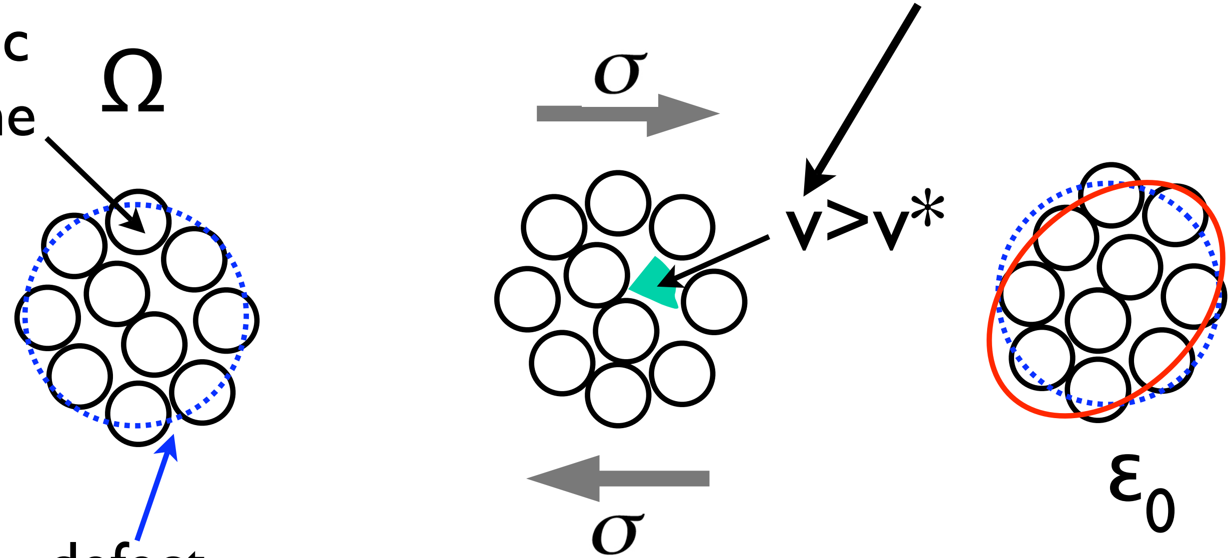
$$\frac{d\varepsilon}{dt} = 2c_f k'_f \frac{\varepsilon_o v_o}{\Omega} \sinh\left(\frac{\varepsilon_o v_o \sigma}{2kT}\right)$$

8 atomic volumes

Newtonian

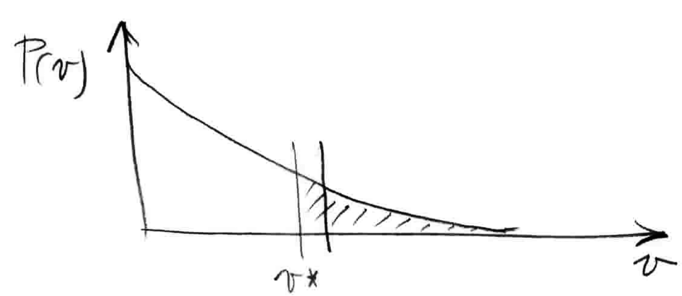
Free volume model

M.H. Cohen and D. Turnbull, J. Chem. Phys. 31, 1164 (1959)



average free volume per atom $v_f = \Omega - \Omega_o$ ← atomic volume at closest packing (infinite viscosity)

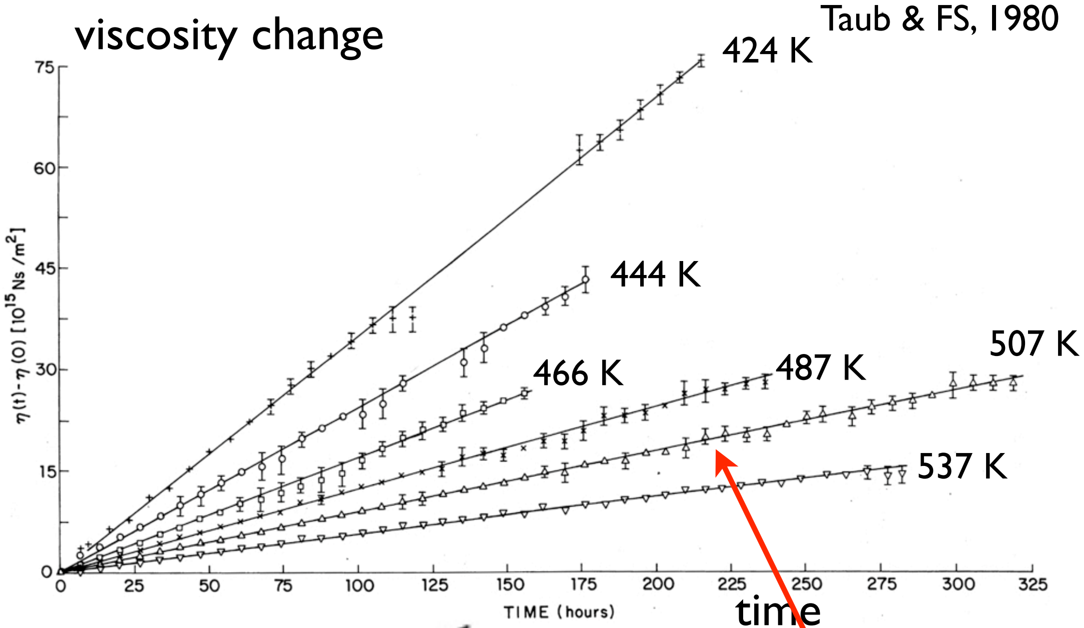
$$c_f \sim \exp\left(-\frac{\gamma v^*}{v_f}\right)$$



$$\eta = \eta_0 \exp\left(\frac{B}{T - T_0}\right)$$

Fulcher-Vogel-Tammann

Structural relaxation kinetics



$$\eta \propto \frac{1}{c_f}$$

$$\frac{d\eta}{dt} \propto -\frac{1}{c_f^2}\frac{dc_f}{dt}$$ = constant

$$\frac{dc_f}{dt} = -k_r c_f^2$$

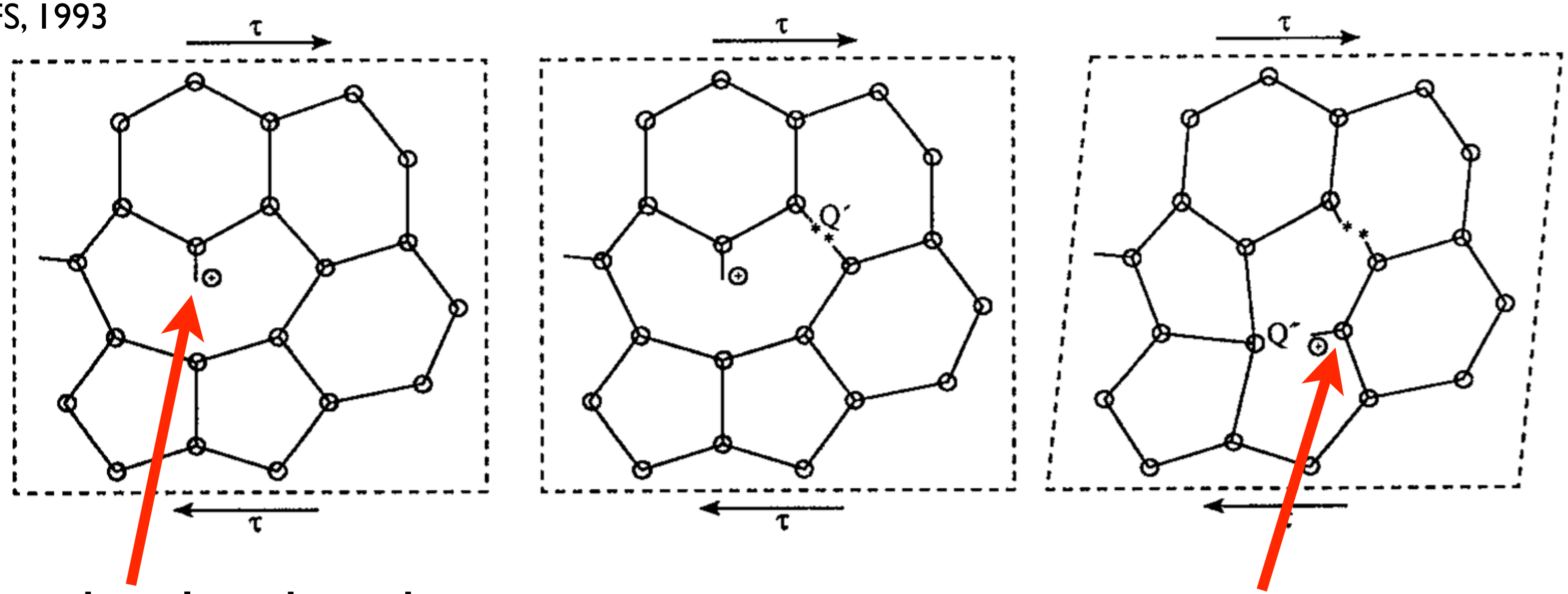
bimolecular annihilation

Structural relaxation kinetics

$$\frac{dc_f}{dt} = -k_r c_f^2$$ bimolecular defect annihilation

seen, as expected, in covalent networks (a-Si)

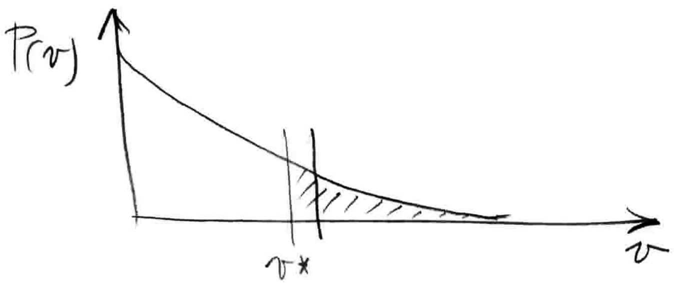
Witvrouw & FS, 1993



dangling bond

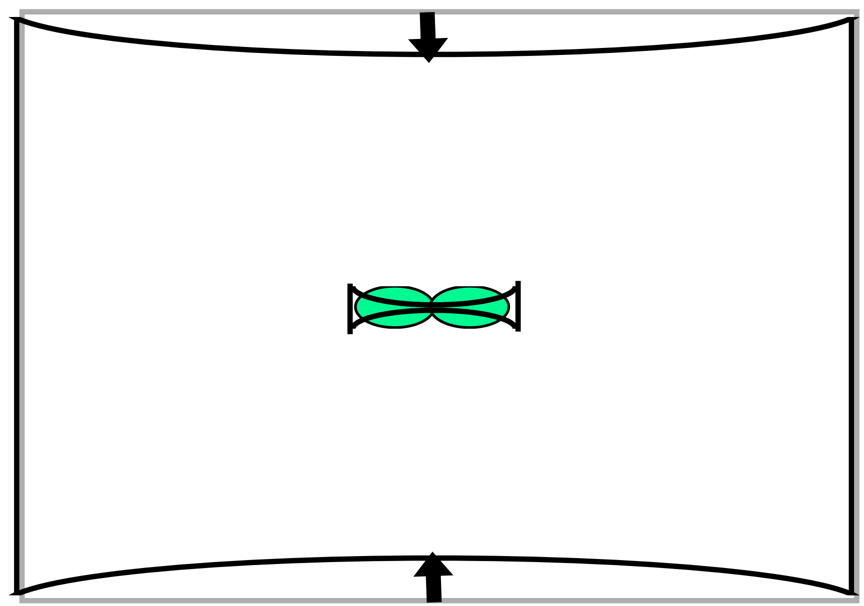
two dangling bonds annihilate to a full bond

Structural relaxation kinetics

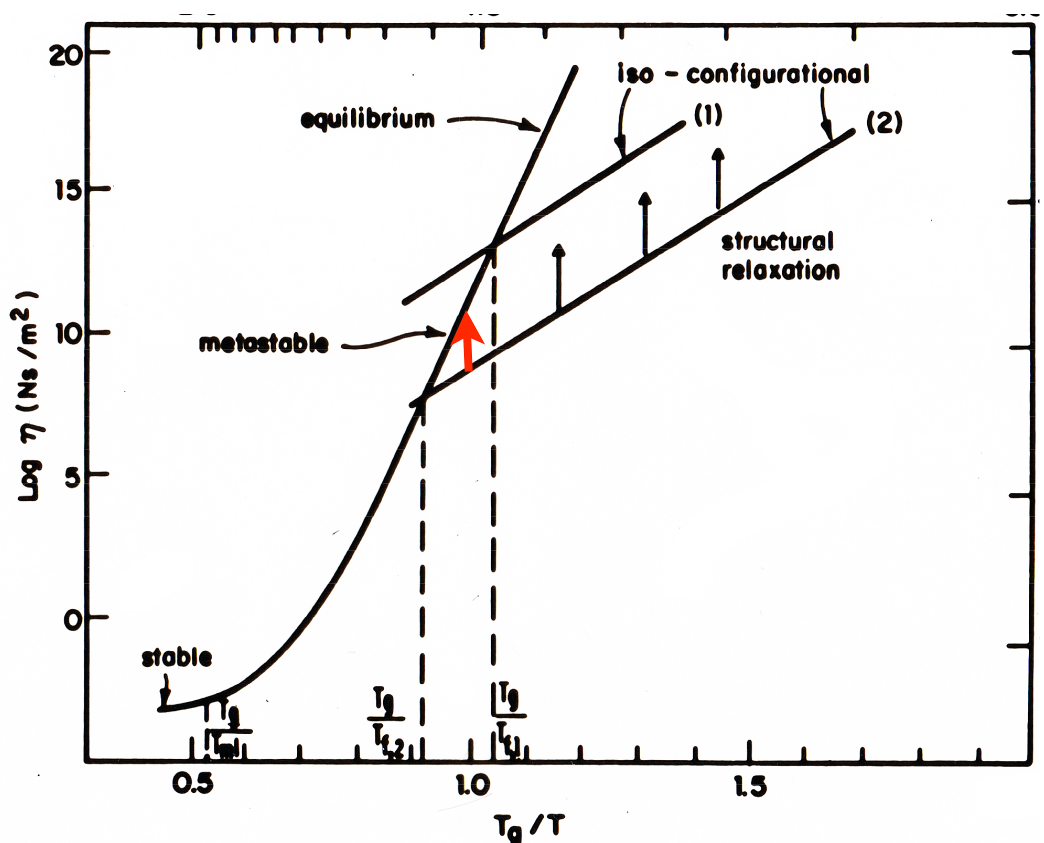


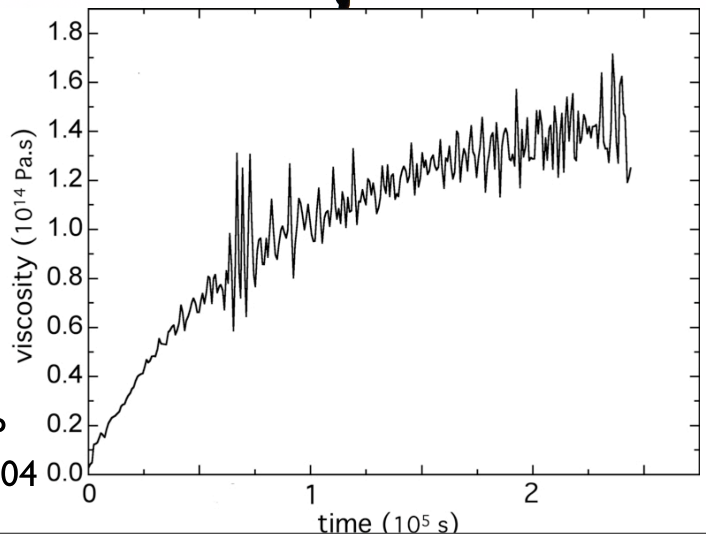
$$\frac{dc_f}{dt} = -k_r c_f^2$$

Bimolecular mechanism
for free volume annihilation



Structural relaxation with saturation

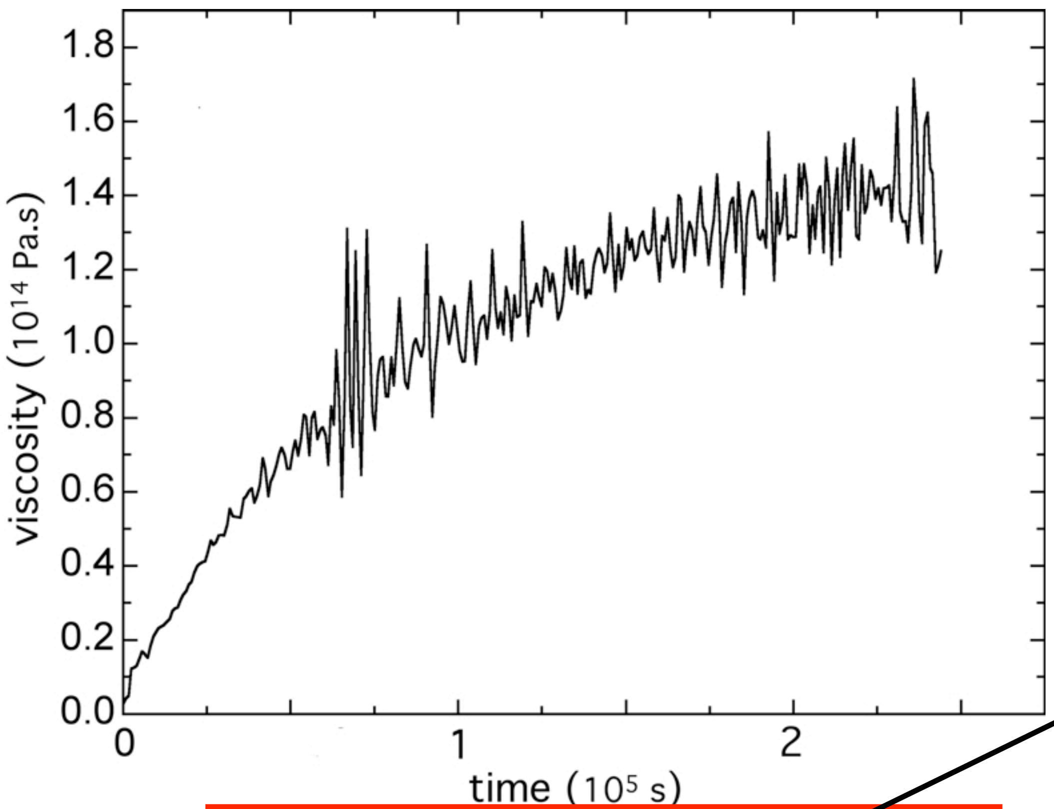




PdNCuiP
Heggen, 2004

Structural relaxation with saturation

Heggen, 2004



bimolecular annihilation (from before)

$$\frac{dc_f}{dt} = -k_r c_f^2$$

$$\frac{dc_f}{dt} = -k_r c_f \left(c_f - c_{f,eq}\right)$$

$$\frac{dc_f}{dt} = -k_r \left(c_f - c_{f,eq}\right)^2$$

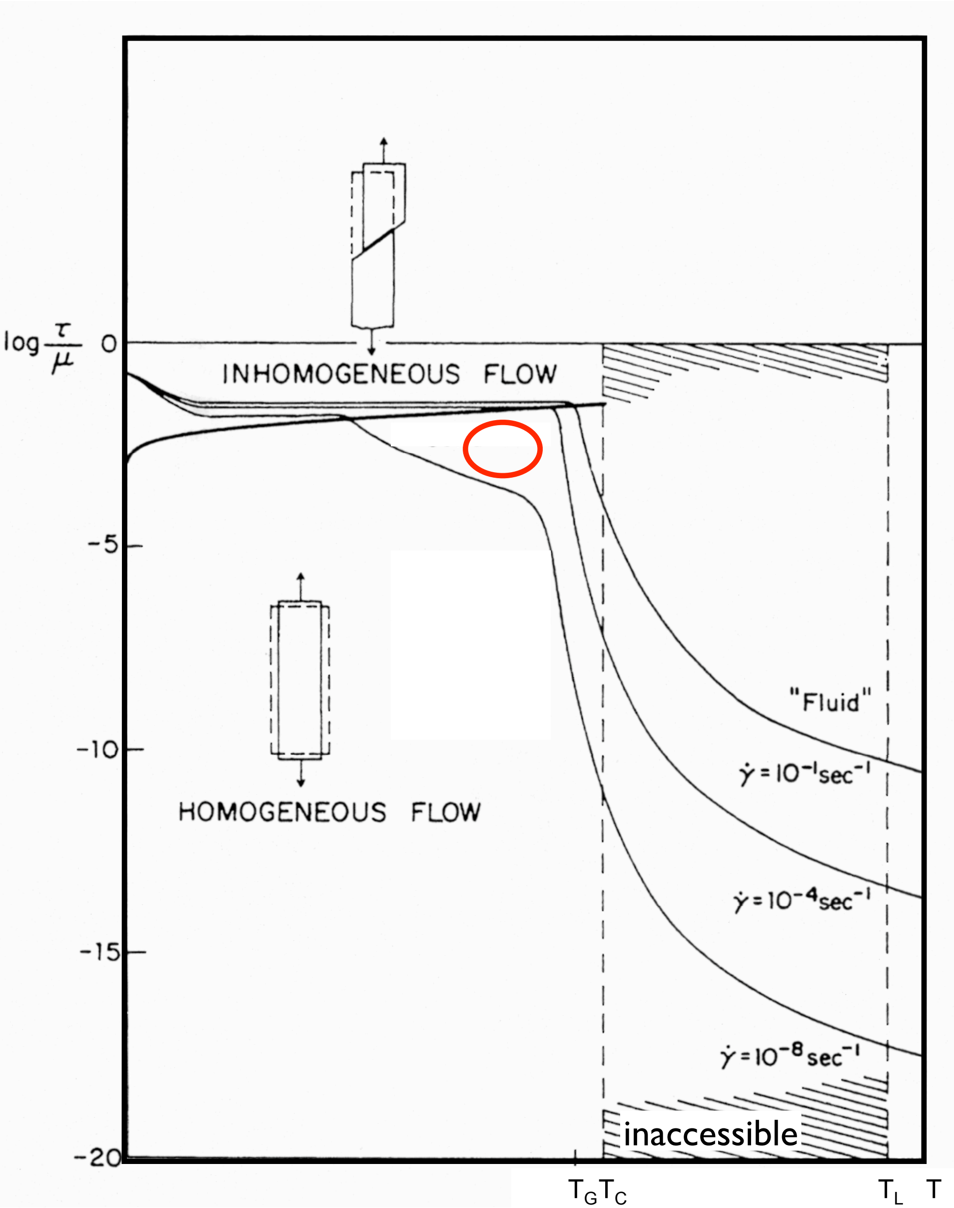
$$\frac{dc_f}{dt} = -k_r c_f^2 + (k_r c_{f,eq}) c_f$$

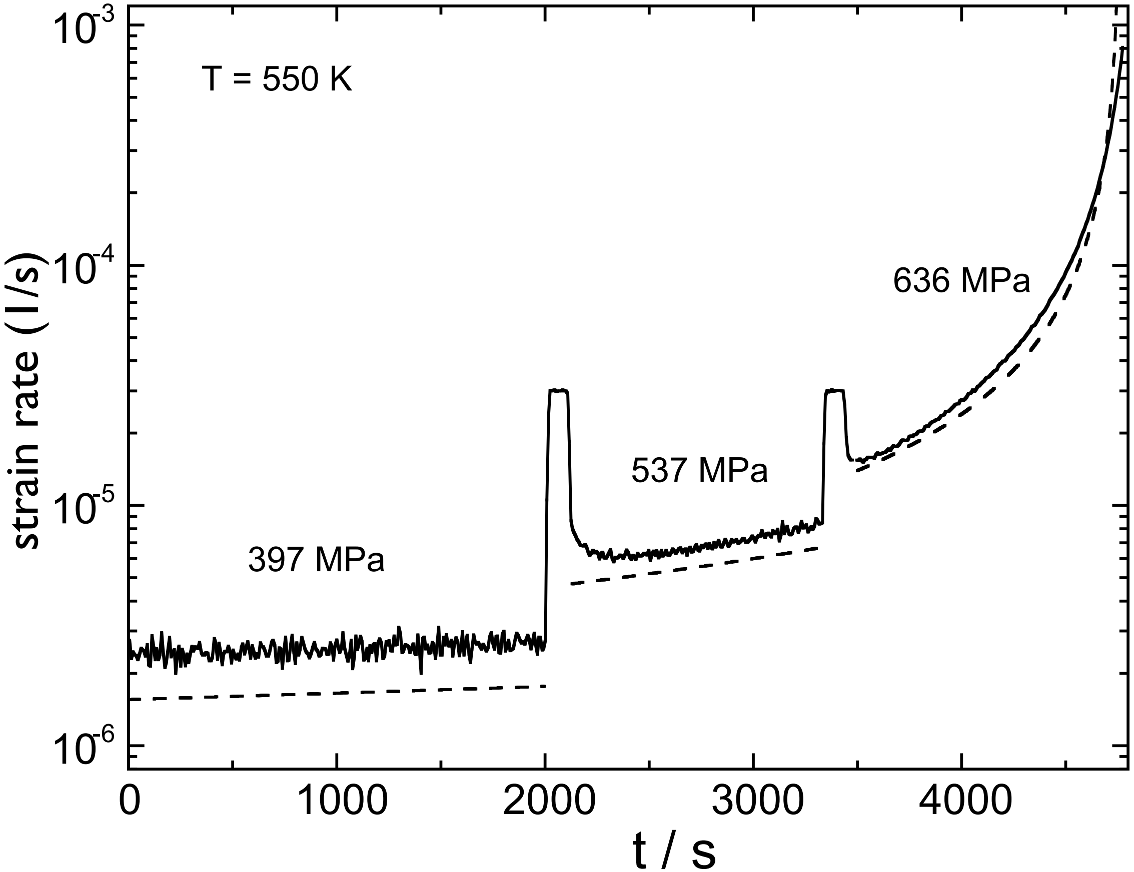
bimolecular annihilation

unimolecular creation

thermal

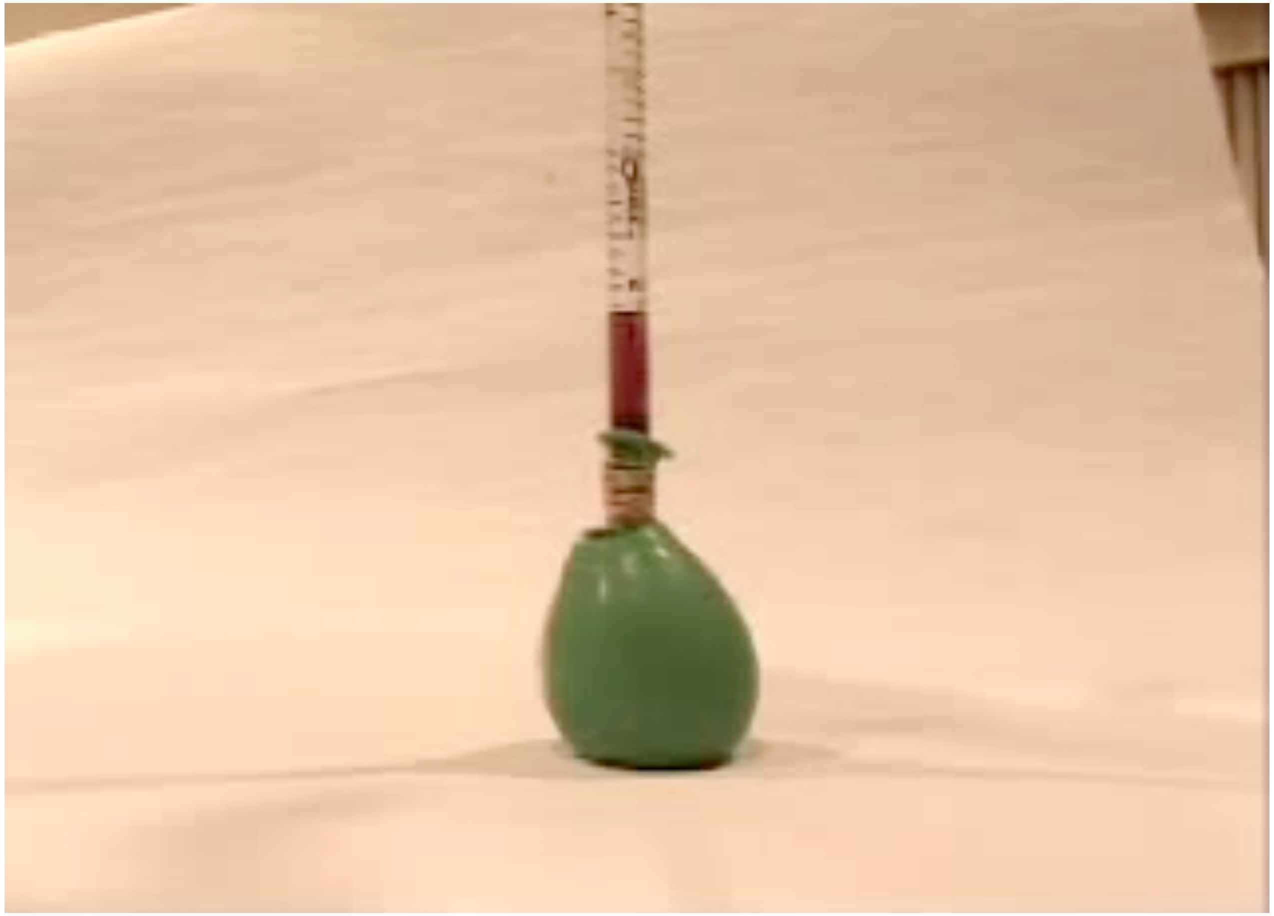
Glass at high stress





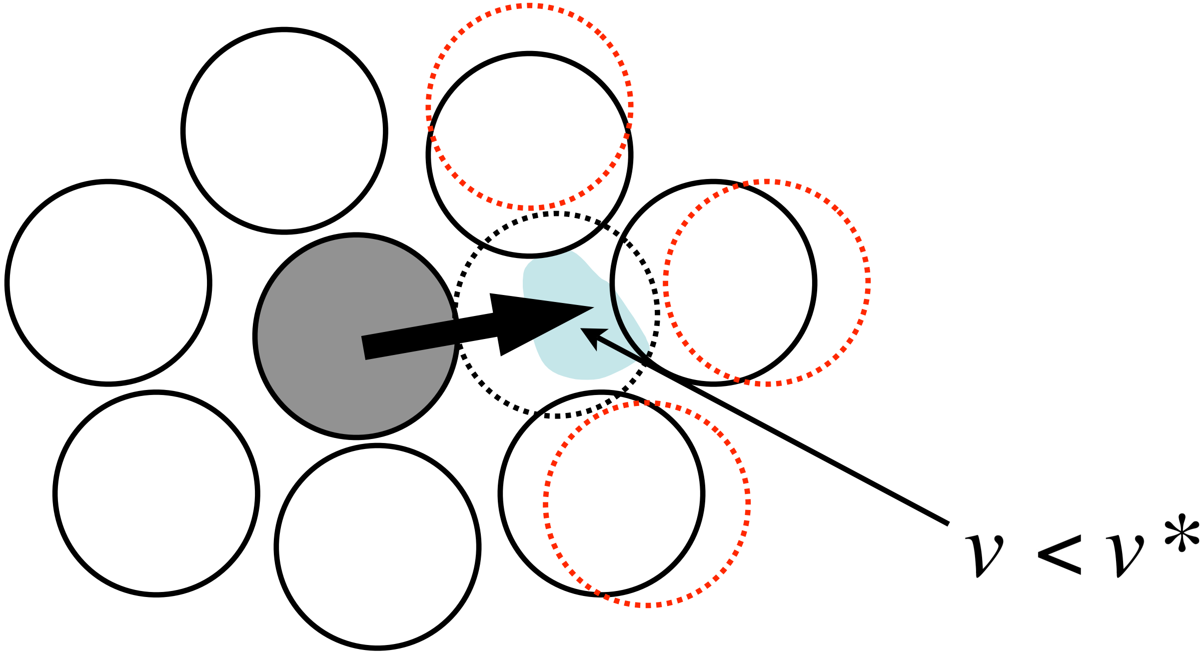
deformation-induced softening

Shear flow causes dilatation



balloon packed with sand
saturated with water

Mechanism for creation of free volume



$$\frac{dv_f}{dt} = 3c_f k_f' \; kT \frac{(1-\nu)}{\mu(1+\nu)} \; \frac{\gamma v^*}{v_f} \left[\cosh\left(\frac{\sigma \varepsilon_o v_o}{2kT} \right) - 1 \right]$$

$\propto \; \sigma^2$ $\qquad \propto \; \sigma \frac{d\varepsilon}{dt}$ $\qquad$ = applied power density

at small stress

Free volume creation parameters

fitted parameter $\dot{v}_f = a_x' \gamma \nu^* \dot{\varepsilon} \sigma$

dilatation model $\dot{v}_f = \frac{1}{8} \frac{\Omega}{S} \frac{\gamma \nu^*}{v_f} \dot{\varepsilon} \sigma$ ← applied power

Work to create one atomic volume of free volume: 12-32 eV
Most energy dissipated as heat

$$a_x' = \frac{1}{8} \frac{\Omega}{v_f S}$$

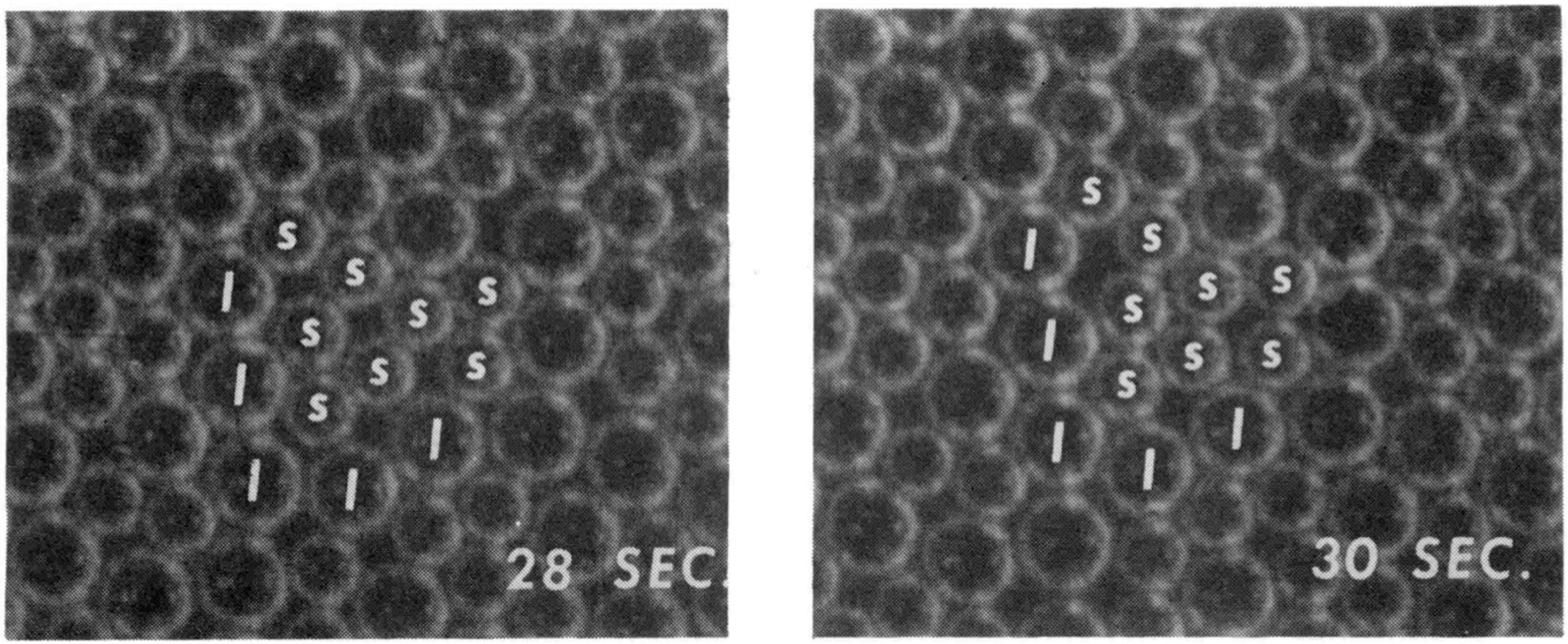
↑ $3.10^{-11} Pa^{-1}$ ↑ $6.10^{-10} Pa^{-1}$

only a small fraction (1/20) of the free volume generated by the dilatation persists

Direct experimental evidence for the structure of the flow defect

Dislocation in a crystal:
diffraction contrast of its strain field
in the electron microscopy

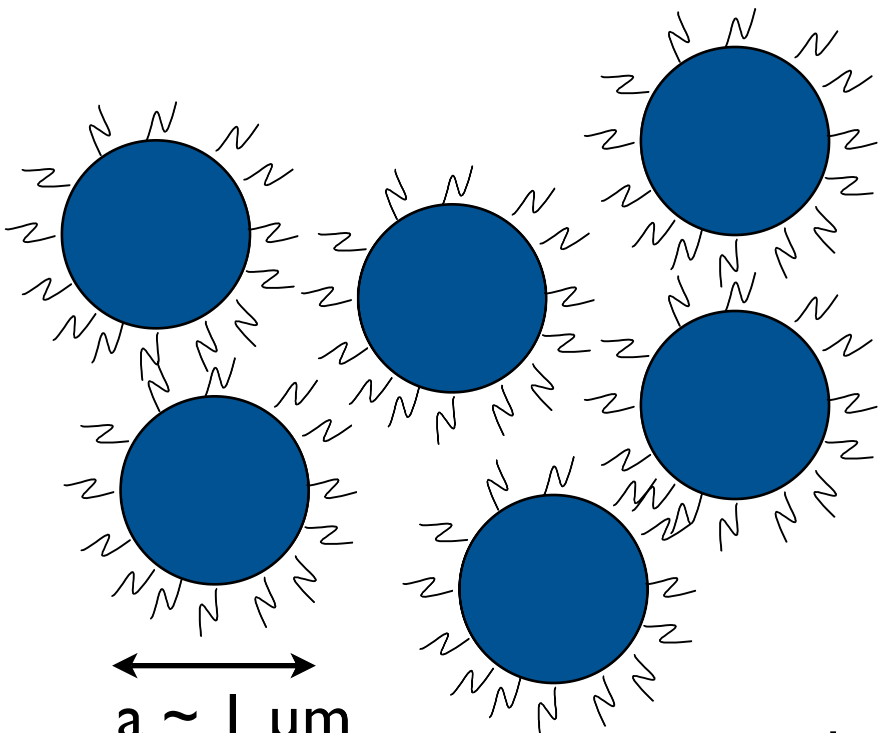
Amorphous bubble raft



Argon, 1979

Three-dimensional "bubble raft"

Colloids



a ~ 1 μm

Big
can be "seen"

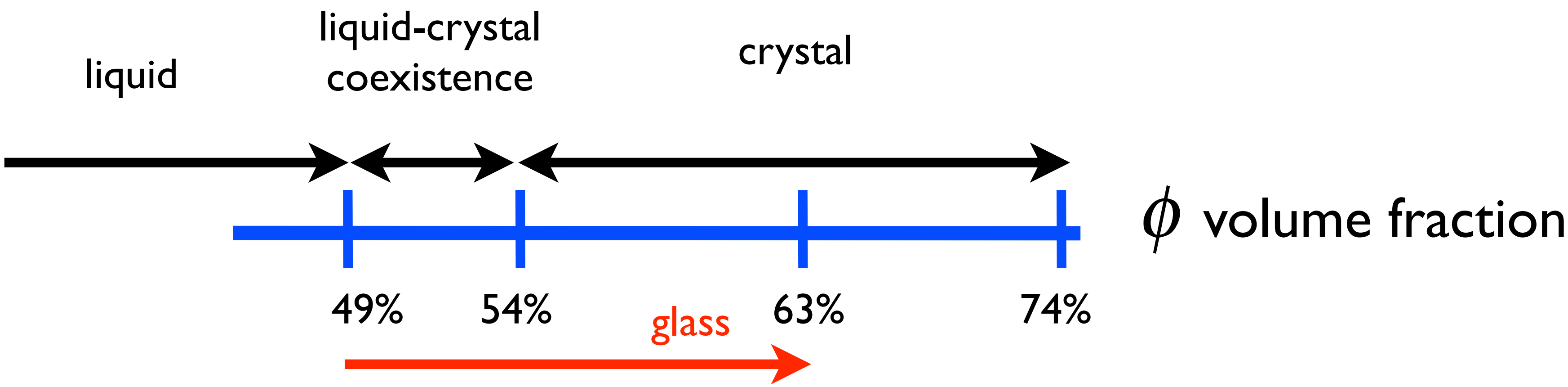
solid particles
in a solvent

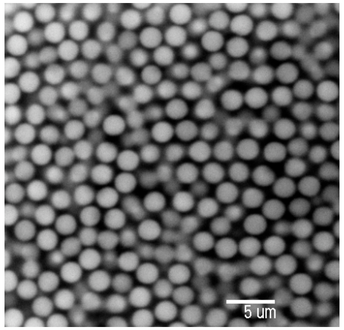
short range repulsion
sometimes charged

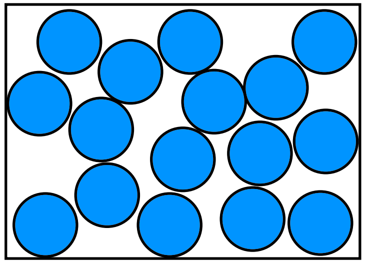
dynamics $\tau = \frac{a^2}{D} = \frac{\eta\, a^3}{kT} = 0.01\text{-}1\ \mathrm{s}$

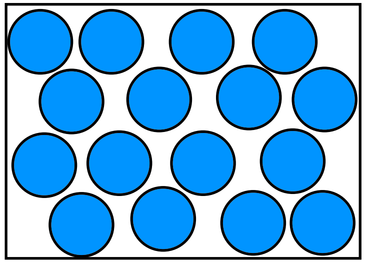
Slow
can be tracked

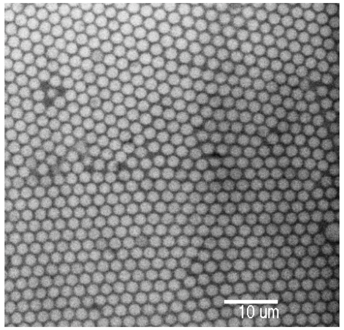
Hard sphere phases











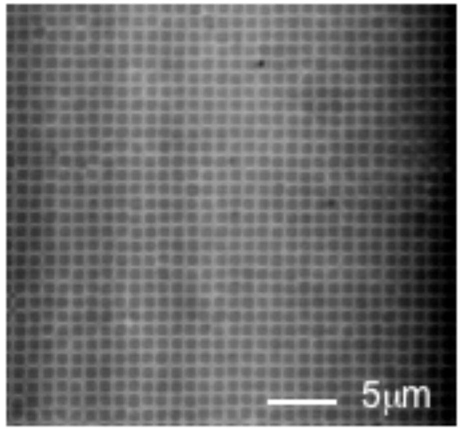
Φ_{max}=0.6366

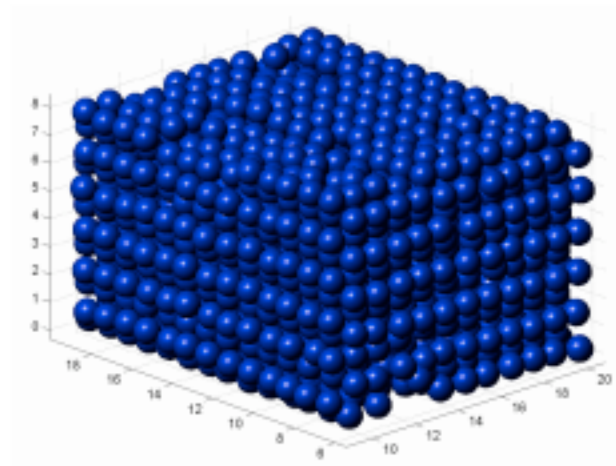
Φ_{max}=0.7405

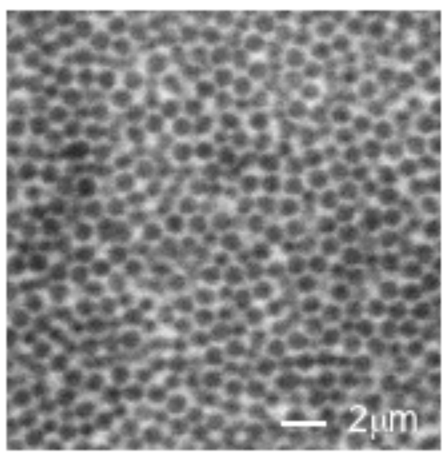
increase Φ ⟷ decrease T

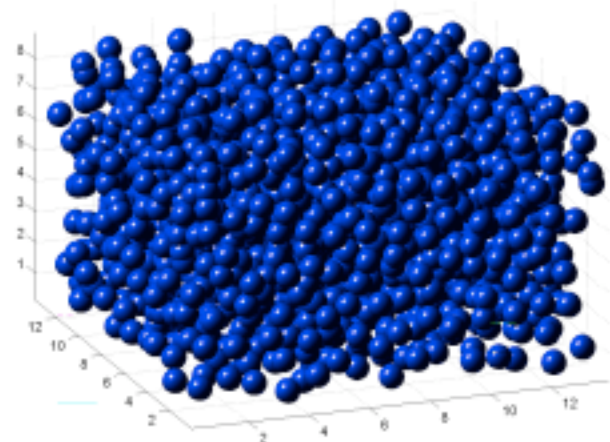
hard spheres — atoms

Crystalline and amorphous colloidal structures

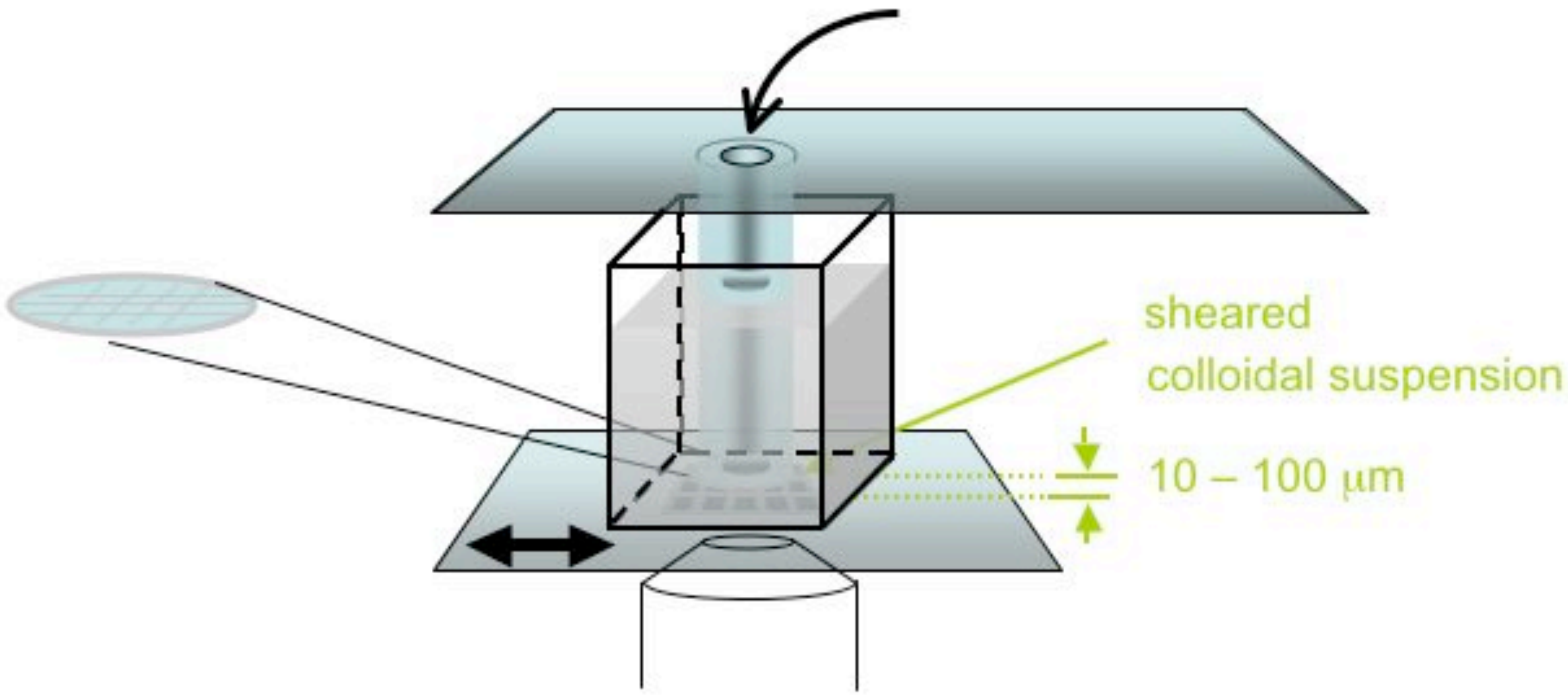


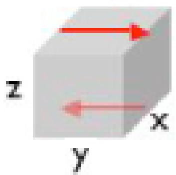




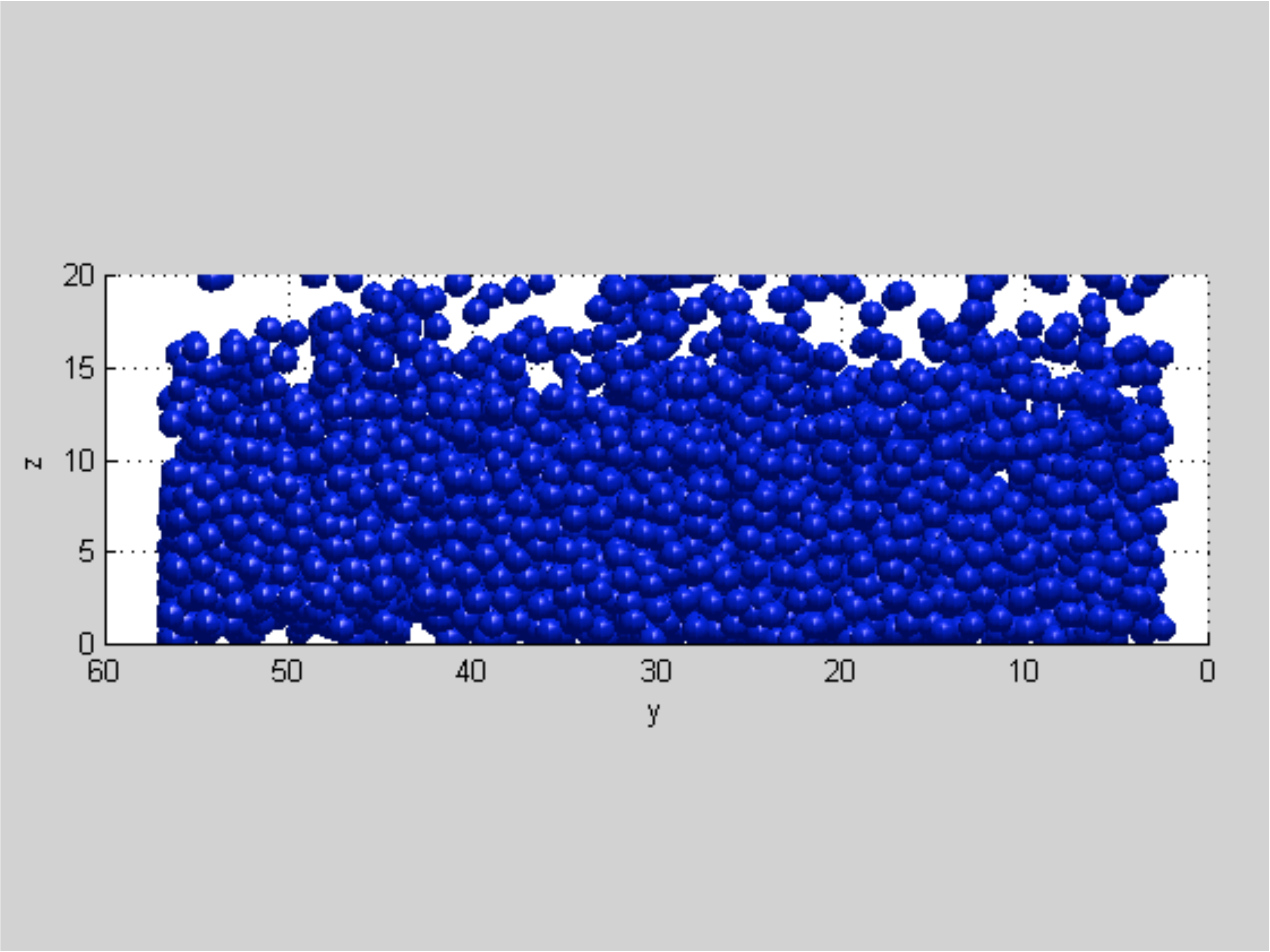


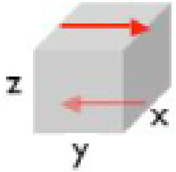
Shear cell





Shearing of a glass

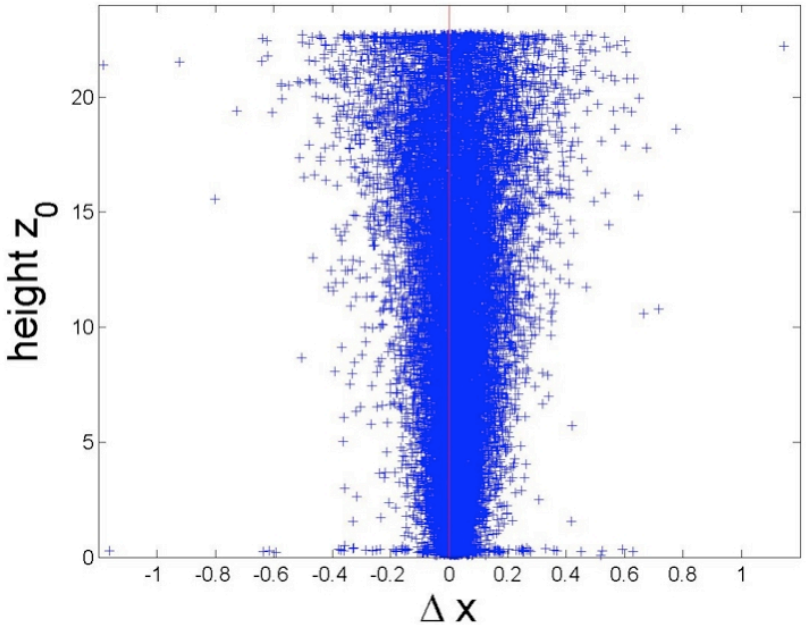




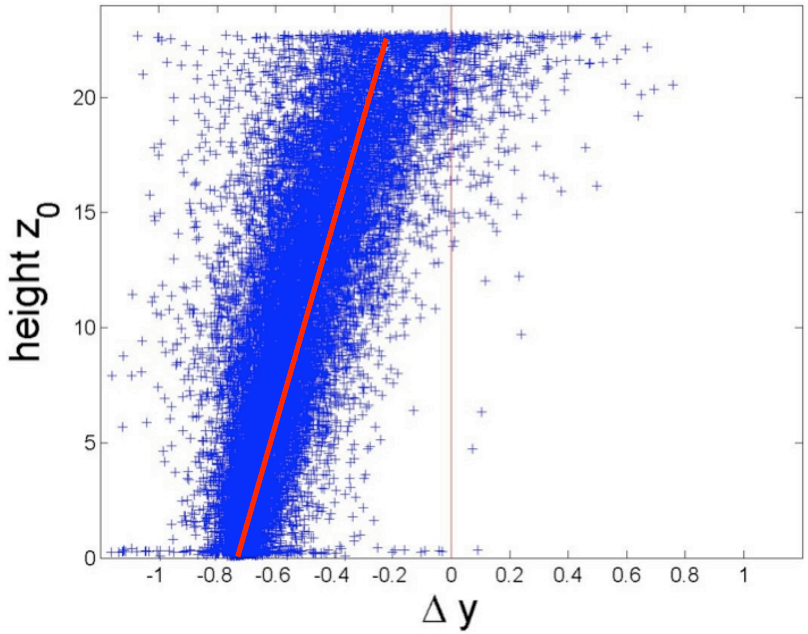
Particle displacements during shear

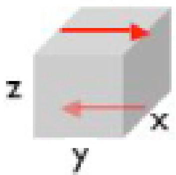
2.5% shear, 10^{-5} s^{-1}

x-displacements

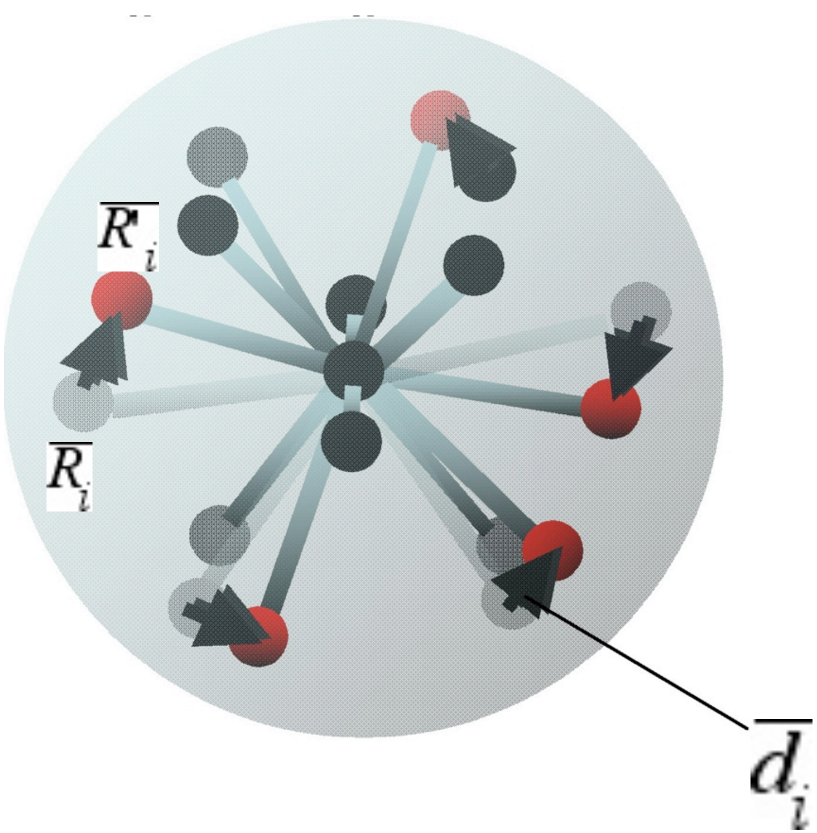


y-displacements





Calculation of the local strain tensor



best self-affine deformation

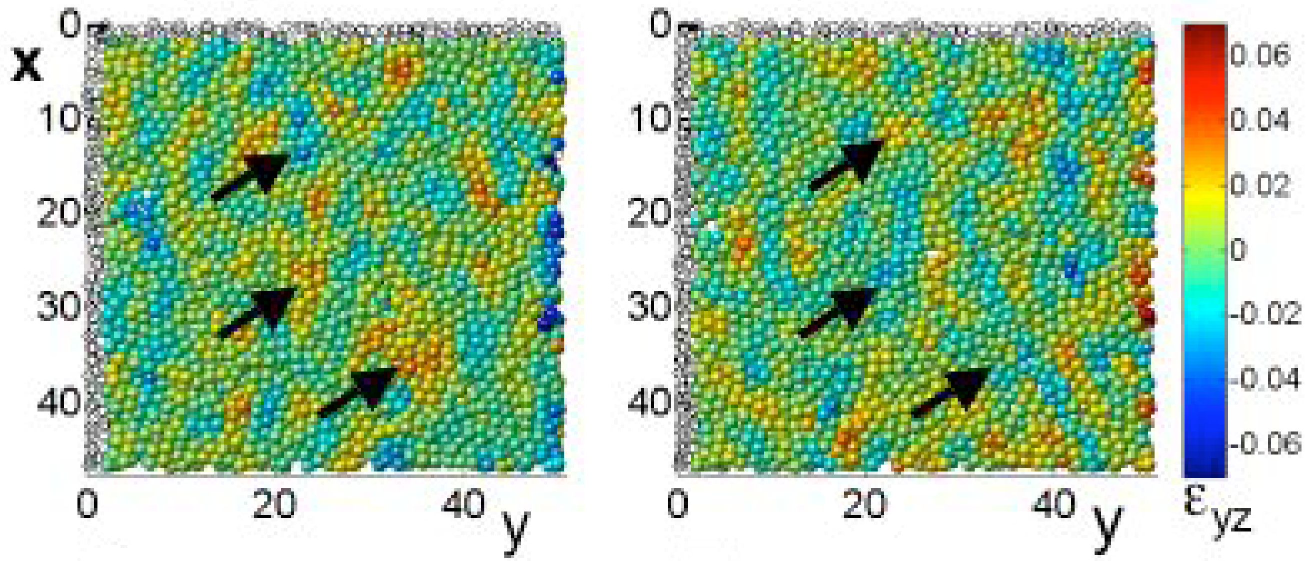
$$\overline{R'}_i = \overline{R}_i + \overline{\overline{\alpha}}.\overline{R}_i$$

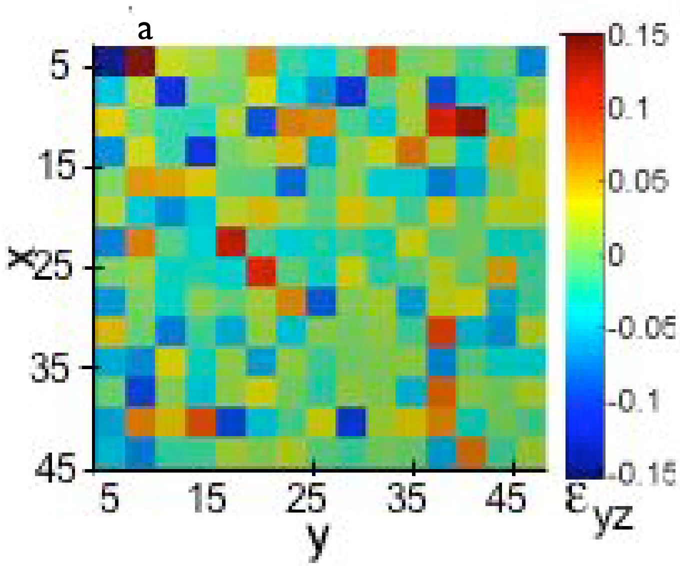
optimize $\overline{\overline{\alpha}}$ by minimizing

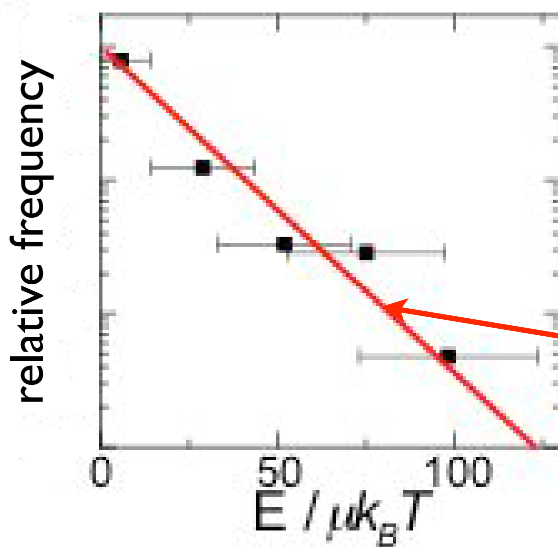
$$D^2 = \sum_i (\overline{d}_i - \overline{\overline{\alpha}}.\overline{R}_i)^2$$

$\overline{\overline{\varepsilon}}$ is the symmetric part of $\overline{\overline{\alpha}}$

Thermal fluctuations of ϵ_{yz} (phonons)





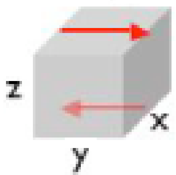


$$\frac{E}{\mu} = \frac{1}{2}\varepsilon_{yz}^2 \ a^3$$

$$f(E) = \exp\left(-\mu \frac{E/\mu}{kT}\right)$$

$$\mu = 0.056Pa$$

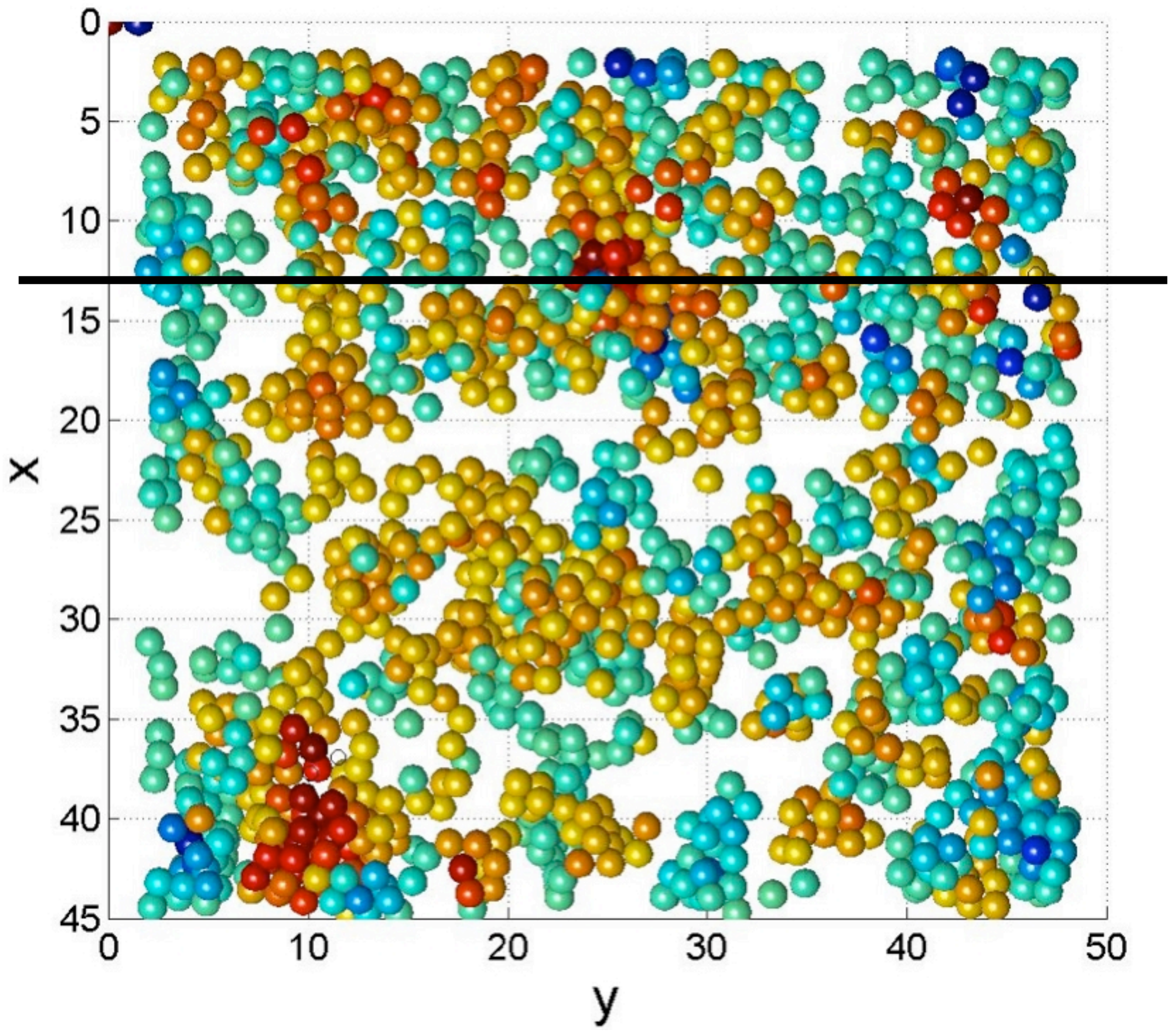
$$\approx \frac{kT}{\Omega}$$

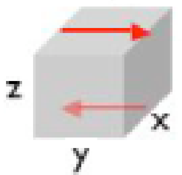


Top view: sites with largest shear strain ϵ_{yz} (+, -)

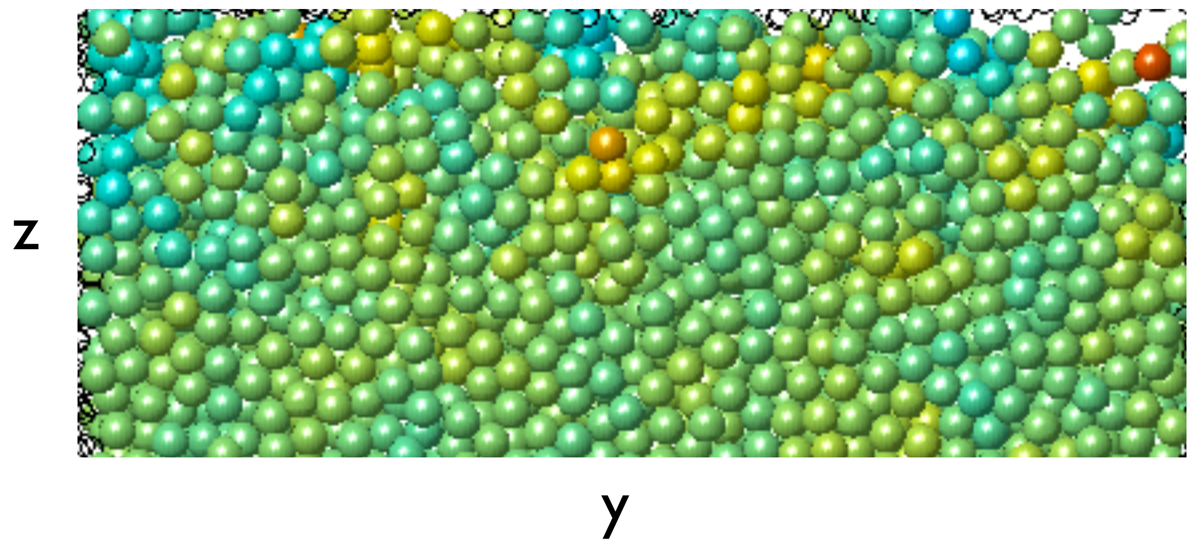
top 5% shear strain in the direction of the applied shear

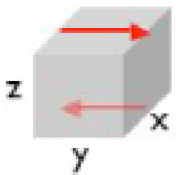
top 5% shear strain opposite to the applied shear



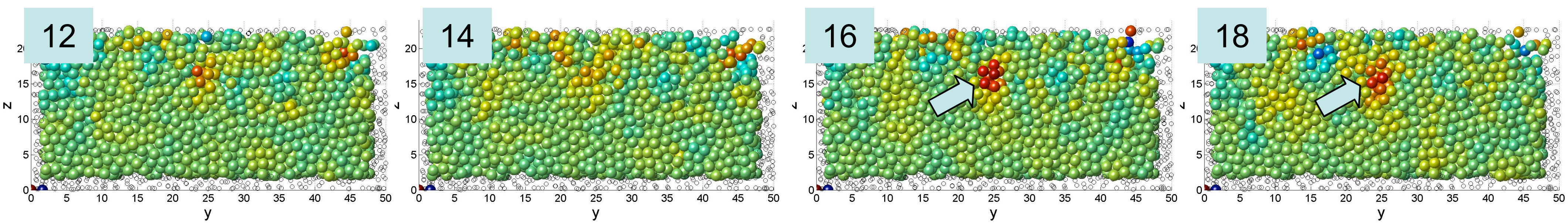


Side view of shear strains ϵ_{yz}

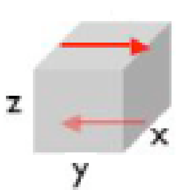




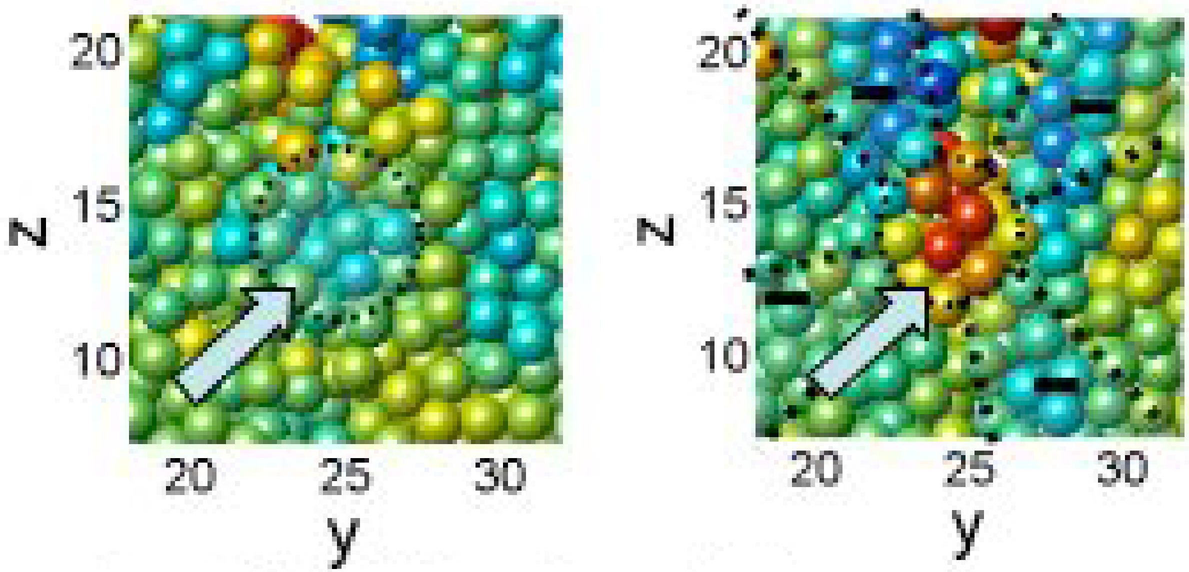
Shear event (ϵ_{yz})

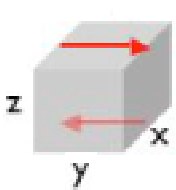


irreversible



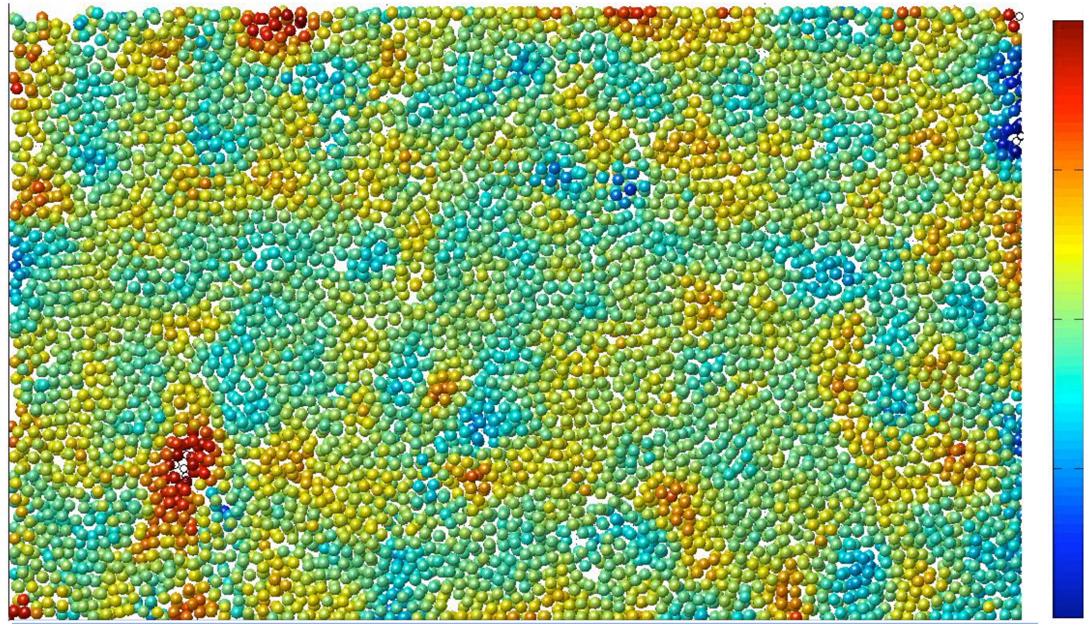
Stress distribution (ϵ_{yz}) around the flow defect



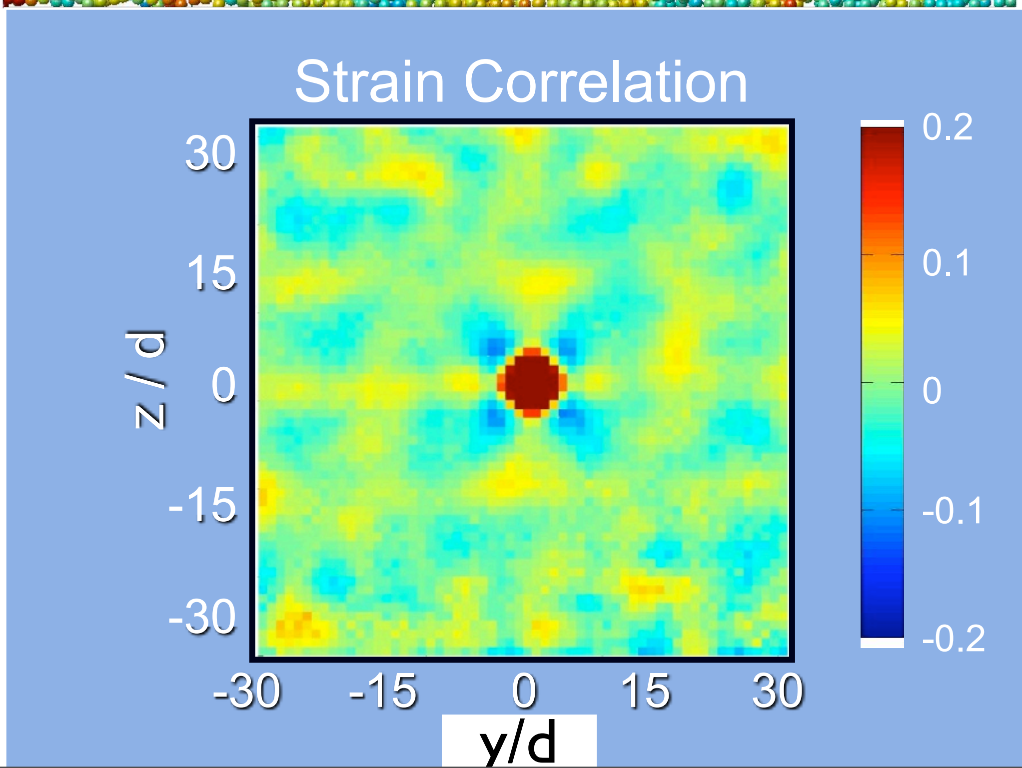


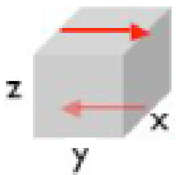
Correlations of ϵ_{yz} around the flow defect

V. Chikkadi, B. Nienhuis and P. Schall (2010)

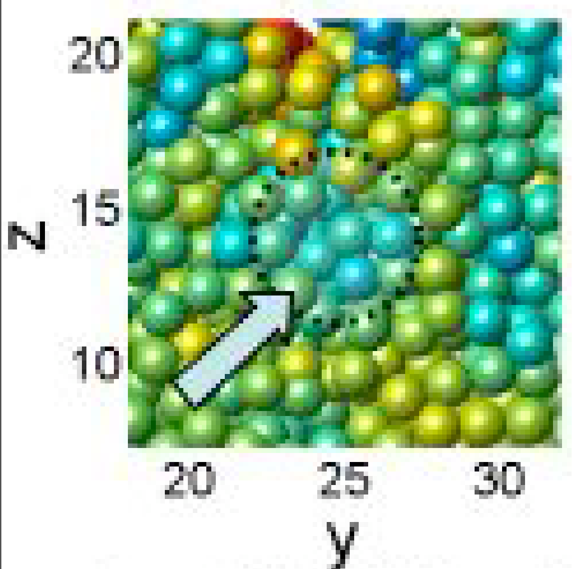


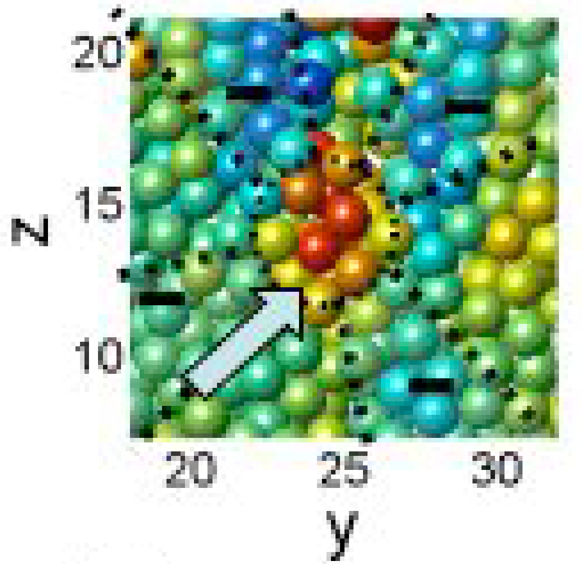
$$C_{\varepsilon_{yz}}(\bar{\Delta}) = \frac{\left\langle \varepsilon_{yz}(\bar{r})\varepsilon_{yz}(\bar{r}+\bar{\Delta})\right\rangle - \left\langle \varepsilon_{yz}\right\rangle^2}{\left\langle \varepsilon_{yz}{}^2\right\rangle - \left\langle \varepsilon_{yz}\right\rangle^2}$$

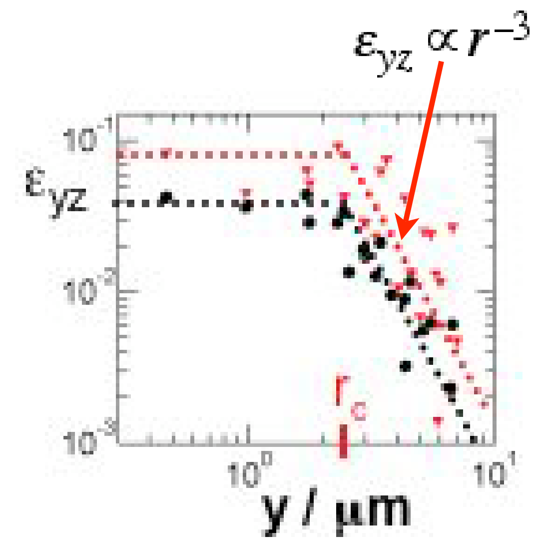


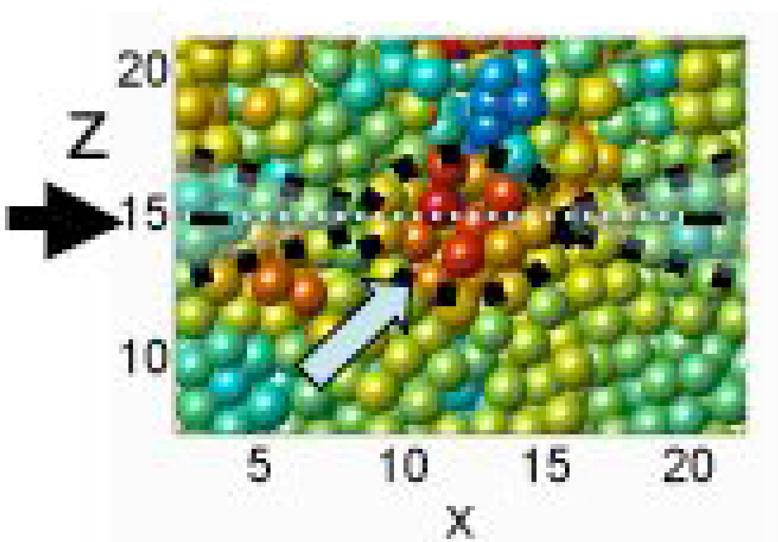


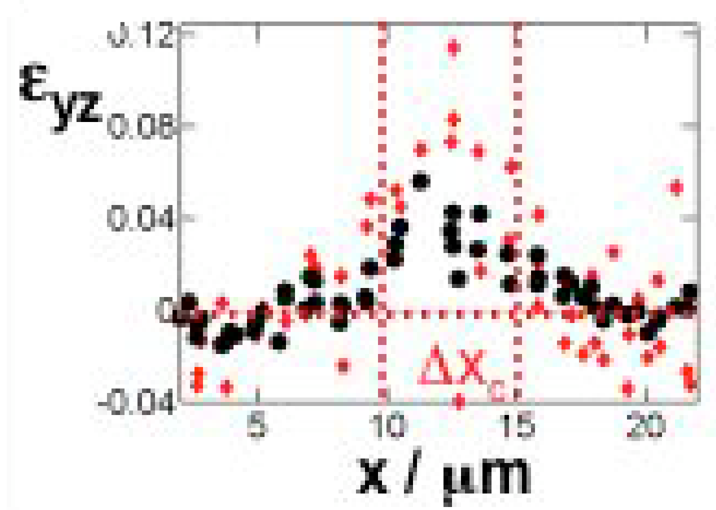
Stress distribution (ϵ_{yz}) around the flow defect

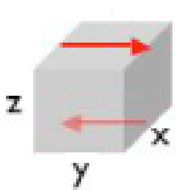






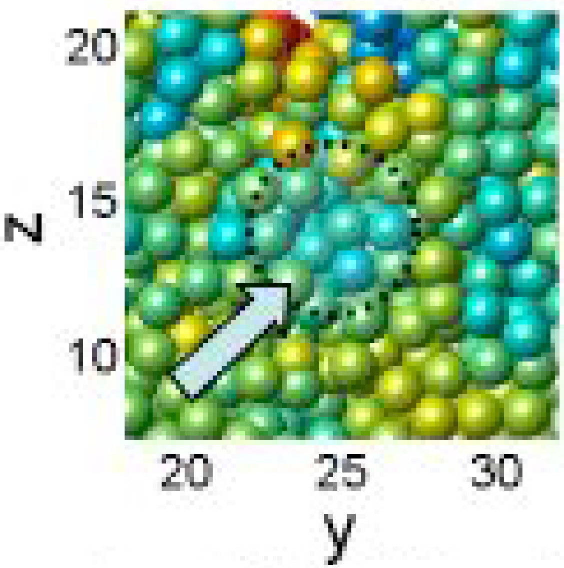


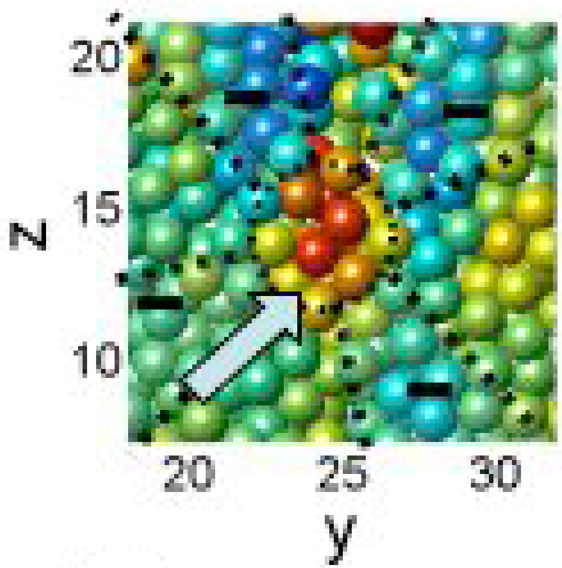


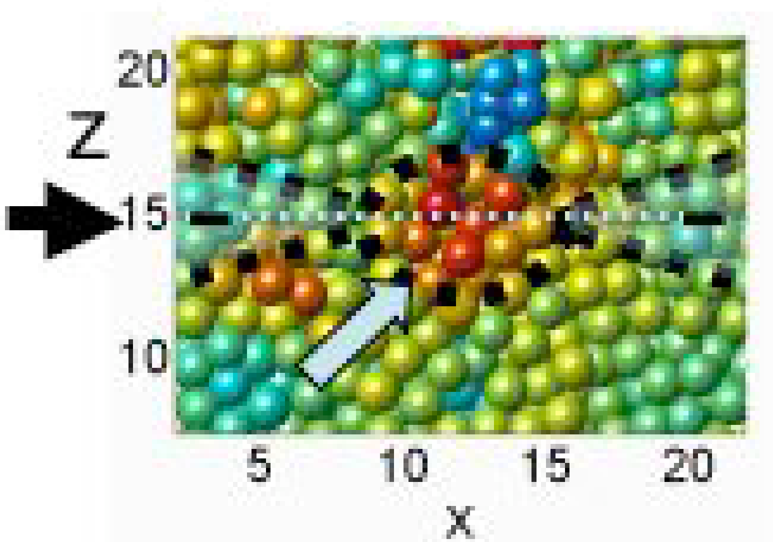


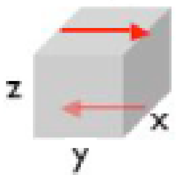
Activation volume

27 particles









$$\varepsilon_0 v_0$$

$$= \sum_{i=1}^{27} \varepsilon_{0,i} v_i$$

unconstrained strain

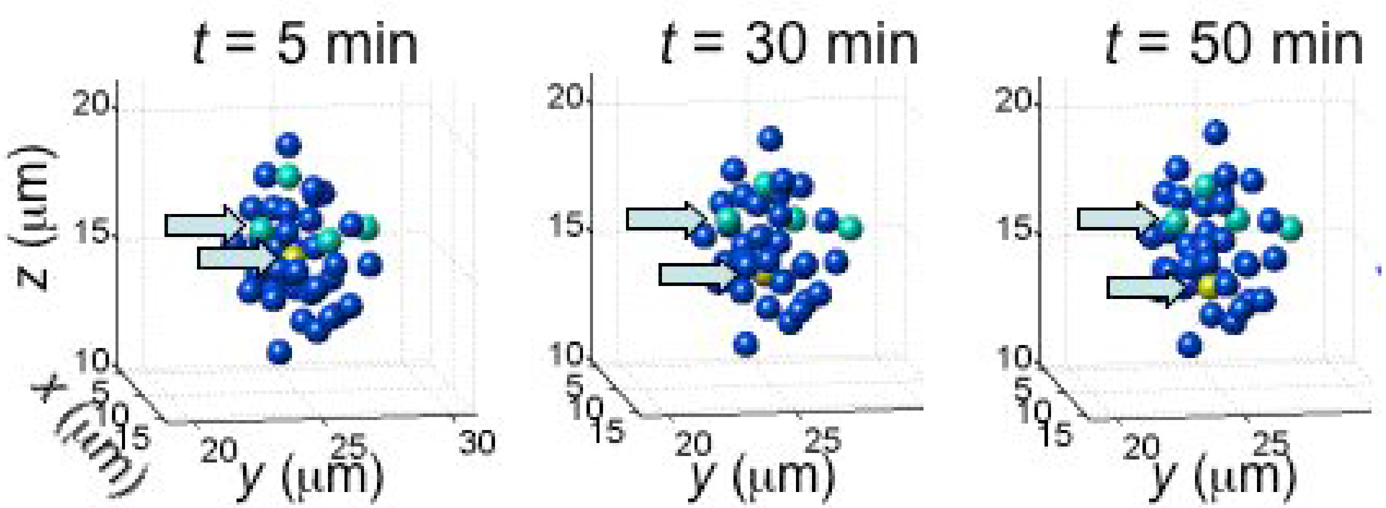
$$= \sum_{i=1}^{27} \frac{15(1-\nu)}{2(4-5\nu)} 2\varepsilon_{yz,i} v_i$$

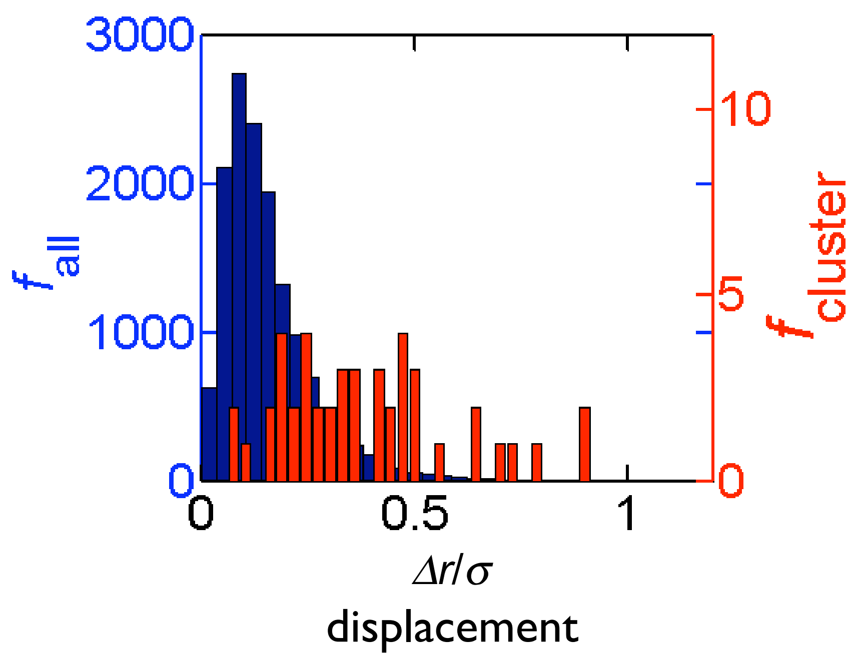
constrained strain (measured)

$$= \Omega \frac{15(1-\nu)}{(4-5\nu)} \sum_{i=1}^{27} \varepsilon_{yz,i}$$

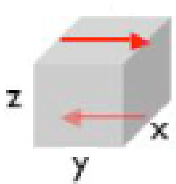
$$= 8.5\,\Omega$$

“Locking” of the shear (irreversibility)





distribution of
particle displacements
at t=30 min

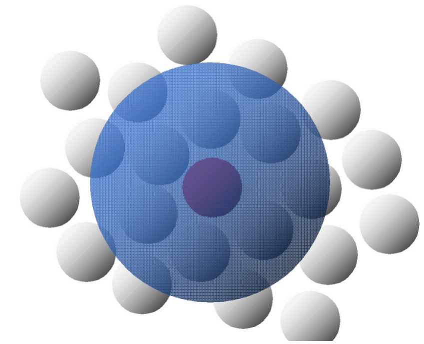


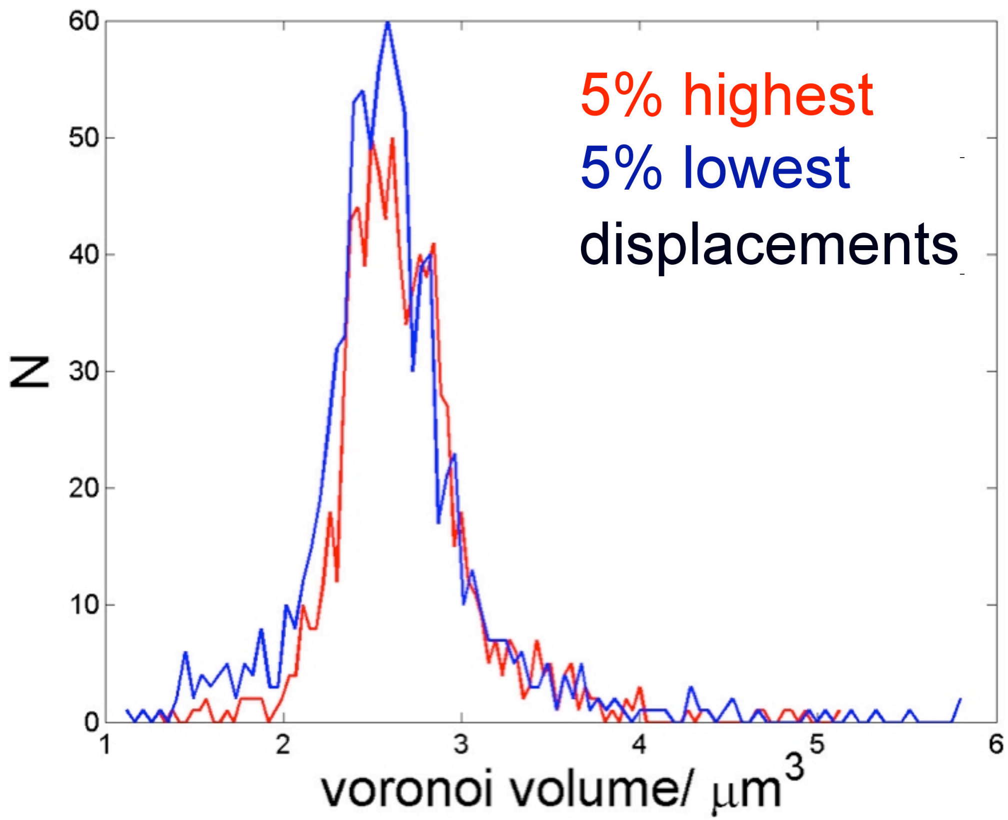
Effect of density (free volume)

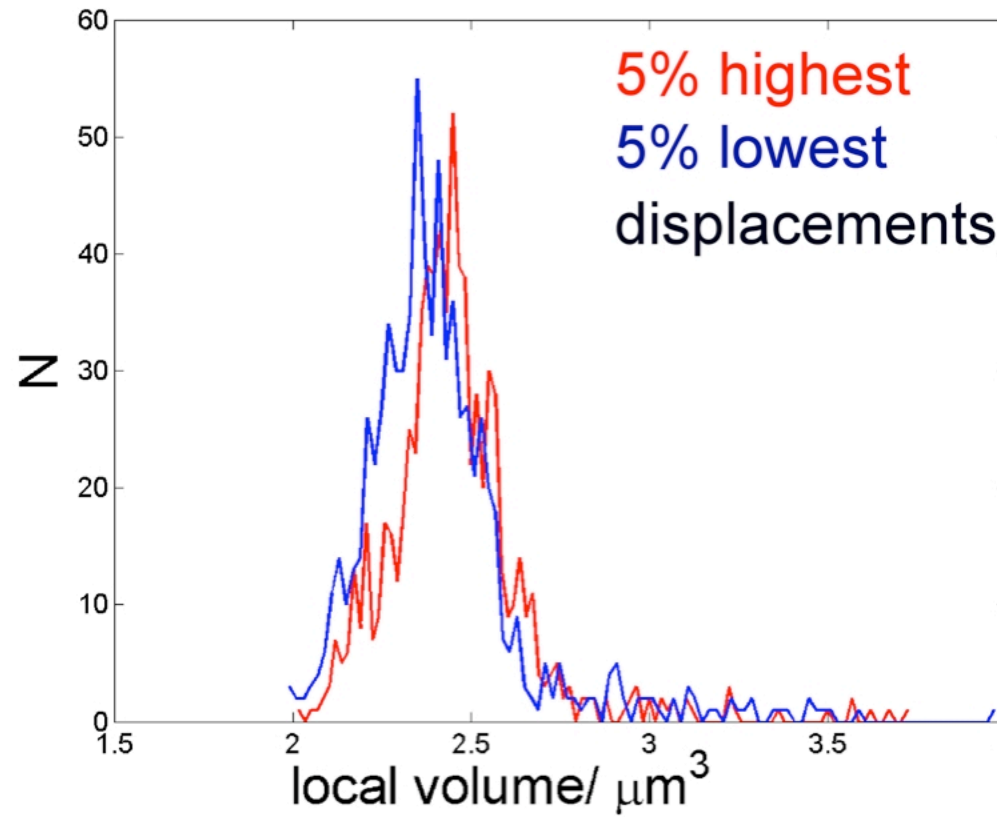
Correlation of flow and free volume

Atomic volume
(Voronoi cell)

Local volume



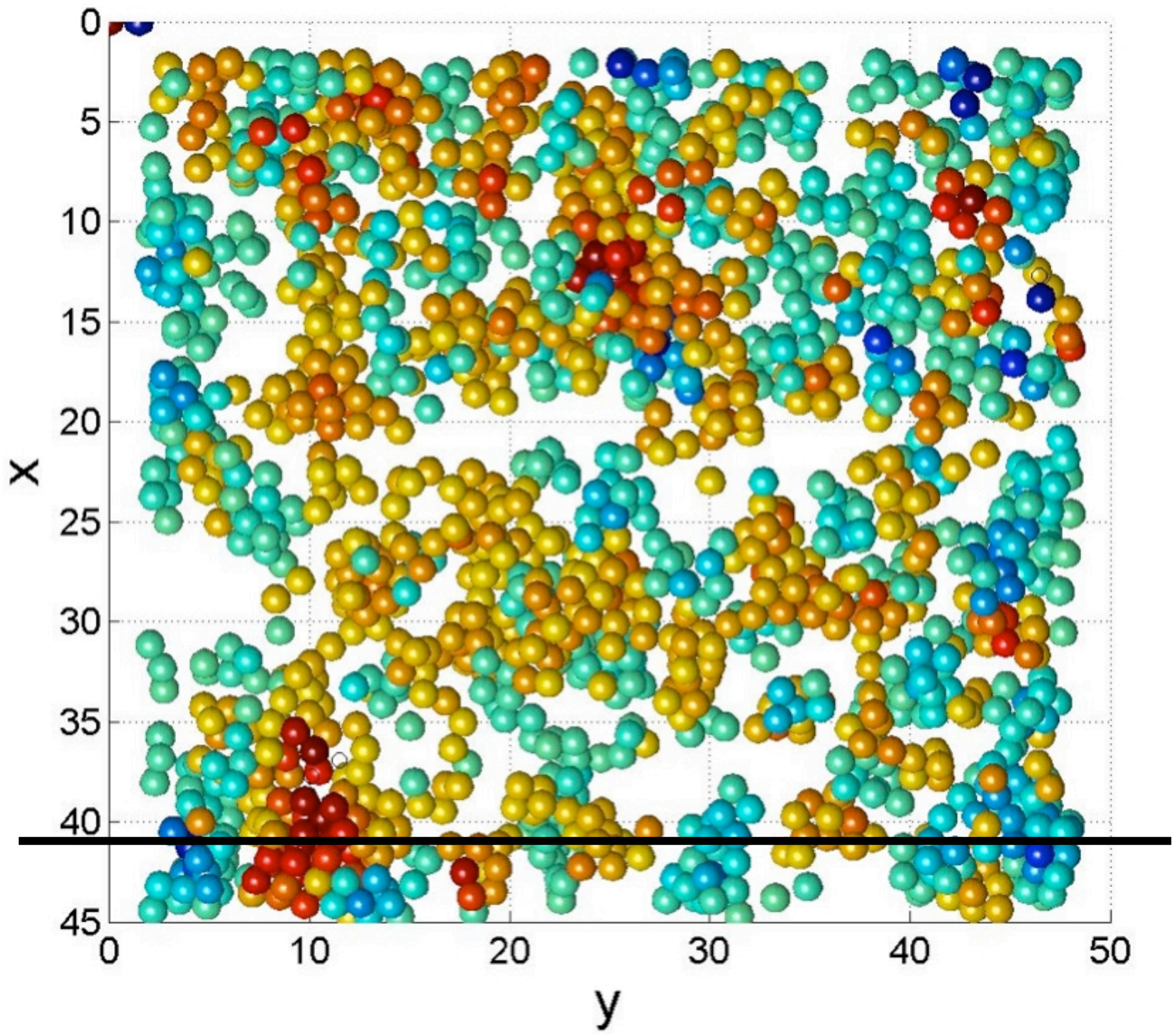


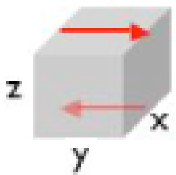


Top view: sites with largest shear strain ϵ_{yz} (+, -)

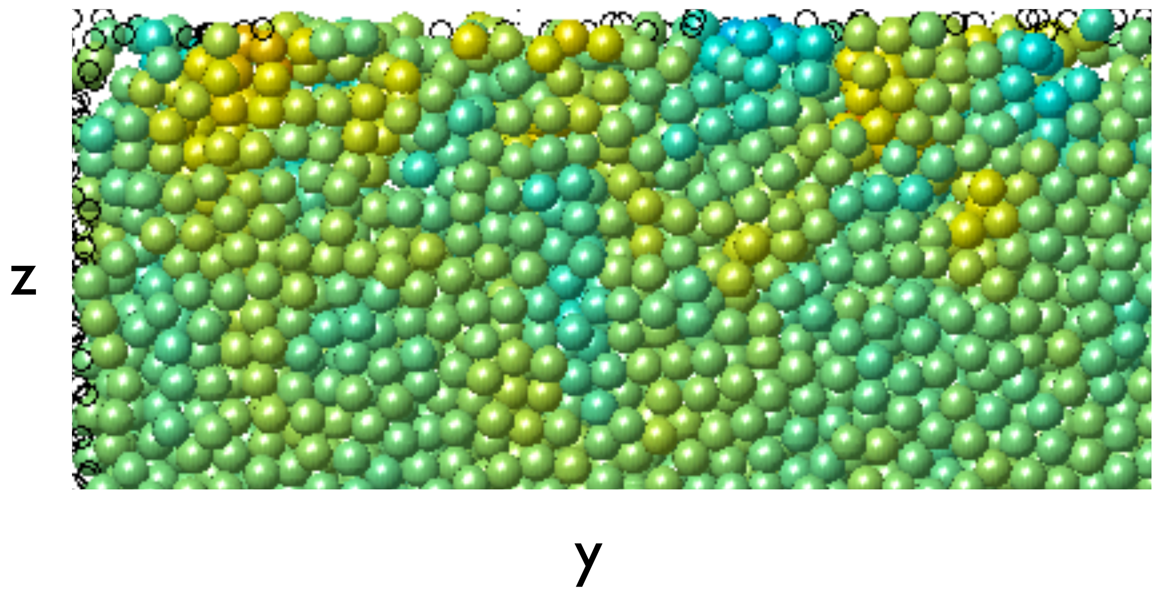
top 5% shear strain in the direction of the applied shear

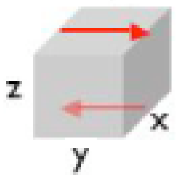
top 5% shear strain opposite to the applied shear



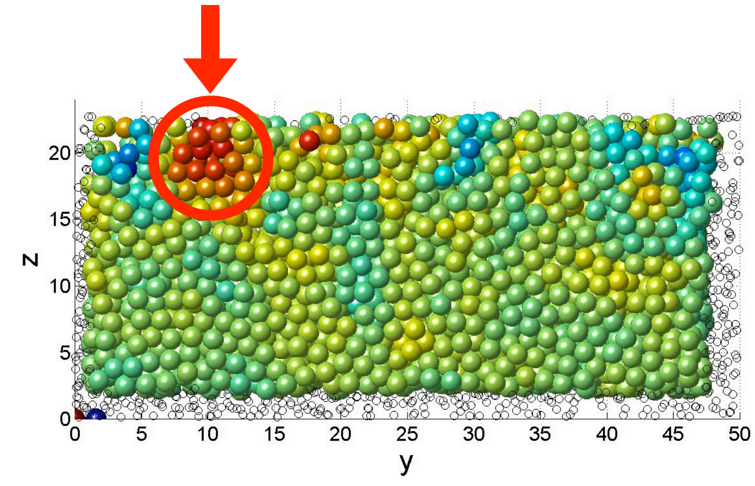


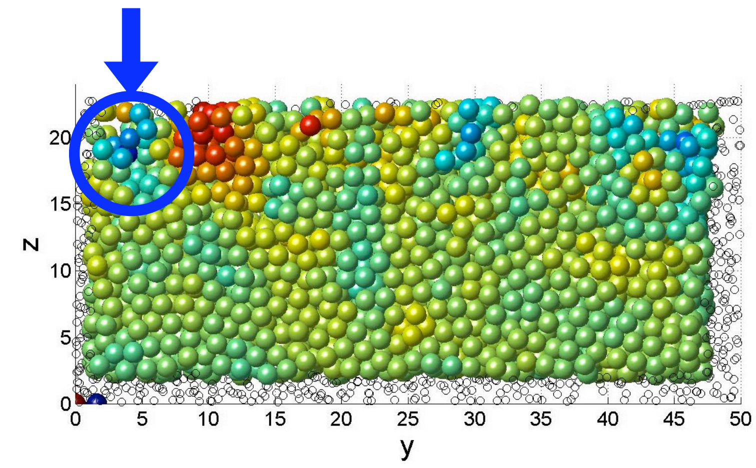
Side view of shear strains ϵ_{yz}

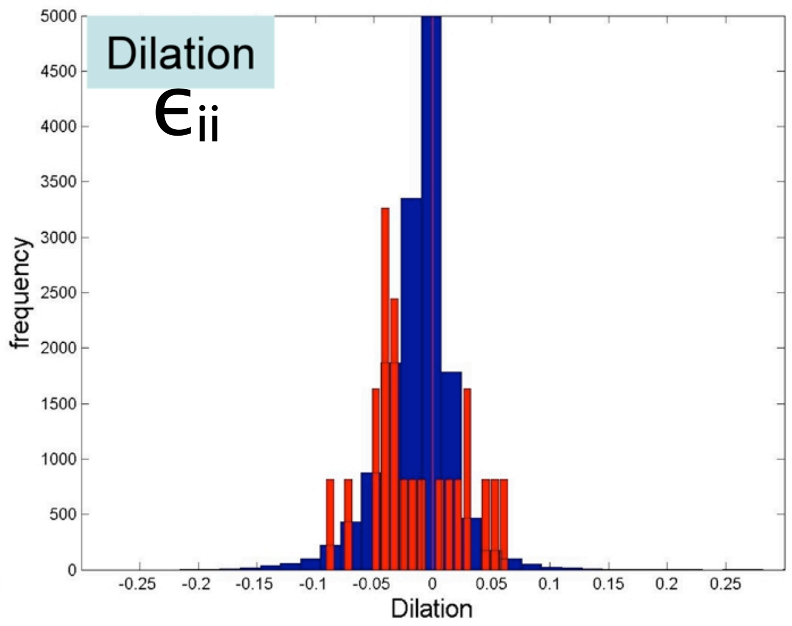


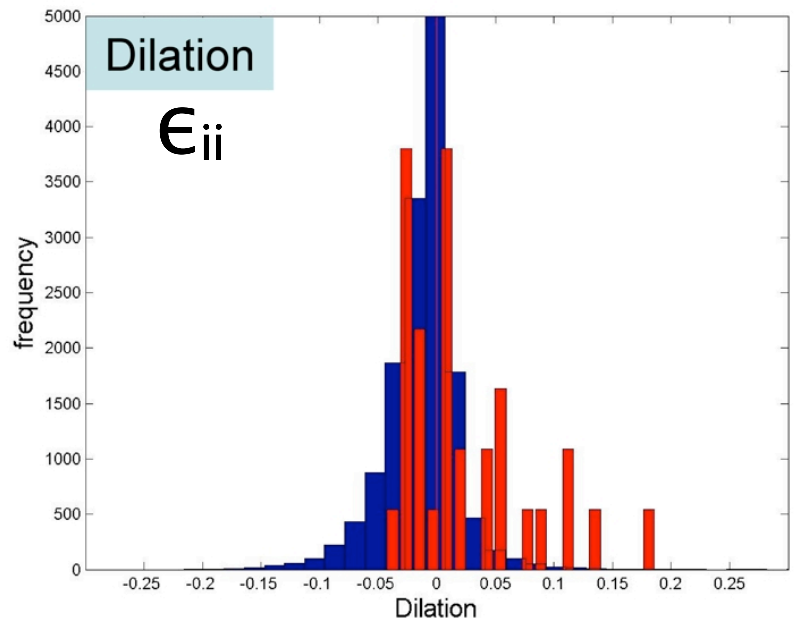


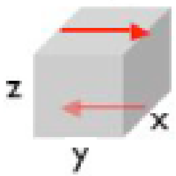
Analysis of a flow defect



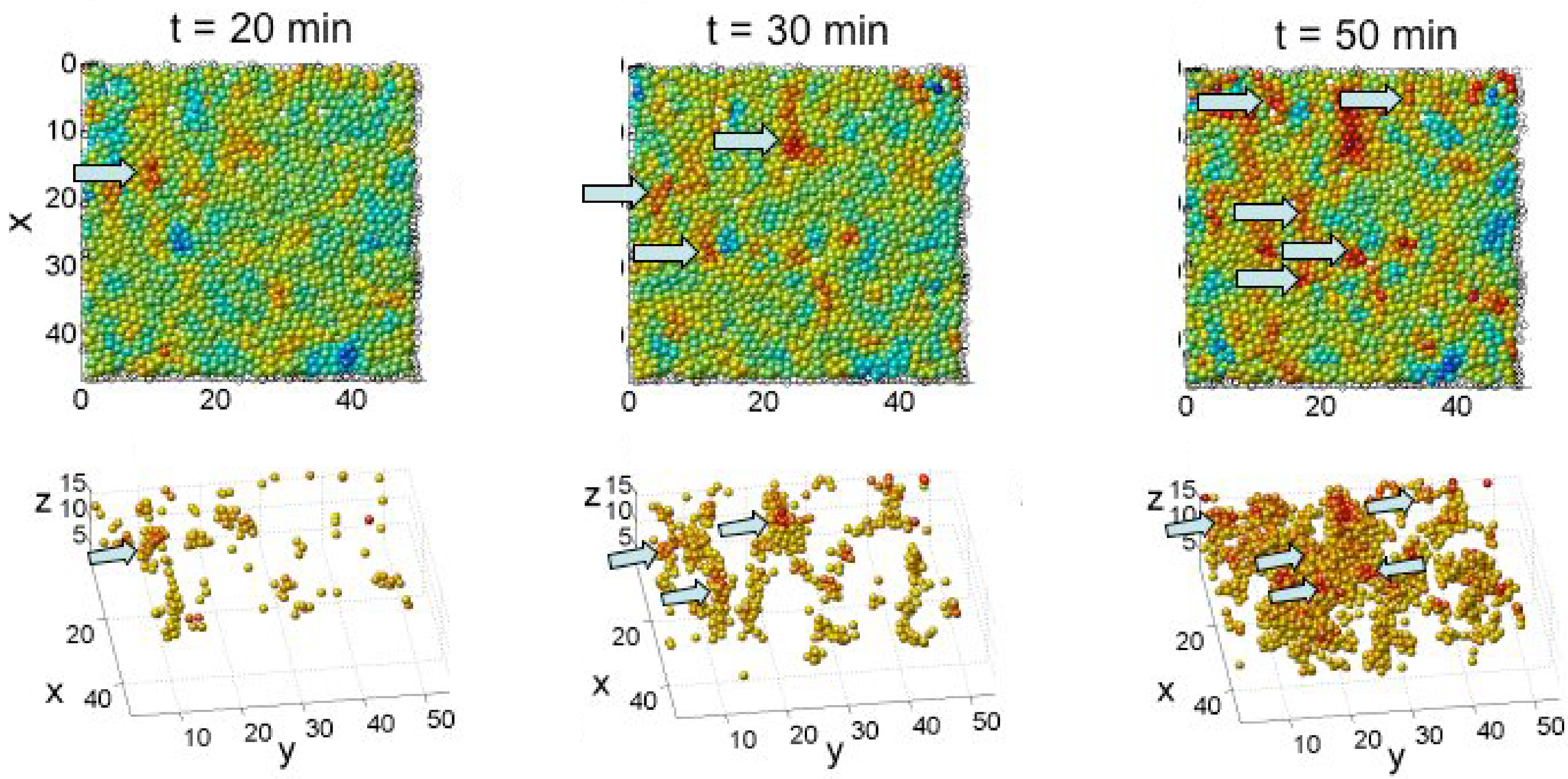


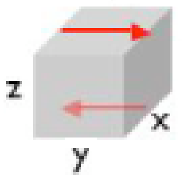






Correlation between shear events





The free volume model

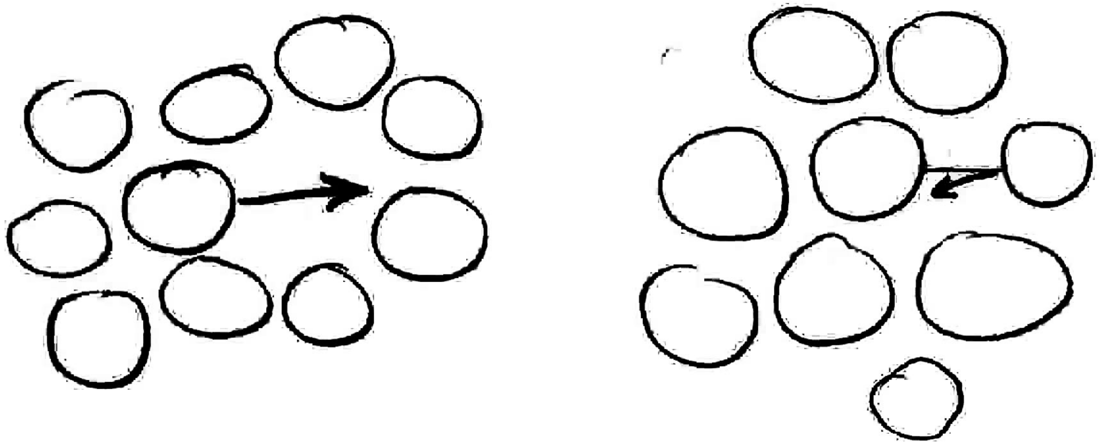
Density is the controlling parameter for hard spheres

The free volume model

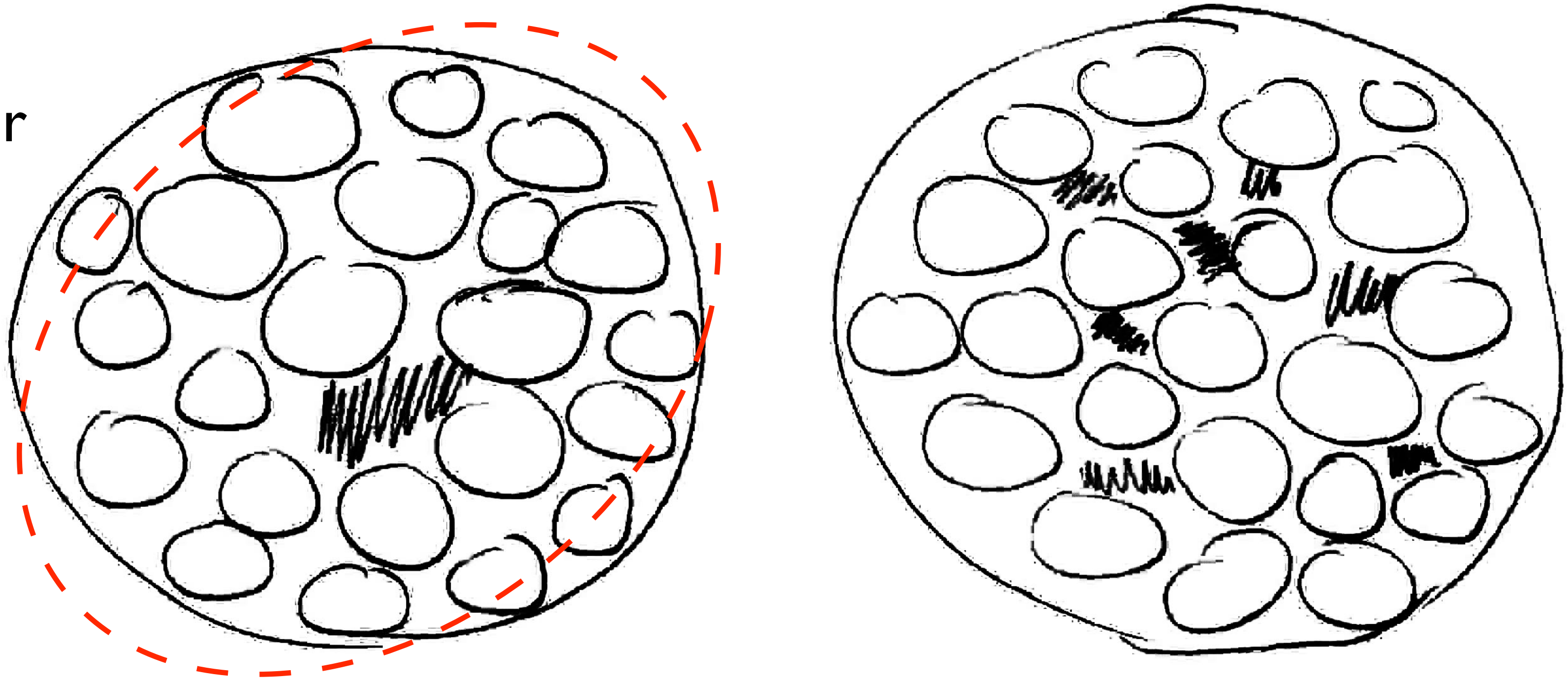
Relation to the shear zone

Original Cohen-Turnbull

diffusion

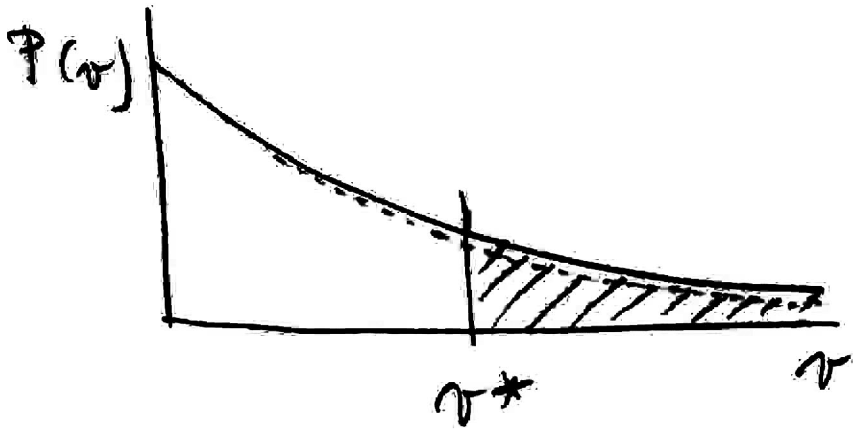


shear zone: larger



The free volume model

Ergodic vs non-ergodic distributions



pressure: non-ergodic rescaling

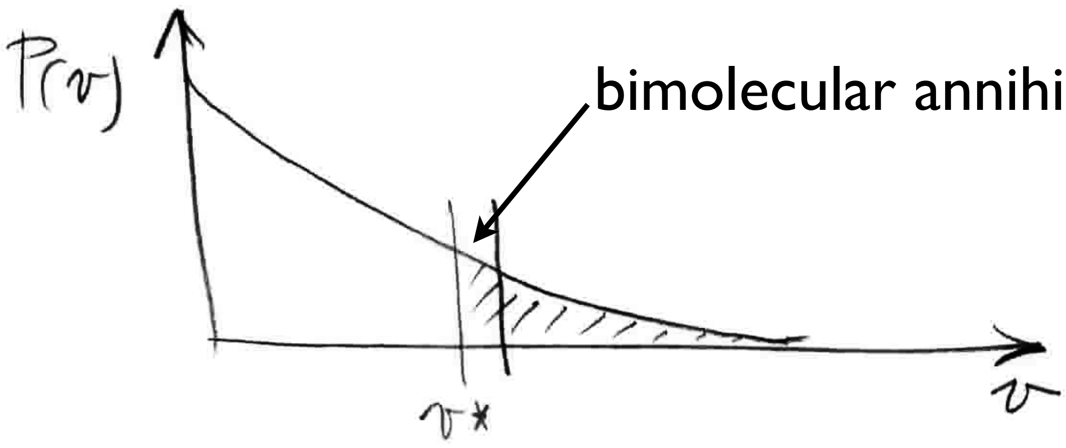
$$\exp\left(-\frac{\gamma v^*}{v_f - \varepsilon v_f}\right)$$

pressure: ergodic redistribution

$$\exp\left(-\frac{\gamma v^*}{v_f - \varepsilon \Omega}\right)$$

The free volume model

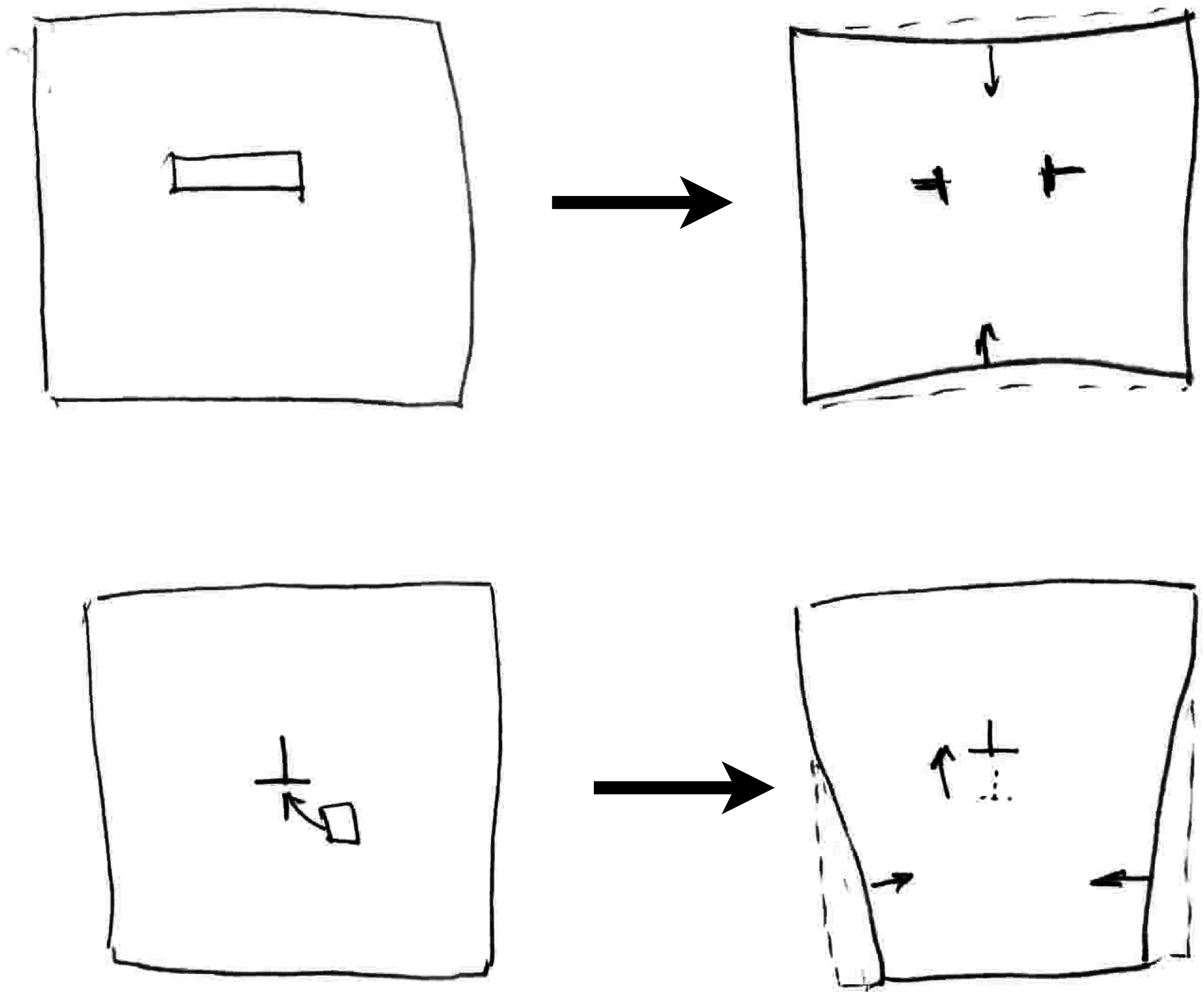
Ergodic vs non-ergodic distributions



Cohen-Grest model: low- and high-free volume clusters

The free volume model

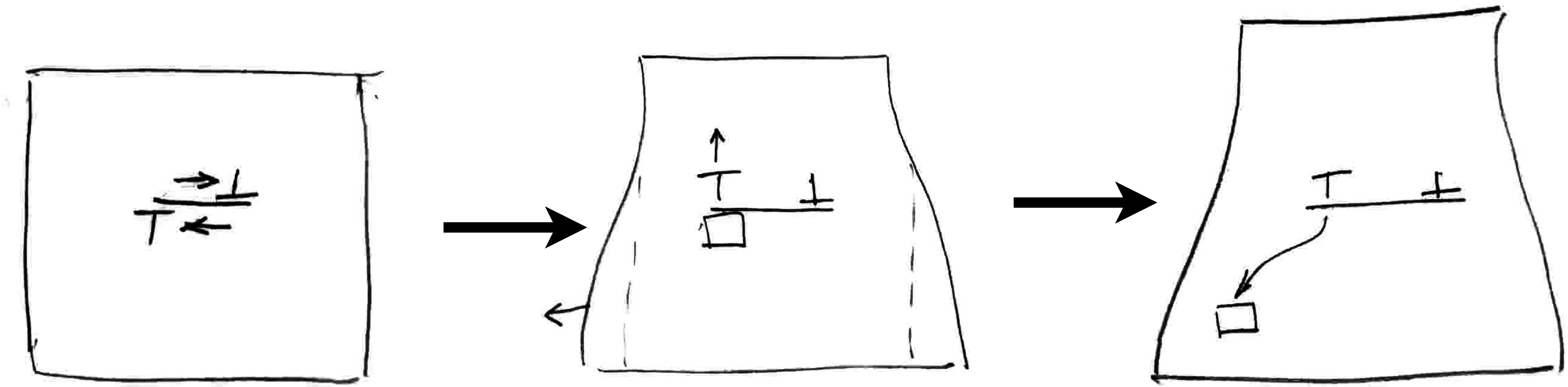
Annihilation and creation of volume: singularities



The free volume model

Annihilation and creation of volume: singularities

shear can create the singularity necessary for annihilation/creation



Acknowledgements

Metallic glass mechanical properties

Alex Donohue
Marc Heggen (FZ Jülich)

Colloid modeling

Peter Schall (now U. Amsterdam)
David Weitz