JMBC Workshop

Jamming and glassy behavior in colloids

2. Flow of glassy materials

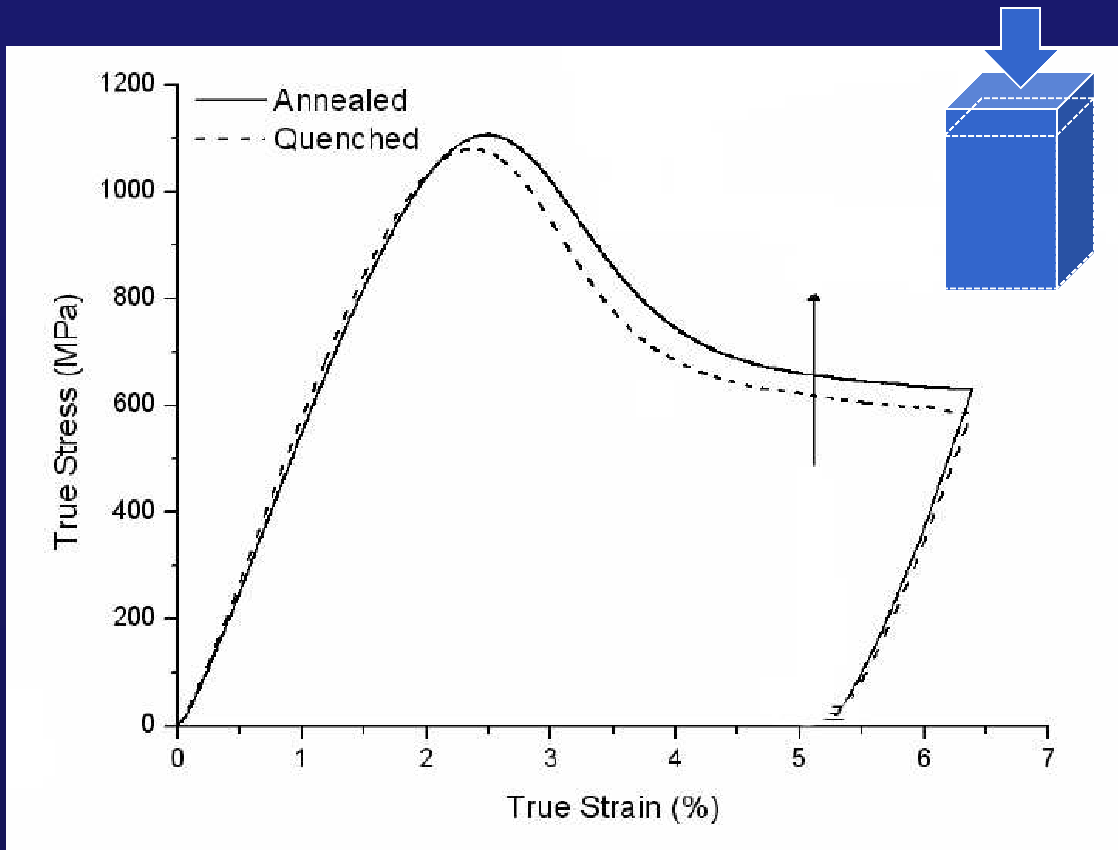
Peter Schall

University of Amsterdam

Macroscopic Stress-Strain Relations

Metallic glass

F



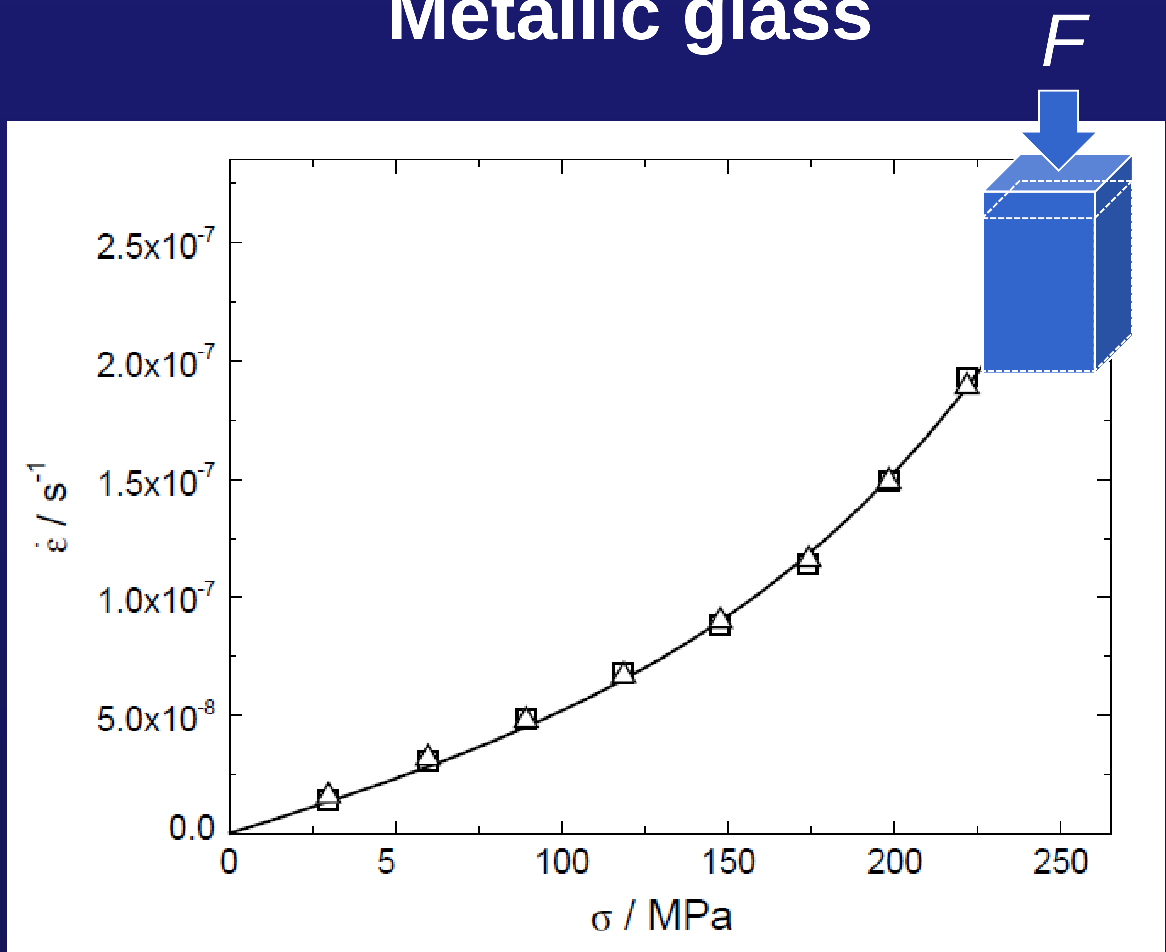
Strain $\frac{\Delta L}{L}$

Stress $\frac{F}{A}$

Constant Strain Rate

Macroscopic Stress-Strain Relations

Metallic glass

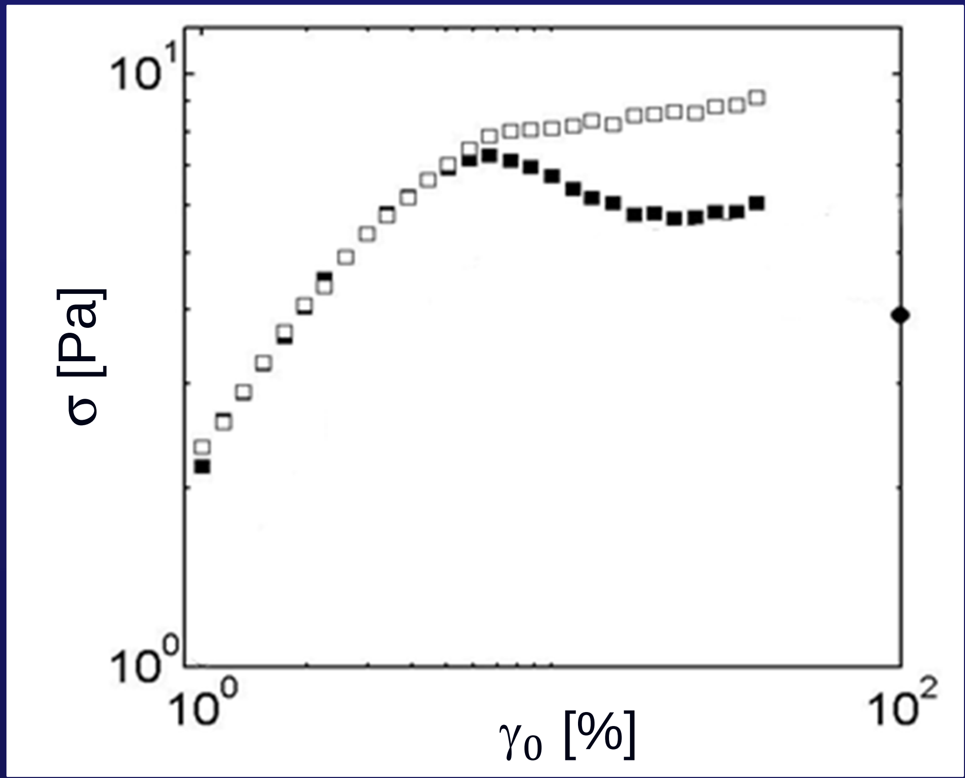


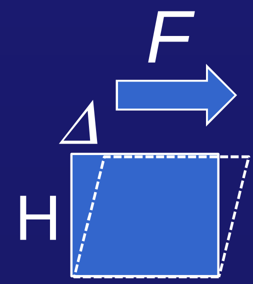
Strain $\frac{\Delta L}{L}$

Stress $\frac{F}{A}$

Constant Stress (Creep)

Macroscopic Stress-Strain Relations
Suspensions





Strain $\frac{\Delta}{H}$

Stress $\frac{F}{A}$

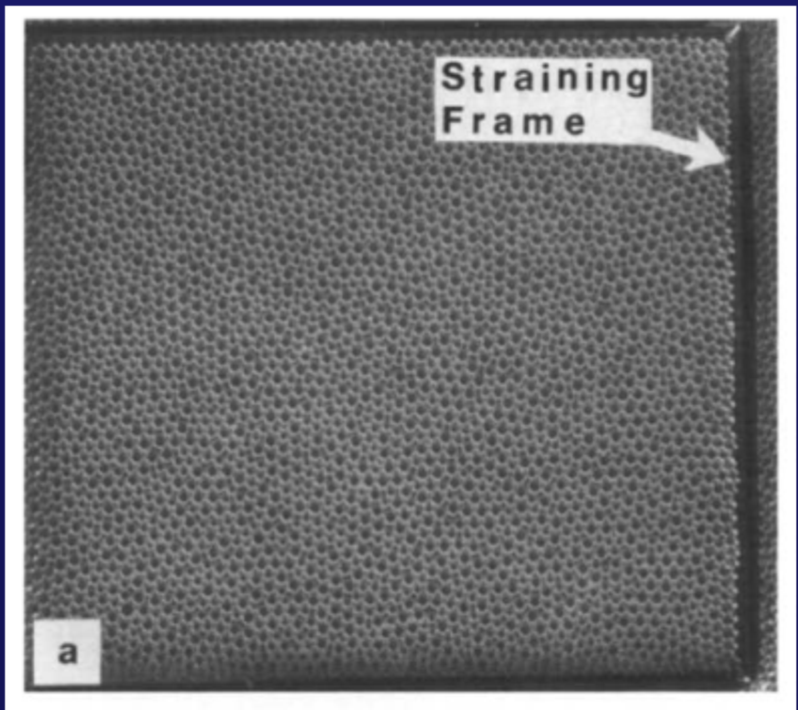
Microscopic Picture?

Bragg – Nye Bubble Raft

Bubble raft experiments

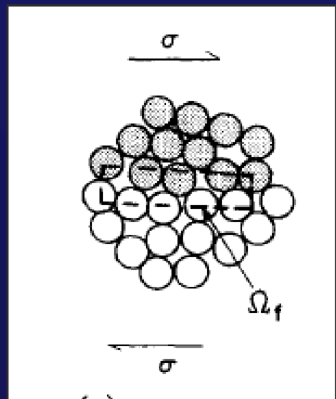
- Bragg-Nye Bubble raft:
  Dislocations and Dislocation motion in crystals (1950's)

- Disordered Bubble raft (Argon, Kuo 1979)
  Shear transformation zones in glasses

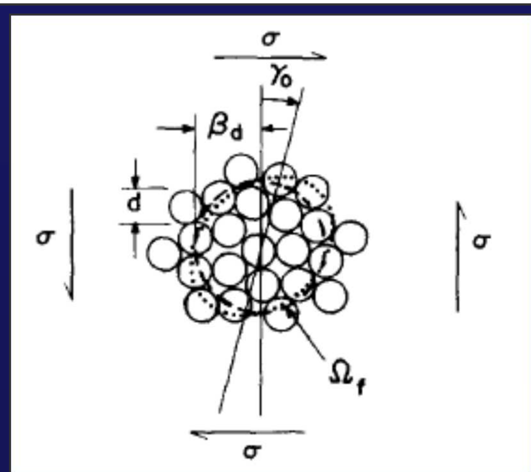


Plastic Flow in a Disordered Bubble Raft (an Analog of a Metallic Glass)

A. S. ARGON and H. Y. KUO*
Massachusetts Institute of Technology, Cambridge, Mass. 02139 (U.S.A.)
(Received November 1, 1978; in revised form December 13, 1978)

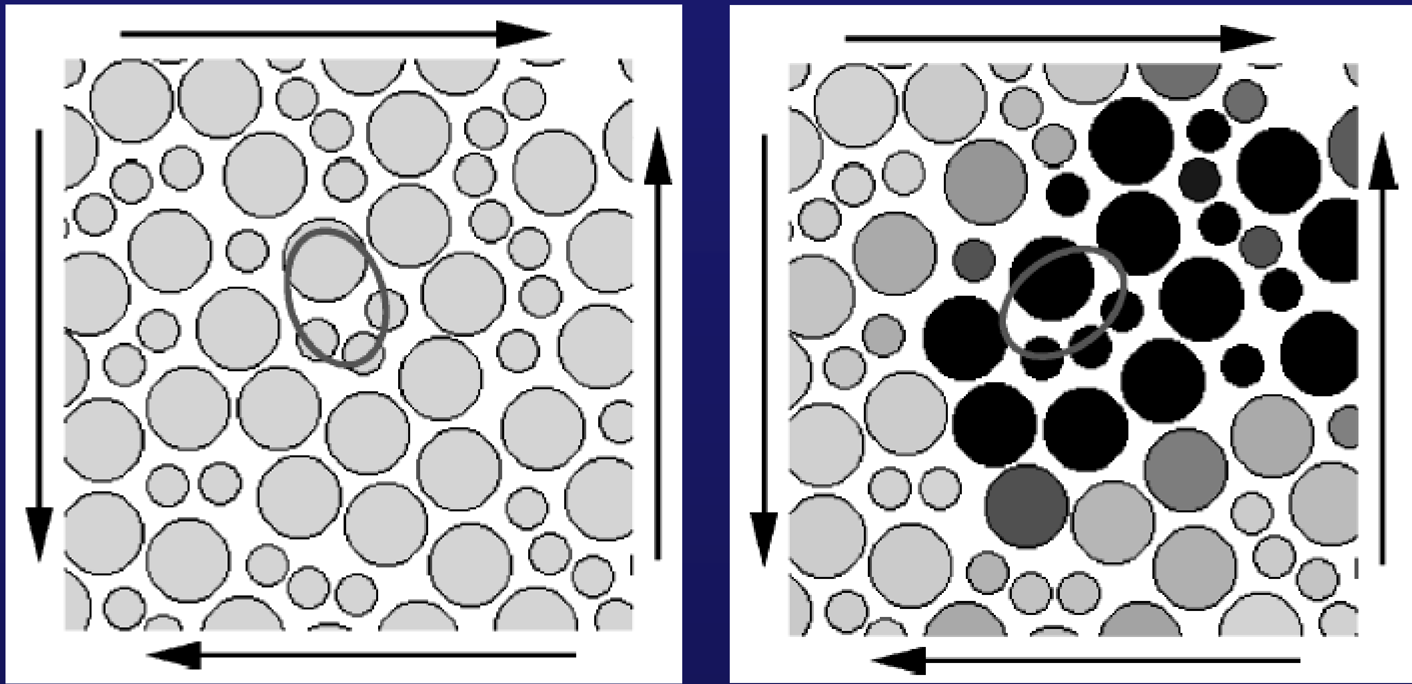


(a)

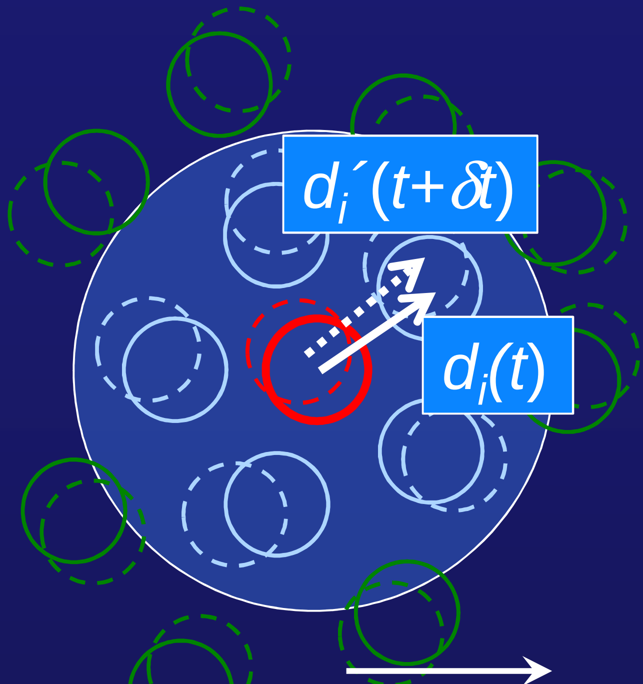


Shear transformation zones

Simulations: Falk and Langer *PRE* 1998



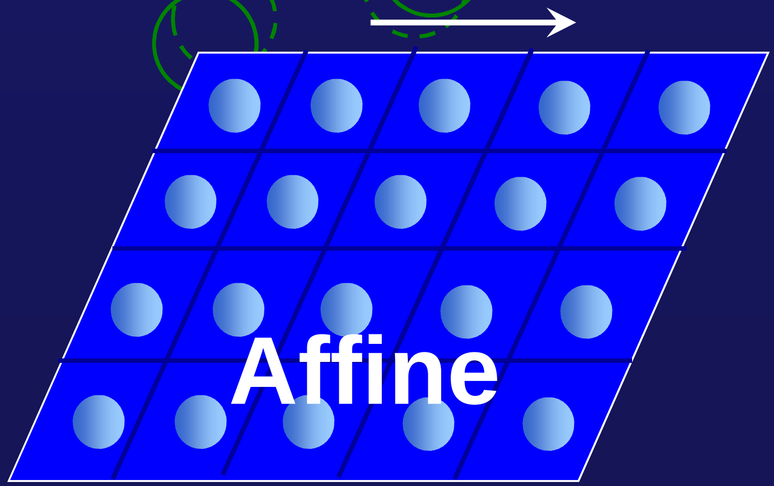
Shear transformation zones

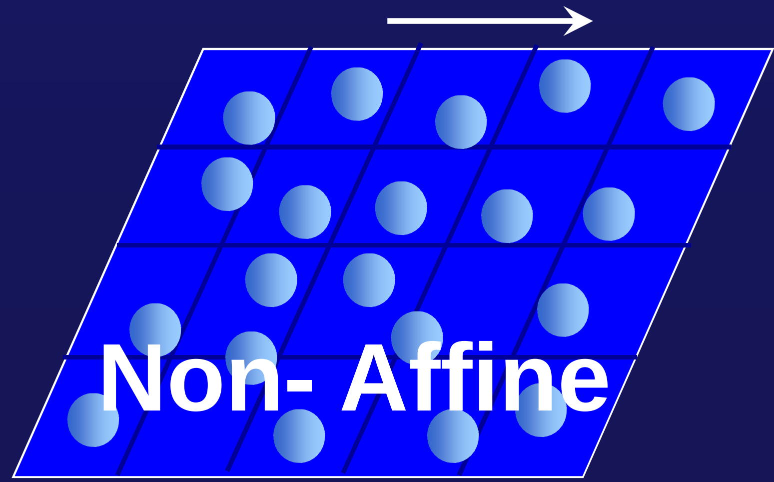


Affine transformation : γ

$$\mathbf{d}_i'^{\,\text{aff}} = \mathbf{d}_i + \gamma \mathbf{d}_i$$

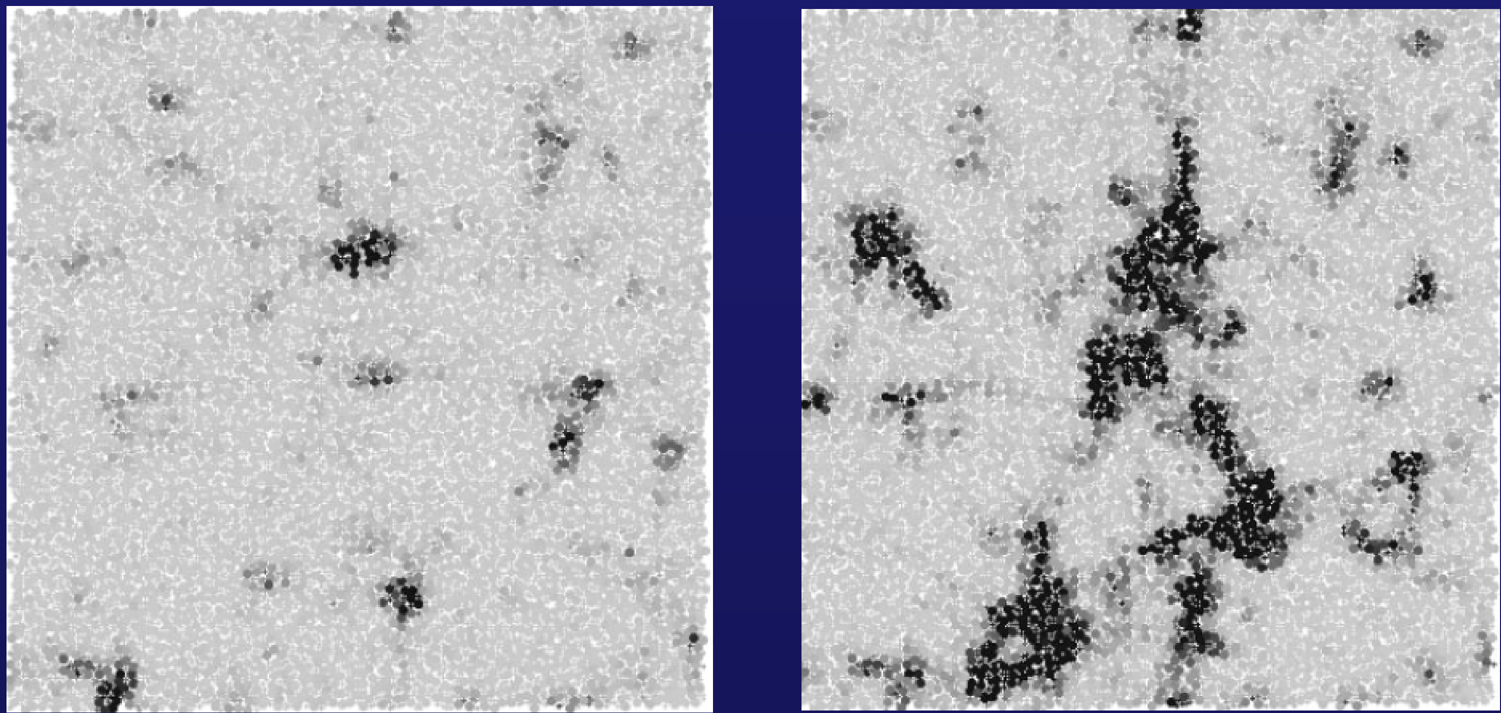
$$D^2_{\min} = \sum^{\text{neighbors}} \underbrace{(\mathbf{d}_i' - \mathbf{d}_i)}_{\text{actual change}} - \underbrace{\gamma \mathbf{d}_i)^2}_{\text{affine change}}$$





Shear transformation zones

$D_{min}^{\;2}$



Time →

Flow by local shear transformations

From Micro to Macro:

Constitutive Models

Constitutive description: Flow equation

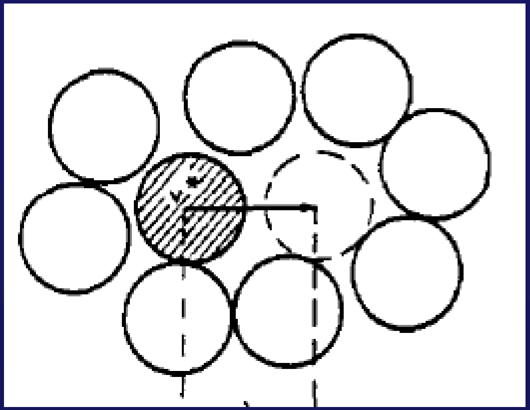
$$\dot{\gamma} = \left(\begin{array}{c}\text{Volume Fraction}\\ \text{of STZ}\end{array}\right) \cdot \left(\begin{array}{c}\text{Strain}\\ \text{per STZ}\end{array}\right) \cdot \left(\begin{array}{c}\text{Rate of STZ}\\ \text{Formation}\end{array}\right)$$

1. Free volume Theory

$$p(v)dv = \frac{\gamma}{v_f} exp\left(-\frac{\gamma}{v_f}\right)$$

Probability for STZ site

$$f = \int_{v^*}^{\infty} p(v)dv = exp\left(-\frac{\gamma v^*}{v_f}\right)$$



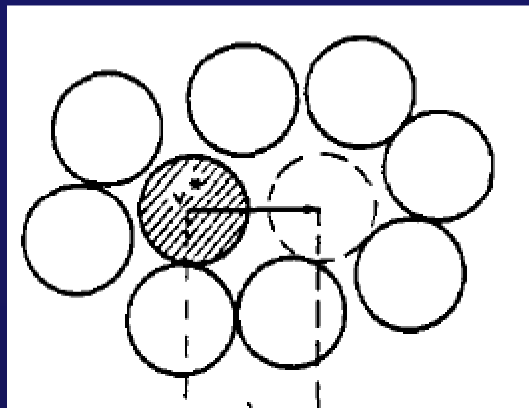
(Spaepen Acta Met. 1977)

Constitutive description: Flow equation

$$\dot{\gamma} = \left(\begin{matrix}\text{Volume Fraction}\\ \text{of STZ}\end{matrix}\right) \cdot \left(\begin{matrix}\text{Strain}\\ \text{per STZ}\end{matrix}\right) \cdot \left(\begin{matrix}\text{Rate of STZ}\\ \text{Formation}\end{matrix}\right)$$

2. Strain per STZ

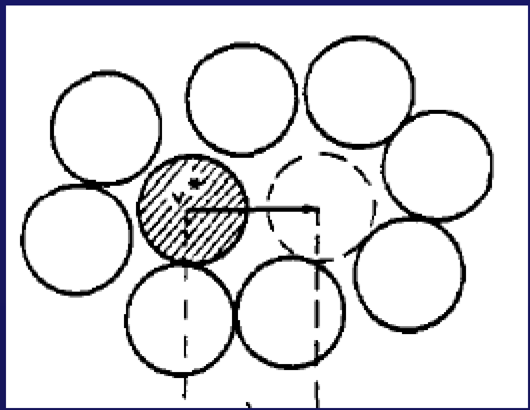
$$\varepsilon_0 \sim 1$$



(Spaepen Acta Met. 1977)

Constitutive description: Flow equation

$$\dot{\gamma} = \begin{pmatrix}\text{Volume Fraction} \\ \text{of STZ}\end{pmatrix} \cdot \begin{pmatrix}\text{Strain} \\ \text{per STZ}\end{pmatrix} \cdot \begin{pmatrix}\text{Rate of STZ} \\ \text{Formation}\end{pmatrix}$$



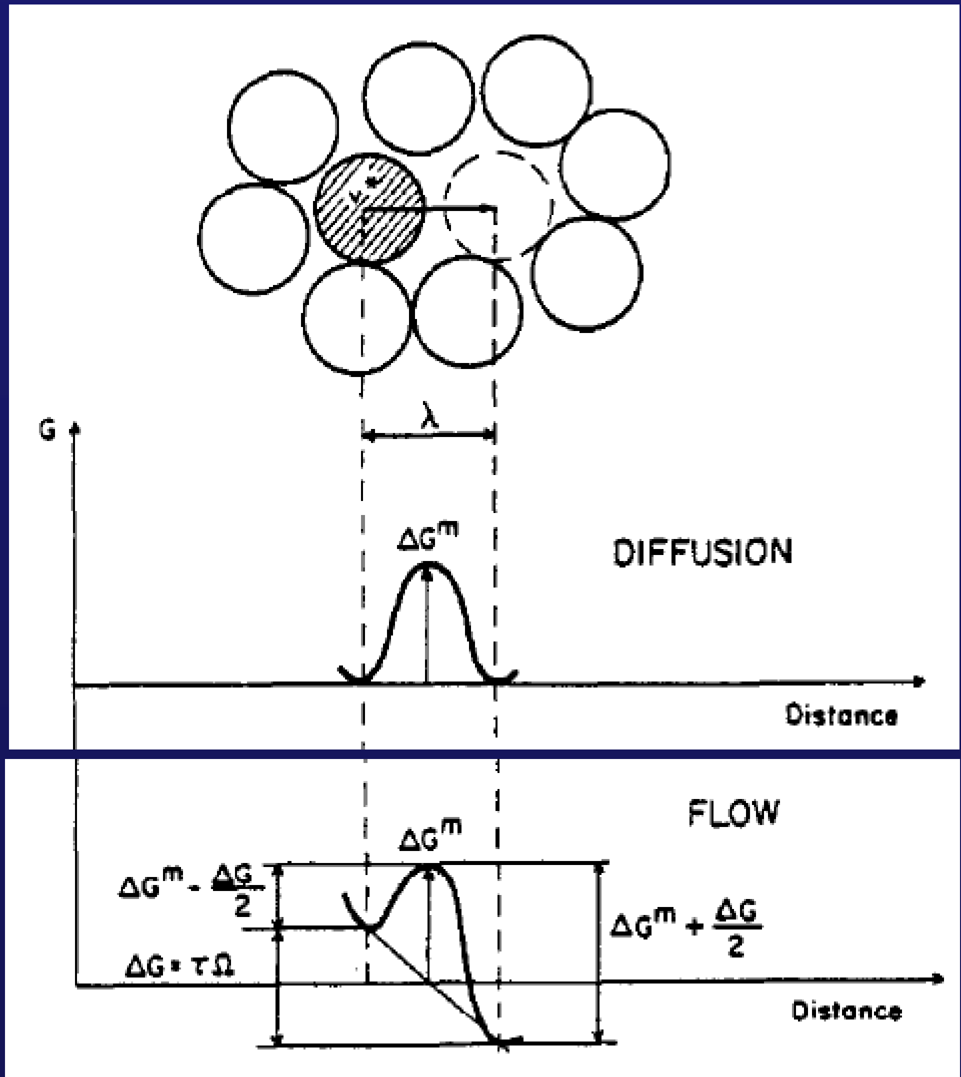
3. Probability of activation

$$P \propto exp\left(-\frac{\Delta G}{kT}\right)$$

Rate of STZ formation

$$R = \nu_0 \, exp\left(-\frac{\Delta G}{kT}\right)$$

Flow equation



Activation volume

$$\Omega = \int \varepsilon \; dV$$

$$P \propto exp\left(-\frac{\Delta G}{kT}\right)$$

forward jump

$$P \propto exp\left(-\frac{\Delta G - \tau\Omega/2}{kT}\right)$$

backward jump

$$P \propto exp\left(-\frac{\Delta G + \tau\Omega/2}{kT}\right)$$

Flow equation

$$\dot{\gamma} = f \cdot \epsilon_0 \cdot \nu_0 \cdot exp(-\frac{\Delta G}{kT})$$

Your turn!

Flow equation under applied stress?

$$\dot{\gamma} = f \cdot \epsilon_0 \cdot \nu_0 \cdot \{exp(-\frac{\Delta G - \sigma\Omega/2}{kT}) - exp(-\frac{\Delta G - \sigma\Omega/2}{kT})\}$$

$$\dot{\gamma} = f \cdot \epsilon_0 \cdot \nu_0 \cdot sinh\{\frac{\sigma\Omega}{2kT}\}\, exp\{-\frac{\Delta G}{kT}\}$$

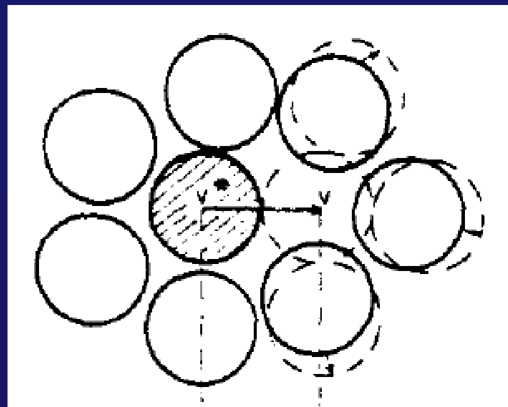
Small applied stress: $sinh\{\frac{\sigma\Omega}{2kT}\} \approx \frac{\sigma\Omega}{2kT}$

Viscosity ?

$$\eta = \frac{\sigma}{\dot{\gamma}} = \frac{kT}{\Omega f \epsilon_0 \nu_0} \cdot exp\{\frac{\Delta G}{kT}\}$$

Flow equation

Structural order parameter: Free volume



create free volume

$v^* - v$

Free volume creation

$$\Delta v^+ = \begin{pmatrix}\text{\#potential} \\ \text{sites}\end{pmatrix} \cdot \begin{pmatrix}\text{net \# forward} \\ \text{jumps}\end{pmatrix} \cdot \begin{pmatrix}\text{Amount of} \\ v_f \text{ created}\end{pmatrix}$$

Free volume annihilation

$$\Delta v^- = \begin{pmatrix}\text{\#potential} \\ \text{sites}\end{pmatrix} \cdot \begin{pmatrix}\text{\#jumps} \\ \text{per sec}\end{pmatrix}$$

Constitutive description

Flow equation

$$\dot{\gamma} = f \cdot \epsilon_0 \cdot \nu_0 \cdot sinh\left\{\frac{\sigma\Omega}{2kT}\right\} exp\left\{-\frac{\Delta G}{kT}\right\}$$

+

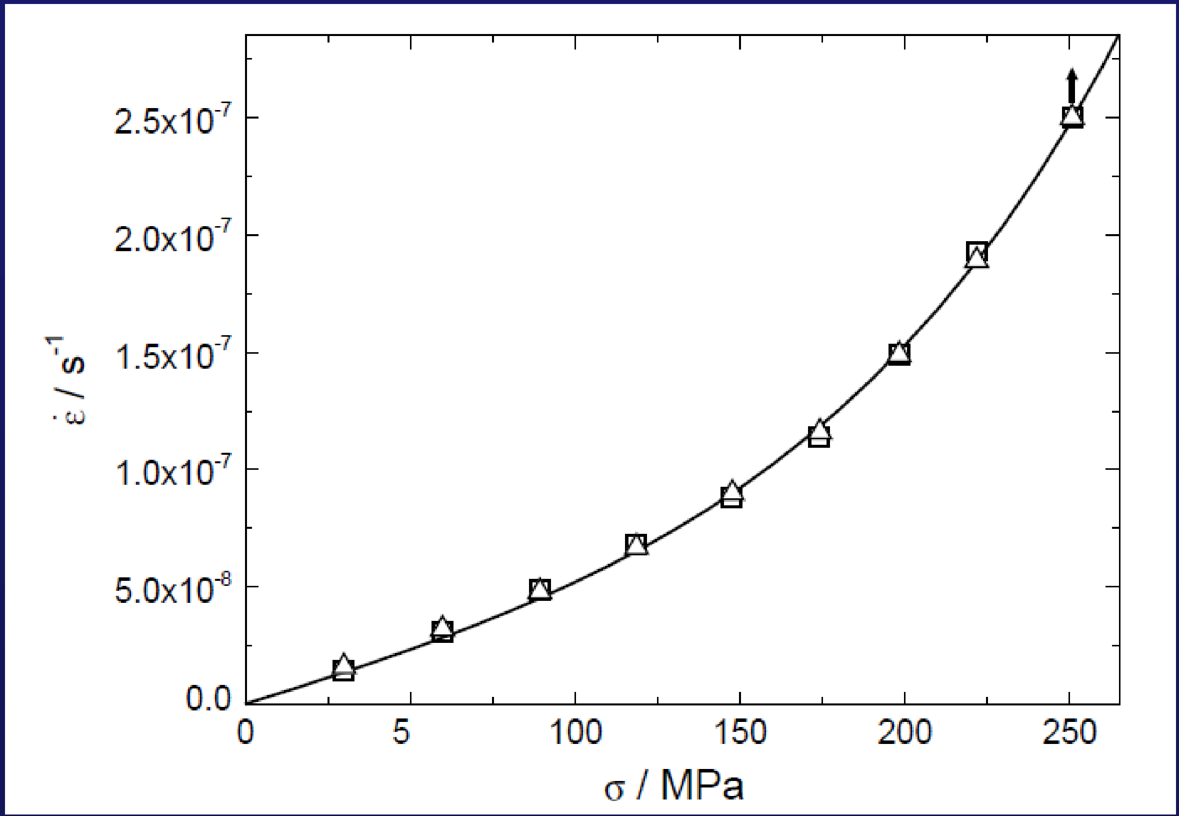
Evolution equations of struct. order parameters

$$\Delta v^+, \Delta v^-$$

$$\dot{\gamma} = \dot{\gamma}(\sigma, T, structure)$$

Constitutive description

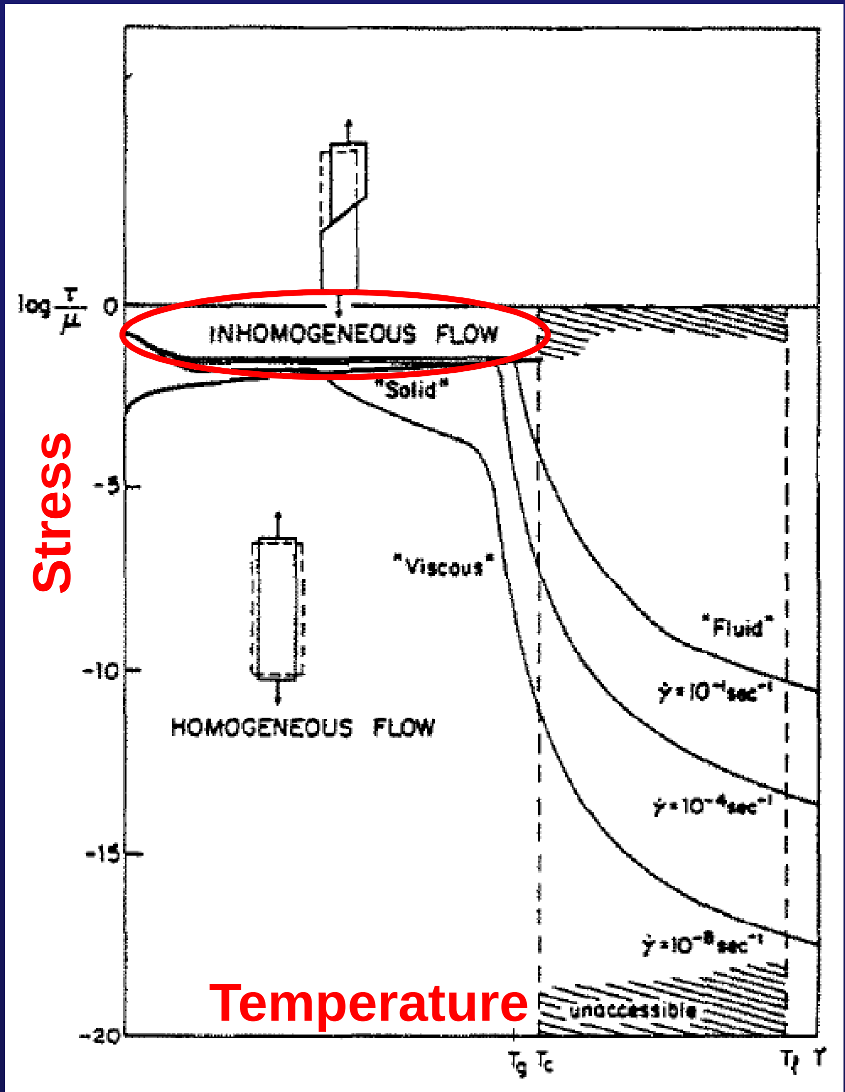
Example: creep test of $Pd_{41}Ni_{10}Cu_{29}P_{20}$ metallic glass



Heggen
et al. 2003

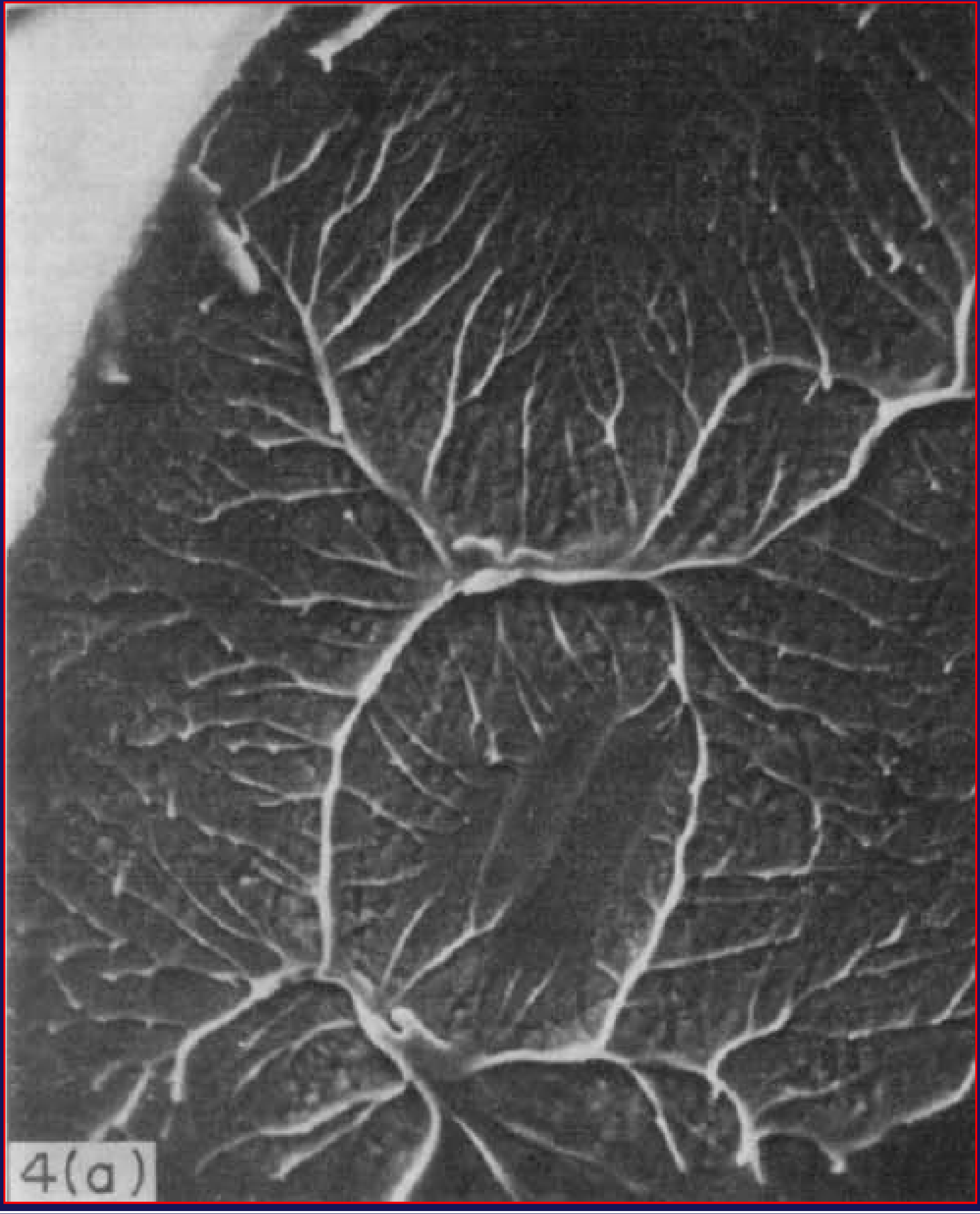
T = 550K

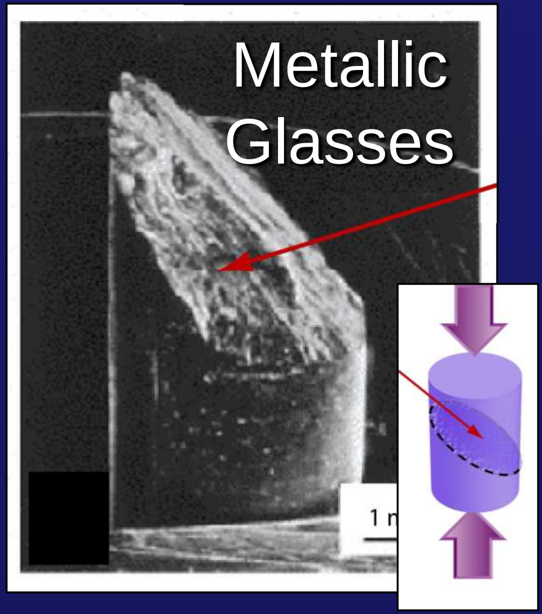
Homogeneous and Inhomogeneous Flow



Deformation Map

Shear banding





Liquefaction?

Shear banding

Suspensions,
Granulates

Liquefaction?

Schall, van Hecke
Ann. Rev. Fluid Mech. 2010

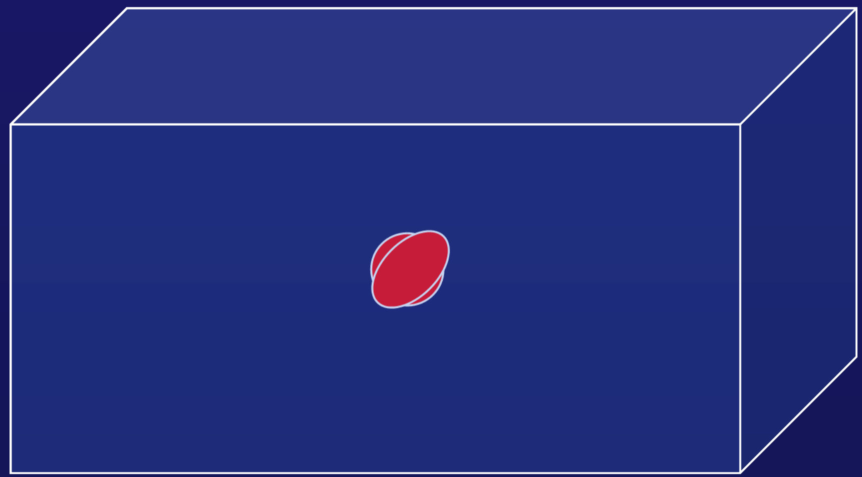
Stress Field

The determination of the elastic field of an ellipsoidal inclusion, and related problems

By J. D. Eshelby

Department of Physical Metallurgy, University of Birmingham

(*Communicated by R. E. Peierls, F.R.S.—Received* 1 *March* 1957)



Elastic Continuum

Stress Field

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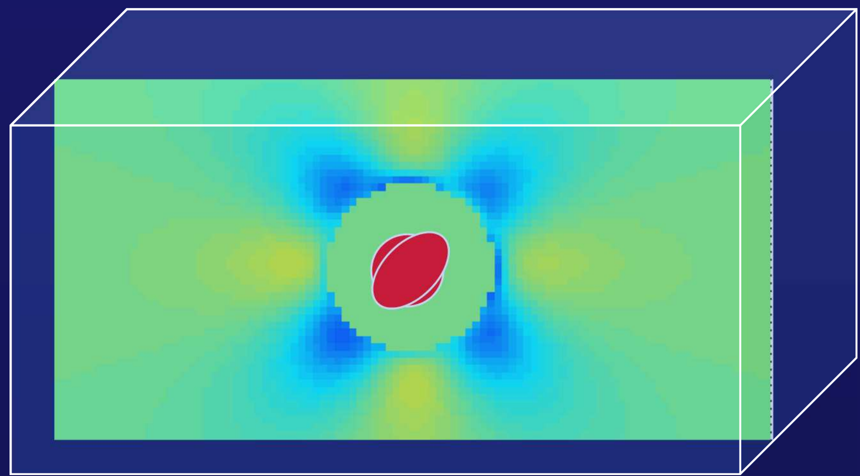
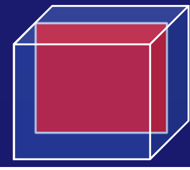


Elastic Continuum

Stress Field



Displacements

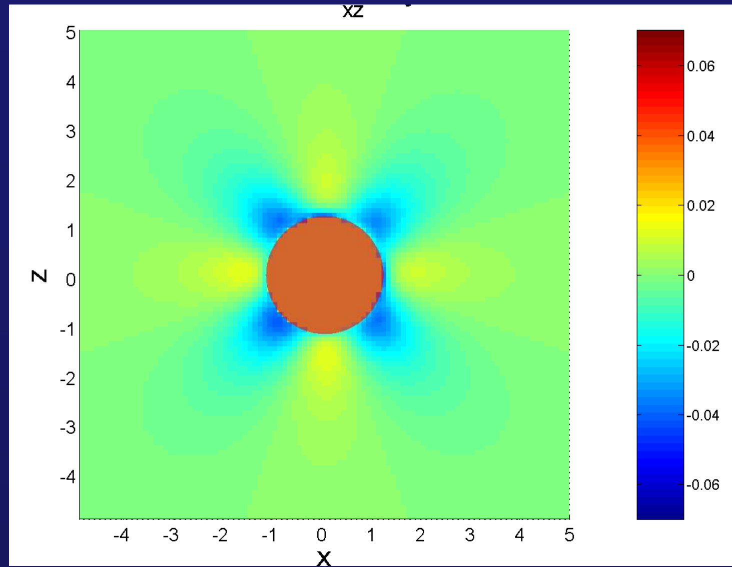
$$u_1 = Aa^3\left\{\frac{x_3}{r^3} + 6c(r^2 - a^2)\left(\frac{5x_1^{\,2}x_3}{r^7} - \frac{x_3}{r^5}\right)\right\}$$

$$u_2 = Aa^3\left\{6c(r^2 - a^2)\left(\frac{5x_1x_2x_3}{r^7}\right)\right\}$$

$$u_3 = Aa^3\left\{\frac{x_1}{r^3} + 6c(r^2 - a^2)\left(\frac{5x_1x_3^{\,2}}{r^7} - \frac{x_1}{r^5}\right)\right\}$$

(Hutchinson 2006)

Strain Field



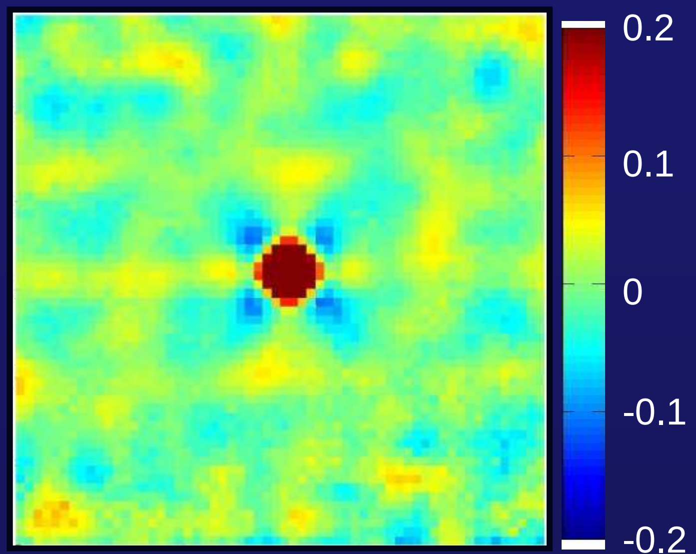
Long-range Strain Field

$$\epsilon_{xz} \propto \frac{1}{r^3}$$

→ Correlations between STZ?

Stress Field

Long-range strain correlations



... are rather the rule than the exception!

- Slowly sheared glasses
- Soft glassy materials

Why such a tough problem?

Computational challenge
Long Length *and* Time scales

Experimental challenge:
No direct atomic imaging of amorphous structures

... both problems solved with Colloidal Glasses