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Phenomenological Approaches to Elasto-Plastic Properties of Glasses: STZ Theory

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Typical Mechanical Behavior

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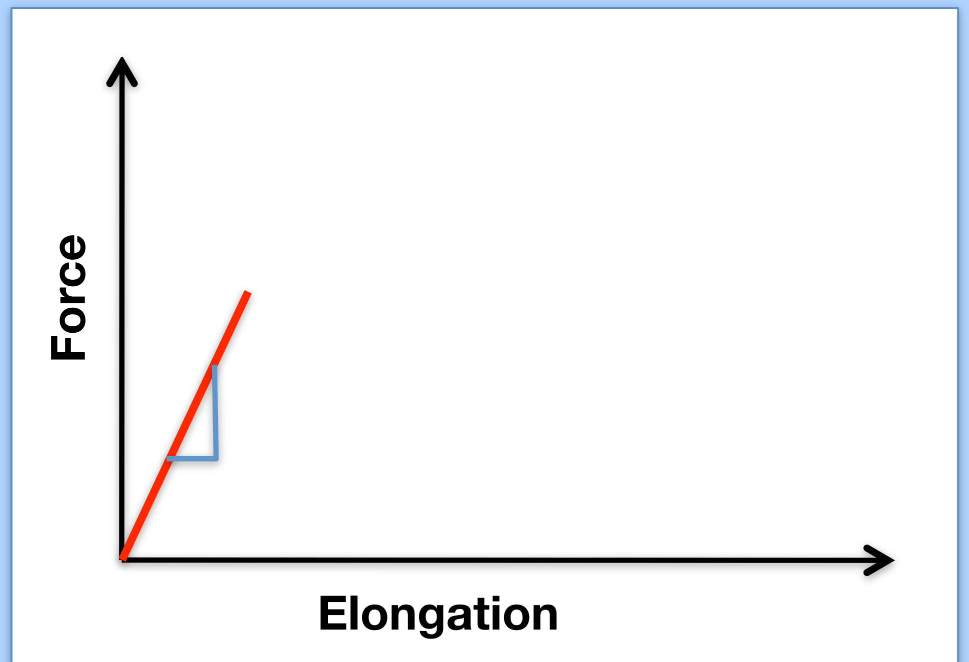
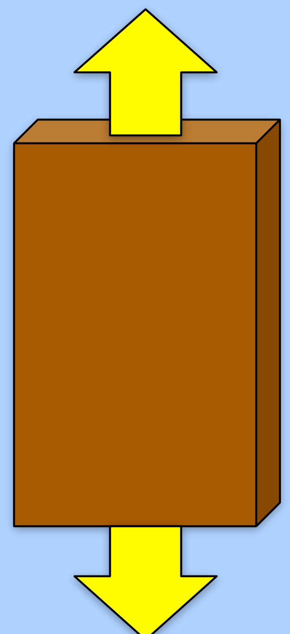
- **What quantities can we measure that give measures of a material's response?**
  - Elastic modulus – stiffness





Outline of Lecture 1

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- Review of Mechanical Properties
- Commentary on Goals
- Mechanics of Plasticity
- Shortcomings of Established Theories
- Eyring Rate Theories of Plasticity
- STZ Theory

Typical Mechanical Behavior

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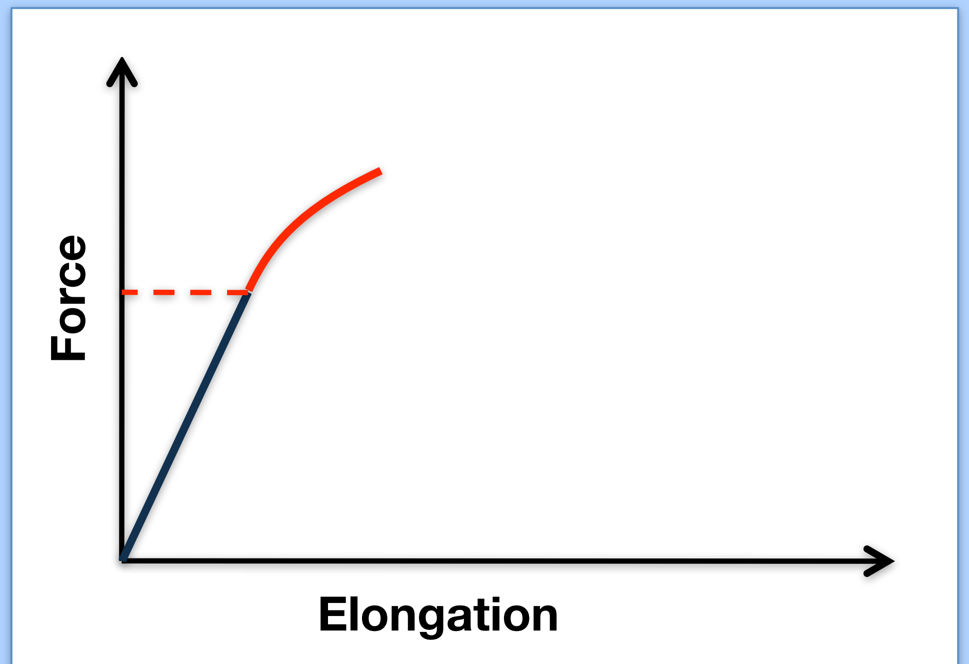
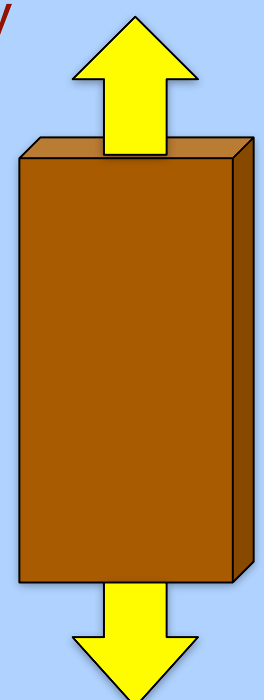
- **What quantities can we measure that give measures of a material's response?**
  - Yield Stress – Onset of Irreversibility





Typical Mechanical Behavior

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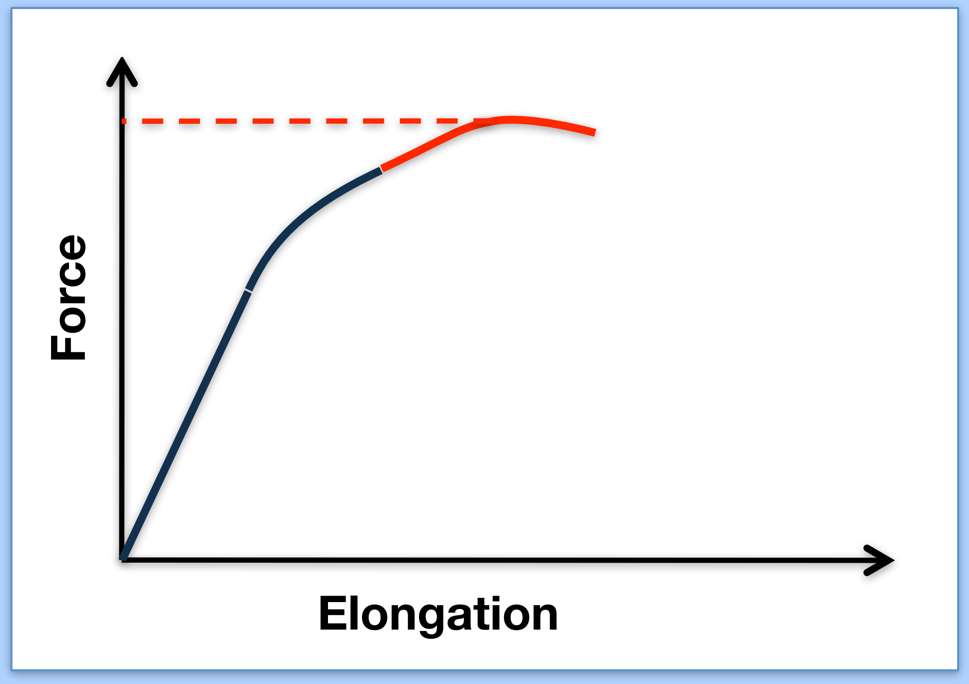
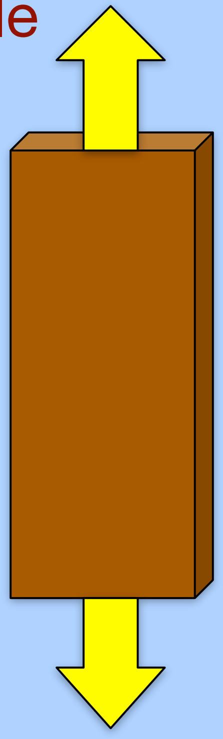
- **What quantities can we measure that give measures of a material's response?**
  - Strength – Maximum stress attainable





Typical Mechanical Behavior

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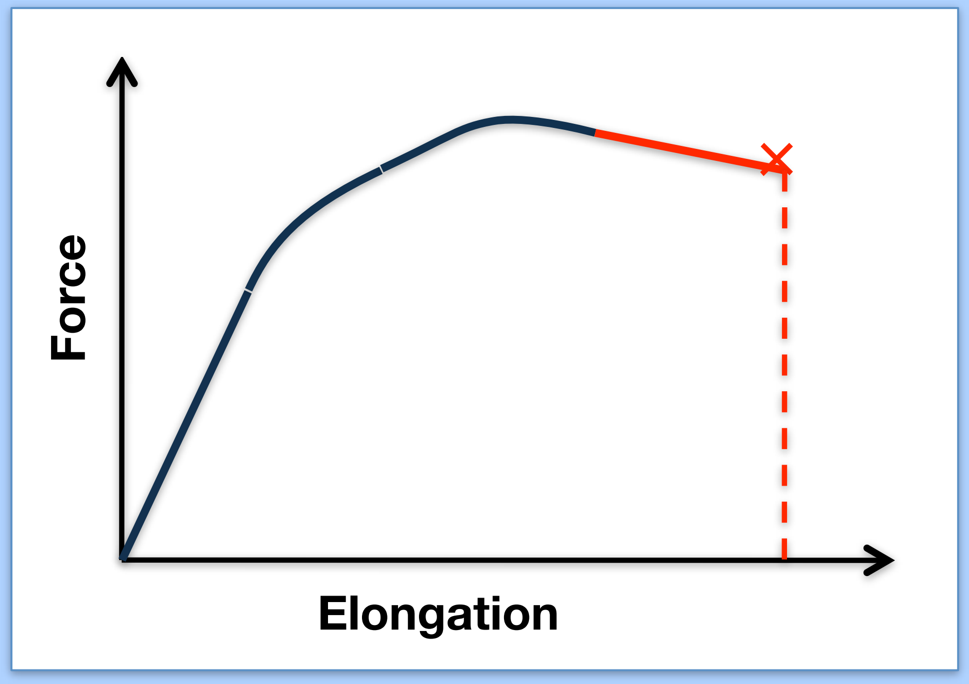
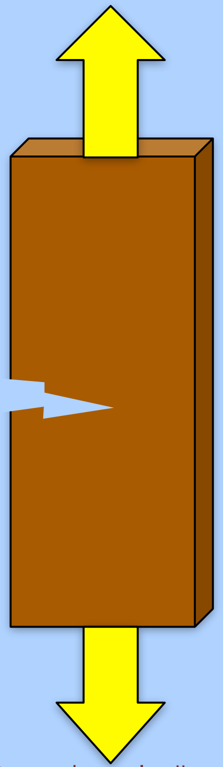
- **What quantities can we measure that give measures of a material's response?**
  - Ductility – Strain to failure





Typical Mechanical Behavior

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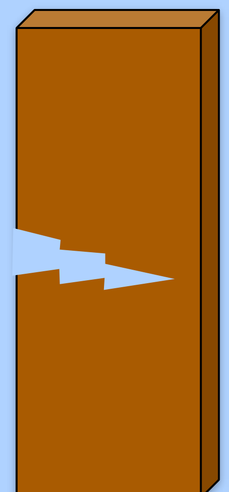
- **What quantities can we measure that give measures of a material's response?**
  - Toughness – Energy expended per unit crack advance



Characterizing Materials

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- **Different loadings can produce different values.**
- **What quantities can we measure that give invariant measures of a material's response?**
    - How do we define and quantify these?
    - What are the origins of these properties?
    - Can we predict these from first principles?
    - Fundamentally, how do we express material response?

Schools of Thought

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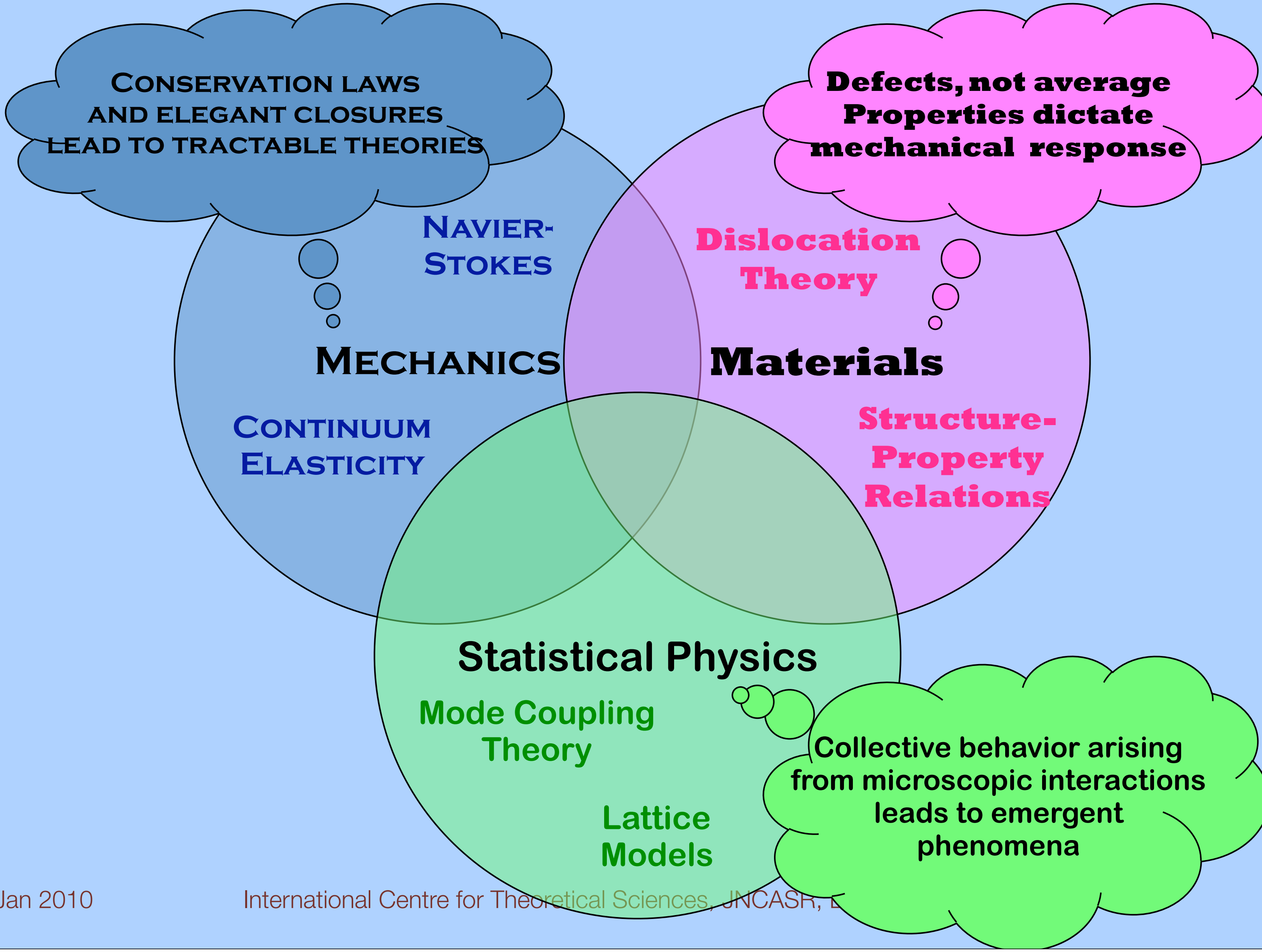

The Grand Challenge

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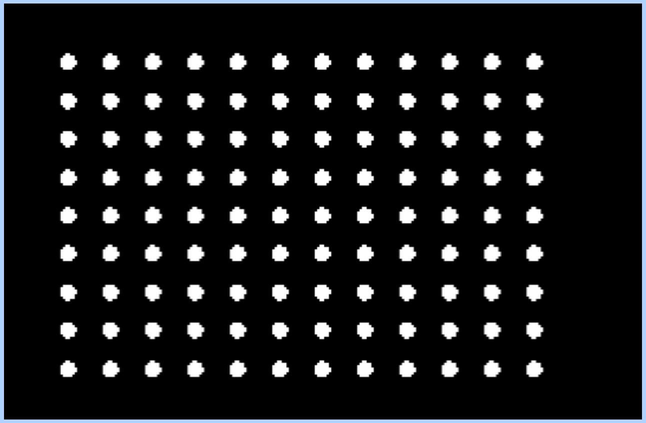
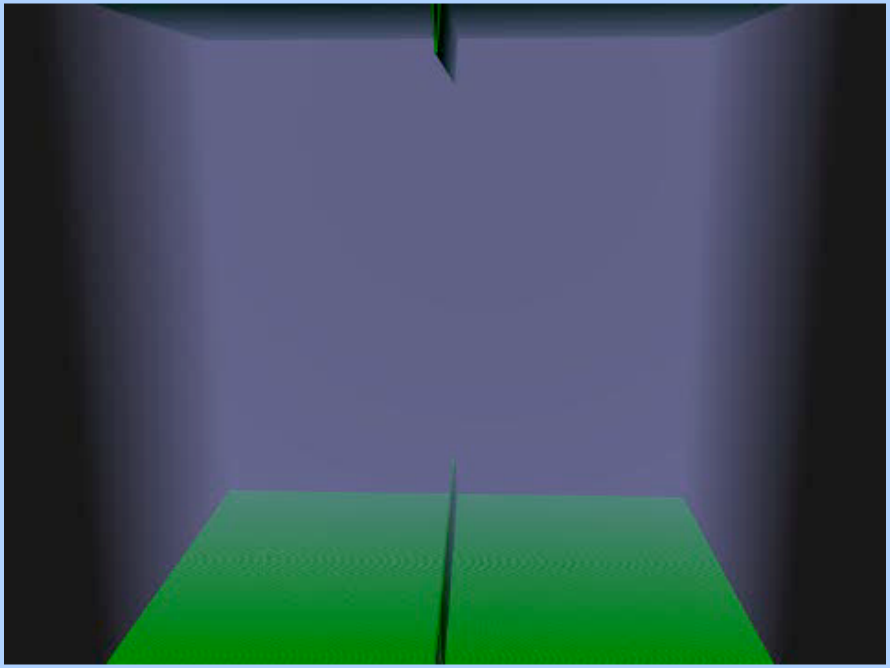
- How do we connect **macro-scale theory** to **micro-scale physics?**

Crystals



M Jessell, P Bons & P Rey 2002
Microstructures Online
http://www.virtualexplorer.com.au/special/meansvolume/contribs/jessell/



Farid Abraham (IBM), Mark Duchaineau and Tomas Diaz De La Rubia (LLNL)

The Grand Challenge

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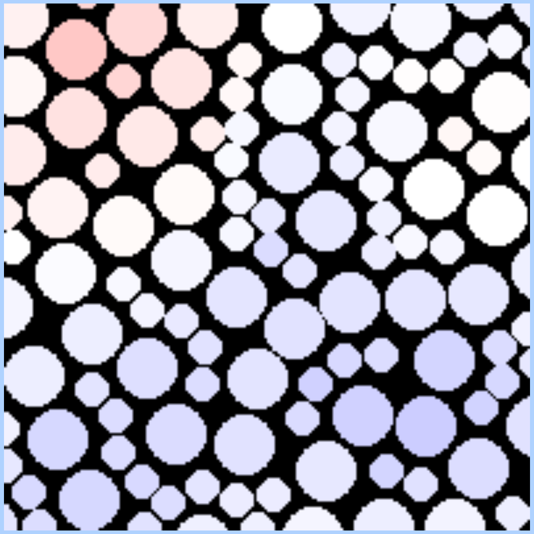
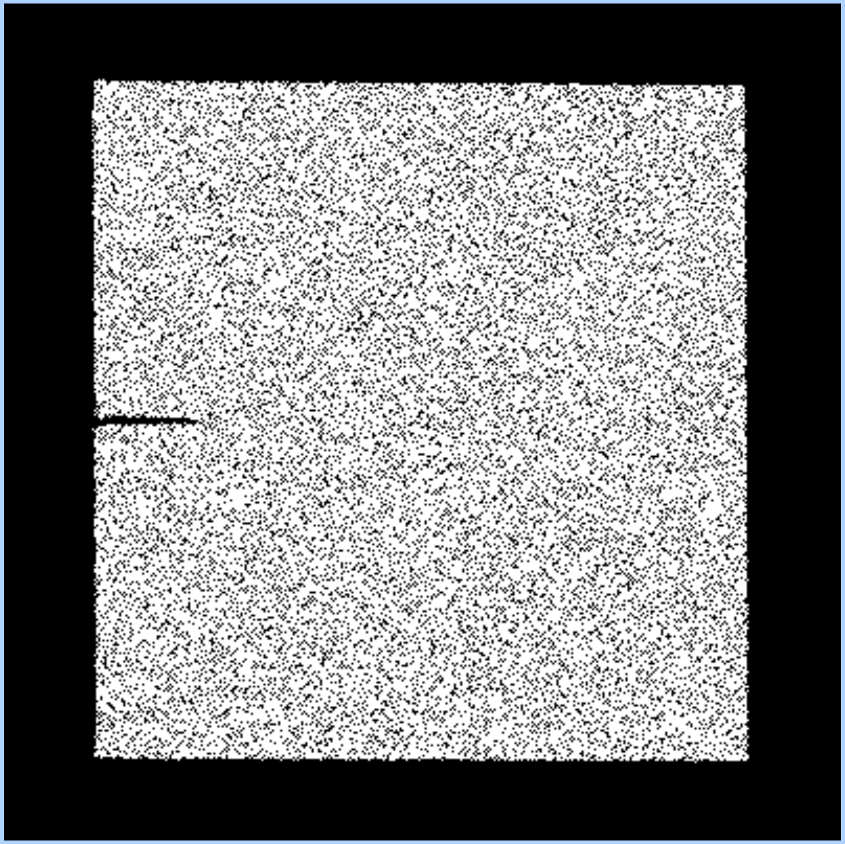
- How do we connect **macro-scale theory** to **micro-scale physics**?

Amorphous Solids



ML Falk, JS Langer, PRE 57, pp. 7192 (1998)



ML Falk, PRB 60, pp. 7062 (1999)

Fundamentals: Strain

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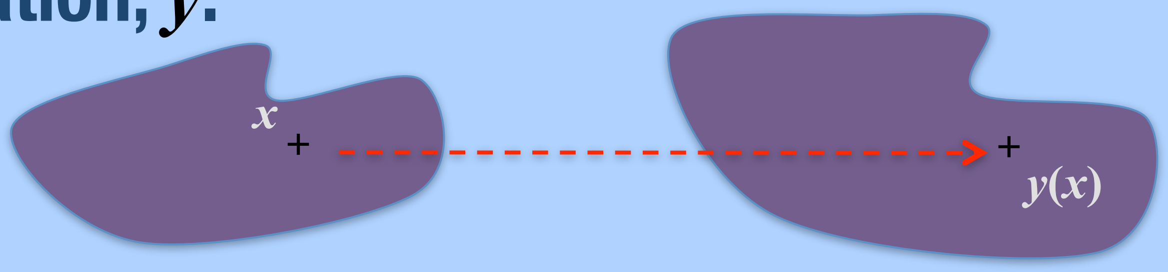
- Consider a body, where each material point is denoted in space by its initial location, $\boldsymbol{x}$.
- After deformation each material point is at a new location, $\boldsymbol{y}$.



- Define the **displacement** as $\boldsymbol{u}(\boldsymbol{x})=\boldsymbol{y}(\boldsymbol{x})-\boldsymbol{x}$
- Define the **deformation gradient** at x as the 3x3 tensor $\mathbf{F}=\nabla y(x)$ or equivalently $F_{ij}=\partial y_i/\partial x_j$

Fundamentals: Strain

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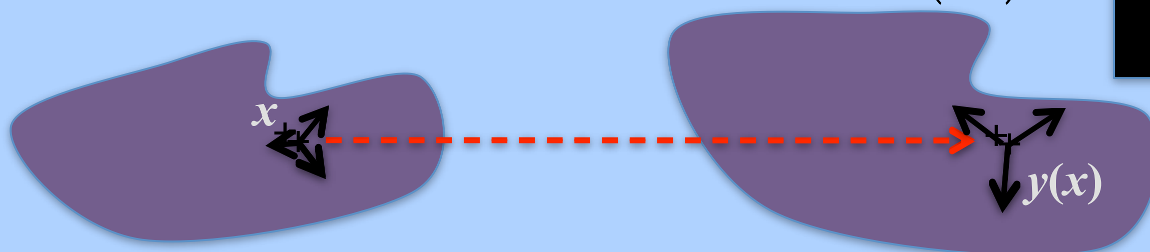
- The **deformation gradient**, **F**, can be used to map a small displacement on the original body to the deformed body as

$$y(x+\delta e) = y(x) + \nabla y \delta e + O(\delta^2)$$

e is a unit vector



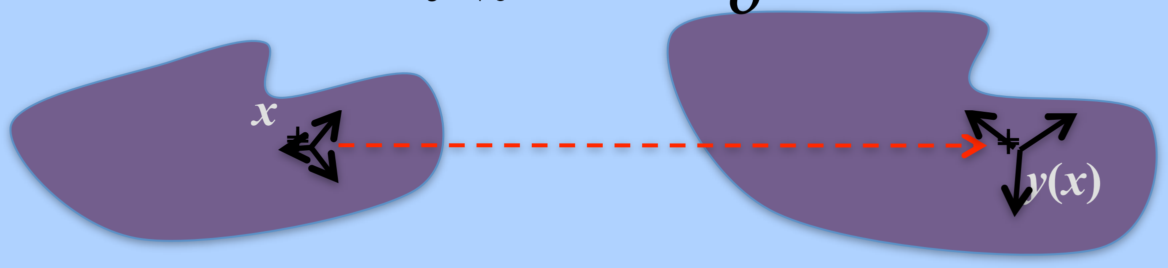
- In other words $y(x+\Delta x) - y(x) \approx \mathbf{F}\Delta x$
- Any orthonormal frame (e_1, e_2, e_3) becomes a linearly independent triad $(\mathbf{F}e_1, \mathbf{F}e_2, \mathbf{F}e_3)$ in the deformed body
- The determinant of this new triad gives the local change in volume due to deformation.

$$det\,\mathbf{F} = \frac{V+\Delta V}{V}$$

Fundamentals: Strain

- We can also use this formalism to extract the changes in length to first order

$$\lim_{\delta \to 0} \frac{\left| y(x+\delta e) - y(x) \right|^2}{\delta^2} = \mathbf{F}e \cdot \mathbf{F}e = \mathbf{F}^T\mathbf{F}$$



- If the body is rigid then $\mathbf{F}$ must be a rotation and $\mathbf{F}^T\mathbf{F} = \mathbf{I}$
- Under more general conditions the on-diagonal terms in the matrix $\mathbf{F}^T\mathbf{F}$ are related to **length changes of "fibers"** along the principal axes, while the off-diagonal elements are related to **changes in angles between these "fibers"**.

Fundamentals: Strain

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- The object **$C=F^TF$** is known as the **Green deformation tensor**
- We can define the **Lagrangian strain** **$E=½(C-I)$**
- Defined in the undeformed body's coordinates.

$$E_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_k}{\partial x_i}\frac{\partial u_k}{\partial x_j}\right]$$

Lagrangian Strain

$$E^*_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial y_j} + \frac{\partial u_j}{\partial y_i} - \frac{\partial u_k}{\partial y_i}\frac{\partial u_k}{\partial y_j}\right]$$

Eulerian Strain

- Strain can be defined in the deformed body's coordinates. This is known as the **Eulerian strain**
- It is typical to consider deformation of solid bodies in a Lagrangian framework.
- Fluid mechanics is typically considered in an Eulerian framework.

Fundamentals: Strain

- **For applications in which the deformation is small, the third term on the RHS is negligible and the deformation can be expressed in terms of an "infinitesimal strain"**

$$\mathrm{E}_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_k}{\partial x_i}\frac{\partial u_k}{\partial x_j}\right]$$

Lagrangian Strain

$$\mathrm{E}^{*}_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial y_j} + \frac{\partial u_j}{\partial y_i} - \frac{\partial u_k}{\partial y_i}\frac{\partial u_k}{\partial y_j}\right]$$

Eulerian Strain

$$\varepsilon_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right]$$

Infinitesimal Strain

Fundamentals: Strain

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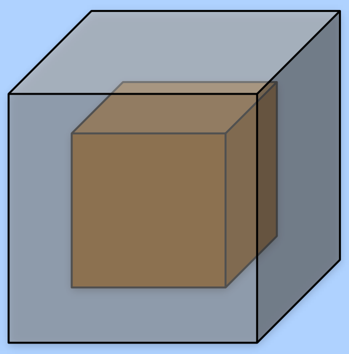
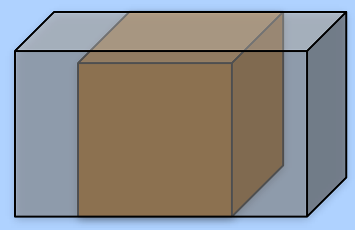
Uniform Dilation



$$\boldsymbol{u}(\boldsymbol{x}) = \alpha(\boldsymbol{x} - \boldsymbol{x}_0)$$

$$\varepsilon_{ij} = \begin{bmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{bmatrix}$$

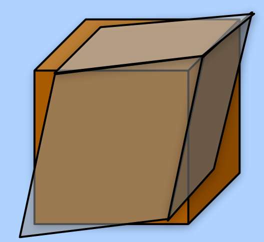
Simple Extension



$$\boldsymbol{u}(\boldsymbol{x}) = \lambda[\boldsymbol{e}_1 \cdot (\boldsymbol{x} - \boldsymbol{x}_0)]\boldsymbol{e}_1$$

$$\varepsilon_{ij} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Pure Shear



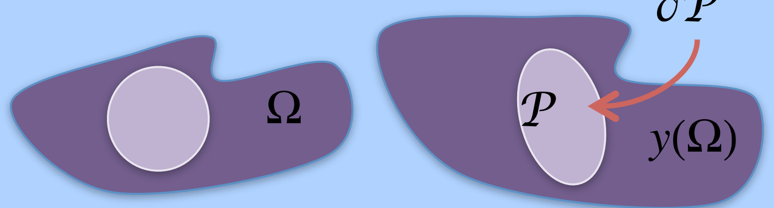
$$\boldsymbol{u}(\boldsymbol{x}) = \begin{array}{l} \gamma\{[\boldsymbol{e}_1 \cdot (\boldsymbol{x} - \boldsymbol{x}_0)]\boldsymbol{e}_2 \\ +[\boldsymbol{e}_2 \cdot (\boldsymbol{x} - \boldsymbol{x}_0)]\boldsymbol{e}_1\} \end{array}$$

$$\varepsilon_{ij} = \begin{bmatrix} 0 & \gamma & 0 \\ \gamma & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Fundamentals: Stress

- The forces on a body can be separated into body and surface forces

$$F(\mathcal{P}) = \int_{\mathcal{P}} \boldsymbol{b}(\boldsymbol{y})d\boldsymbol{V}_y + \int_{\partial\mathcal{P}} \boldsymbol{s}(\boldsymbol{y},\boldsymbol{n}(\boldsymbol{y}))d\boldsymbol{A}_y = \int_{\mathcal{P}} \rho(\boldsymbol{y})\ddot{\boldsymbol{u}}(\boldsymbol{y})d\boldsymbol{V}_y$$



- Cauchy's Theorem: ∃a sym. tensor σ_{ij} such that

$$\boldsymbol{s}(\boldsymbol{y},\boldsymbol{n}(\boldsymbol{y})) = \sigma(\boldsymbol{y}) \cdot \boldsymbol{n}(\boldsymbol{y})$$

- Which, by the divergence theorem implies that

$$0 = \int_{\mathcal{P}} [\rho(\boldsymbol{y})\ddot{\boldsymbol{u}}(\boldsymbol{y}) - \boldsymbol{b}(\boldsymbol{y}) - \nabla \cdot \sigma] d\boldsymbol{V}_y \qquad \rho\ddot{u}_i = b_i + \frac{\partial \sigma_{ij}}{\partial x_j}$$

- In equilibrium this reduces to

$$\boxed{b_i + \frac{\partial \sigma_{ij}}{\partial x_j} = 0}$$

Fundamentals: Thermodynamics

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- **Work done (integrate force x velocity)**

$$\mathcal{W} = \int_{\mathcal{P}} \left[b_i \dot{u}_i + \frac{\partial \sigma_{ij}}{\partial x_j} \dot{u}_i \right] dV = \int_{\mathcal{P}} \left[b_i \dot{u}_i - \sigma_{ij} \frac{\partial \dot{u}_i}{\partial x_j} \right] dV = \int_{\mathcal{P}} \left[b_i \dot{u}_i - \sigma_{ij} \dot{\varepsilon}_{ij} \right] dV$$

- **If energy stored in the material per unit volume is denoted ψ then the energy dissipated is**

$$\mathcal{D} = \int_{\mathcal{P}} \left[b_i \dot{u}_i - \sigma_{ij} \dot{\varepsilon}_{ij} - \dot{\psi} \right] dV \geq 0$$

The Missing Ingredients

- At this point, assuming 3D, we have a **displacement field** from which we can derive the strain (3 unknowns)
- We have a **stress** (6 unknowns)
- We also have **equilibrium** (3 equations)
- Since the problem remains **underdetermined** we need a set of equations that will relate the stresses to the strains, and thereby to the displacement field.
- These equations are known as **constitutive equations**.

$$\varepsilon_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right]$$

$$b_i + \frac{\partial \sigma_{ij}}{\partial x_j} = 0$$

Linear Elasticity

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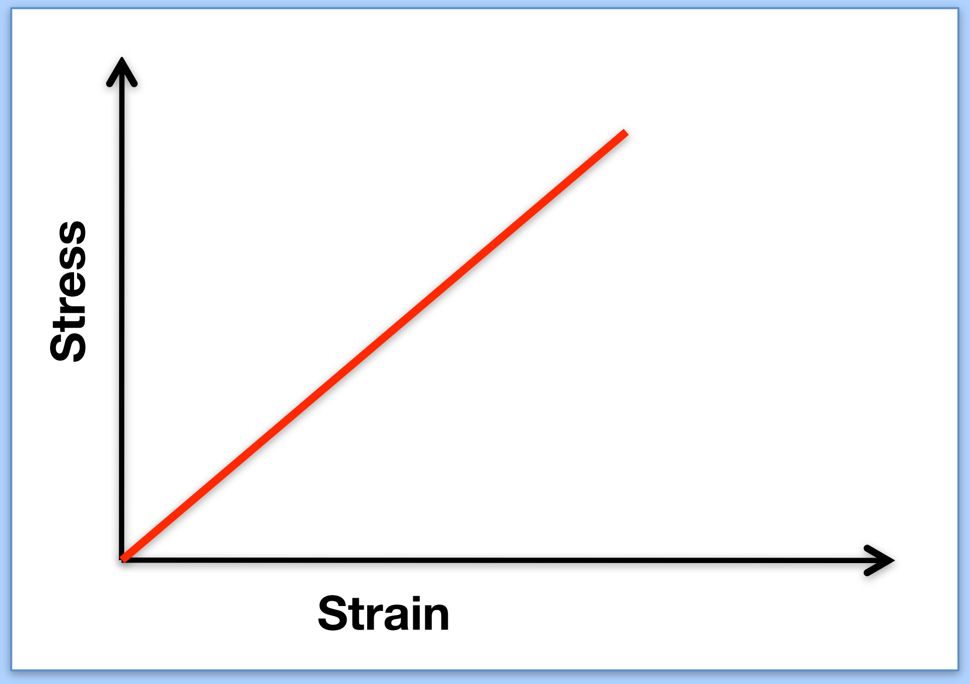
- Linear elasticity is the simplest constitutive equation and assumes proportionality between stress and strain



Linear Elasticity

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- **Linear elasticity is the simplest constitutive equation and assumes proportionality between stress and strain**

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}, \qquad \sigma_{ij} = \frac{\partial\psi}{\partial\varepsilon_{ij}}$$

- **If the material is isotropic this reduces to a simpler equation**

$$\sigma_{ij} = 2\mu\varepsilon_{ij} + \lambda\varepsilon_{kk}\delta_{ij}$$

- **Here μ is the shear modulus and the bulk modulus K is related to μ and λ by**

$$\tfrac{1}{3}\sigma_{ii} = \left(\tfrac{2}{3}\mu + \lambda\right)\varepsilon_{ii} = K\varepsilon_{ii}$$

- **Since the energy per unit volume is given by** $\psi = \tfrac{1}{2}\varepsilon_{ij}C_{ijkl}\varepsilon_{kl}$ **assuming no body forces**

$$d = \sigma_{ij}\dot{\varepsilon}_{ij} - \dot{\psi} = 0$$

Viscoelasticity

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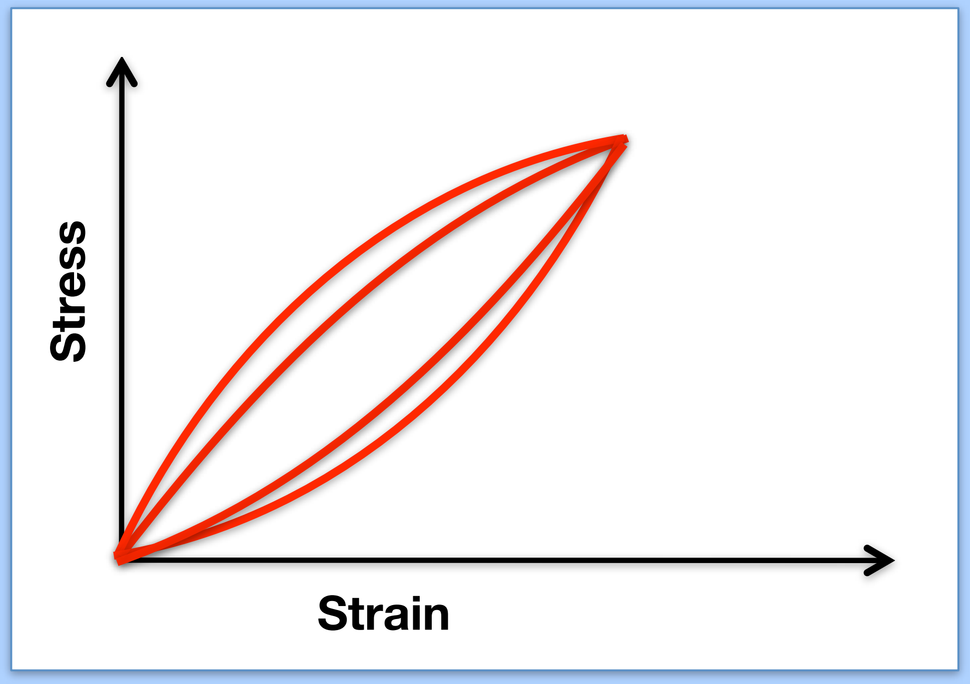
- **Viscoelasticity introduces dissipation by allowing the stress to be strain rate dependent**



Viscoelasticity

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- Viscoelasticity introduces dissipation by allowing the stress to be strain rate dependent

$$\sigma_{ij} = \frac{\partial \psi}{\partial \varepsilon_{ij}} + \sigma_{ij}^{diss}$$

- To assure compliance with 2nd law of thermodynamics

$$d = \left(\frac{\partial \psi}{\partial \varepsilon_{ij}} + \sigma_{ij}^{diss} \right) \dot{\varepsilon}_{ij} - \dot{\psi} \;=\; \frac{\partial \psi}{\partial \varepsilon_{ij}} \dot{\varepsilon}_{ij} + \sigma_{ij}^{diss} \dot{\varepsilon}_{ij} - \dot{\psi} \;=\; \sigma_{ij}^{diss} \dot{\varepsilon}_{ij} \;\geq\; 0$$

- One reasonable choice would be

$$\sigma_{ij}^{diss} = \eta \dot{\varepsilon}_{ij}$$

- Which we could cast as a "dissipative potential"

$$\phi = \tfrac{1}{2} \eta \dot{\varepsilon}^2 , \quad \sigma^{diss} = \frac{\partial \phi}{\partial \dot{\varepsilon}}$$

- Any choice of ϕ that is convex and minimized at 0 will satisfy thermodynamics

Plasticity

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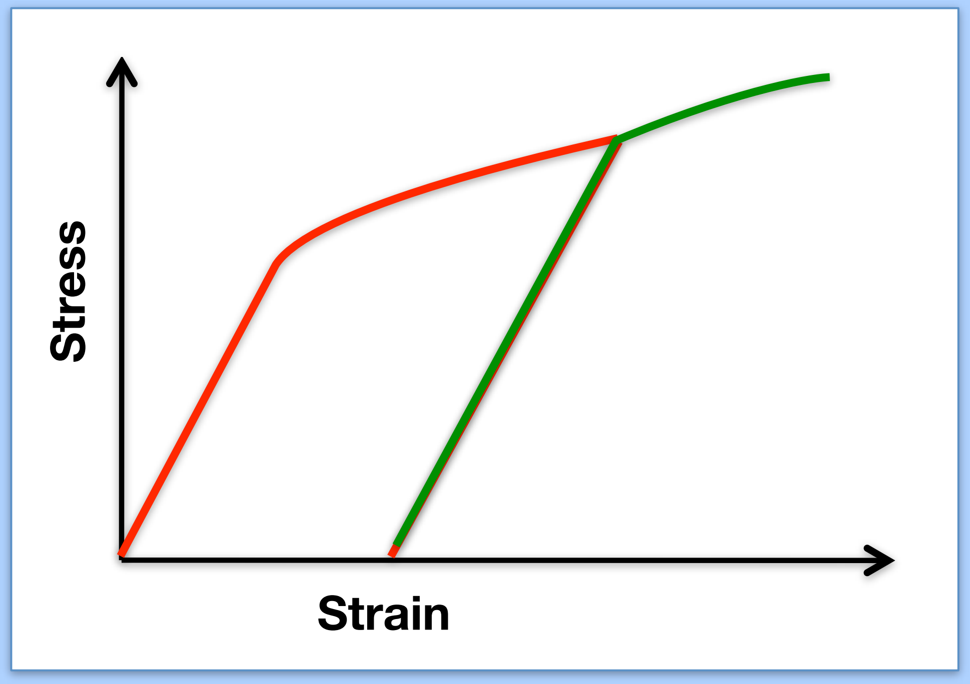
- **In plasticity (as opposed to elasticity) the material deforms irreversibly.**



Plasticity

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- In plasticity (as opposed to elasticity) the material deforms irreversibly.
- This implies that the material does not retain memory of the initial state.
- This argues for models in which the change in the internal state of the material is an intrinsic feature of the theory.

The Yield Surface

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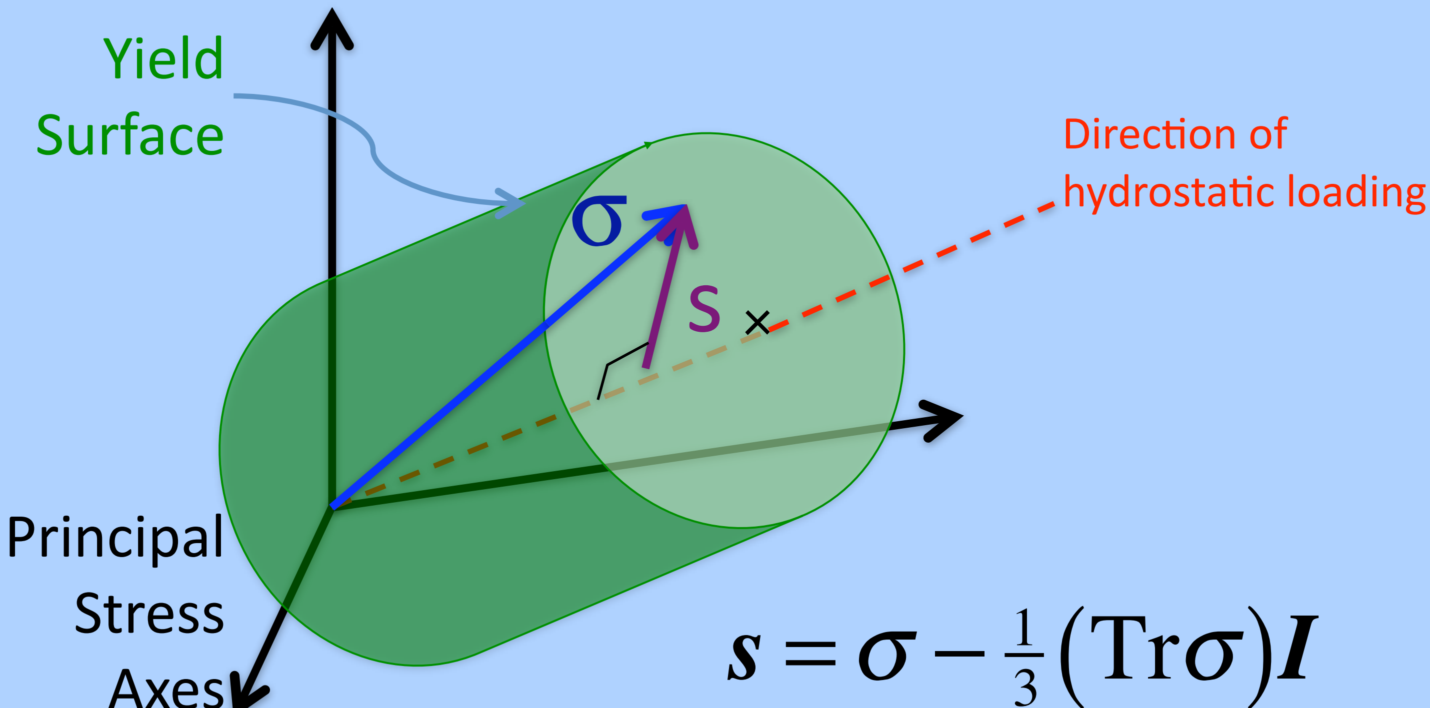
- Deformation takes place in shear, not dilation, so the operative stress is the deviatoric stress, s



$$s = \sigma - \tfrac{1}{3}(\mathrm{Tr}\,\sigma)I$$

Plasticity

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- Traditional plasticity theories consider the yield stress to be an intrinsic material property

$$\varepsilon[\boldsymbol{u}] = \varepsilon^{el} + \varepsilon^{pl}$$

$$\sigma = \boldsymbol{C}\varepsilon^{el} = \boldsymbol{C}\left(\varepsilon[\boldsymbol{u}] - \varepsilon^{pl}\right)$$

- To determine how the plastic strain evolves it is postulated that there exists a yield criterion $f(\sigma,\zeta)$ such that

$$f(\sigma,\zeta) = |s| - \zeta$$

$$f(\sigma,\zeta) < 0: \quad \text{purely elastic response}$$

$$f(\sigma,\zeta) = 0: \quad \zeta \text{ evolves to remain on yield surface}$$

Plasticity

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- **Two functions describe how the yield surface will evolve**

$$\dot{\varepsilon}^{pl} = \dot{\gamma}\frac{\partial f(\sigma,\zeta)}{\partial \sigma} = \dot{\gamma}\boldsymbol{N}(\sigma,\zeta),\ \dot{\gamma} \geq 0$$

$$\dot{\zeta} = \dot{\gamma}\boldsymbol{h}(\sigma,\zeta)$$

- **Given these assumptions we want to determine the unknown strain increment $\dot{\gamma}$ when we are on the yield surface**

$$0 = \dot{f} = \frac{\partial f}{\partial \sigma}\cdot\dot{\sigma} + \frac{\partial f}{\partial \zeta}\dot{\zeta} = \frac{\partial f}{\partial \sigma}\cdot \boldsymbol{C}\left(\dot{\varepsilon} - \dot{\varepsilon}^{pl}\right) + \frac{\partial f}{\partial \zeta}\dot{\zeta}$$

$$0 = \boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon} - \dot{\gamma}\boldsymbol{N}\cdot\boldsymbol{C}\boldsymbol{N} + \dot{\gamma}\frac{\partial f}{\partial \zeta}\boldsymbol{h}$$

$$\dot{\gamma} = \frac{\boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon}}{\boldsymbol{N}\cdot\boldsymbol{C}\boldsymbol{N} - \frac{\partial f}{\partial \zeta}\boldsymbol{h}} = \frac{\boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon}}{\boldsymbol{N}\cdot\boldsymbol{C}\boldsymbol{N} + \boldsymbol{H}(\sigma,\zeta)},\ when\ \boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon} > 0$$

Perfect Plasticity

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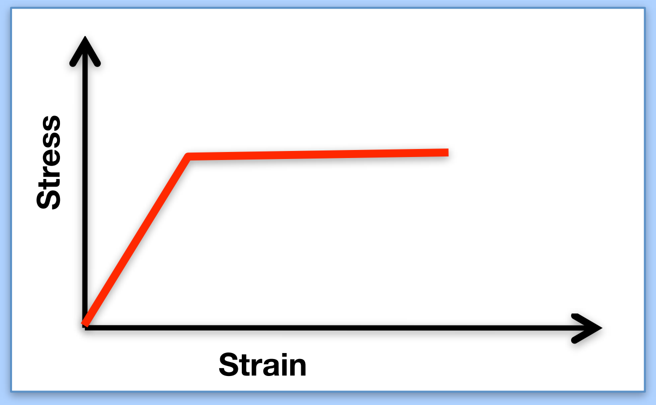
- Consider one particular case where H=0

$$\dot{\varepsilon}^{pl} = \dot{\gamma}\frac{\partial f(\sigma,\zeta)}{\partial\sigma} = \dot{\gamma}N(\sigma,\zeta),\ \dot{\gamma}\geq 0$$

$$\dot{\zeta} = 0$$



- Given these assumptions we want to determine the unknown strain increment $\dot{\gamma}$ when we are on the yield surface

$$\dot{\gamma} = \frac{\boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon}}{\boldsymbol{N}\cdot\boldsymbol{C}\boldsymbol{N}},\ \text{when } \boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon} > 0$$

$$\dot{\sigma} = \boldsymbol{C}\left(\dot{\varepsilon} - \dot{\varepsilon}^{pl}\right) = \begin{cases} 0, & \boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon} > 0 \\ \boldsymbol{C}\dot{\varepsilon}, & \boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon} \leq 0 \end{cases}$$

Isotropic Hardening

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- Consider one particular case where H=h=const

$$\dot{\varepsilon}^{pl} = \dot{\gamma}\frac{\partial f(\sigma,\zeta)}{\partial\sigma} = \dot{\gamma}N(\sigma,\zeta),\ \dot{\gamma} \geq 0$$

$$\dot{\zeta} = \dot{\gamma}\mathrm{h}$$

- Given these assumptions we want to determine the unknown strain increment $\dot{\gamma}$ when we are on the yield surface

$$\dot{\gamma} = \frac{\boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon}}{\boldsymbol{N}\cdot\boldsymbol{C}\boldsymbol{N}+\mathrm{h}},\ \text{when } \boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon} > 0$$

$$\dot{\sigma} = \boldsymbol{C}\left(\dot{\varepsilon} - \dot{\varepsilon}^{pl}\right) = \begin{cases} \left(\dfrac{\mathrm{h}\boldsymbol{C}\dot{\varepsilon}}{\boldsymbol{N}\cdot\boldsymbol{C}\boldsymbol{N}+\mathrm{h}}\right), & \boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon} > 0 \\ \boldsymbol{C}\dot{\varepsilon}, & \boldsymbol{N}\cdot\boldsymbol{C}\dot{\varepsilon} \leq 0 \end{cases}$$

A Critical Assessment

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- **What is missing from this picture of plasticity?**
  - Rate dependence
  - A relation between the internal variables (in this case the yield stress ζ) and microscopic physics of deformation and microstructural evolution
  - As such the theory remains entirely empirical
- **At present we don't have tools suitable for abstracting our understanding of material microstructure to inform continuum theory.**

Eyring Rate Theory

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- Eyring developed a formalism whereby one can treat plasticity the same way we would chemical kinetics

$$\dot{\varepsilon}^{pl} = n\Omega R(s)\frac{\mathbf{s}}{s} \qquad R(s) = f\, exp\left(-\frac{\Delta G_m - s\Omega}{kT}\right)$$

n=number of plasticity carriers (dislocations)

R=biased rate of transitions that couple to shear

- Note that forward and backward hopping are both possible

$$\dot{\varepsilon}^{pl} = n\Omega\left[R(s) - R(-s)\right]\frac{\mathbf{s}}{s} = 2n\Omega f\, exp\left(-\frac{\Delta G_m}{kT}\right) sinh\left(\frac{s\Omega}{kT}\right)\frac{\mathbf{s}}{s}$$

Free Volume Theory

F. Spaepen, Acta Metall. 25, 407 (1977)

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- Posited that "flow defects" are present in the metallic glass

$$\dot{\varepsilon}^{pl} = n\Omega\left[R(s) - R(-s)\right]\frac{\mathbf{s}}{s} = 2n\Omega f\, exp\left(-\frac{\Delta G_m}{kT}\right) sinh\left(\frac{s\Omega}{kT}\right)\frac{\mathbf{s}}{s}$$

- The number density is proportional to a material property called "free volume" which is both created and destroyed during flow.

$$n = \exp\left(-\gamma v^{*}/v_f\right)$$

$$\dot{v}_f = nfv^{*}\, exp\left(-\frac{\Delta G_m}{kT}\right)\left\{\frac{\gamma}{v_f}\frac{kT}{S}\left[cosh\left(\frac{s\Omega}{kT}\right) - 1\right] - \frac{1}{n_D}\right\}$$

Critique of Free Volume Theory

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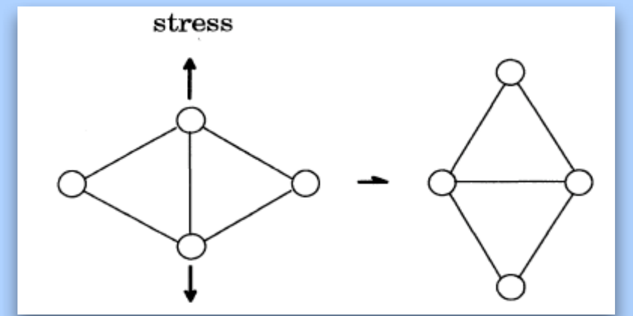
$$\dot{\varepsilon}^{pl} = n\Omega\left[R(s) - R(-s)\right]\frac{\mathbf{s}}{s} = 2n\Omega f\, exp\left(-\frac{\Delta G_m}{kT}\right) sinh\left(\frac{s\Omega}{kT}\right)\frac{\mathbf{s}}{s}$$

$$n = \exp\left(-\gamma v^* / v_f\right)$$

$$\dot{v}_f = -nfv^*\, exp\left(-\frac{\Delta G_m}{kT}\right)\left\{\frac{\gamma}{v_f}\frac{kT}{S}\left[cosh\left(\frac{s\Omega}{kT}\right) - 1\right] - \frac{1}{n_D}\right\}$$

- There is no reasonable zero temperature limit.
- No accounting for induced anisotropies in the glass.



Tomida and Egami, PRB 48, 3048 (1991)

2D Simulation System

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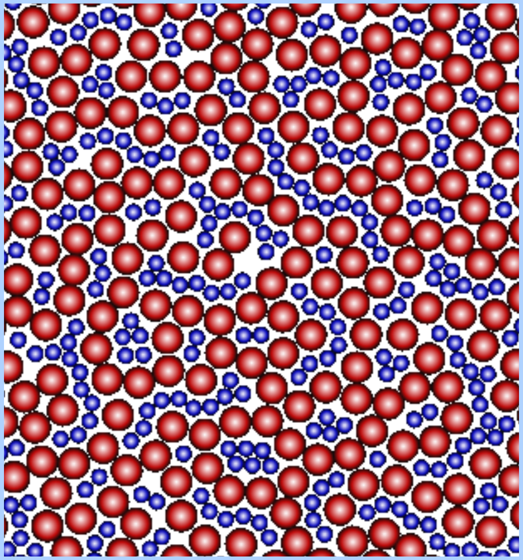
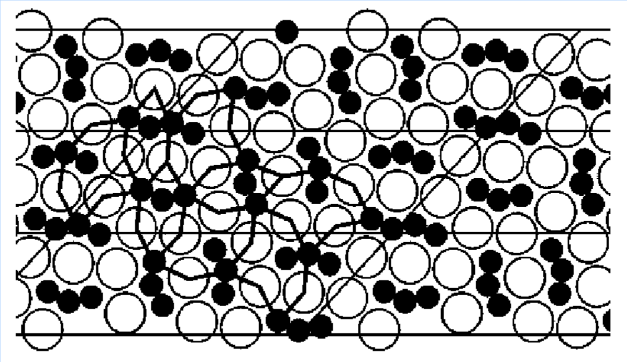
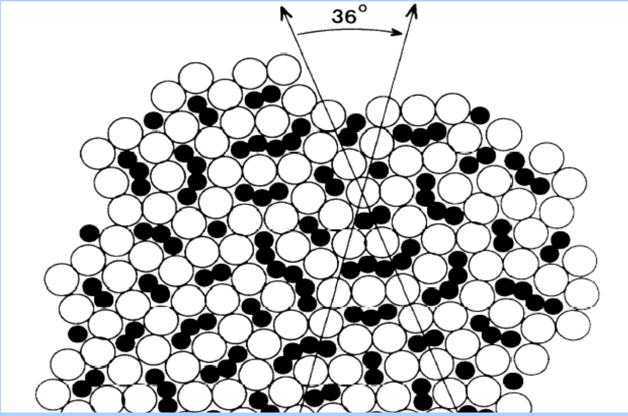


(Lancon et al, Europhys. Lett, 1986)



Lee, Swendsen, Widom (2001)



Widom, Strandburg, Swendsen (1987)

- 2D binary Lennard-Jones 12-6 potential
- Binary system with quasi-crystalline packing
  45:55 composition, 20,000-80,000 atoms
- $T_{MCT} \approx 0.325$

Stress-Strain Response

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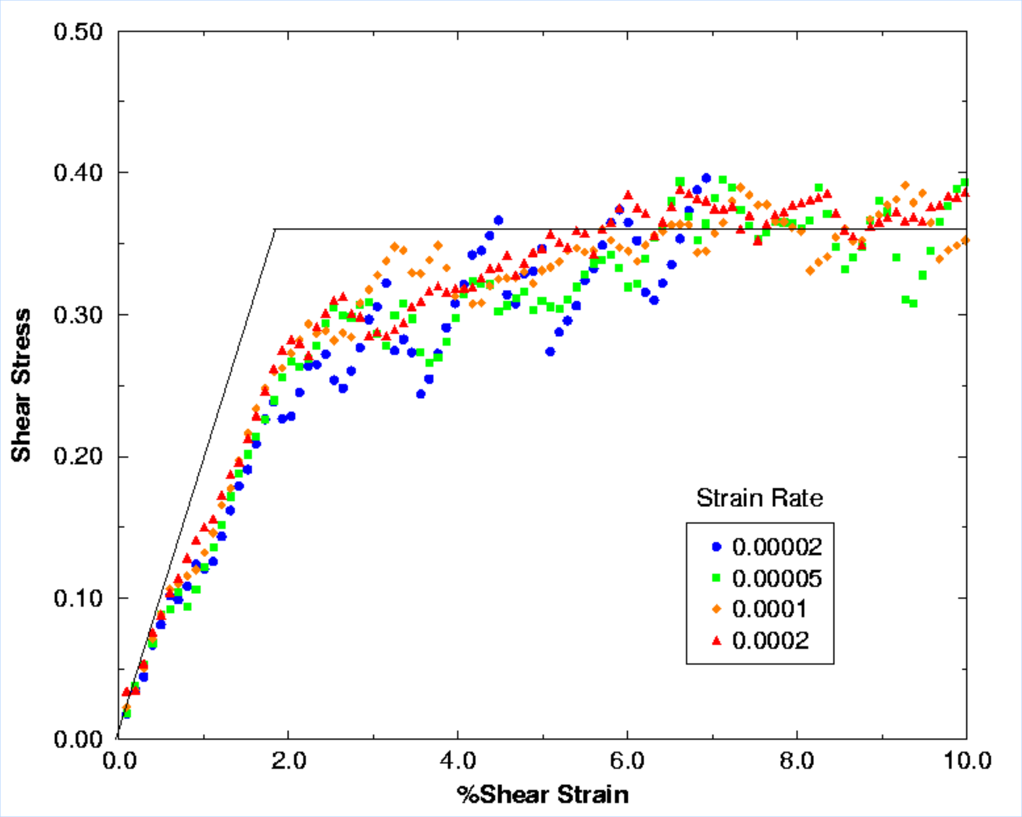
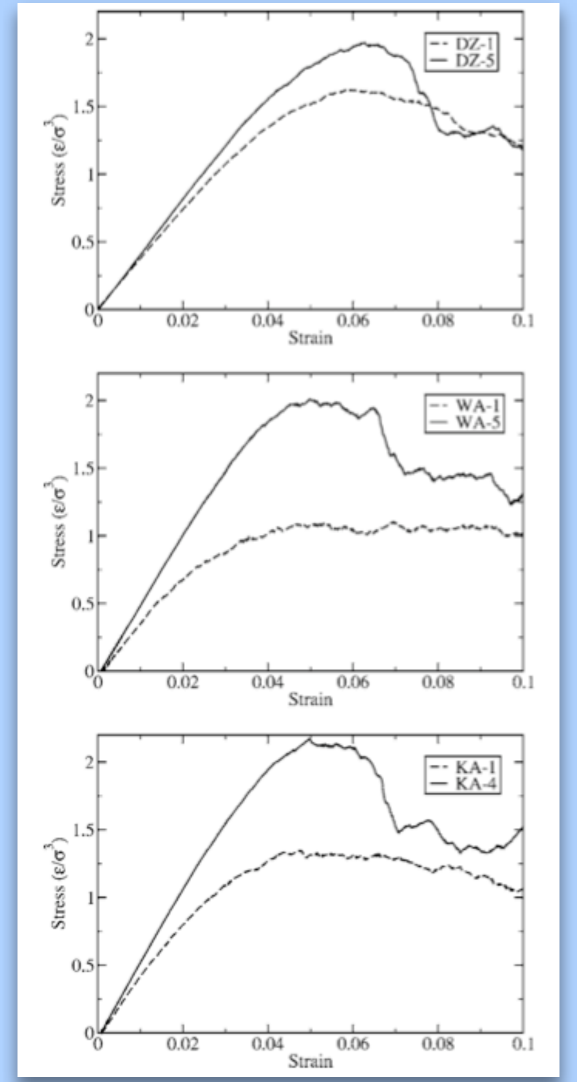


MLF and JS Langer, PRE, Vol. 57, pp. 7192-7205 (1998)



Yunfeng Shi and MLF, PRB 73, 214201 (2006)

Diverging Time Scale

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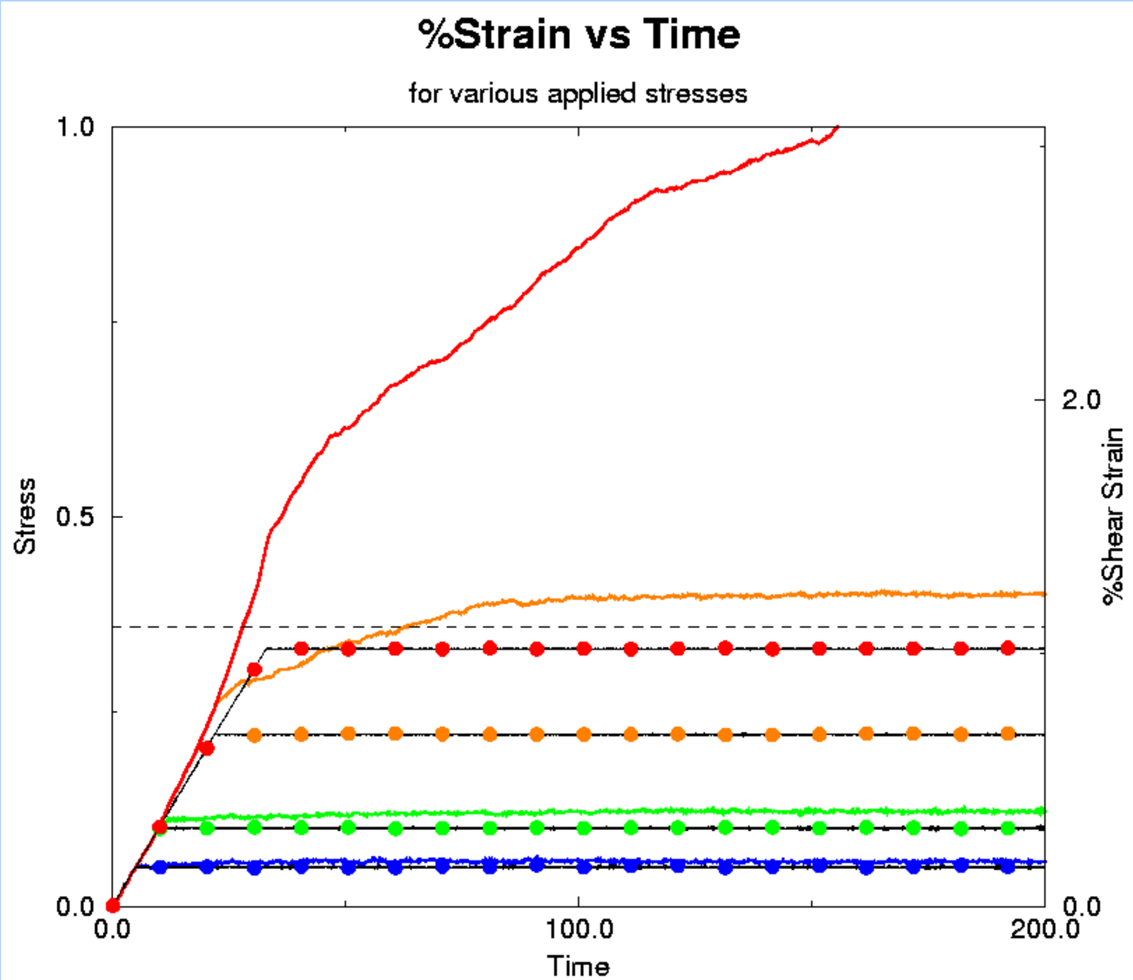

MLF and JS Langer, PRE, Vol. 57, pp. 7192-7205 (1998)

Anelasticity / Bauschinger Effect

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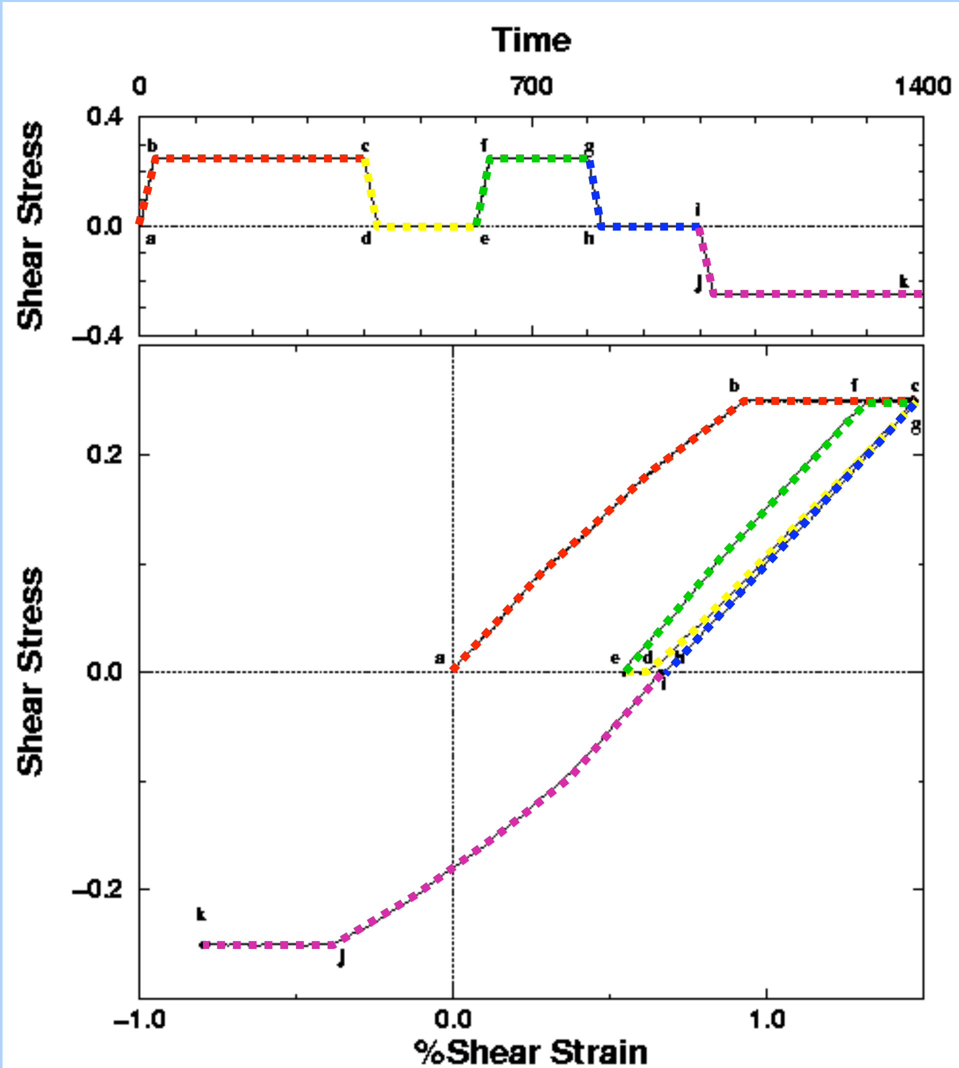

MLF and JS Langer, PRE, Vol. 57, pp. 7192-7205 (1998)

Shear Induced Anisotropy in Granular Media

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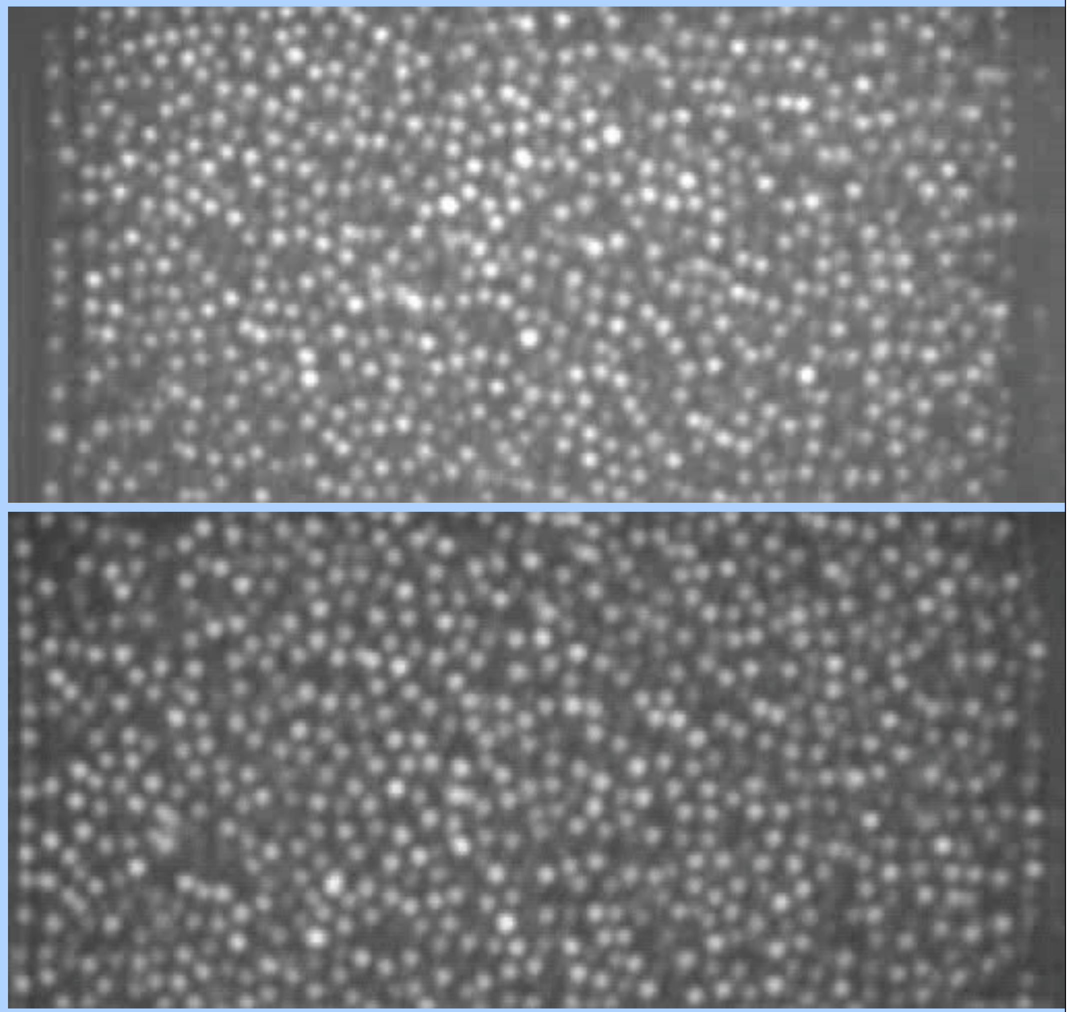
(experiments by W. Losert and M. Toyia)

- Taylor-Couette cell
- 102mm inner cylinder
- 44mm gap
- 1mm beads
  or 2mm beads
- Inner cylinder rotated 4-8 mm/s
- Top surface monitored with high speed camera
- Torque measured at inner cylinder



MLF, M. Toiya, W. Losert, arxiv:0802.1752 (2008)

STZ Picture

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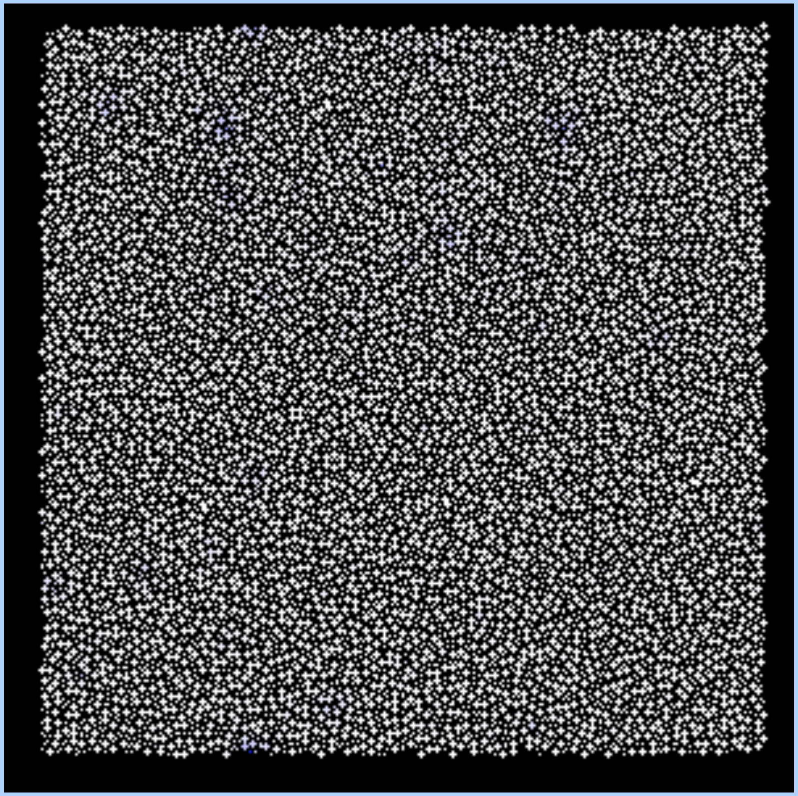

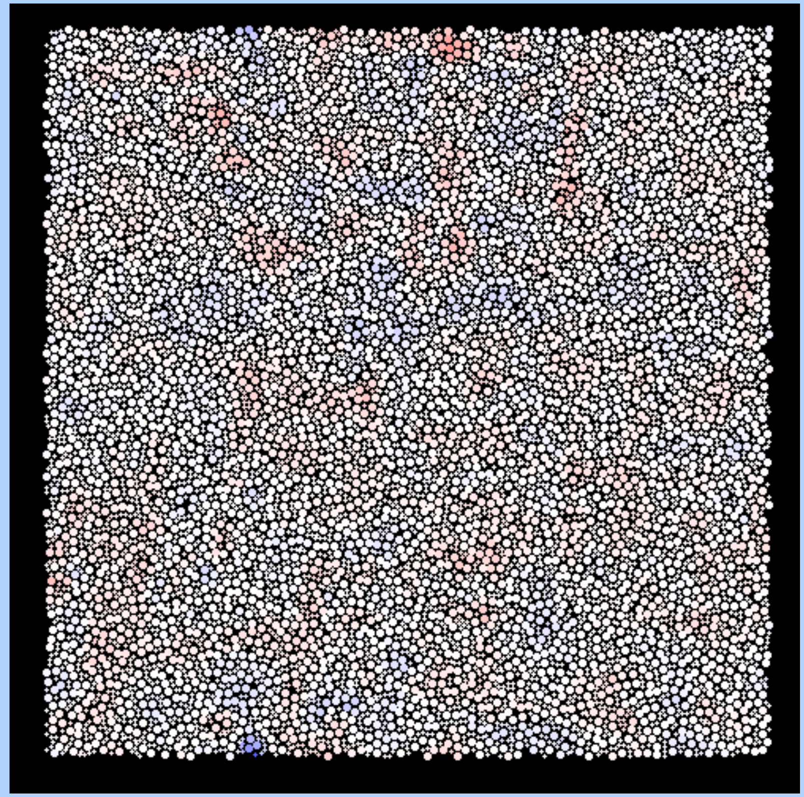

STZ Picture

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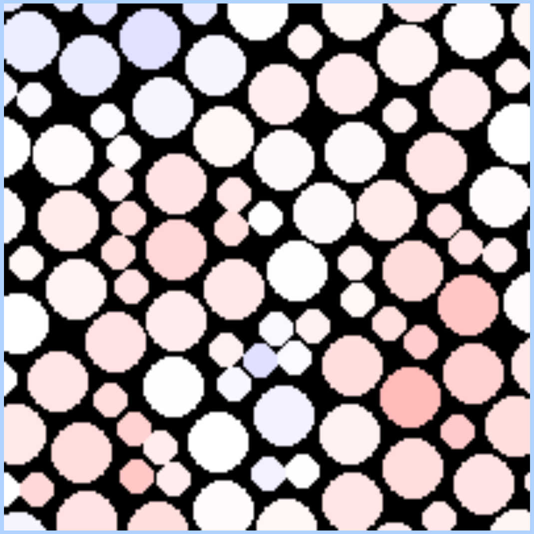

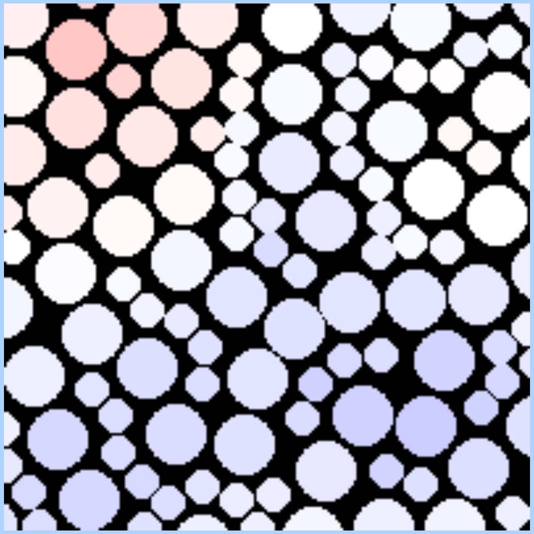

- STZs have a particular orientation. They are susceptible to shear to the extent that the shear is along this direction.
- STZs are reversible until their environment rearranges. They behave as 2-state systems.
- STZs are transient. They can be created and destroyed by neighboring plastic activity.

The STZ Model

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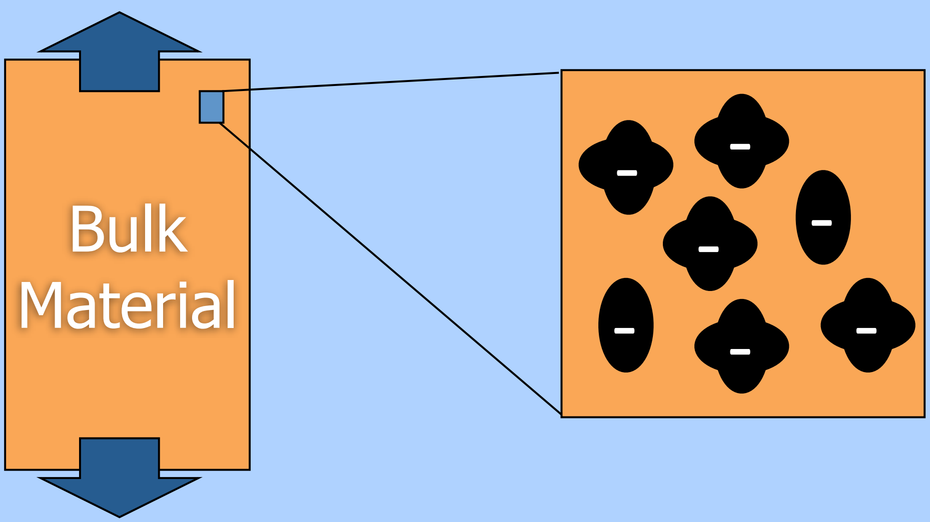
Plastic Strain Rate Proportional to Flips

$$\dot{\epsilon}^{pl} = \epsilon_0 \left[R_-(s)n_- - R_+(s)n_+\right]$$

Flip Rates

Shear Stress



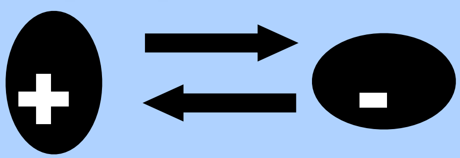
The STZ Model

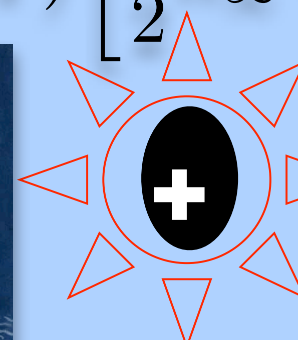
- **Plastic Strain Rate Proportional to Flips**

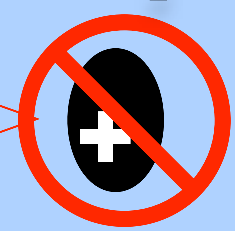
$$\dot{\epsilon}^{pl} = \epsilon_0 \left[R_-(s) n_- - R_+(s) n_+ \right]$$

- **Master Equation for Densities**

$$\dot{n}_\pm = R_\mp n_\mp - R_\pm n_\pm + \Gamma(s, n_\pm, T) \left[\frac{1}{2} n_\infty - n_\pm \right]$$







The STZ Model

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- **Plastic Strain Rate Proportional to Flips**

$$\dot{\epsilon}^{pl} = \epsilon_0 \left[R_-(s) n_- - R_+(s) n_+ \right]$$

- **Master Equation for Densities**

$$\dot{n}_+ = +R_- n_- - R_+ n_+ + \Gamma \left[\frac{1}{2} n_\infty - n_+ \right]$$

$$\dot{n}_- = -R_- n_- + R_+ n_+ + \Gamma \left[\frac{1}{2} n_\infty - n_- \right]$$

$$\Lambda = n_+ + n_- \qquad m = \frac{n_+ - n_-}{\Lambda}$$

The STZ Model

WHITING SCHOOL OF ENGINEERING
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- Plastic Strain Rate Proportional to Flips

$$\dot{\epsilon}^{pl} = \epsilon_0 \left[R_-(s) n_- - R_+(s) n_+ \right]$$

$$\dot{\epsilon}^{pl} = \epsilon_0 \Lambda \mathcal{C}(s) \left[\mathcal{T}(s) - m \right]$$

- Master Equation for Densities

$$\dot{n}_+ = +R_- n_- - R_+ n_+ + \Gamma \left[\frac{1}{2} n_\infty - n_+ \right]$$

$$\dot{n}_- = -R_- n_- + R_+ n_+ + \Gamma \left[\frac{1}{2} n_\infty - n_- \right]$$

$$\Lambda = n_+ + n_- \quad m = \frac{n_+ - n_-}{\Lambda}$$

$$\mathcal{C} \equiv \frac{R_- + R_+}{2}$$

$$\mathcal{T} \equiv \frac{R_- - R_+}{R_- + R_+}$$

The STZ Model

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- **Plastic Strain Rate Proportional to Flips**

$$\dot{\epsilon}^{pl} = \epsilon_0 \Lambda \mathcal{C}(s) \left[\mathcal{T}(s) - m \right]$$

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$$\dot{n}_+ = +R_- n_- - R_+ n_+ + \Gamma \left[\frac{1}{2} n_\infty - n_+ \right]$$

$$\dot{n}_- = -R_- n_- + R_+ n_+ + \Gamma \left[\frac{1}{2} n_\infty - n_- \right]$$

$$\dot{\Lambda} = \dot{n}_+ + \dot{n}_- = \Gamma [n_\infty - \Lambda]$$

The STZ Model

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- **Plastic Strain Rate Proportional to Flips**

$$\dot{\epsilon}^{pl} = \epsilon_0 \Lambda \mathcal{C}(s) \left[\mathcal{T}(s) - m \right]$$

- **Master Equation for Densities**

$$\dot{\Lambda} = \Gamma [n_\infty - \Lambda]$$

$$\dot{m} = \frac{2\dot{\epsilon}^{pl}}{\Lambda \epsilon_0} - m\Gamma$$

The STZ Model

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- **Plastic Strain Rate Proportional to Flips**

$$\dot{\epsilon}^{pl} = \epsilon_0 \Lambda \mathcal{C}(s)\left[\mathcal{T}(s) - m\right]$$

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$$\dot{\Lambda} = \Gamma[n_\infty - \Lambda] \qquad \dot{m} = \frac{2\dot{\epsilon}^{pl}}{\Lambda \epsilon_0} - m\Gamma$$

The n_∞ parameter is the ratio of annihilation to creation and sets the equilibrium defect density. This is identified with the "Effective Temperature" χ.

Langer (2004)

The STZ Model

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- **Plastic Strain Rate Proportional to Flips**

$$\dot{\epsilon}^{pl} = \epsilon_0 \Lambda \mathcal{C}(s) \left[\mathcal{T}(s) - m\right]$$

- **Master Equation for Densities**

$$\dot{\Lambda} = \Gamma[e^{-1/\chi} - \Lambda] \qquad \dot{m} = \frac{2\dot{\epsilon}^{pl}}{\Lambda \epsilon_0} - m\Gamma$$

The n_∞ parameter is the ratio of annihilation to creation and sets the equilibrium defect density. This is identified with the "Effective Temperature" χ.

Langer (2004)

The STZ Model

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- **Plastic Strain Rate Proportional to Flips**

$$\dot{\epsilon}^{pl} = \epsilon_0 e^{-1/\chi} \mathcal{C}(s) \left[\mathcal{T}(s) - m \right]$$

- **Master Equation for Densities**

$$\Lambda = e^{-1/\chi} \qquad \dot{m} = 2\mathcal{C}(s)[\mathcal{T}(s) - m] - m\Gamma$$

We can simplify by noting that Λ approaches $e^{-1/\chi}$ in steady state.

The STZ Model

- **Finding Γ**

$$\begin{aligned} \dot{\epsilon}^{pl} &= \epsilon_0 e^{-1/\chi} \mathcal{C}(s) \left[\mathcal{T}(s) - m \right] \\ \dot{m} &= 2\mathcal{C}(s)[\mathcal{T}(s) - m] - m\Gamma \end{aligned}$$

- **To satisfy 2nd law, need to ensure that energy is dissipated not created**

$$\begin{aligned} \Gamma &= \Gamma^T(T) + \Gamma^M(s, \chi, m) \\ s\,\dot{\epsilon}^{pl} &= \epsilon_0 e^{-1/\chi} \frac{d\psi(m)}{dt} + Q(s, \chi, m) \\ Q(s, \chi, m) &= \epsilon_0 e^{-1/\chi} \Gamma^M(s, \chi, m) \end{aligned}$$

The STZ Model

- **Finding Γ**

$$\begin{aligned}\dot{\epsilon}^{pl} &= \epsilon_0 e^{-1/\chi}\mathcal{C}(s)\left[\mathcal{T}(s) - m\right]\\ \dot{m} &= 2\mathcal{C}(s)[\mathcal{T}(s) - m] - m\Gamma\end{aligned}$$

- **Substitute our dynamical equations into the expression and solve for Γ^{M} self consistently**

$$\begin{aligned}\Gamma &= \Gamma^{T}(T) + \Gamma^{M}(s,\chi,m)\\ s\,\dot{\epsilon}^{pl} &= \epsilon_0 e^{-1/\chi}\frac{d\psi(m)}{dm}\dot{m} + Q(s,\chi,m)\\ Q(s,\chi,m) &= \epsilon_0 e^{-1/\chi}\Gamma^{M}(s,\chi,m)\end{aligned}$$

The STZ Model

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- **Finding Γ**

$$\begin{aligned} \dot{\epsilon}^{pl} &= \epsilon_0 e^{-1/\chi}\mathcal{C}(s)\left[\mathcal{T}(s) - m\right] \\ \dot{m} &= 2\mathcal{C}(s)[\mathcal{T}(s) - m] - m\Gamma \end{aligned}$$

- **Substitute our dynamical equations into the expression and solve for Γ^{M} self consistently**

$$\Gamma = \frac{\mathcal{C}(s)\left[s - \psi'(m)\right]\left[\mathcal{T}(s) - m\right] + \Gamma^{T}}{1 - m\psi'(m)}$$

- **To ensure that the numerator is positive we choose** $\psi'(m) = \xi(m) = \mathcal{T}^{-1}(m)$

The STZ Model

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- **Finding Γ**

$$\dot{\epsilon}^{pl} = \epsilon_0 e^{-1/\chi} \mathcal{C}(s) \left[\mathcal{T}(s) - m\right]$$
$$\dot{m} = 2\mathcal{C}(s)[\mathcal{T}(s) - m] - m\Gamma$$

- **Substitute our dynamical equations into the expression and solve for Γ self consistently**

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- **To ensure that the numerator is positive we choose** $\psi'(m) = \xi(m) = \mathcal{T}^{-1}(m)$

Dynamic Jamming Transition (T=0)

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$$\dot{\epsilon}^{pl} = \epsilon_0 e^{-1/\chi} \mathcal{C}(s) \left[\mathcal{T}(s) - m\right]$$

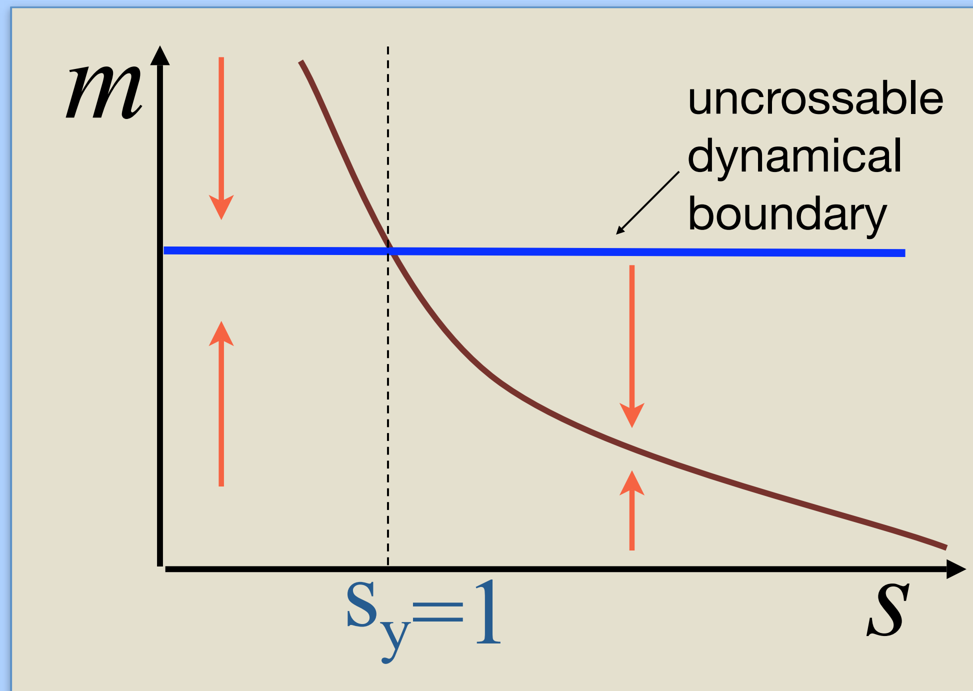
$$\dot{m} = 2\mathcal{C}(s)[\mathcal{T}(s) - m][1 - s\, m]$$

In this limit

$$\Gamma = s\dot{\epsilon}^{pl}$$

Also Assume

$$\mathcal{T}(s) = \text{sign}(s)$$



Rate Constants R_+ and R_-

- The least well-established part of the model are the stress dependences of R_+ and R_-
- For **high T** the Eyring forms make sense

$$R_{\pm}(s) = \nu\, exp\left(-\frac{\Delta G \pm s\Omega}{k_B T}\right)$$

$$\mathcal{C}(s) = \nu\, e^{\frac{-\Delta G}{k_B T}}\, cosh\left(\frac{s\Omega}{k_B T}\right)$$

$$\mathcal{T}(s) = tanh\left(\frac{s\Omega}{k_B T}\right)$$

Rate Constants R_+ and R_-

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- The least well-established part of the model are the stress dependences of R_+ and R_-
- For near zero T we do not expect STZ flips under reverse loading

$$R_\pm(s) = f(\pm s)\Theta(s)$$

$$\mathcal{T}(s) = \mathrm{sign}(s)$$

- $\mathcal{C}$ is some symmetric function of s

Diverging Time Scale

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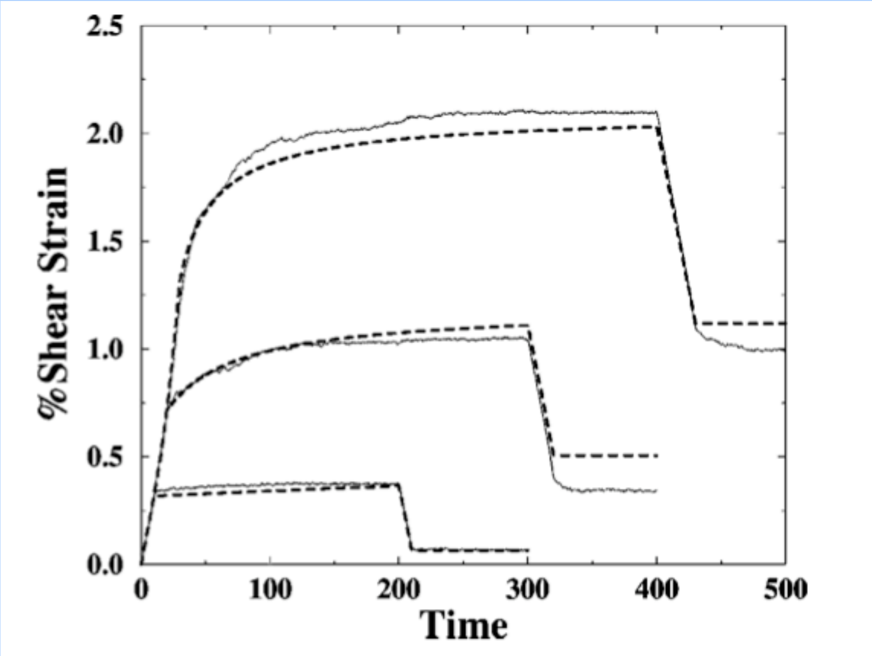
- The equations can be solved analytically at constant s and a diverging time scale emerges.



$$m = \frac{1 - e^{-t/\tau}}{1 - s\, e^{-t/\tau}}$$

$$\tau \equiv \frac{1}{2\mathcal{C}(s)(1-s)}$$

MLF and JS Langer, PRE, Vol. 57, pp. 7192-7205 (1998)

Anelasticity / Bauschinger Effect

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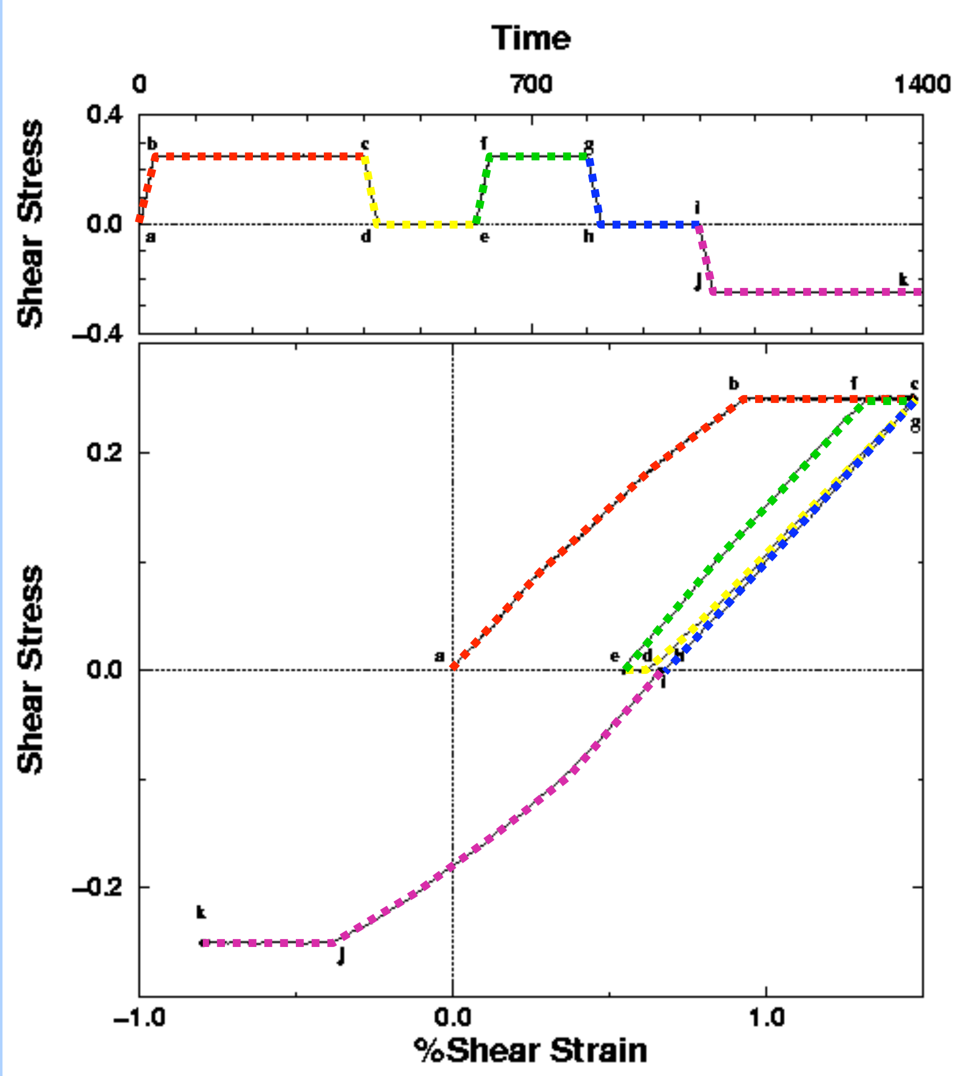
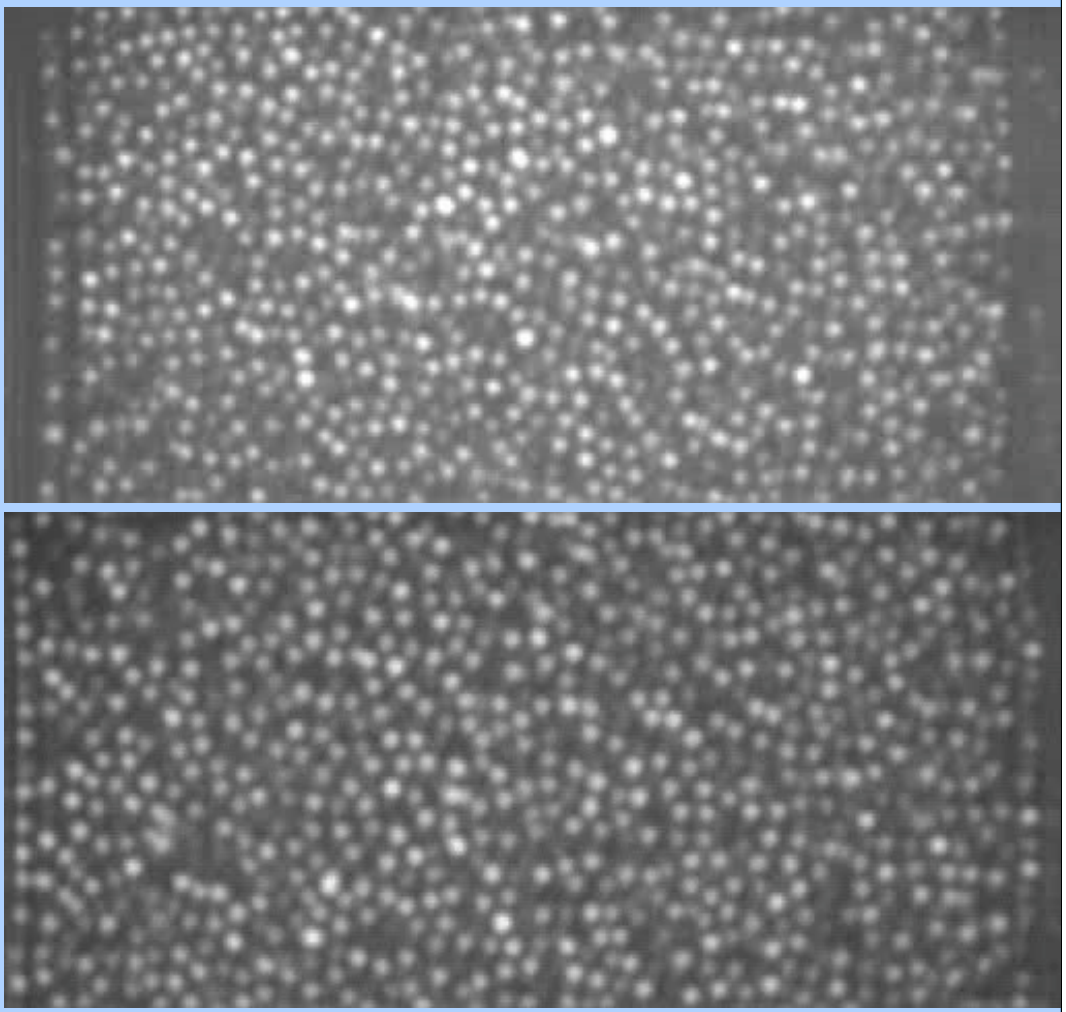


MLF and JS Langer, PRE, Vol. 57, pp. 7192-7205 (1998)

Shear Induced Anisotropy in Granular Media

(experiments by W. Losert and M. Toyia)

- Taylor-Couette cell
- 102mm inner cylinder
- 44mm gap
- 1mm beads
  or 2mm beads
- Inner cylinder rotated 4-8 mm/s
- Top surface monitored with high speed camera
- Torque measured at inner cylinder



MLF, M. Toiya, W. Losert, arxiv:0802.1752 (2008)

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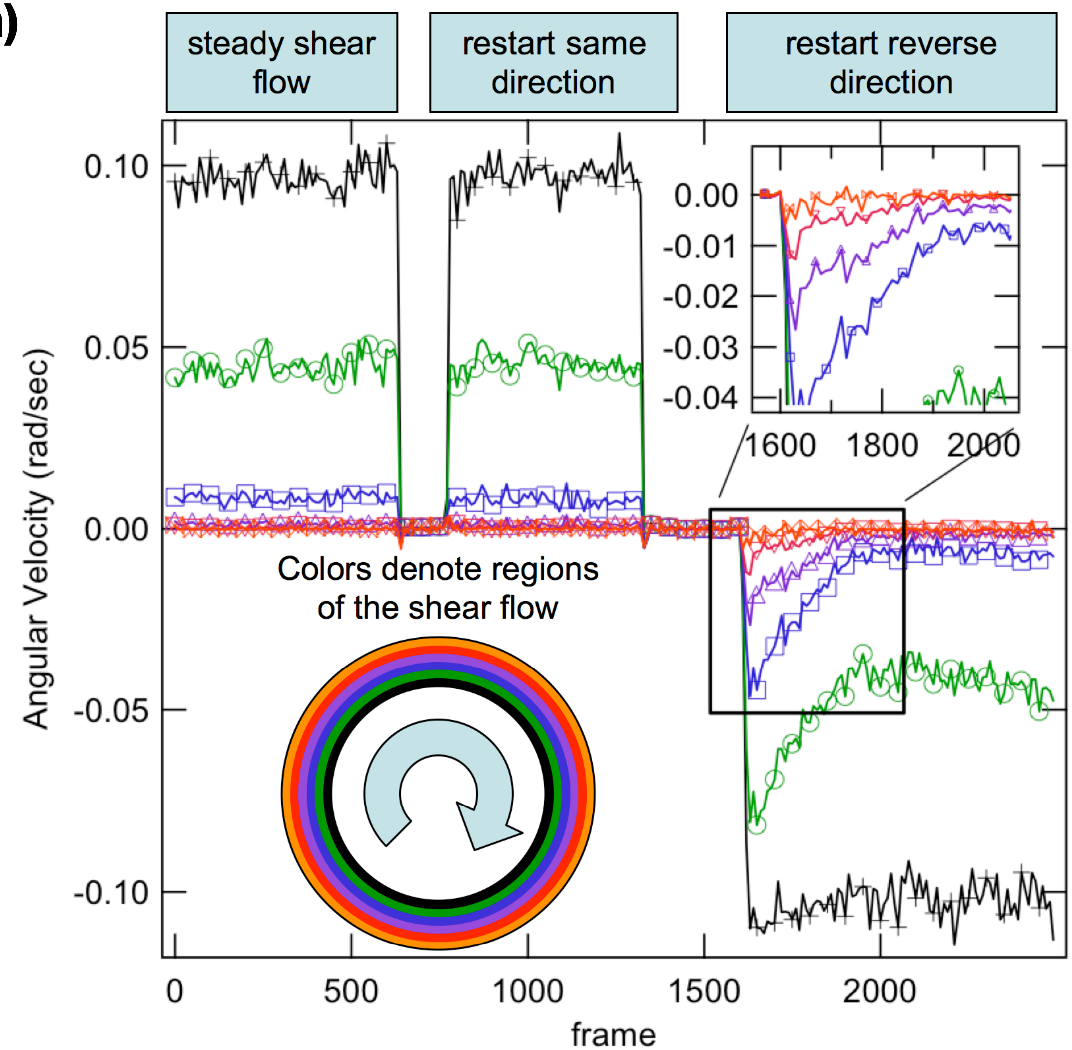

MLF, M. Toiya, W. Losert, arxiv:0802.1752 (2008)

STZ Model: Transient granular flow

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- No internal time scale, requires everything to be slaved to the motion of the inner cylinder. So a' denotes da/dΘ, where Θ is the angle of the inner cylinder.
- The stress is inhomogeneous $\sigma_{r\theta}(r)$.
- We can assume that through cyclic loading the dilational degrees of freedom, described by χ, are in steady state.
- However, during the transient following reversal the orientational degrees of freedom, described by m, are not.

$$\varepsilon'_{r\theta}\left(s_{r\theta},m_{r\theta}\right)=e^{-1/\chi_\infty}f\left(s_{r\theta},m_{r\theta}\right)=\gamma\varepsilon_0 C\left(\frac{s_{r\theta}}{s_y}\right)\left[\mathrm{sign}\left(s_{r\theta}\right)-m\right]\mathrm{sign}\left(\frac{d\Theta}{dt}\right)$$

$$m'\left(\tilde{s},m\right)=\frac{\varepsilon'_{r\theta}\left(s_{r\theta},m\right)}{\varepsilon_0}\left(1-\frac{s_{r\theta}m}{s_y}\right)$$

MLF, M. Toiya, W. Losert, arxiv:0802.1752 (2008)

STZ Model: Transient granular flow

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$$\varepsilon'_{r\theta}\left(s_{r\theta},m_{r\theta}\right)=e^{-1/\chi_\infty}f\left(s_{r\theta},m_{r\theta}\right)=\gamma\varepsilon_0 C\left(\frac{s_{r\theta}}{s_y}\right)\left[\operatorname{sign}\left(s_{r\theta}\right)-m\right]\operatorname{sign}\left(\frac{d\Theta}{dt}\right)$$

$$m'\left(\tilde{s},m\right)=\frac{\varepsilon'_{r\theta}\left(s_{r\theta},m\right)}{\varepsilon_0}\left(1-\frac{s_{r\theta}m}{s_y}\right)$$

- **We must also define the function C**
  Bouchbinder, Procaccia and Langer, PRE 75, 036107 (2007)

$$C\left(\tilde{s};\zeta\right)=\frac{\left|\tilde{s}\right|^{\zeta+1}}{\sqrt{2\pi\zeta}}\exp\left[-\zeta\left(\left|\tilde{s}\right|-1\right)\right]+\left(\left|\tilde{s}\right|-1-\zeta^{-1}\right)P\left(\zeta+1,\zeta\left|\tilde{s}\right|\right)$$

- **Now 4 parameters must be specified**
  - The radius, r_y, at which $s=s_y$.
    (116mm for 1mm beads, 127mm for 2mm beads)
  - The stress distribution of the STZs, ζ. (100)
  - The strain per STZ, ε_0. (4% for 1mm beads, 0.5% for 2mm beads)
  - γ, the attempt frequency per rate of rotation of the inner cylinder, $d\Theta/dt$. (18000)

MLF, M. Toiya, W. Losert, arxiv:0802.1752 (2008)

Comparison to Experimental Data

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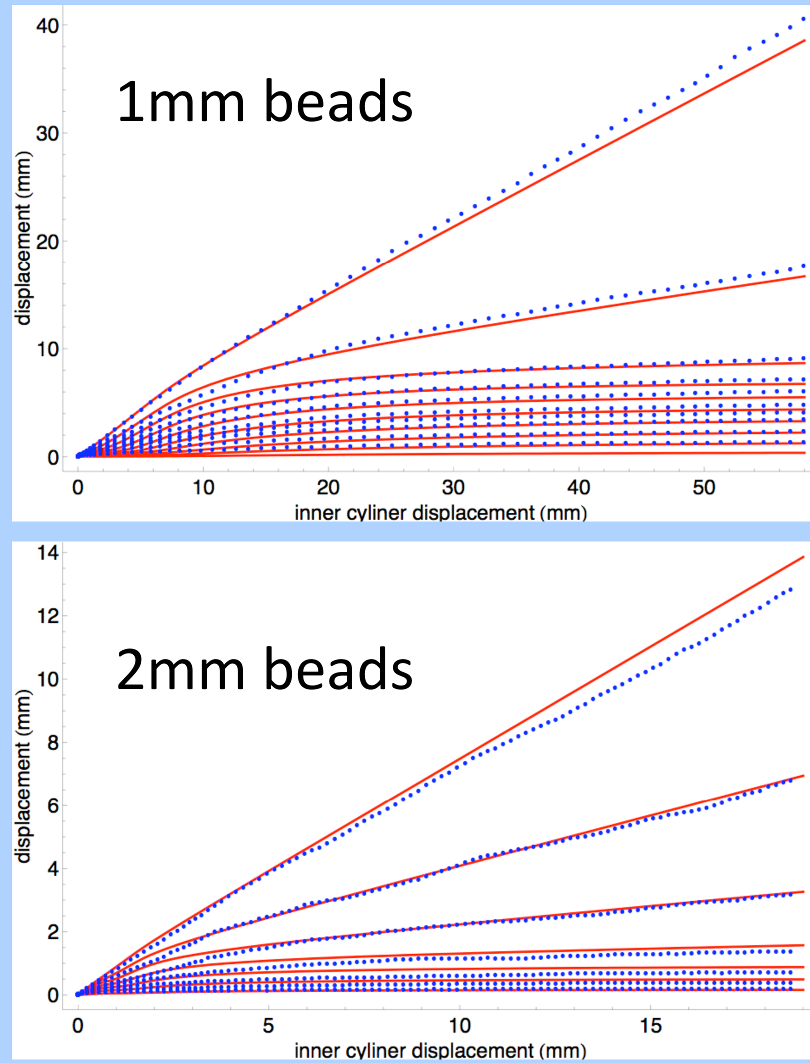
- The blue dots represent experimental measurements of displacement at a specified radial position, plotted as a function of the inner cylinder displacement subsequent to shear reversal.

- The red lines are the STZ predictions given the assumptions on the previous slides.



MLF, M. Toiya, W. Losert, arxiv:0802.1752 (2008)

Stress vs. Time (blue=data, red=theory)

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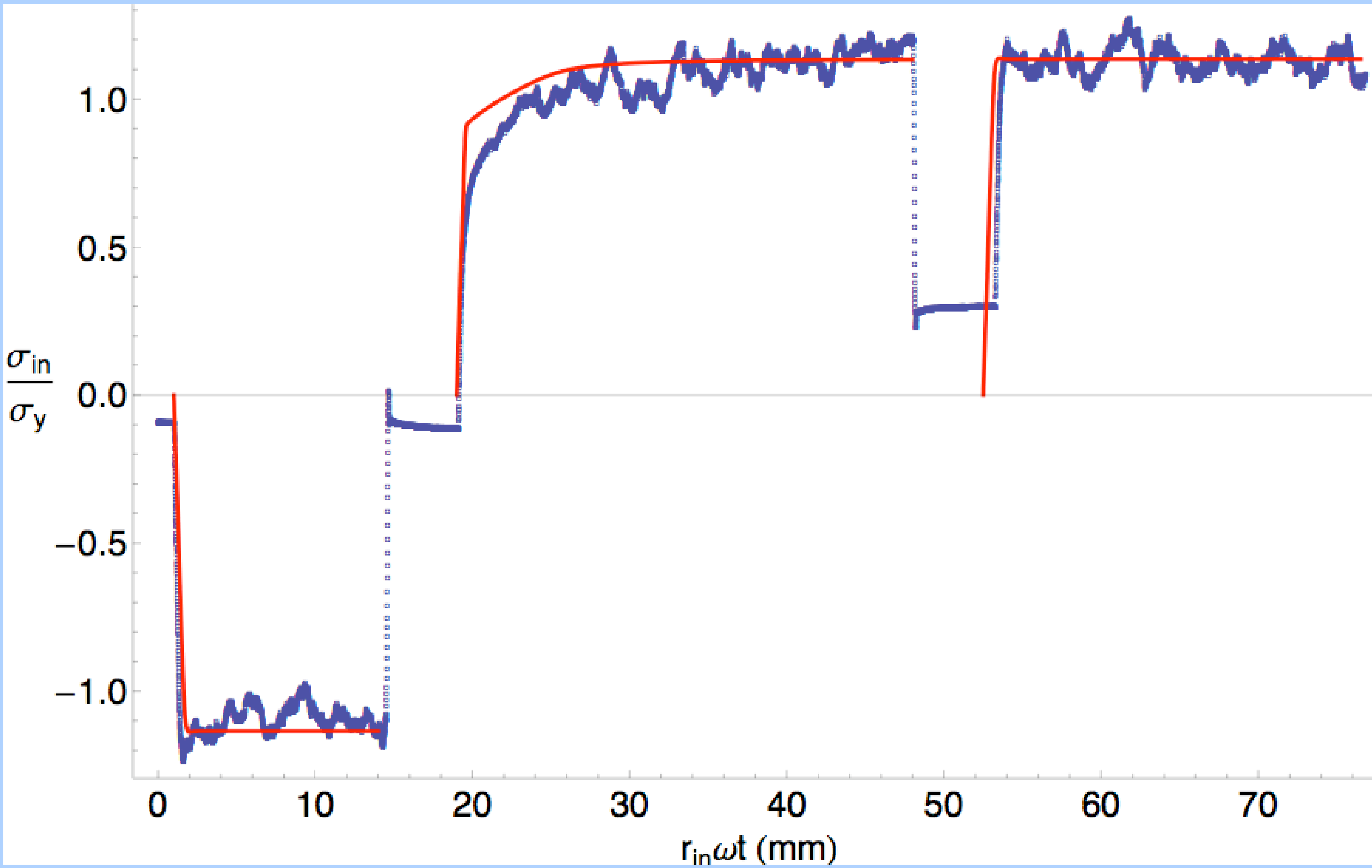
NB: time is multiplied by displacement rate of inner cylinder



MLF, M. Toiya, W. Losert, arxiv:0802.1752 (2008)

STZ Comparison to Shear of a-Si

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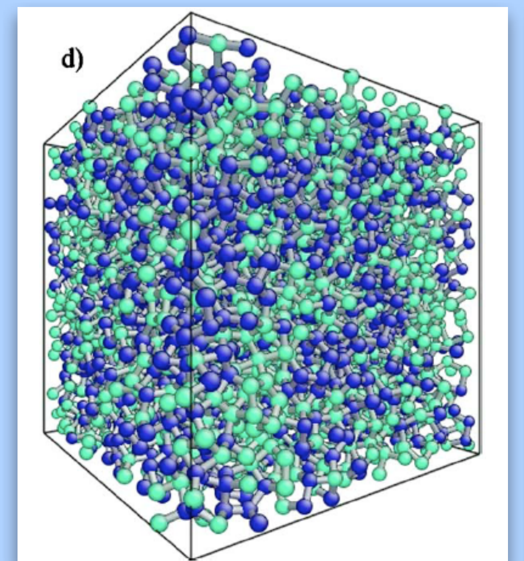

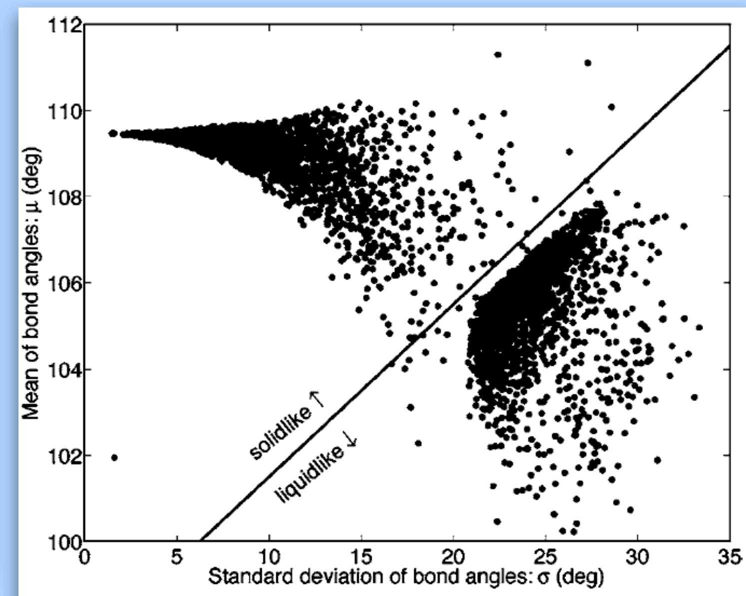

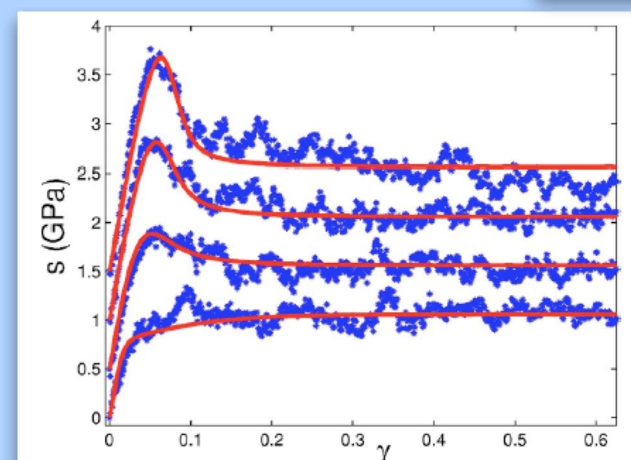

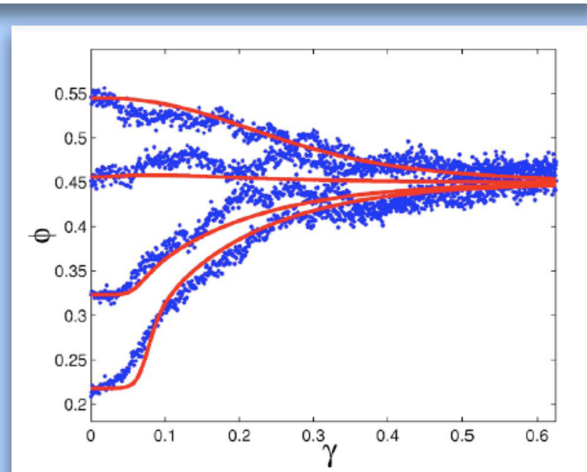

Amorphous Silicon forms 5-fold coordinated liquid-like regions that facilitate shear.

Requires χ dynamics

Demkowicz and Argon, PRB 72, 245205 (2005).

Bouchbinder, Langer and Procaccia, PRE 75, 036108 (2007).

Summing Up

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- **We need constitutive theories of plastic response in order to predict mechanical response past the elastic regime.**
- **Most engineering mechanics based theories are not based on specific micromechanisms, which prevents direct connection to the underlying physics**
- **Shear Transformation Zone Theory is an attempt to build a phenomenological theory with such a connection.**
- **The theory exhibits the following behaviors that are seen in simualtion and experiment**
  - A range of behavior from perfectly plastic to shear softening
  - Plastic hysteresis (Bauschinger effects)
  - Existence of a dynamically emerging yield stress
  - Diverging timescale for deformation near the yield stress
- **The million dollar question: Are STZ's real? Do local 2 state systems exist in some sense and control deformation?**

End of Lecture 1

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