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A Thermodynamic Formulation of the STZ Theory of Deformation in Amorphous Solids

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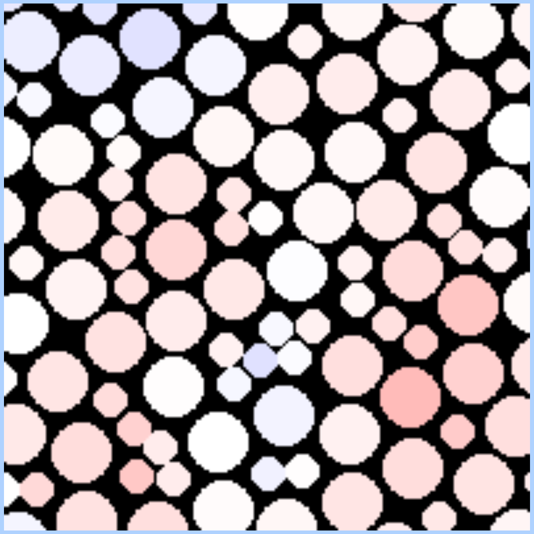

Thermodynamics and STZs

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- **Briefly review the shear transformation zone theory of amorphous plasticity.**
- **Apply the non-equilibrium thermodynamics framework just presented to an STZ system in order to**
  - Constrain the theory
  - Relate the microscopic degrees of freedom the relevant "effective temperature" associated with these degrees of freedom
- **See Falk, Langer, Annual Reviews of Condensed Matter Physics (in press) arXiv:1004.4684**

Micro-mechanical Observations 1

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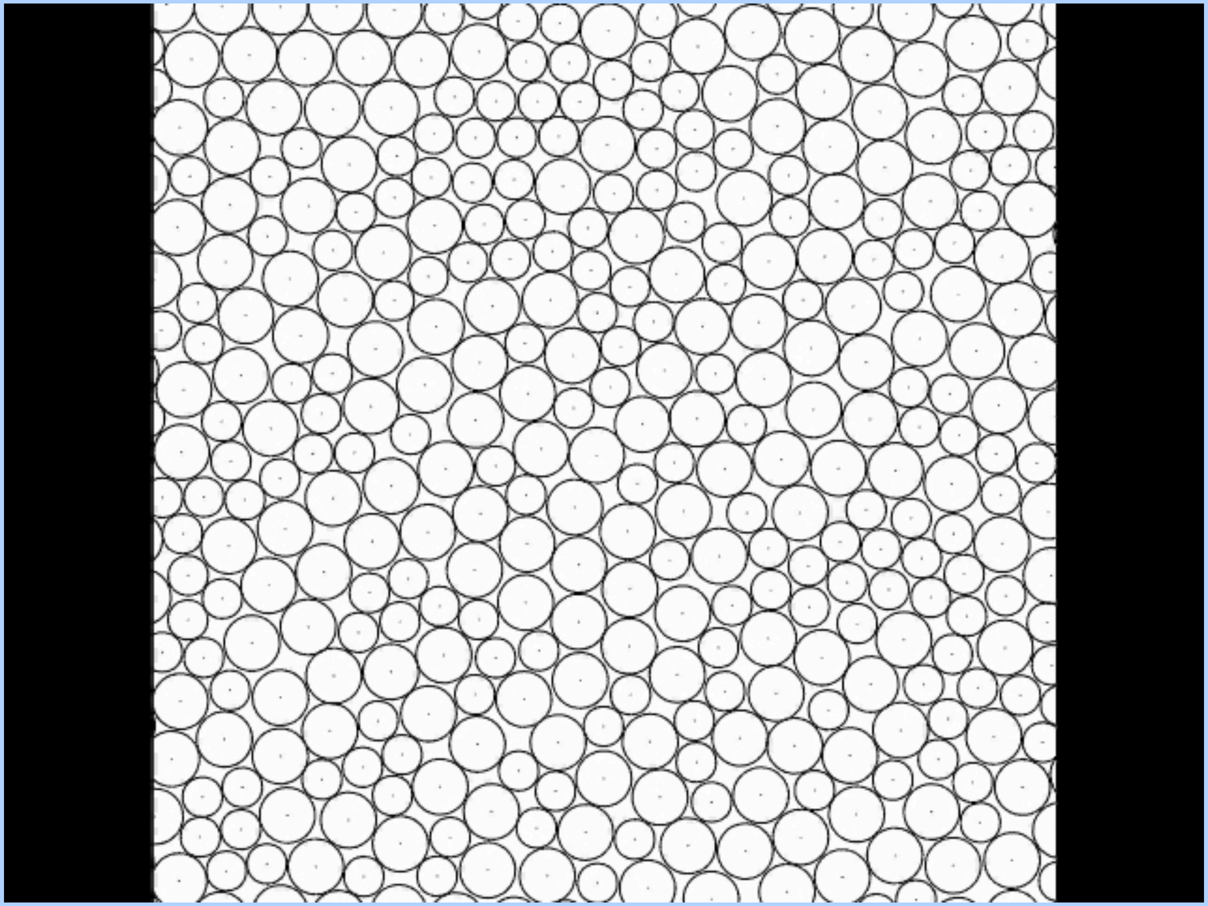
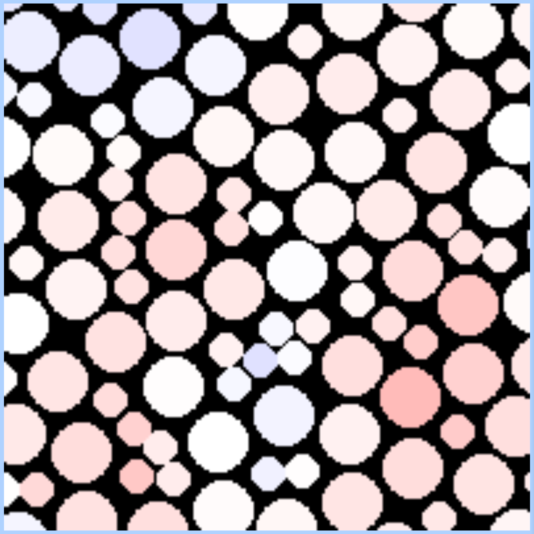
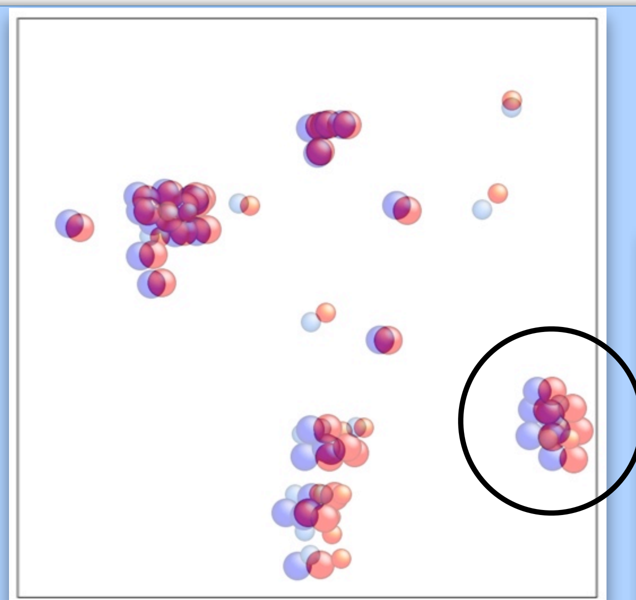


Simulation by T.K. Haxton and A.J. Liu, PRL 99, 195701 (2007)

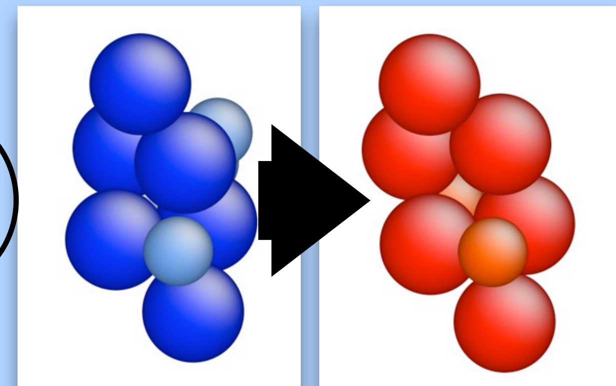
Shear Transformation Zones



Falk, Langer, PRE (1998)



Falk, Maloney, EPJB (2010)



Postulates:

- 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.

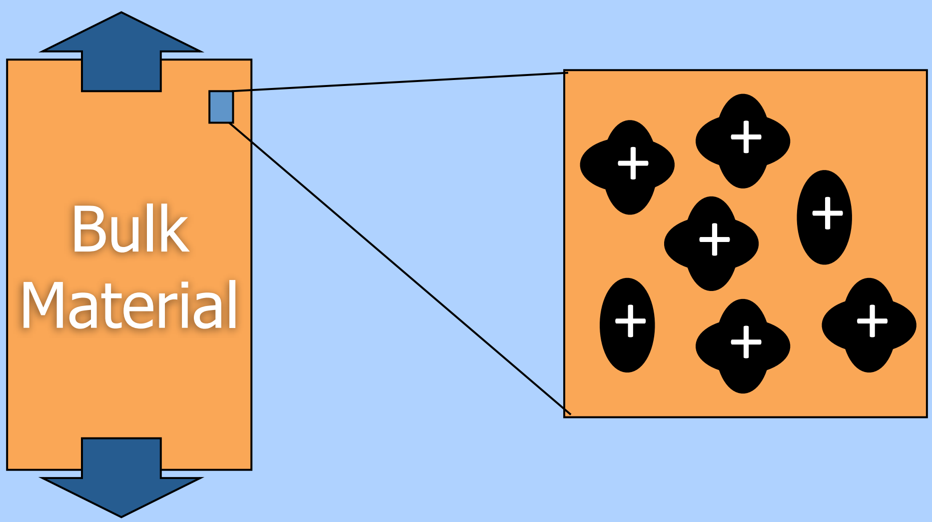
Deformation by STZs

Next consider the shear response by assuming plastic strain rate to be proportional to STZ Flips

$$\dot{\epsilon}^{pl} = v_0[R(s)n_- - R(-s)n_+]$$

Flip Rates

Shear Stress



Deformation by STZs

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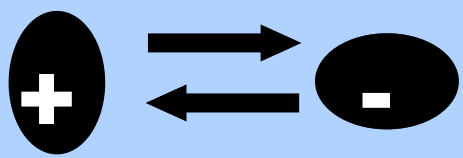
- **Plastic Strain Rate Proportional to Flips**

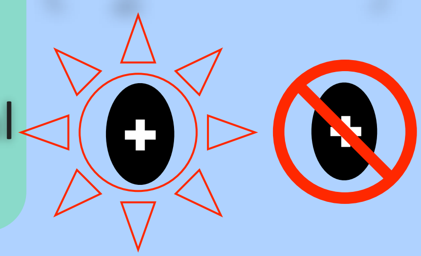
$$\dot{\epsilon}^{pl} = v_0[R(s)n_- - R(-s)n_+]$$

- **Master Equation for Densities**

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



Rate of Mechanical Mixing



Re-expressing the Master Eq

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- **Plastic Strain Rate Proportional to Flips**

$$\dot{\epsilon}^{pl} = v_0[R(s)n_- - R(-s)n_+]$$

- **Master Equation for Densities**

$$\dot{n}_+ = +R(s)\,n_- - R(-s)\,n_+ + \Gamma\left[\frac{n_{eq}}{2} - n_+\right]$$
$$\dot{n}_- = -R(s)\,n_- + R(-s)\,n_+ + \Gamma\left[\frac{n_{eq}}{2} - n_-\right]$$

$$\Lambda = \frac{n_+ + n_-}{(N/V)} \qquad m = \frac{n_+ - n_-}{n_+ + n_-}$$

In a full tensorial model Λ would be a scalar, but $\boldsymbol{m}$ would be a tensor $\boldsymbol{m}_{ij}$ that describes the second moment of the STZ orientational distribution.

Re-expressing the Master Eq

- **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**

$$\dot{\Lambda} = \dot{n}_+ + \dot{n}_- = \Gamma(s, \Lambda, m) [\Lambda_{eq} - \Lambda]$$

$$\dot{m} = 2\mathcal{C}(s) \left[\mathcal{T}(s) - m \right] - \Gamma(s, \Lambda, m) \frac{\Lambda_{eq}}{\Lambda} m$$

- **need to come up with way to obtain Λ_{eq} and Γ**
- **original guess for Γ was $s\, \dot{\epsilon}^{pl}$**

Thermodynamics of a Deforming System

Bouchbinder, Langer PRE, 80 031131,031132 (2009)

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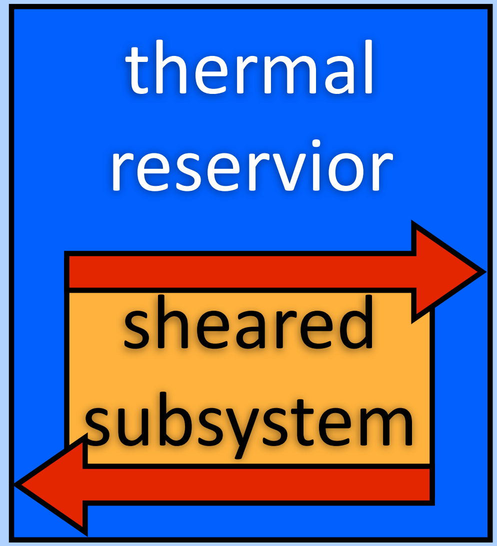
- Consider a thermally isolated system consisting of a deforming subsystem with energy U_C and entropy S_C in contact with a thermal reservoir of energy U_R and entropy S_R.



- Define

$$\chi \equiv \left(\frac{\partial U_C}{\partial S_C}\right)_{\sigma,\{\Lambda\}} \neq \theta \equiv \left(\frac{\partial U_R}{\partial S_R}\right)$$

- And $U^{tot} = U_C\left(S_C, s, \{\Lambda\}\right) + U_R(S_R)$

$\{\Lambda\}$ represents all the internal state variables needed to describe the subsystem.

- By 1st Law $2\,V\,s\,\dot{\epsilon}^{tot} = \dot{U}^{tot}$

The First Law of Thermodynamics

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$$2\,V\,s\,\dot{\epsilon}^{tot} = \dot{U}^{tot}$$

$$2\,V\,s\left(\dot{\epsilon^{el}} + \dot{\epsilon^{pl}}\right) = \dot{U^{tot}} = \left(\frac{\partial U_C}{\partial \epsilon^{el}}\right)\dot{\epsilon^{el}} + \ldots$$

- If $2\,V\,s = \left(\partial U_C / \partial \epsilon^{el}\right)$ then elastic terms cancel and we find

$$2\,V\,s\,\dot{\epsilon}^{pl} = \chi \dot{S}_C + \sum_\alpha \left(\frac{\partial U_C}{\partial \Lambda_\alpha}\right)_{S_C} \dot{\Lambda}_\alpha + \theta \dot{S}_R$$

How to Apply the Second Law?

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- **Clausius-Duhem Inequality states** $\dot{S} \geq 0$
- **Coleman-Noll (1963)**
  - Axiomatic approach takes the Clausius-Duhem statement to be the definition of entropy and temperature.
  - We can apply this to a system with two temperatures.
- **See Bouchbinder, Langer (2009) for details.**

Enforcing the Second Law

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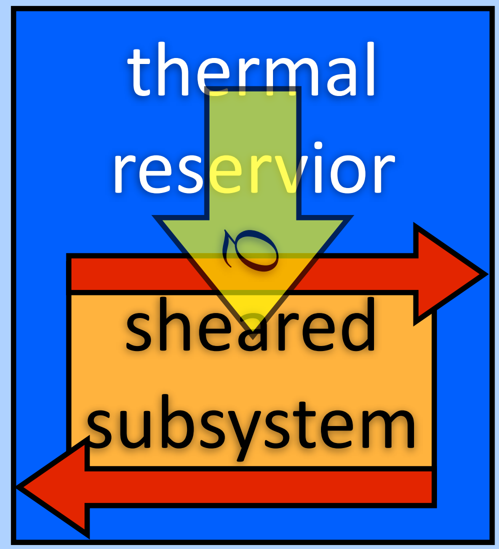
- **This leaves us with the requirement that the work done exceeds the amount of energy stored in internal degrees of freedom.**

$$\mathcal{W}(s,\{\Lambda\}) \equiv 2\,V\,s\,\dot{\epsilon}^{pl} - \sum_{\alpha} \left(\frac{\partial U_C}{\partial \Lambda_\alpha}\right)_{S_C} \dot{\Lambda}_\alpha \geq 0$$

- **And the first law becomes**

$$\chi \dot{S}_C = \mathcal{W}(s,\{\Lambda\}) + Q$$



but this is simply energy conservation, and when we define the specific heat as
$V\,c_{eff} \approx \chi(\partial S_C/\partial \chi)$
the first law reduces to

$$V\,c_{eff}\,\dot{\chi} = \mathcal{W}(s,\{\Lambda\}) + Q$$

Constraining Λ_{eq} and Γ

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- We can write down an expression for configurational entropy

$$S_C = N\Lambda - N\Lambda \ln \Lambda + N\Lambda\psi(m) + S_1(U_1)$$

- and the configurational energy

$$U_C = N\Lambda\, e_Z + U_1(S_1)$$

- from these and the equations of motion we derive an expression for the rate of plastic work

$$\mathcal{W}(s, \{\Lambda\}) \equiv 2\, V\, s\, \dot{\epsilon}^{pl} - \sum_{\alpha} \left(\frac{\partial U_C}{\partial \Lambda_\alpha} \right)_{S_C} \dot{\Lambda}_\alpha \geq 0$$

Constraining Λ_{eq} and Γ

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$$\frac{\mathcal{W}}{V} = 2\Lambda\mathcal{C}(s)[\mathcal{T}(s) - m]\left[sv_0 + \chi\frac{\partial\psi}{\partial m}\right] - \left[e_z + \chi\ln\Lambda - \chi\psi(m) + \chi m\frac{\partial\psi}{\partial m}\right]\dot{\Lambda} - \Gamma\chi\Lambda m\frac{\partial\psi}{\partial m} \geq 0$$

- **We can assure the work is non-negative if each term is non-negative.**

ψ **must be an even function peaked at 0**

Constraining Λ_{eq} and Γ

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$$\frac{\mathcal{W}}{V} = 2\Lambda\mathcal{C}(s)[\mathcal{T}(s) - m]\left[sv_0 + \chi\frac{\partial\psi}{\partial m}\right]$$

$$-\left[e_z + \chi\ln\Lambda - \chi\psi(m) + \chi m\frac{\partial\psi}{\partial m}\right]\dot{\Lambda}$$

$$-\Gamma\chi\Lambda m\frac{\partial\psi}{\partial m} \geq 0$$

Basic Form:

$$-\frac{\partial F_Z}{\partial\Lambda}\dot{\Lambda}$$

- **The second term will be even if the term in brackets goes to zero at $\Lambda = \Lambda_{eq}$ implying**

$$\Lambda_{eq} = \nu(m)\exp(-e_z/\chi)$$

$$\nu(m) = \exp\left[\psi(m) - m\frac{\partial\psi}{\partial m}\right]$$

Constraining Λ_{eq} and Γ

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$$\frac{\mathcal{W}}{V} = 2\,\Lambda\,\mathcal{C}(s)[\mathcal{T}(s) - m]\left[sv_0 + \chi\frac{\partial\psi}{\partial m}\right]$$
$$-\left[e_z + \chi\ln\Lambda - \chi\psi(m) + \chi m\frac{\partial\psi}{\partial m}\right]\dot{\Lambda}$$
$$-\Gamma\chi\Lambda m\frac{\partial\psi}{\partial m} \geq 0$$

- **Similarly the first term will be even if the unknown term goes to zero when $\mathcal{T}(s) = m$**

$$\frac{\partial\psi}{\partial m} = -\frac{v_0}{\chi}\xi(m) \qquad \mathcal{T}[\xi(m)] = m$$

"Athermal" Limit

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- We will discuss the theory in the "athermal" limit; when annealing (aging) is negligible on the time scale of the experiment.
- In this limit there is only one relevant physical rate, the rate of plastic dissipation, which must be positive definite.
- The heat flow out of the system must also be proportional to the rate of plastic work, and we can write an equation for the evolution of χ.
- If we also assume we are in the low strain rate limit, there must be a well defined lower bound for χ_{ss}, more than likely this value $\chi_0 = k_B T_g$.

$$c_{eff}\dot{\chi} \propto \mathcal{W} \times \left[1 - \frac{\chi}{\chi_0}\right]$$

- The rate of mixing must also be proportional to the rate of work per STZ

$$\frac{\mathcal{W}}{V} = 2\,\Lambda\,\mathcal{C}(s)[\mathcal{T}(s) - m]s v_0 = \Gamma\,\Lambda\,v_0\,s_0$$

STZ Equations of Motion

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

$$\dot{m} = 2\mathcal{C}(s)[\mathrm{sign}(s) - m]\left(1 - \frac{s\,m}{s_0}\right)$$

$$\dot{\Lambda} = \frac{2\mathcal{C}(s)\,s}{s_0}[\mathrm{sign}(s) - m][\Lambda - e^{\psi(0) - ez/\chi}]$$

$$\dot{\chi} = \frac{2\,s}{c_{eff}}\epsilon_0 \Lambda \mathcal{C}(s)[\mathrm{sign}(s) - m]\left[1 - \frac{\chi}{\chi_0}\right]$$

Yield in the "Athermal" Limit

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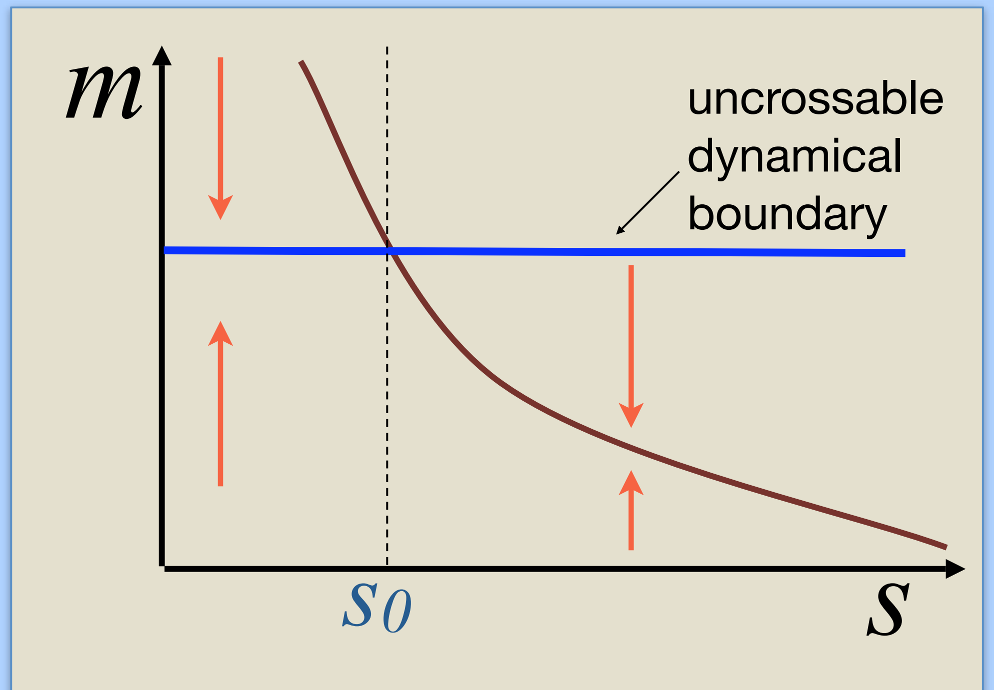
$$\dot{\epsilon}^{pl} = \epsilon_0 \nu(0) e^{-ez/\chi} \mathcal{C}(s)[\mathrm{sign}(s) - m]$$

$$\dot{m} = 2\mathcal{C}(s)[\mathrm{sign}(s) - m]\left(1 - \frac{s\,m}{s_0}\right)$$



Development of a Shear Band

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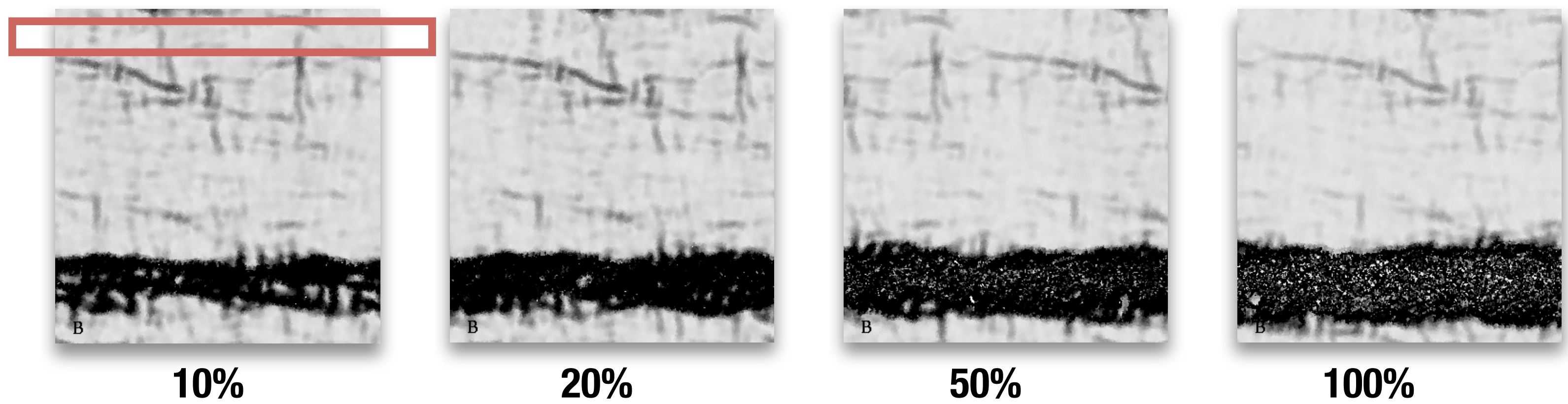

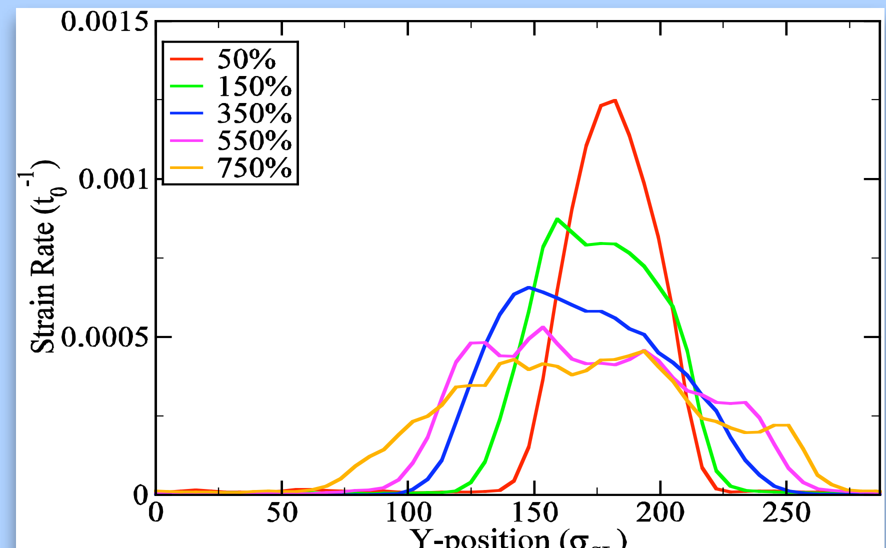

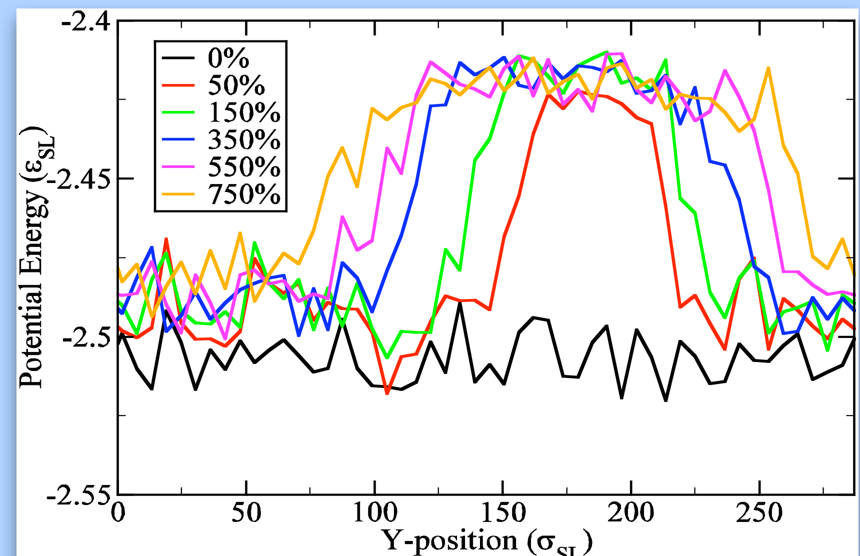

Y Shi, MB Katz, H Li, MLF, PRL, 98, 185505 (2007)

Relating χ to the microstructure

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- Consider a linear relation between the χ parameter and the local internal energy

$$C_1\,\chi = U - U_0$$

$$\dot{\epsilon}^{pl} = \exp(-e_Z/\chi)\,f(s)$$

- Is there an underlying scaling?

$$\frac{\dot{\epsilon}^{pl}(y)}{\dot{\epsilon}_b} = \exp\left(\frac{e_Z}{\chi_b} - \frac{e_Z}{\chi(y)}\right)$$

$$\ln\left(\frac{\dot{\epsilon}^{pl}(y)}{\dot{\epsilon}_b}\right) = \frac{e_Z}{\chi_0(\dot{\epsilon}^{pl})} - \frac{C_1\,e_Z}{U(y) - U_0}$$

Scaling verifies the hypothesis

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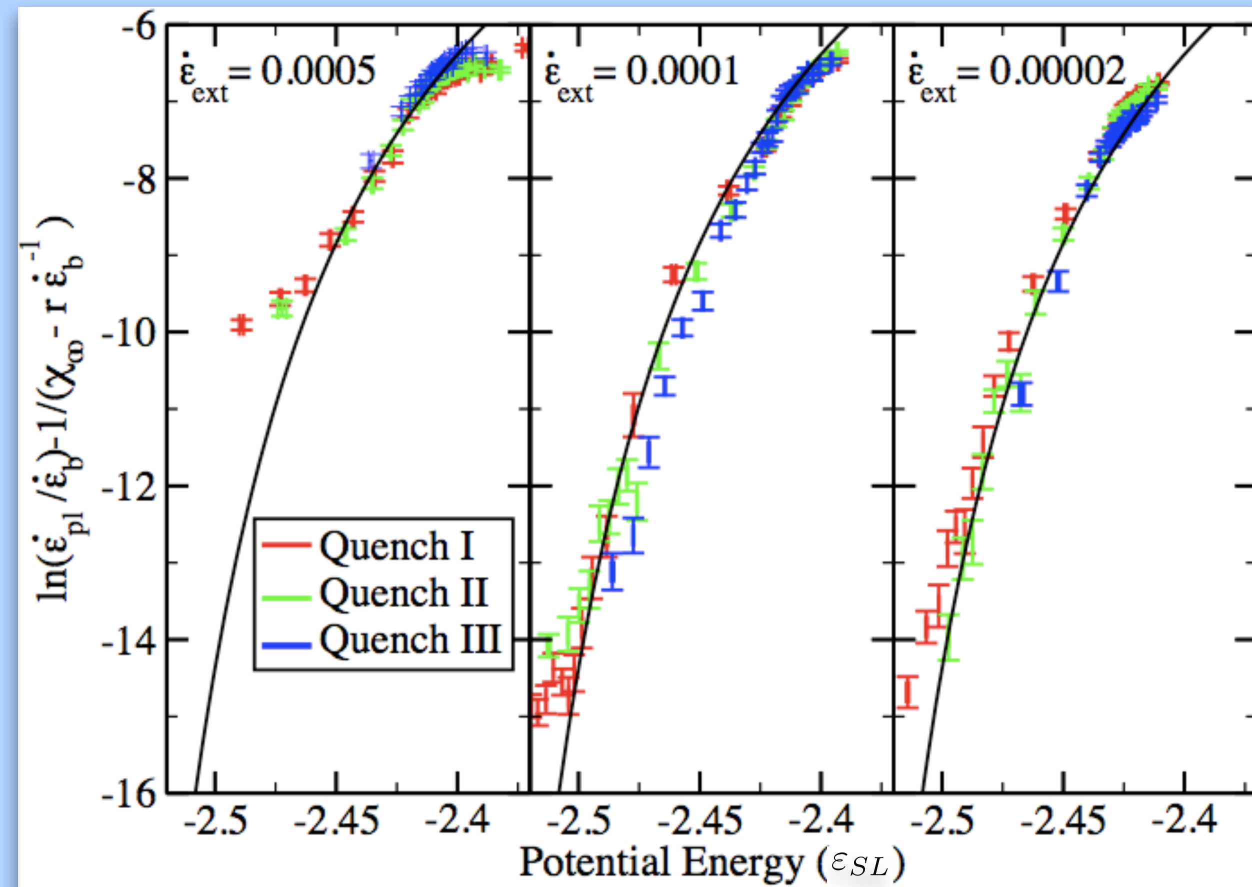

- **Assuming,** $\chi_0 \approx k_B T_g$ **, e_Z=1.9ε**

Y Shi, MB Katz, H Li, MLF, PRL, 98, 185505 (2007)

Numerical Results

(M Lisa Manning and JS Langer, PRE, 76, 056106(2007))

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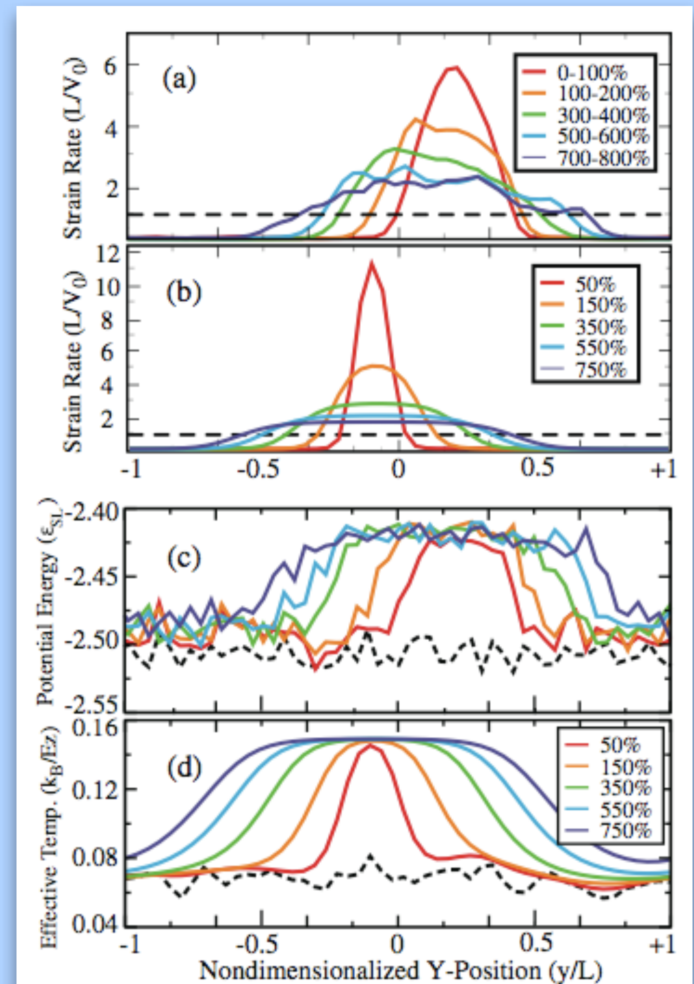
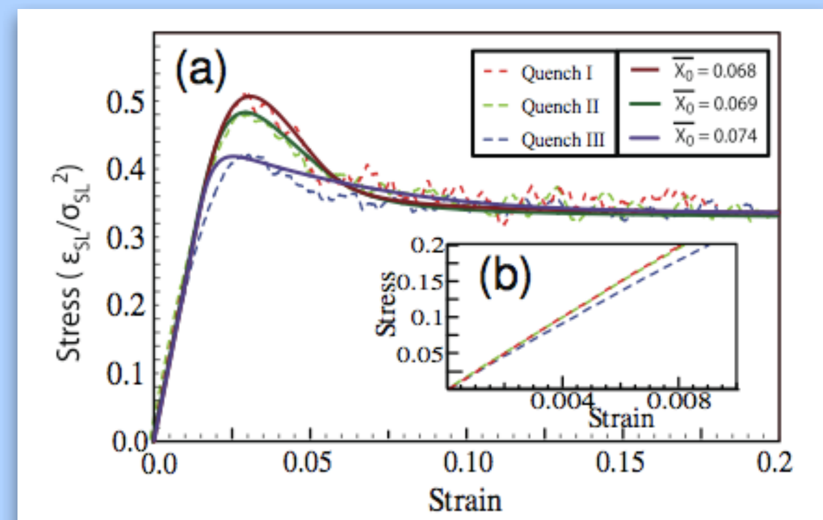
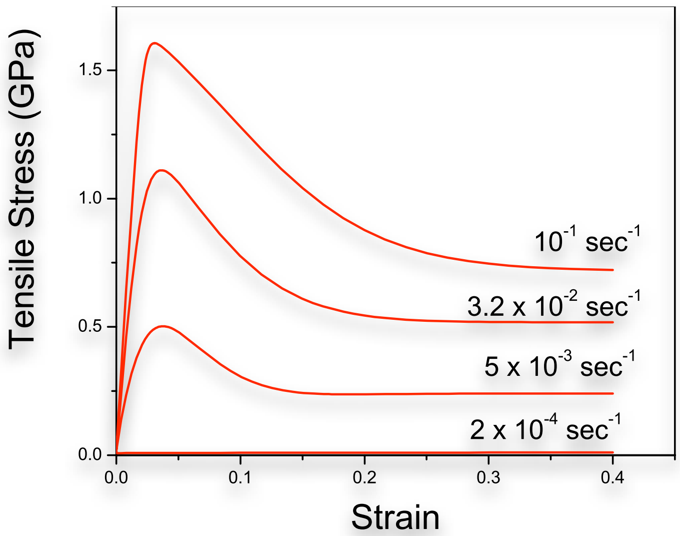
- These equations closely reproduce the details of the strain rate and structural profiles during band formation

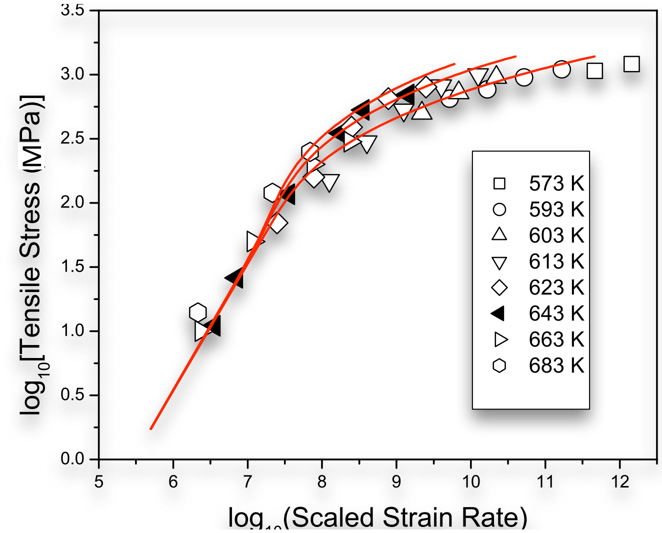


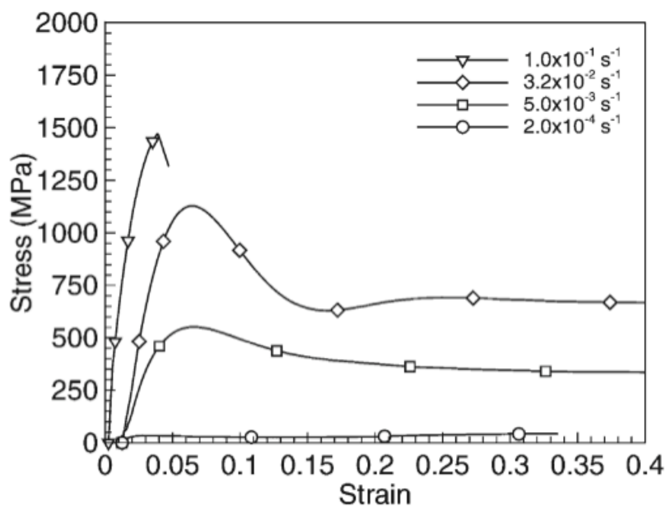


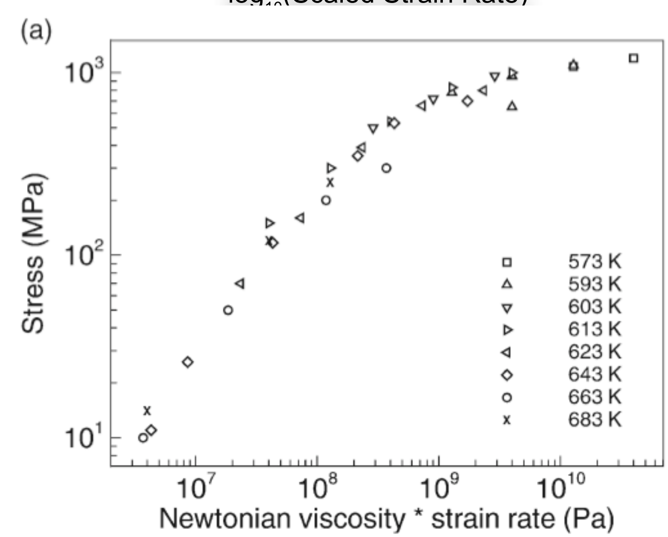
Metallic Glass Deformation

Lu, Ravichandran, Johnson, Acta Mat 51, 3429 (2003)









Shear Induced Anisotropy in Granular Media

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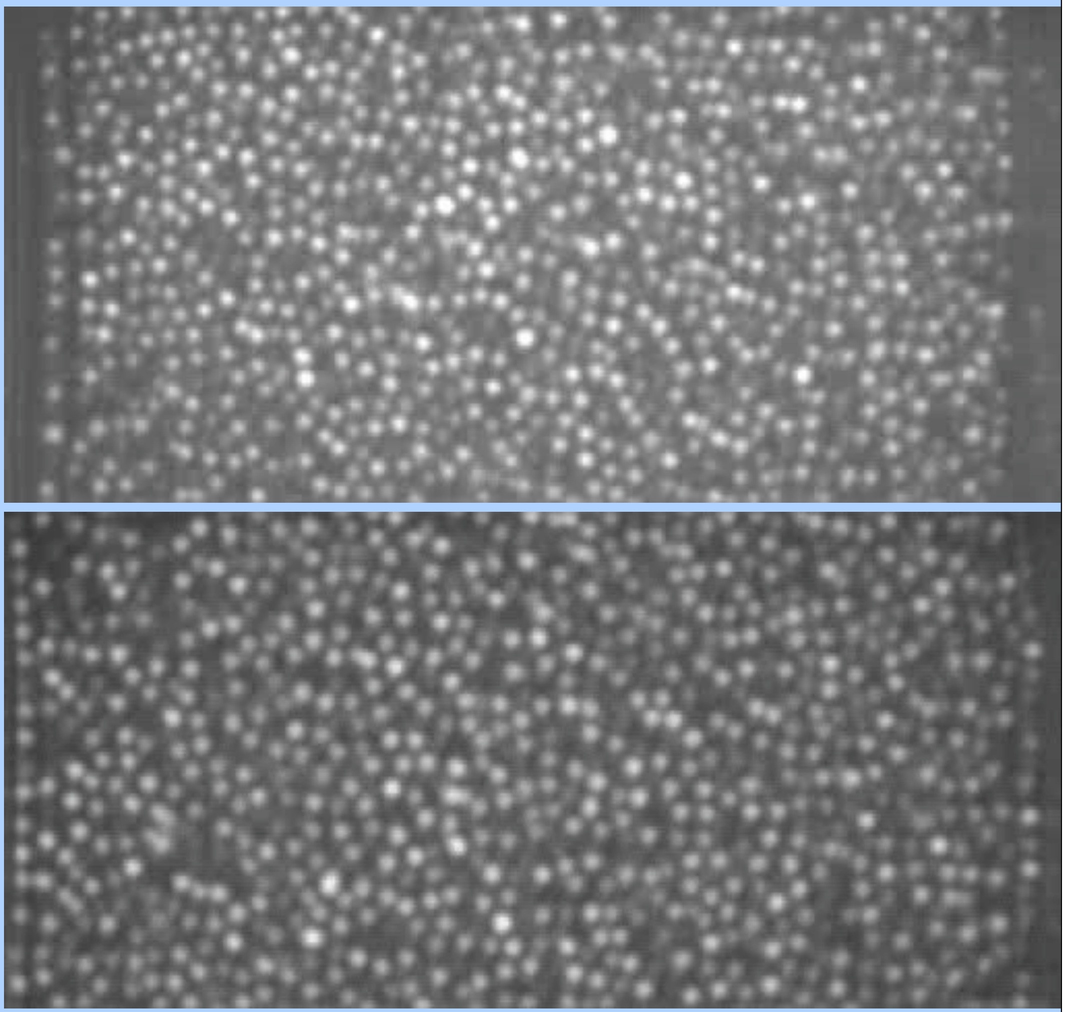
(experiments by W. Losert and M. Toyia)

- 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)

Comparison to Granular Flow Data

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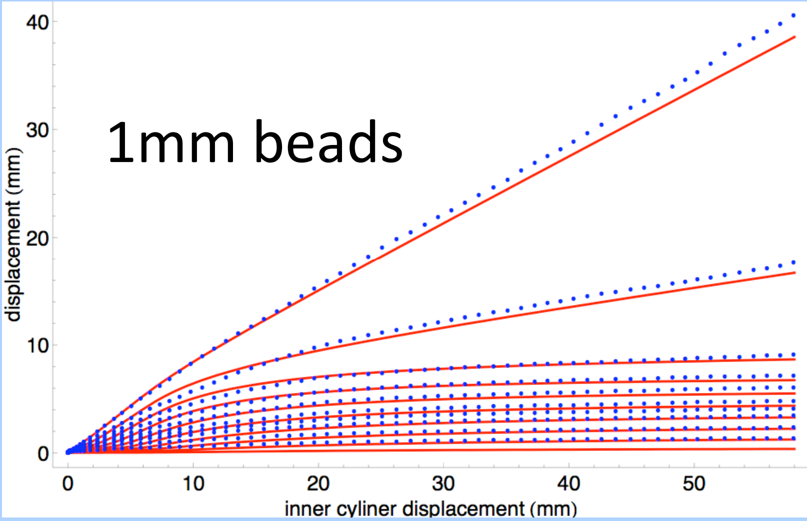
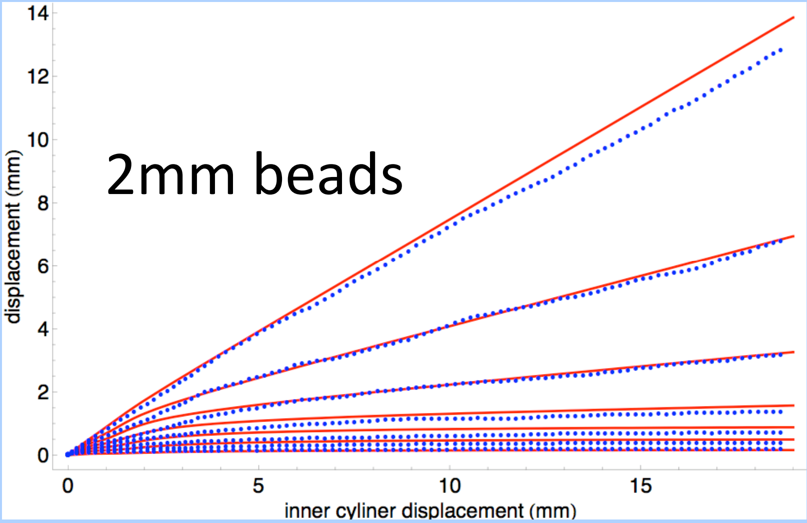
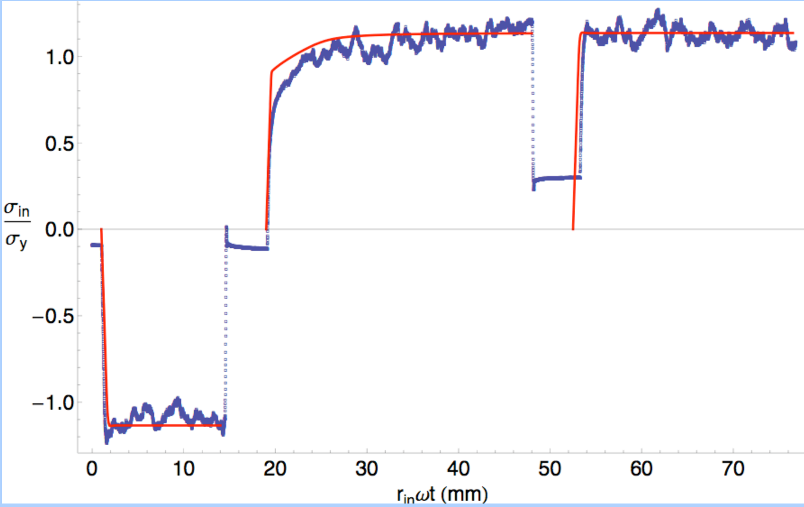
- **The blue dots represent experimental measurements of displacement at a specified radial position, plotted as a function of the inner cylinder displacement subsequent to shear reversal.**

- **The red lines are the STZ predictions.**







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

STZ Comparison to Shear of a-Si

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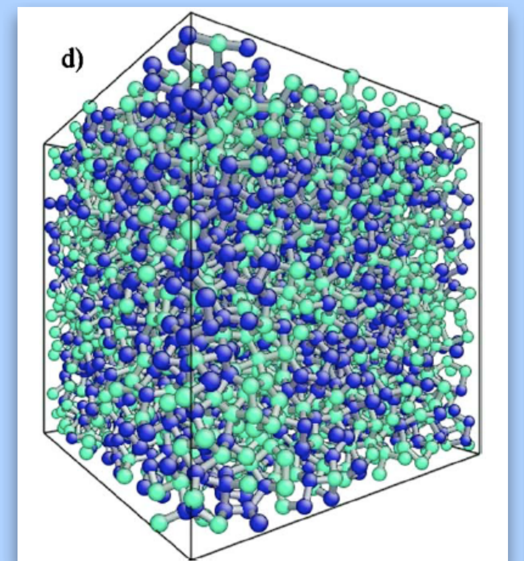
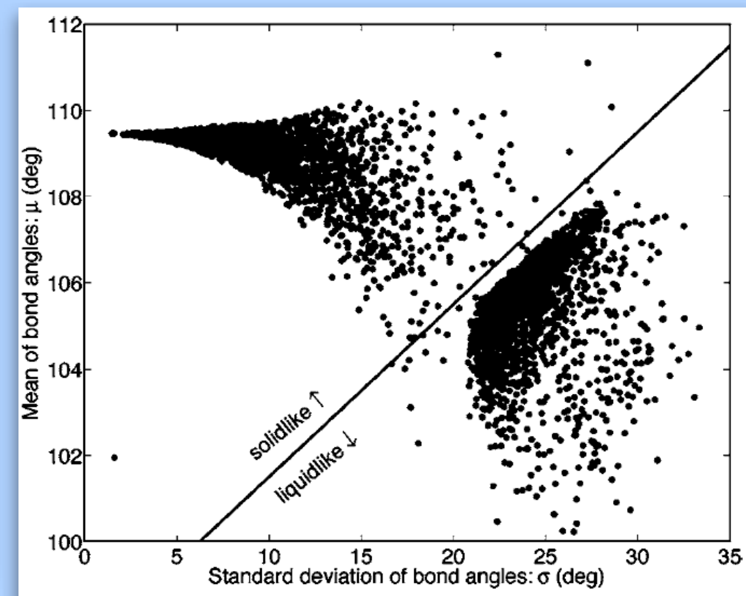
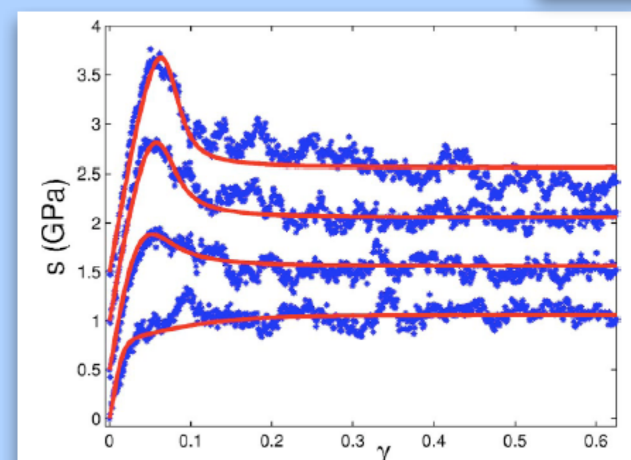
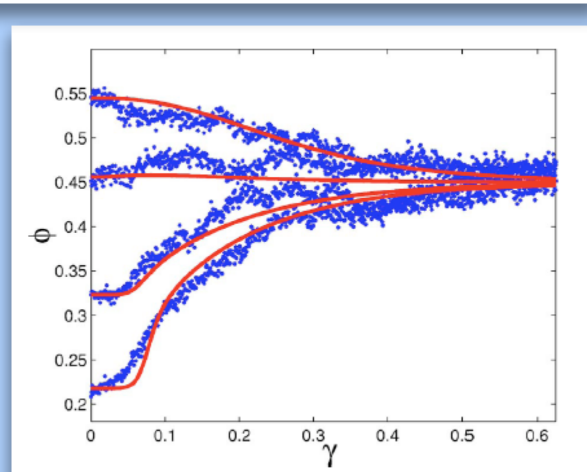




Amorphous Silicon forms 5-fold coordinated liquid-like regions that facilitate shear.

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.**
- **Shear Transformation Zone Theory is an attempt to build a thermodynamically based phenomenological theory with a connection to the microscopic physics of deformation.**
- **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 (transition from creep to superplastic flow ⇒ nonlinear rheology)
  - Diverging time scale for deformation near the yield stress
- **Are STZ's ephemeral or persistent?**
- **How can we more precisely connect atomic scale to parameters?**
- **What is the physically correct form for R(s)?**