The Relationship Between Localization and Percolation in Simulated Systems

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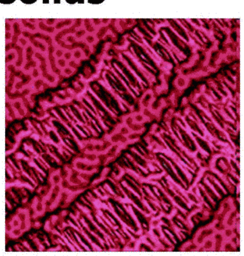
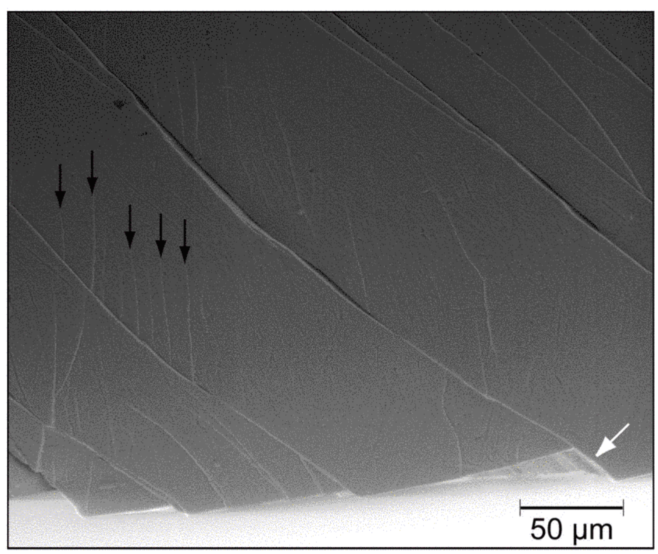
Strain Localization
is an important failure mode in non-crystalline solids



Craze in a block copolymer (PCHE/PE) film, Veeco NanoTheatre(2004)



SEM Image of Shear Bands Formed in Bending Metallic Glass, Hufnagel, El-Deiry, Vinci (2000)

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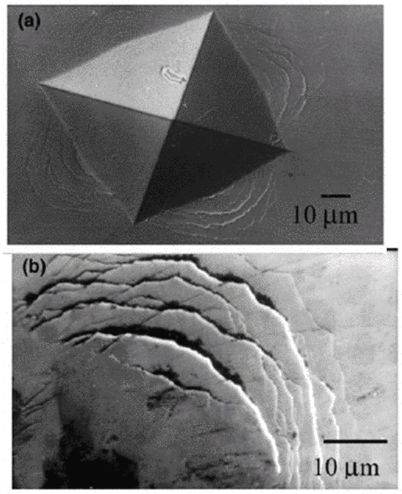
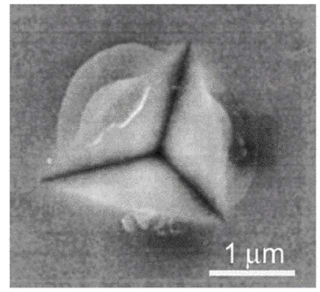
Indentation for Characterizing Metallic Glass Mechanical Response





"Nanoindentation studies of shear banding in fully amorphous and partially devitrified metallic alloys"
Mat. Sci. Eng. A (2005)
A.L. Greer., A. Castellero, S.V. Madge, I.T. Walker, J.R. Wilde

"Hardness and plastic deformation in a bulk metallic glass"
Acta Materialia (2005)
U. Ramamurty, S. Jana, Y. Kawamura, K. Chattopadhyay

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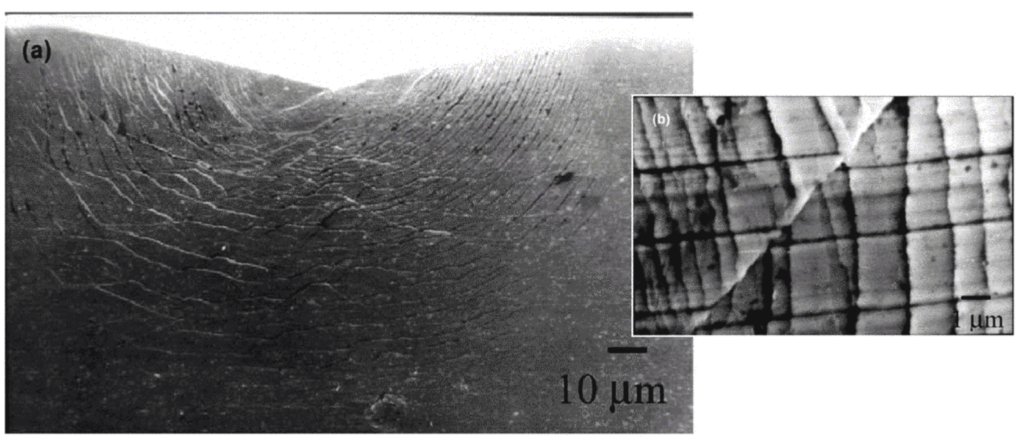
Indentation for Characterizing Metallic Glass Mechanical Response



"Hardness and plastic deformation in a bulk metallic glass"
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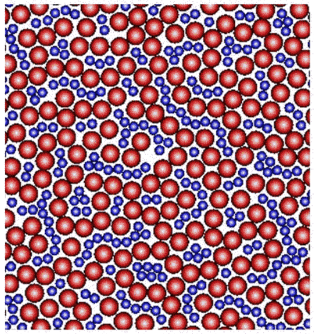
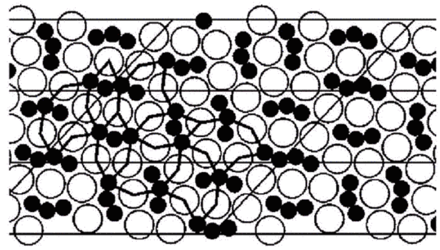
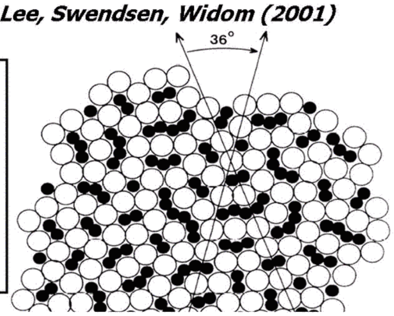
2D Simulation System





Lee, Swendsen, Widom (2001)



Widom, Strandburg, Swendsen (1987)

- 2D binary Lennard-Jones 12-6 potential
- Binary system with quasi-crystalline packing *(Lancon et al, Europhys. Lett, 1986)*

45:55 composition, 20' 000 atoms

- $T_{MCT} \approx 0.325$

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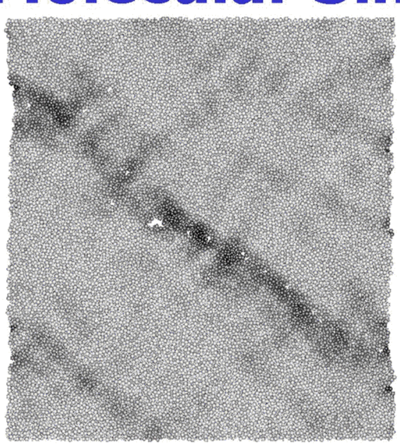
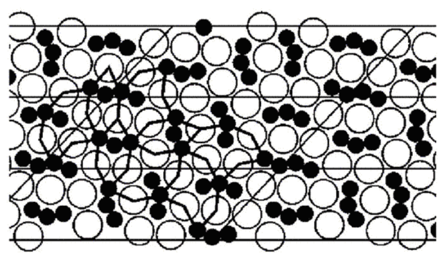
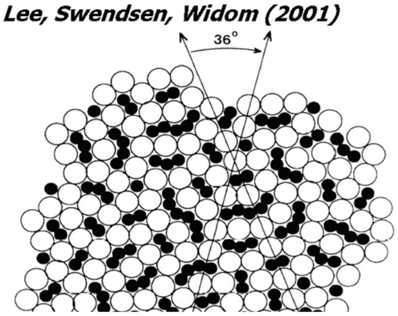
Molecular Simulation System





Lee, Swendsen, Widom (2001)



Widom, Strandburg, Swendsen (1987)

- Simple system that exhibits shear localization
- 2D systems can be studied at a larger spatial dimension

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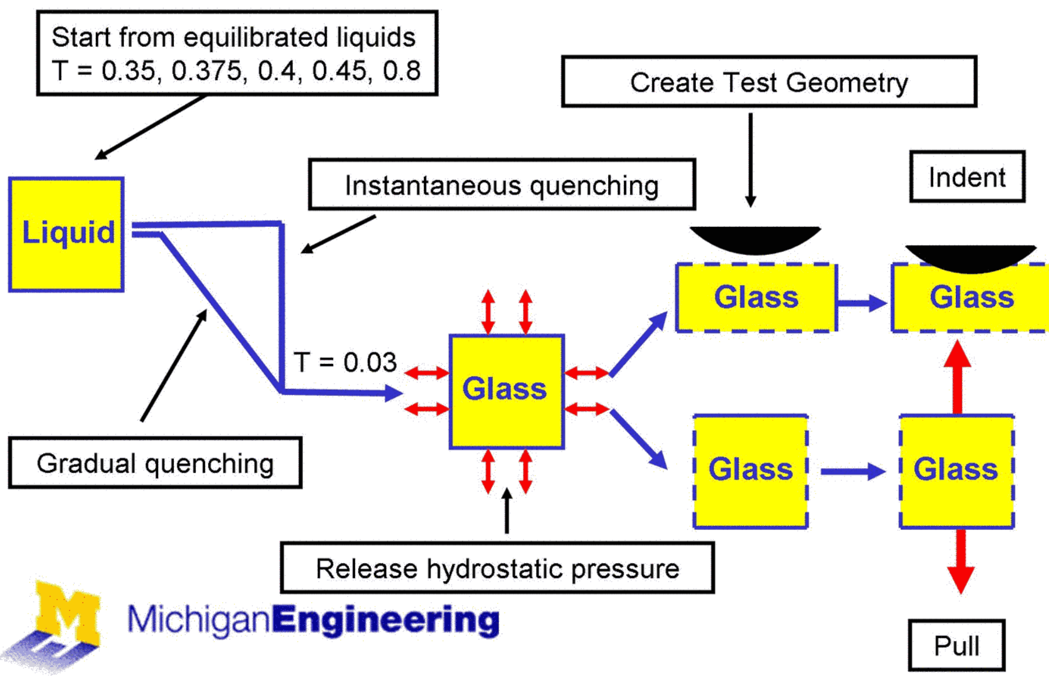
Preparation of Glasses



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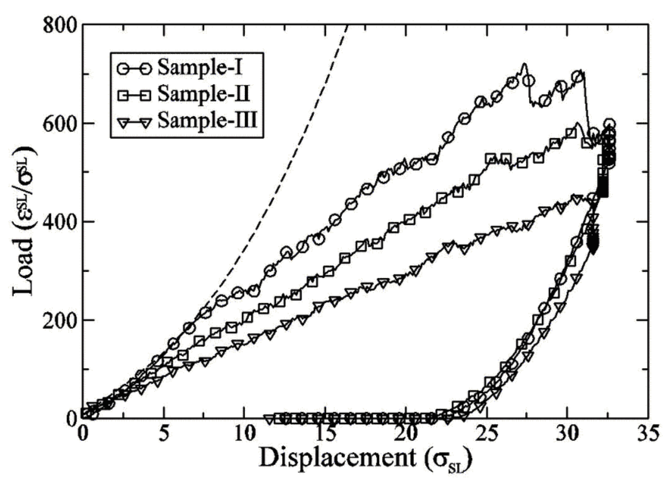
Nanoindentation of Three Glasses

- Sample I – Quenched over 0.5 μs
- Sample II – Quenched over 10ns
- Sample III – Quenched instantaneously and annealed for 0.1ns



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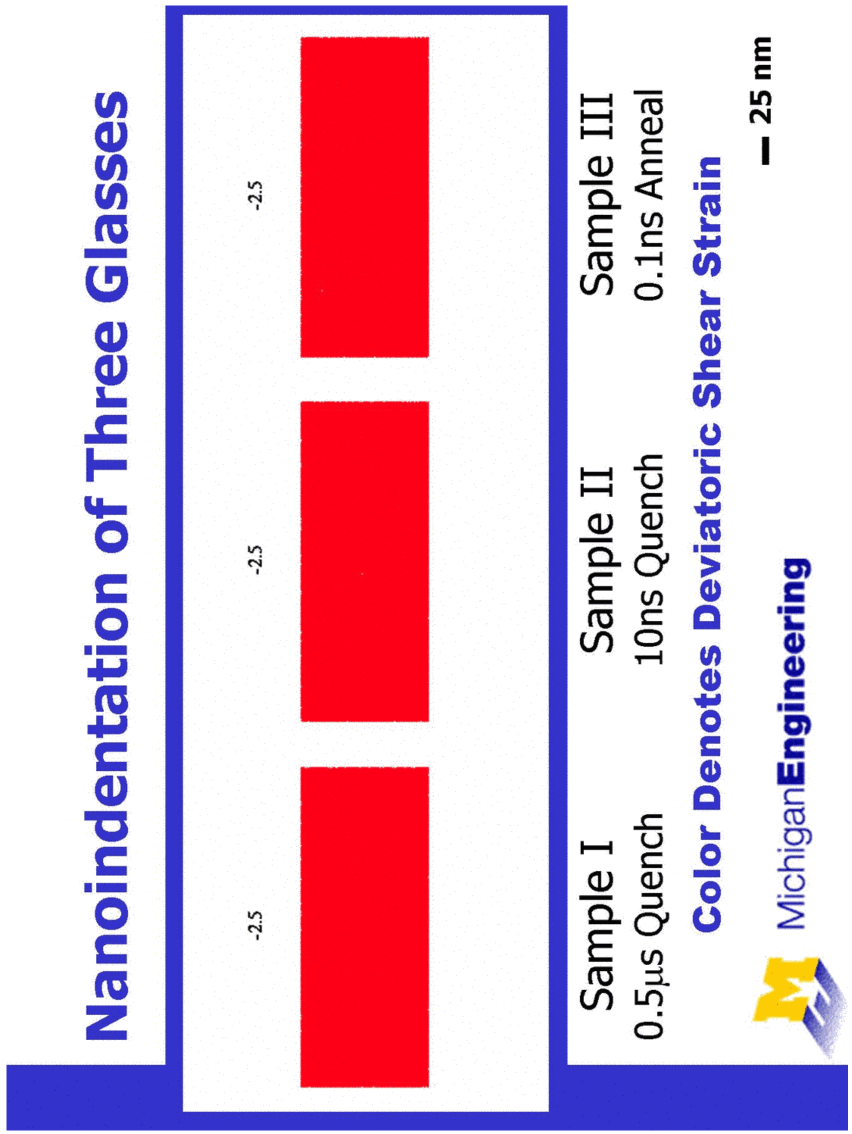
Nanoindentation of Three Glasses
-2.5
-2.5
-2.5
Sample I
0.5μs Quench
Sample II
10ns Quench
Sample III
0.1ns Anneal
Color Denotes Deviatoric Shear Strain
25 nm
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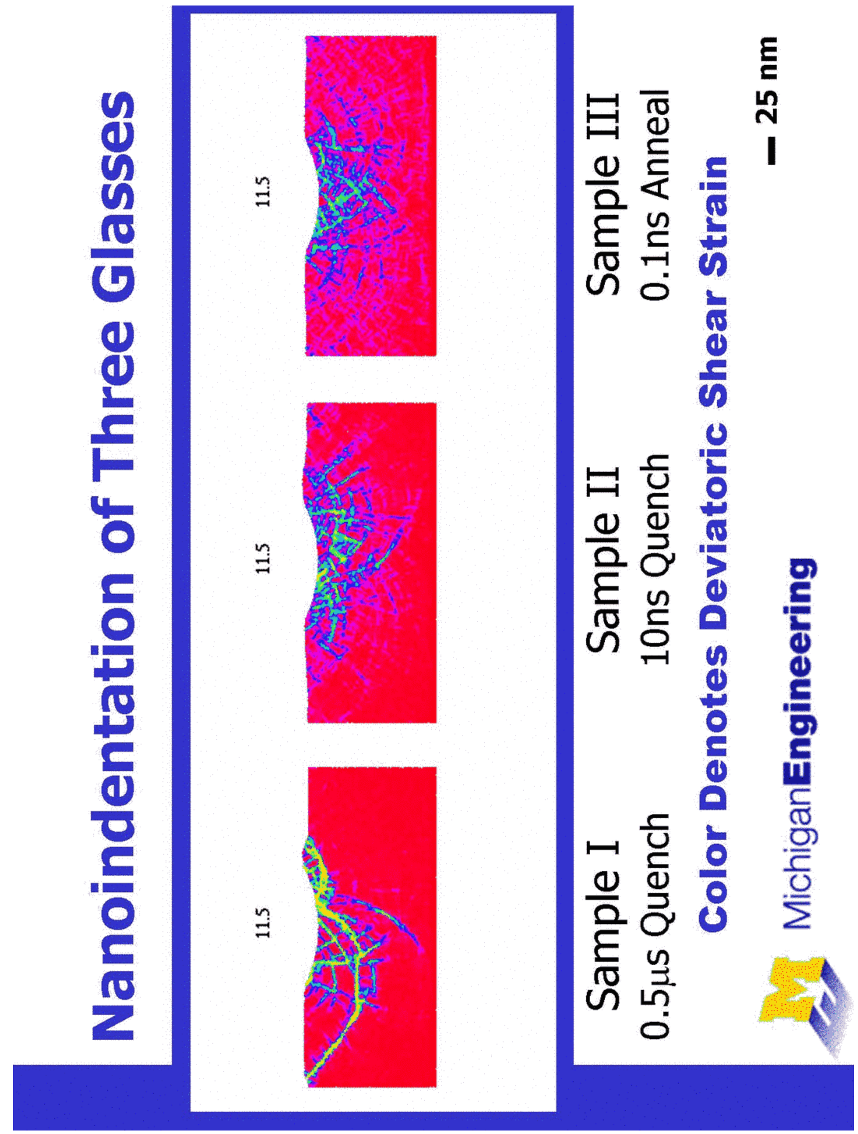
Nanoindentation of Three Glasses
11.5
11.5
11.5
Sample I
0.5μs Quench
Sample II
10ns Quench
Sample III
0.1ns Anneal
Color Denotes Deviatoric Shear Strain
25 nm
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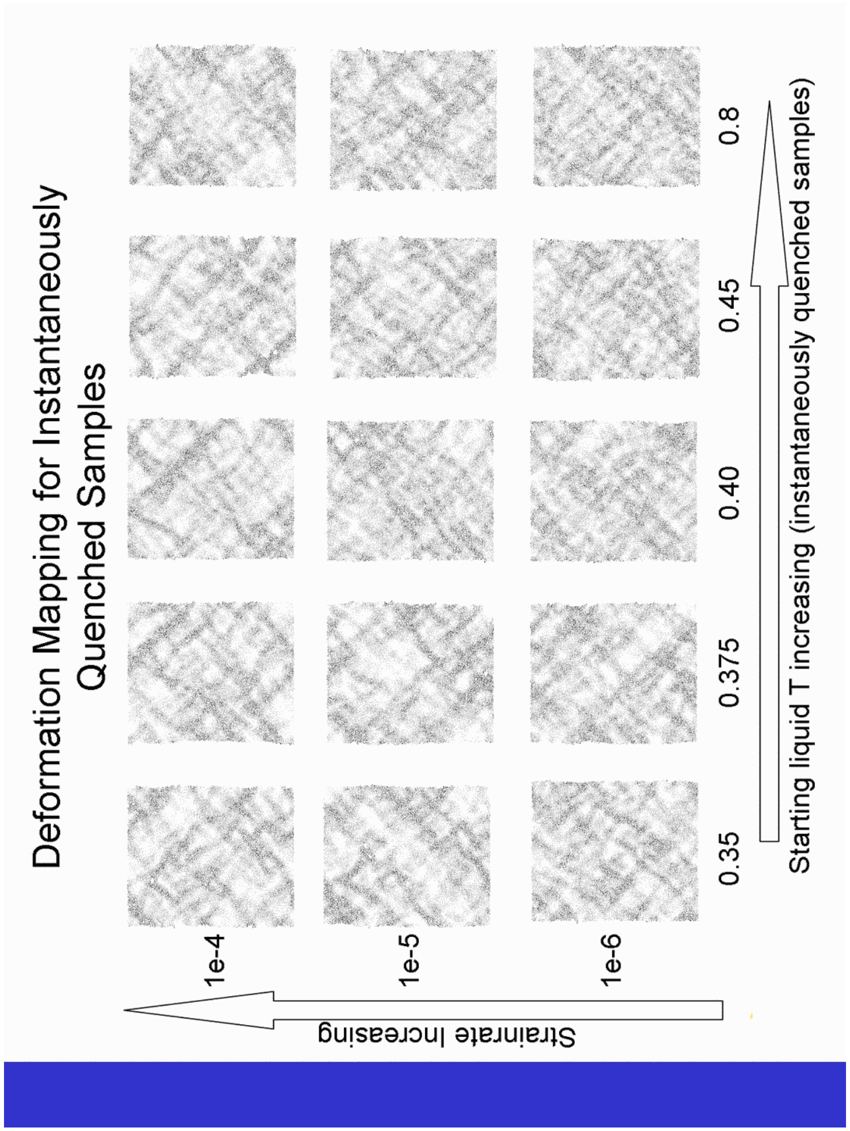
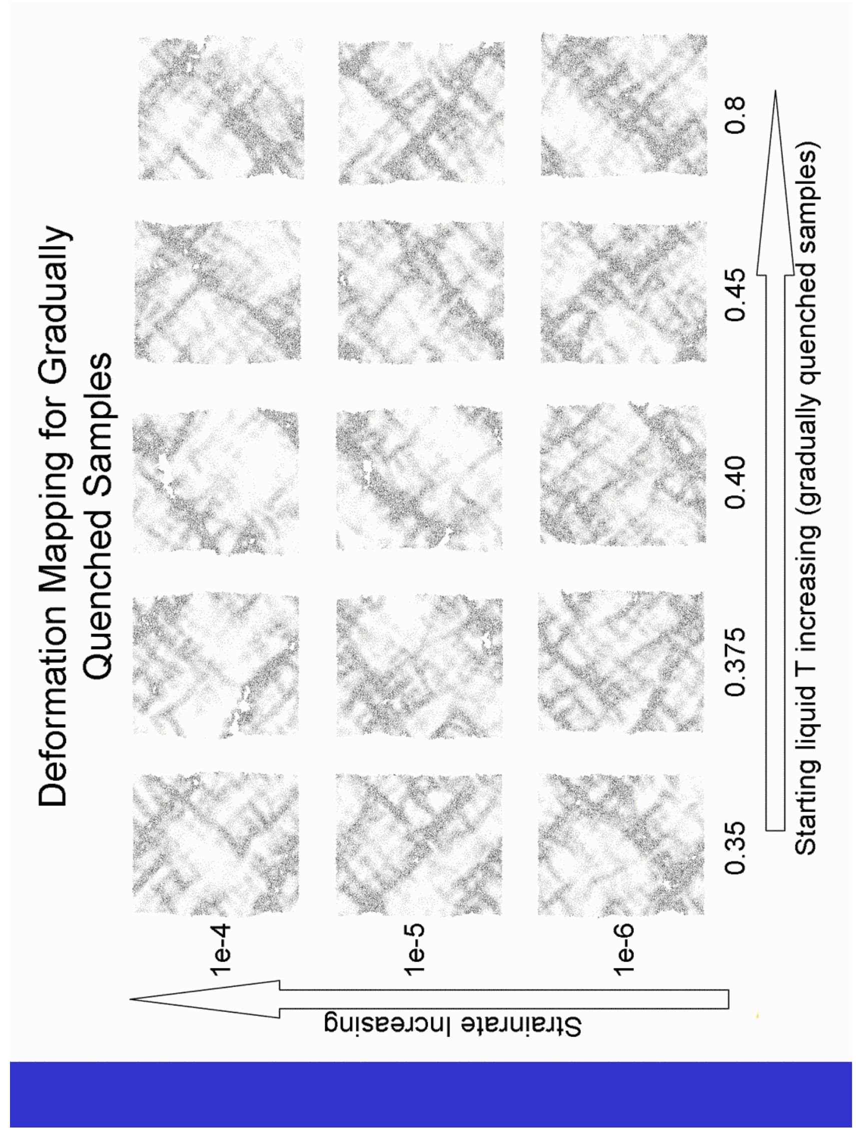
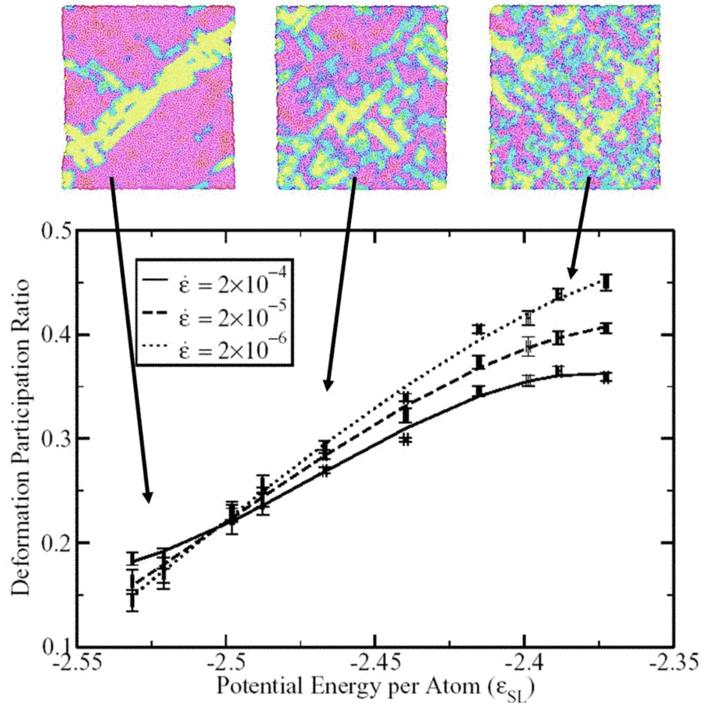

Deformation Mapping for Instantaneously Quenched Samples
1e-4
1e-5
1e-6
0.35
0.375
0.40
0.45
0.8
Starting liquid T increasing (instantaneously quenched samples)
Strainrate Increasing


Deformation Mapping for Gradually Quenched Samples
1e-4
1e-5
1e-6
0.35
0.375
0.40
0.45
0.8
Starting liquid T increasing (gradually quenched samples)
Strainrate Increasing

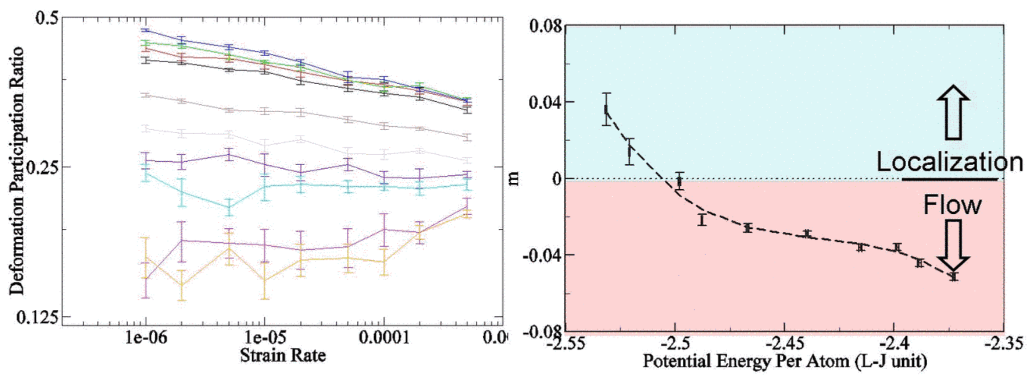
Quantification of Shear Localization

Participation Ratio

- Participation Ratio: Percentage of material with a local shear strain larger than the nominal strain
- Low strain rate favors homogenous deformation in instantaneously quenched samples
- Low strain rate favors inhomogeneous deformation in gradually quenched samples.



Strain-rate Sensitivity of DPR



$$DPR \approx A\dot{\varepsilon}^{m}$$

For $\dot{\varepsilon} \to 0$ and system size $\to \infty$

$m < 0$: homogenous deformation

$m >= 0$: localized deformation

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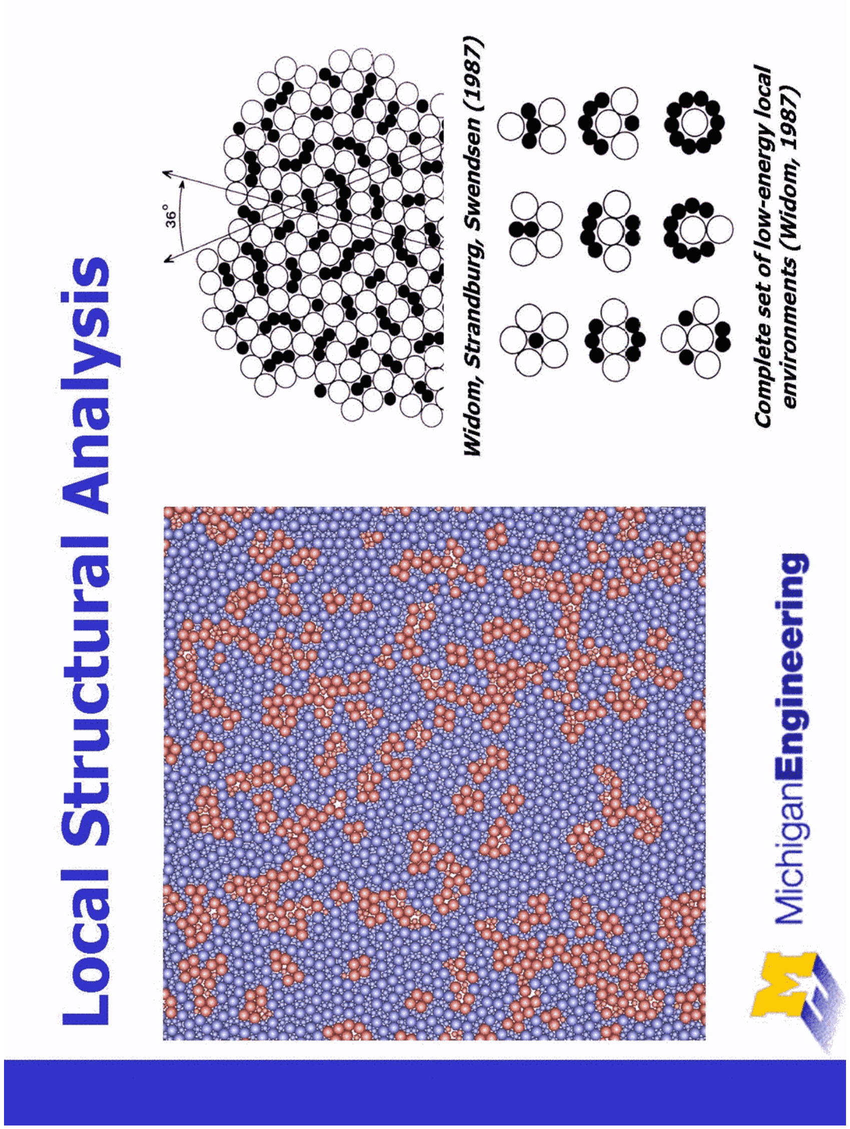
Local Structural Analysis
36°
Widom, Strandburg, Swendsen (1987)
Complete set of low-energy local environments (Widom, 1987)
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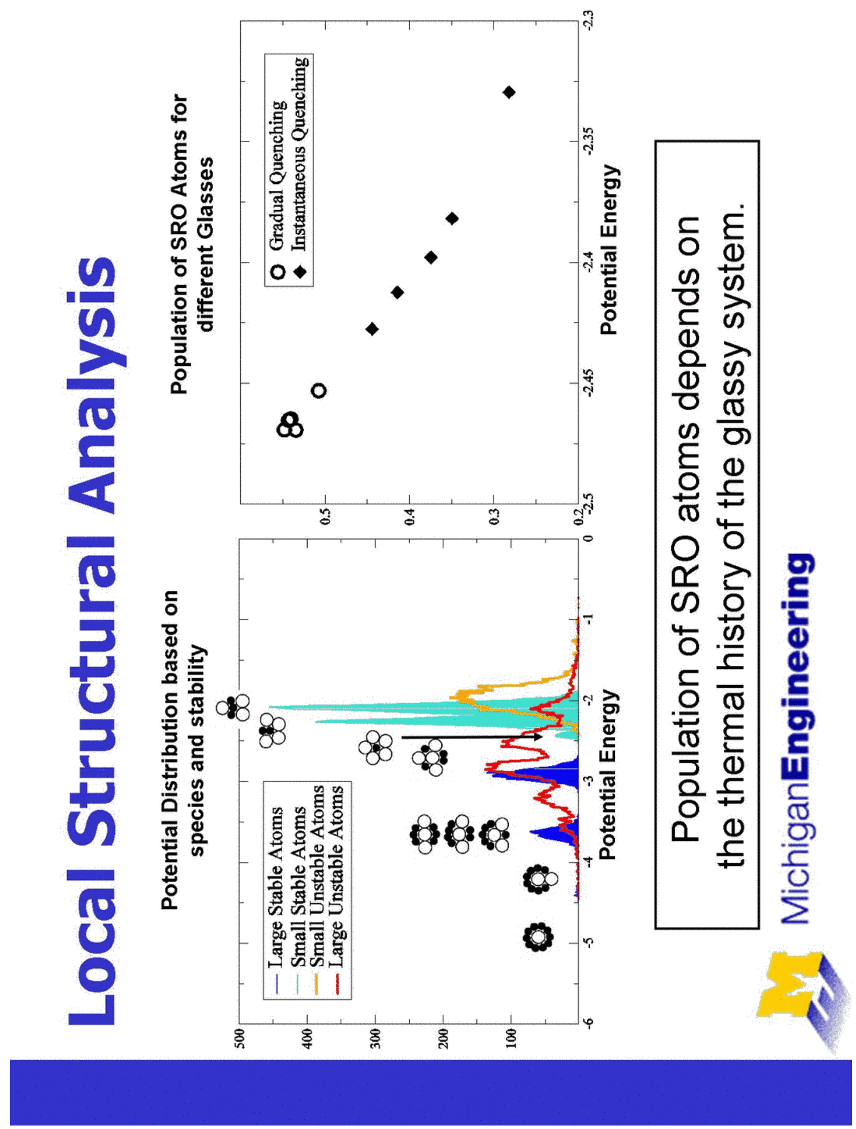
Local Structural Analysis
Potential Distribution based on species and stability
Large Stable Atoms
Small Stable Atoms
Small Unstable Atoms
Large Unstable Atoms
Potential Energy
Population of SRO Atoms for different Glasses
Gradual Quenching
Instantaneous Quenching
Potential Energy
Population of SRO atoms depends on the thermal history of the glassy system.
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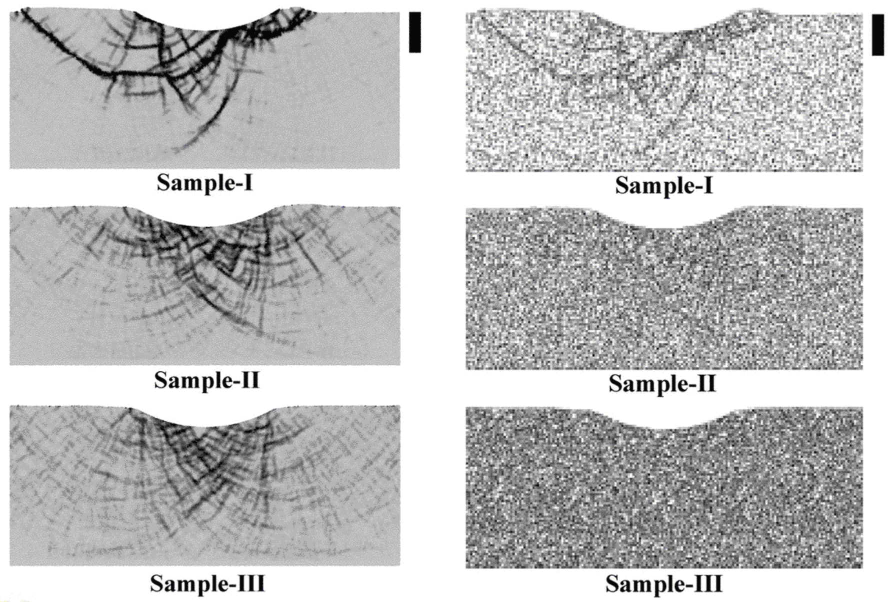
Structural Signature of Localization in Nanoindentation



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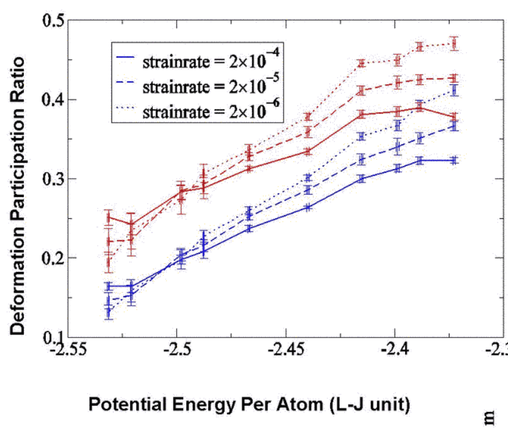
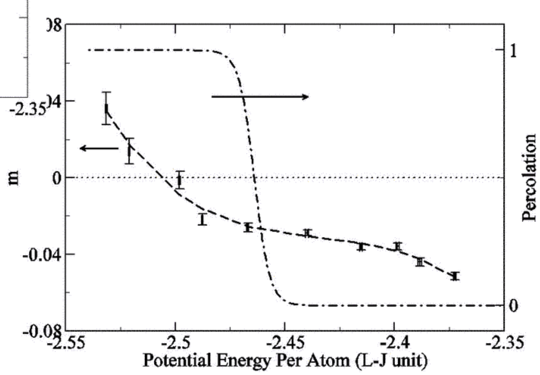
Local Structure and Deformation



- Stable atom cluster may prevent flowing
- Problem: stable atom cluster may not be rigid



Red lines: unSRO atoms

Blue lines: SRO atoms

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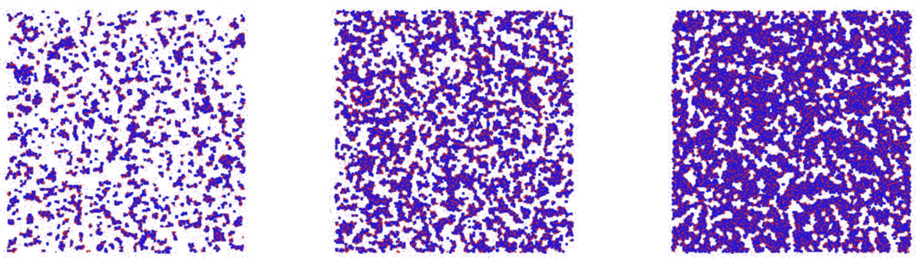
K-core Percolation of SRO

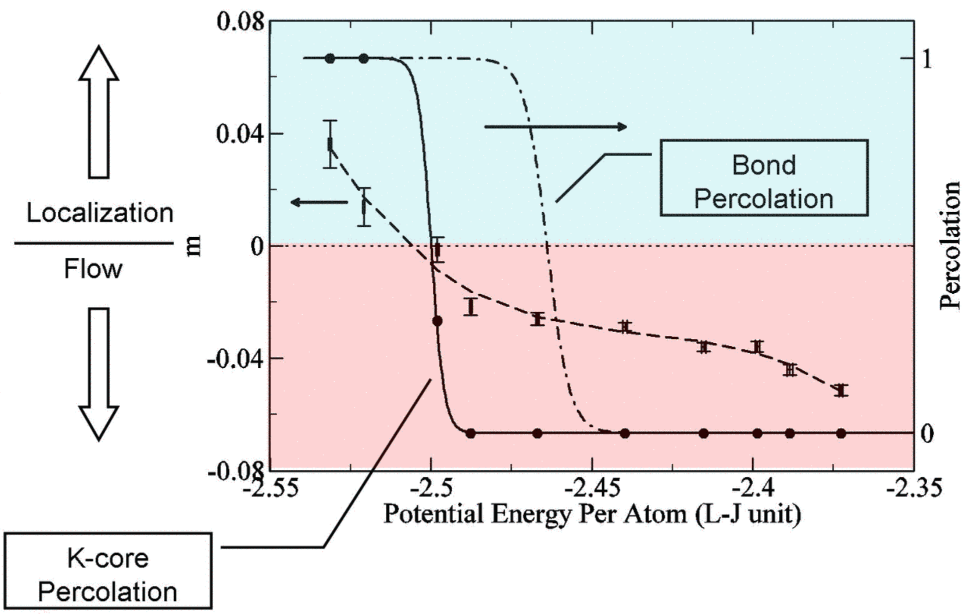
Mechanically unstable

Mechanically stable

Schwarz, Liu and Chayes, arXiv:cond-mat/0410595, 2004



K-core Percolation and Localization



Summary

- Simulated glasses with higher degrees of SRO demonstrated a stronger tendency toward localization.
- In more rapidly quenched samples localization appears to decrease at lower strain rates.
- In more slowly quenched samples localization appears to increase at lower strain rates.
- The transition from homogeneous to localized deformation in the quasi-static limit corresponds to the K-core Percolation of a stable backbone of material with quasi-crystal-like short range order.

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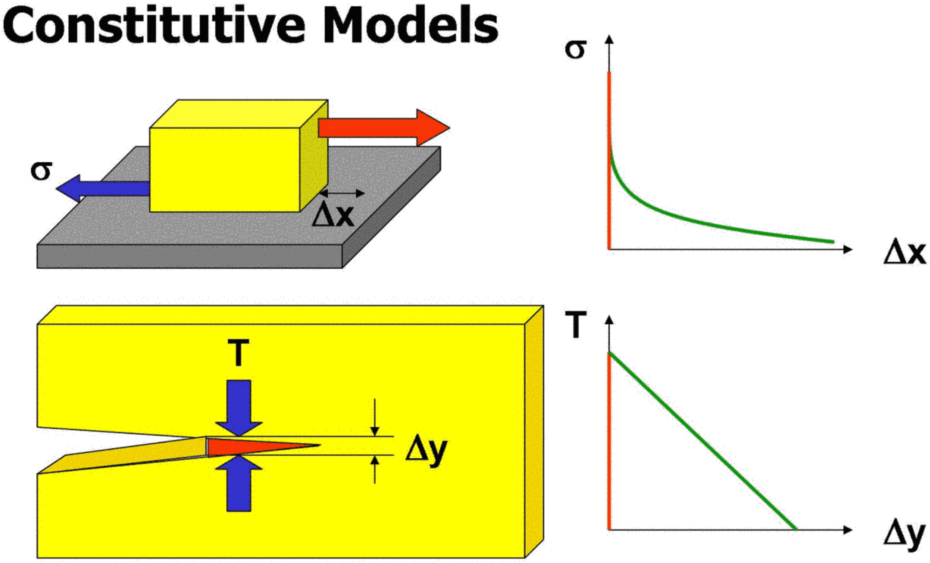
What do friction, fracture and shear bands have in common?

Constitutive Models



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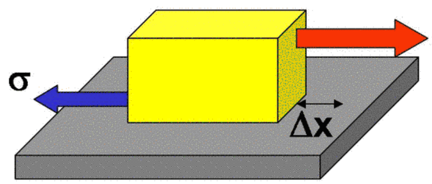
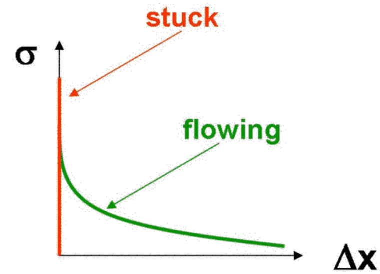
Constitutive Models

The Problem…





- Most of these systems involve a "stuck" or "jammed" state and a "flowing" or "slipping" state.
- Simple constitutive laws often include discontinuities.
- This complicates the analysis of instabilities and other properties that can sensitively depend on the dynamic transition between jammed and flowing states.

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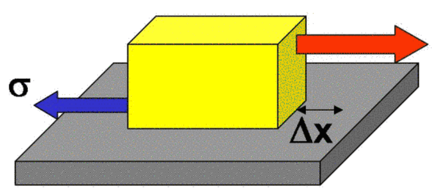
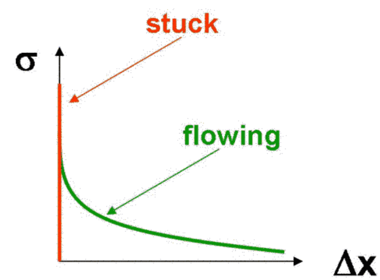
Rate and State Formulations

The Solution?





- These transitions arise due to internal degrees of freedom not represented in, e.g. Coulomb Friction Law
- Rate and State formulations attempt to capture the essential physics of these hidden degrees of freedom.
- Examples: Dieterich (1978), Rice and Ruina (1983).
- But the issue arises: What do these new degrees of freedom represent? (e.g. contact area in Dieterich)

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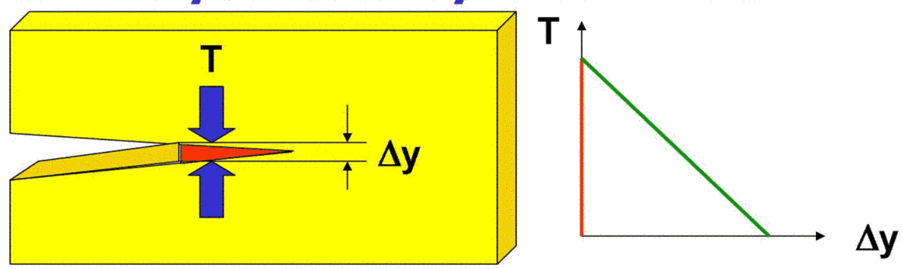
Rate and State Plasticity

STZ Theory for Non-crystalline Solids



- A number of such models exist in the context of plastic deformation primarily aimed at modeling crystals.
- Crystal deformation is difficult to relate to microscopics because of the nature of the defect (D-2 object).
- STZ theory attempts this for non-crystals by making some simplifying assumptions, e.g. that the defect is D=0 and has zero mobility.

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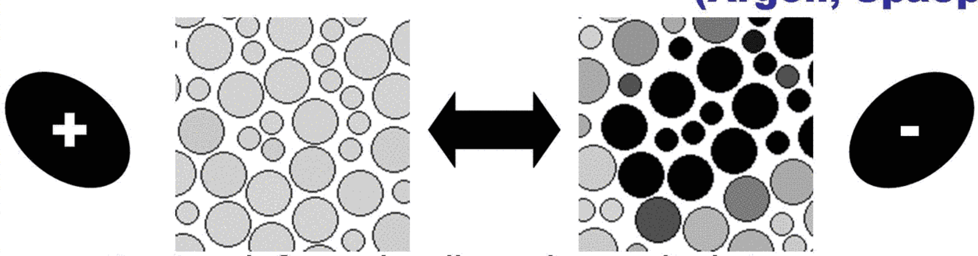
Shear Transformation Zones

(Argon, Spaepen)



- Region deforms locally under applied stress
- Region may reverse its rearrangement if stress is reversed shortly thereafter
- Deformation becomes permanent after some amount of additional rearrangement
- Stress in opposite direction produces deformation <u>in different regions</u>

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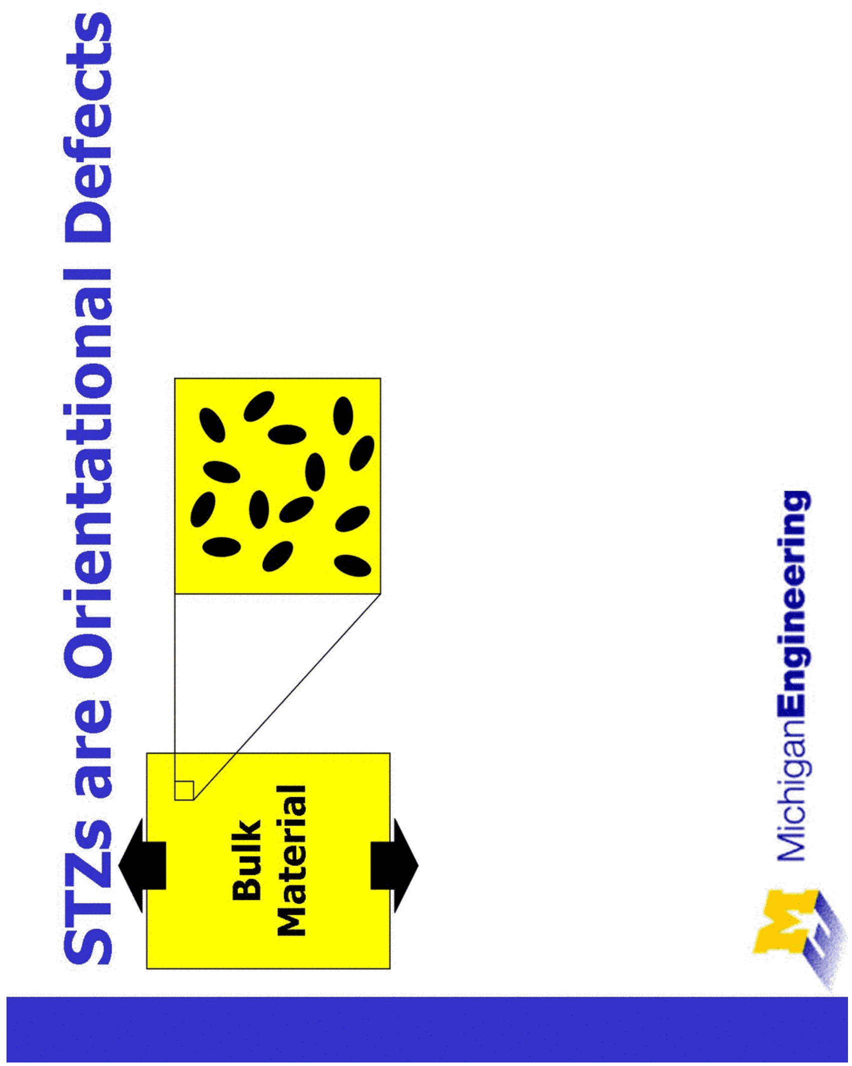
STZs are Orientational Defects
Bulk Material
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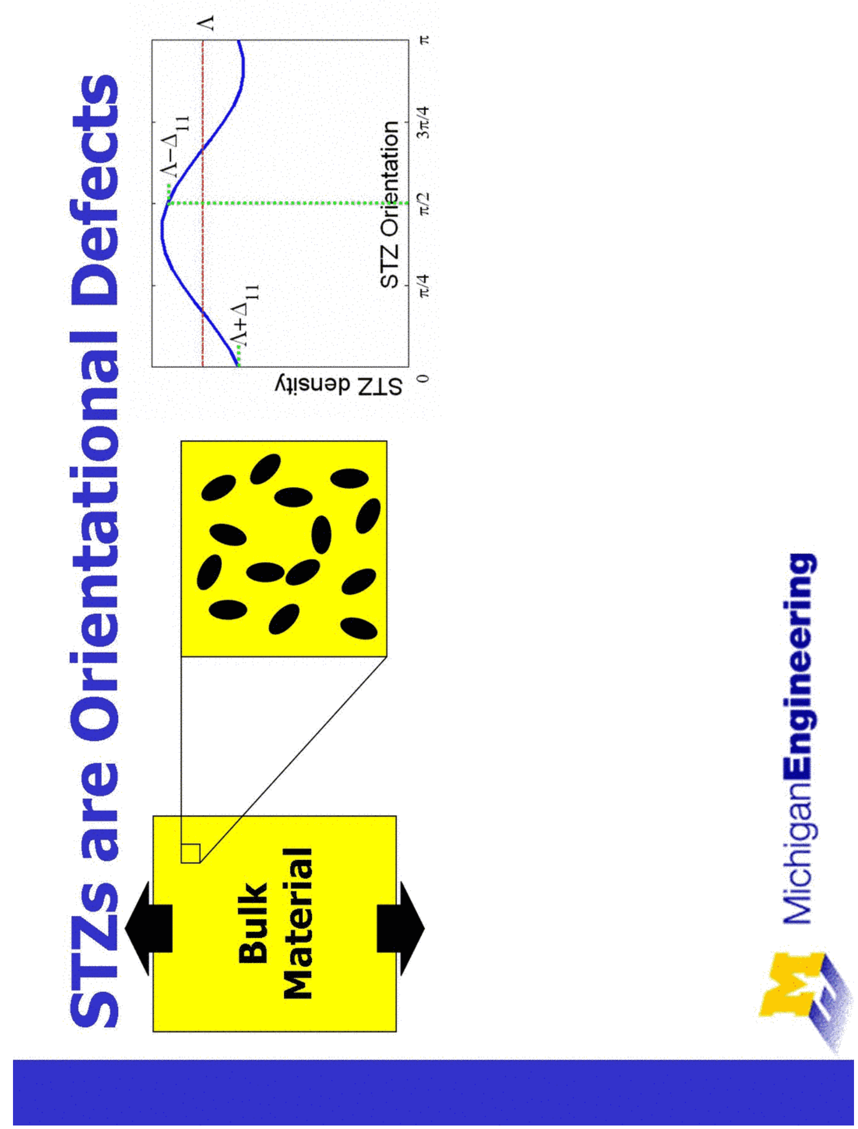
STZs are Orientational Defects
Bulk Material
STZ density
STZ Orientation
Λ
Λ+Δ11
Λ−Δ11
0
π/4
π/2
3π/4
π
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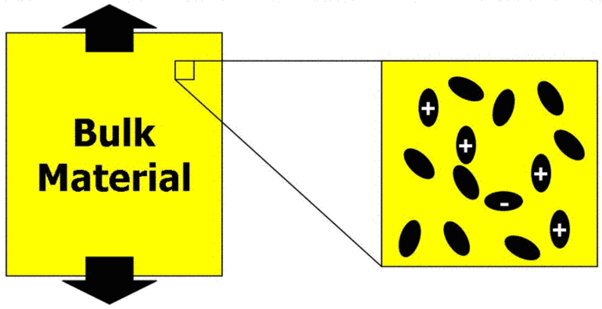
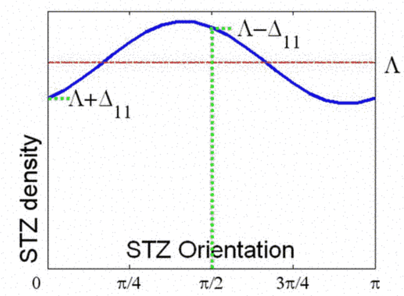
STZs are Orientational Defects





- Simplifying to shear only along x and y principal axes:

$$n_+ = \frac{n_\infty}{2}\left(\Lambda + \Delta_{11}\right)$$

$$n_- = \frac{n_\infty}{2}\left(\Lambda + \Delta_{22}\right) = \frac{n_\infty}{2}\left(\Lambda - \Delta_{11}\right)$$

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The STZ Model

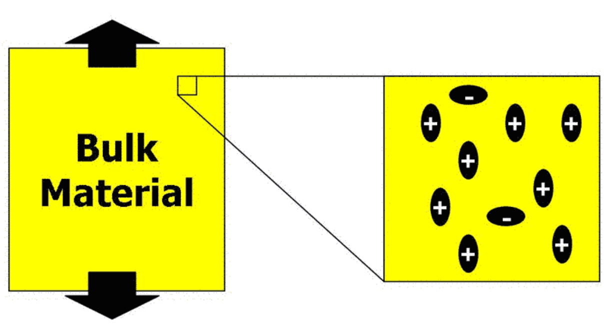
Plastic Strain Rate Proportional to Flips

$$\dot{\varepsilon}^{pl} = \frac{\varepsilon_0}{n_\infty}\left[R_-(s)\,n_- - R_+(s)\,n_+\right]$$

ε_0/n_∞= volume per STZ

Flip Rates

Deviatoric Stress



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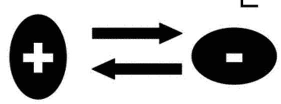
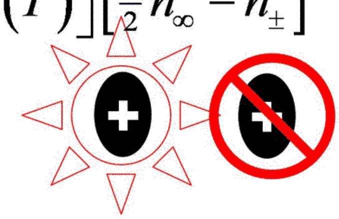
ε_0/n_∞= volume per STZ

Master Equation for Densities

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





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For the state of the system to depend only upon the strain history in the low T, low rate limit, the same rate function must control both annihilation and creation

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The STZ Model

Plastic Strain Rate Proportional to Flips

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This provides a closure for Γ assuming that the First Law of Thermodynamics is obeyed and that Γ is proportional to the rate of dissipation.

L. Pechenik (2003)

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The STZ Model

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The n_∞ parameter is the ratio of annihilation to creation and sets the equilibrium defect density.

This is identified with the "Granular Temperature" χ.

Langer (2004)

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The STZ Model

Plastic Strain Rate Proportional to Flips

$$\dot{\varepsilon}^{pl} = \frac{\varepsilon_0}{n_\infty}\left[R_-(s)\,n_- - R_+(s)\,n_+\right]$$

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Langer (2004)

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Master Equation for Densities

$$\dot{n}_\pm = R_\mp n_\mp - R_\pm n_\pm + \left[\Gamma(s,n_\pm)+\rho(T)\right]\left[\tfrac{1}{2}e^{-1/\chi} - n_\pm\right]$$

χ has its own dynamics. Shear drives it to a high value (χ_∞) while thermal fluctuations drive it to a low value ($\chi_T = kT/E_{STZ}$).

Langer (2004)

The STZ Model

Plastic Strain Rate Proportional to Flips

$$\dot{\varepsilon}^{pl} = \frac{\varepsilon_0}{n_\infty}\left[R_-(s)n_- - R_+(s)n_+\right]$$

ε_0/n_∞ = volume per STZ

Master Equation for Densities

$$\dot{n}_\pm = R_\mp n_\mp - R_\pm n_\pm + \left[\Gamma(s,n_\pm)+\rho(T)\right]\left[\tfrac{1}{2}e^{-1/\chi} - n_\pm\right]$$

$$\frac{\tau_0 c_0}{\varepsilon_0}\dot{\chi} = e^{-1/\chi}\Gamma(\chi_\infty - \chi) + \kappa\rho(T)e^{-\beta/\chi}(\chi_T - \chi) + \ell^2\nabla^2\chi$$

Length scale introduced by the diffusion of the granular temperature.

Langer (2004)

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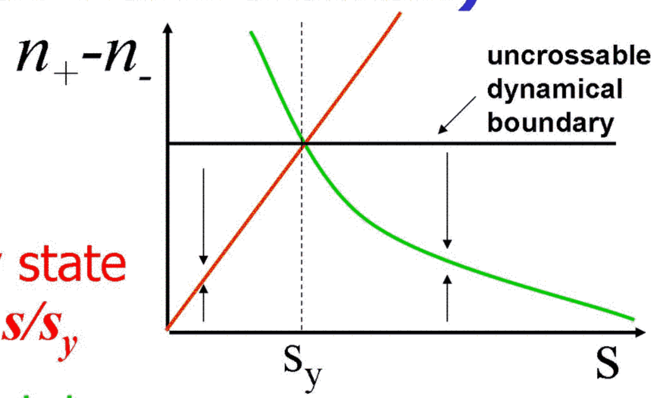
Dynamic Transition from Hardening to Flow (Quasilinear Formulation)



Jammed steady state

$n_+ - n_- = (n_+ + n_-)\, s/s_y$

Flowing steady state

$n_+ - n_- = s_y/s,\ n_+ + n_- = n_\infty$

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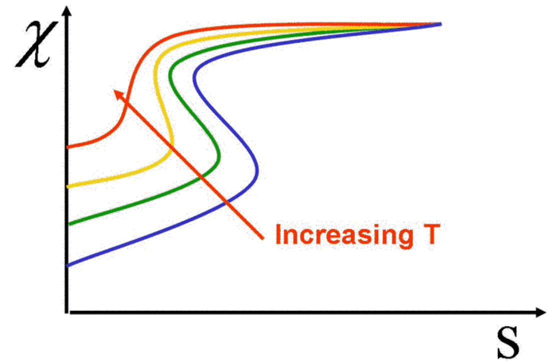
Dynamic Transition from Hardening to Flow (Quasilinear Formulation)

At low T, granular temperature, χ, is double valued as a function of stress implying the possibility of 2 phase coexistence between jamming (creep) and flow.



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Current Investigations

- Is this a good model for the observed localization?
- Is this a unique or optimal model?
- Does χ map directly onto %SRO?
- Can this model help quantify the role of internal degrees of freedom in the softening process?
- Does this have any bearing on localization in other (e.g., granular) materials?

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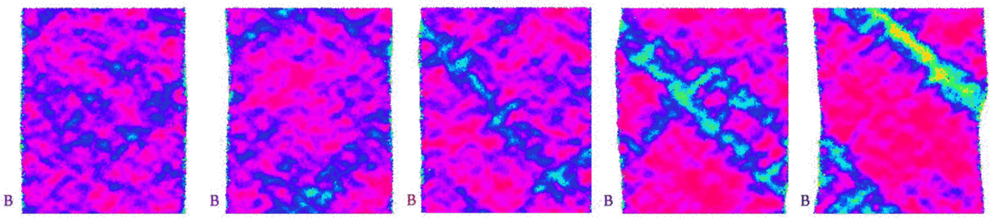
How does this vary with dimensionality?



0.01M 0.1M 0.5M 1M ~3 M

- Repeated in 3D binary LJ glass using 50:50 Wahnstrom potential
- Strain rate $1 \times 10^{-5}\ t_0^{-1}$
- Shown, Quench time: 3.33 T_{MCT} to 0.1 T_{MCT}.

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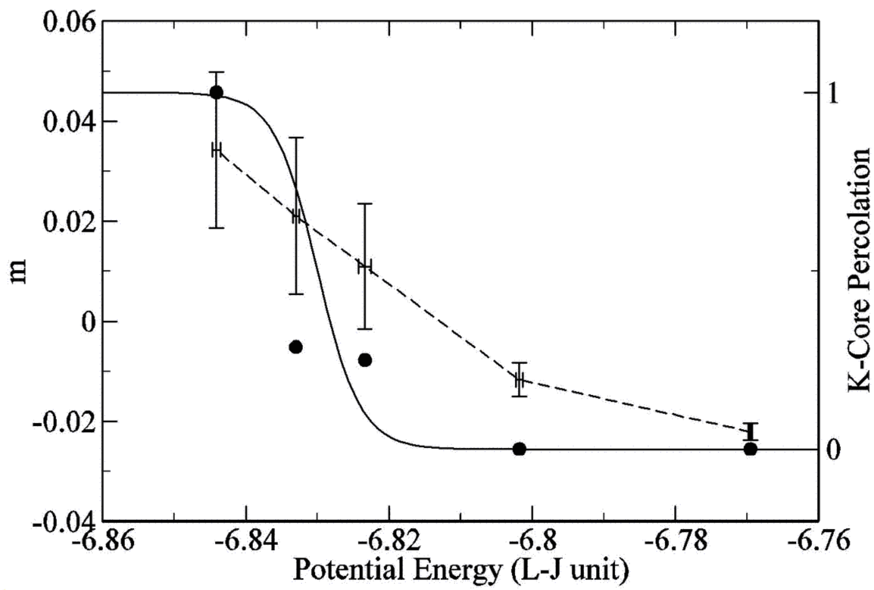
How does this vary with dimensionality?



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