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Simulating Plastic Localization in Metallic Glasses

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Outline

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- **Shear Bands In Amorphous Solids**
  - Structural Analysis
  - STZ Analysis
- **Fracture in Amorphous Solids**

Shear Bands in Metallic Glass

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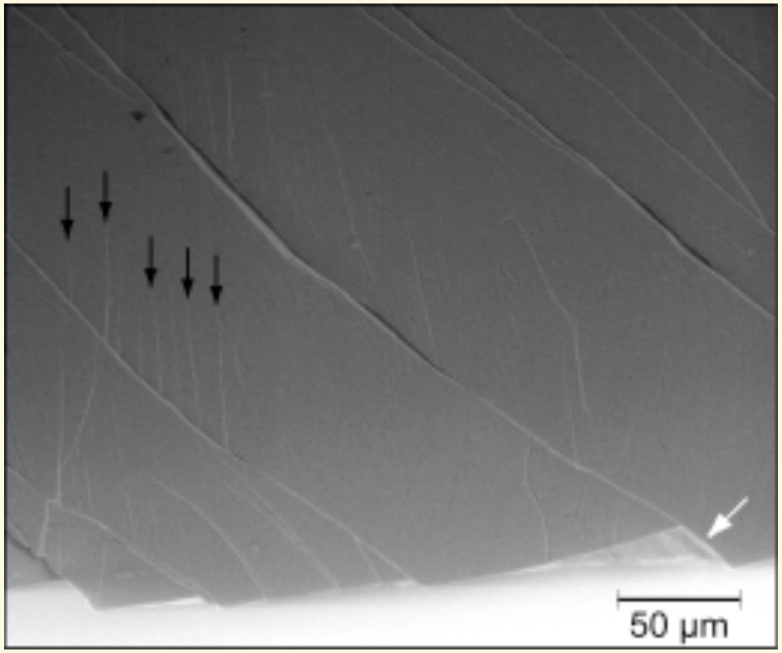
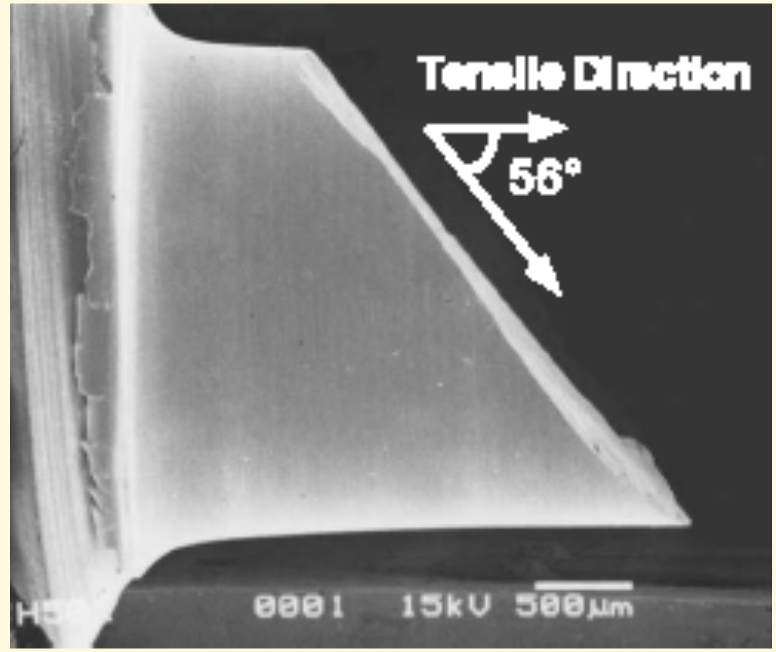
strain localization (shear banding) is the primary failure mode



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



Quasistatic Fracture Specimen
Mukai, Nieh, Kawamura, Inoue, Higashi (2002)

Indentation Testing of Metallic Glass

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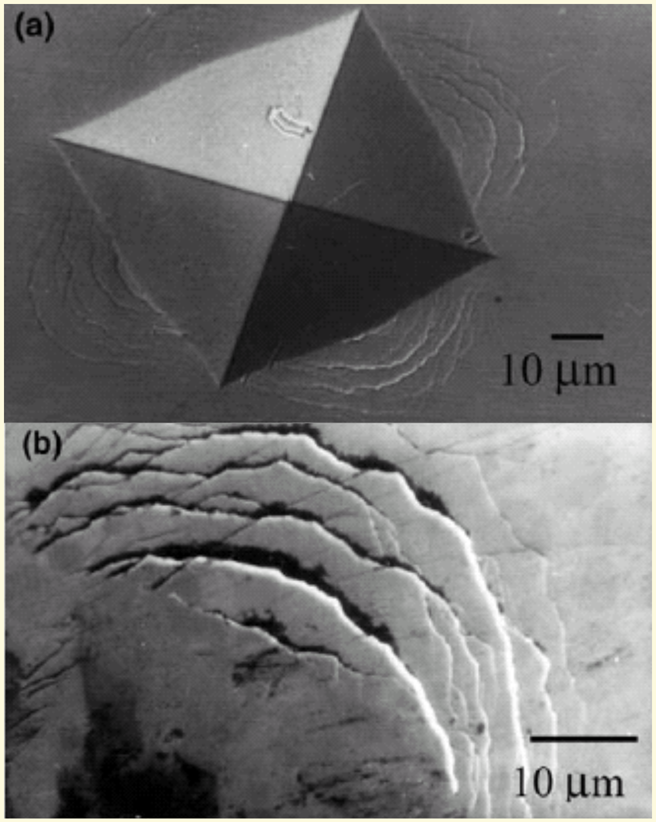
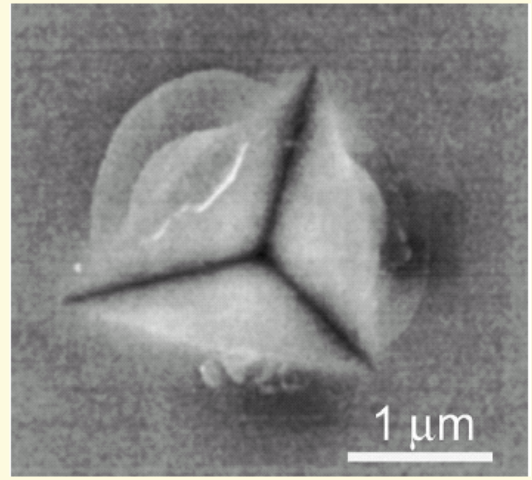


"Hardness and plastic deformation in a bulk metallic glass"
Acta Materialia (2005)
U. Ramamurty, S. Jana, Y. Kawamura, K. Chattopadhyay



"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

Simulated System: 3D Binary Alloy

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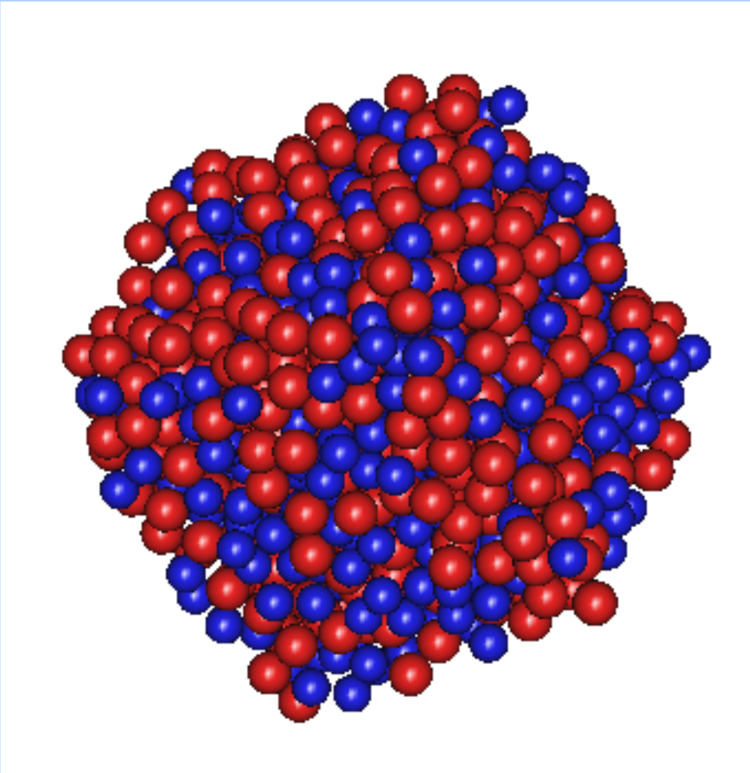

- **Wahnstrom Potential (PRA, 1991)**
- **Rough Approximation of $Nb_{50}Ni_{50}$**
- **Lennard-Jones Interactions**
- **Equal Interaction Energies**
- **Bond Length Ratios:**
  - $a_{NiNi} \sim {}^{5}/_{6}\, a_{NbNb}$
  - $a_{NiNb} \sim {}^{11}/_{12}\, a_{NbNb}$
- **T_g ~ 1000K**
- **Studied previously in the context of the glass transition (Lacevic, *et. al.* PRB 2002)**

- **Unlike crystalline systems, it is not possible to skip simulating the processing step**
- **Glasses were created by quenching at 3 different rates: 50K/ps, 1K/ps and 0.02 K/ps**

Metallic Glass Nanoindentation

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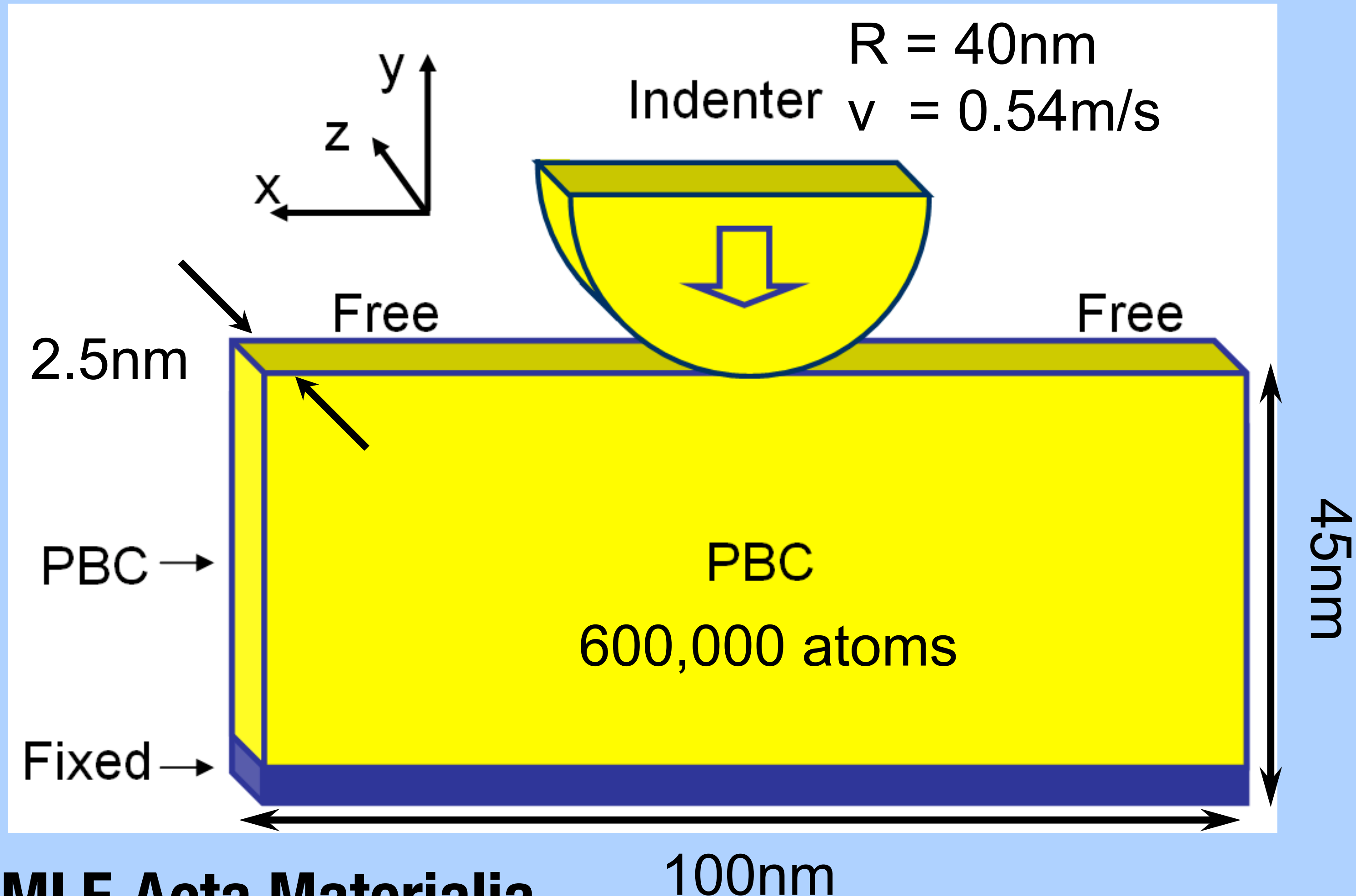
Simulations performed using molecular dynamics code across 64 nodes of a parallel cluster



Y. Shi, MLF, Acta Materialia, 55, 4317 (2007)

Metallic Glass Nanoindentation

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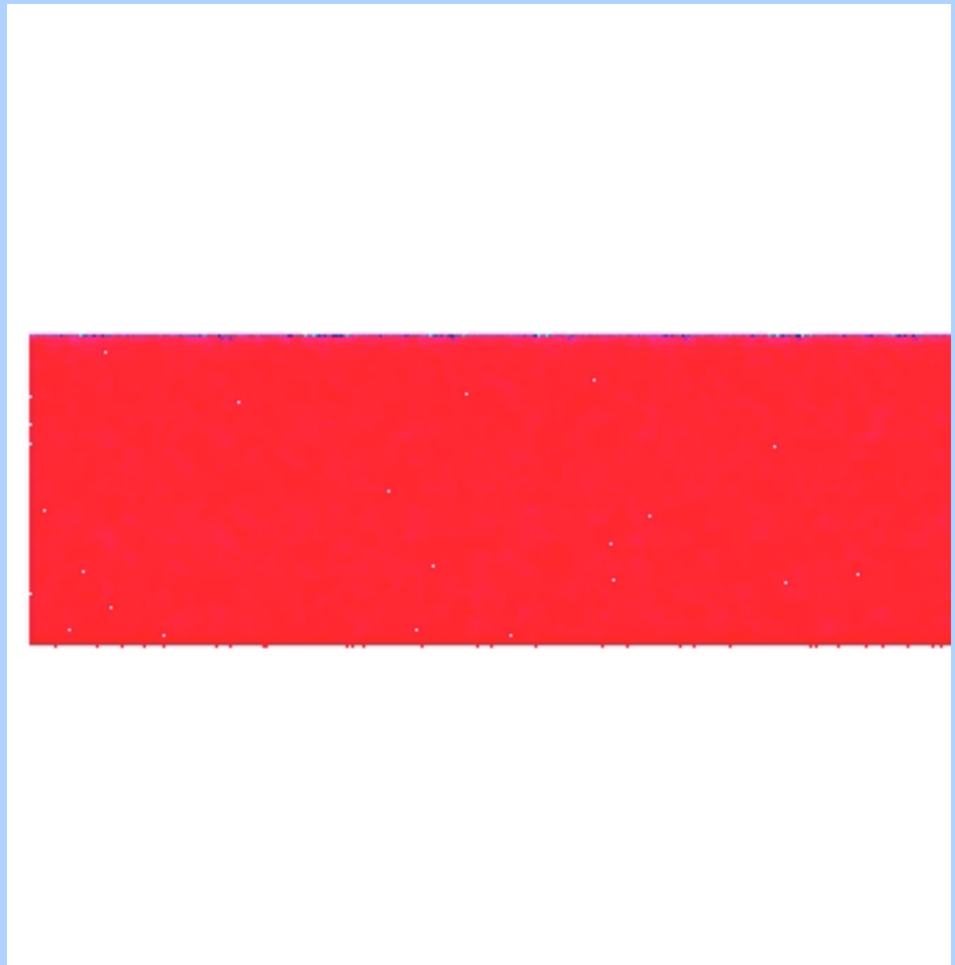
color = deviatoric strain

0%

40%



Y. Shi, MLF, Acta Materialia, 55, 4317 (2007)

Metallic Glass Nanoindentation

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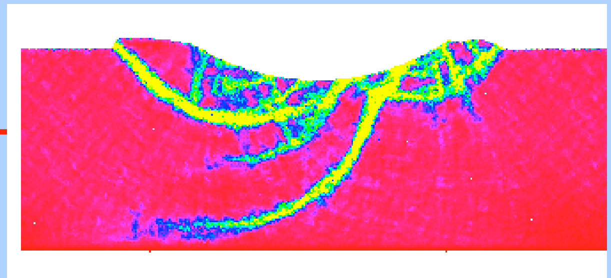
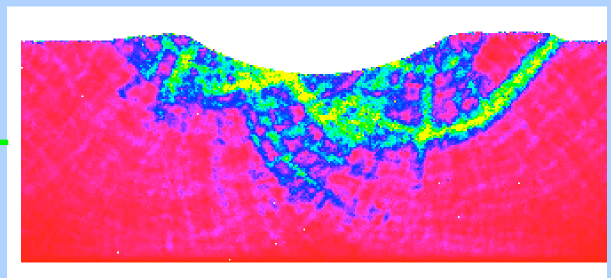
Sample I



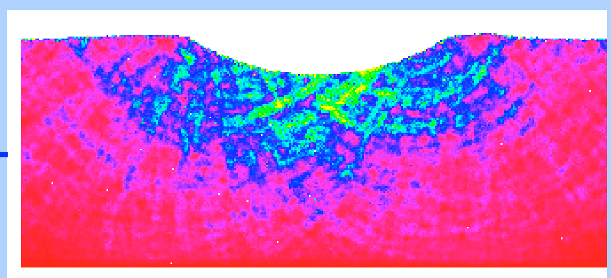
0.02 K/ps

Sample II

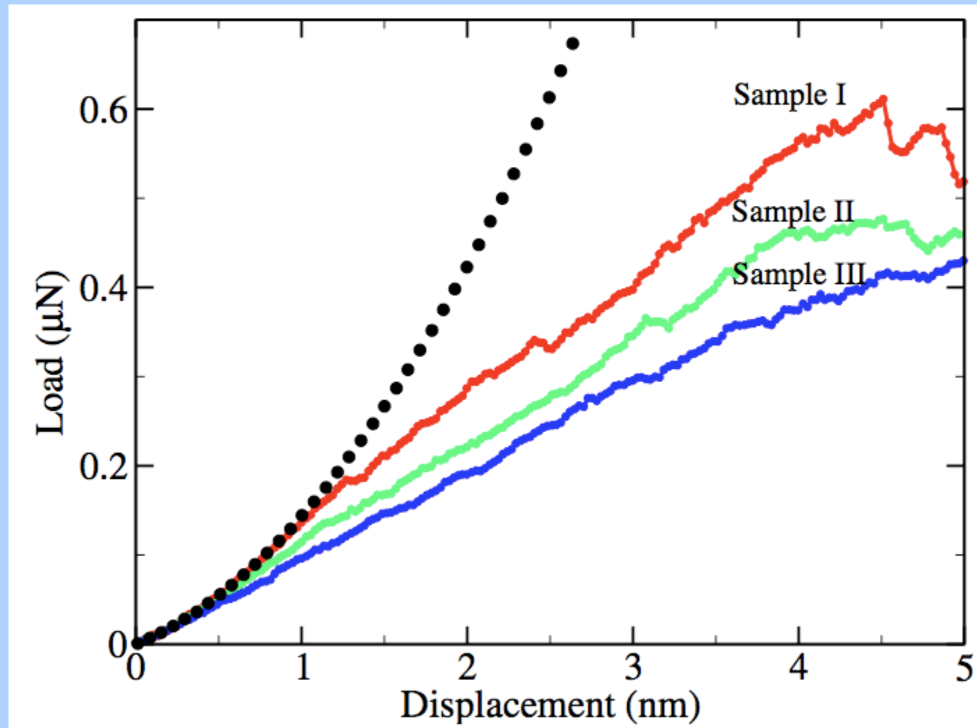


1K/ps

Sample III



50K/ps



Y. Shi, MLF, Acta Materialia, 55, 4317 (2007)

Metallic Glass Nanoindentation

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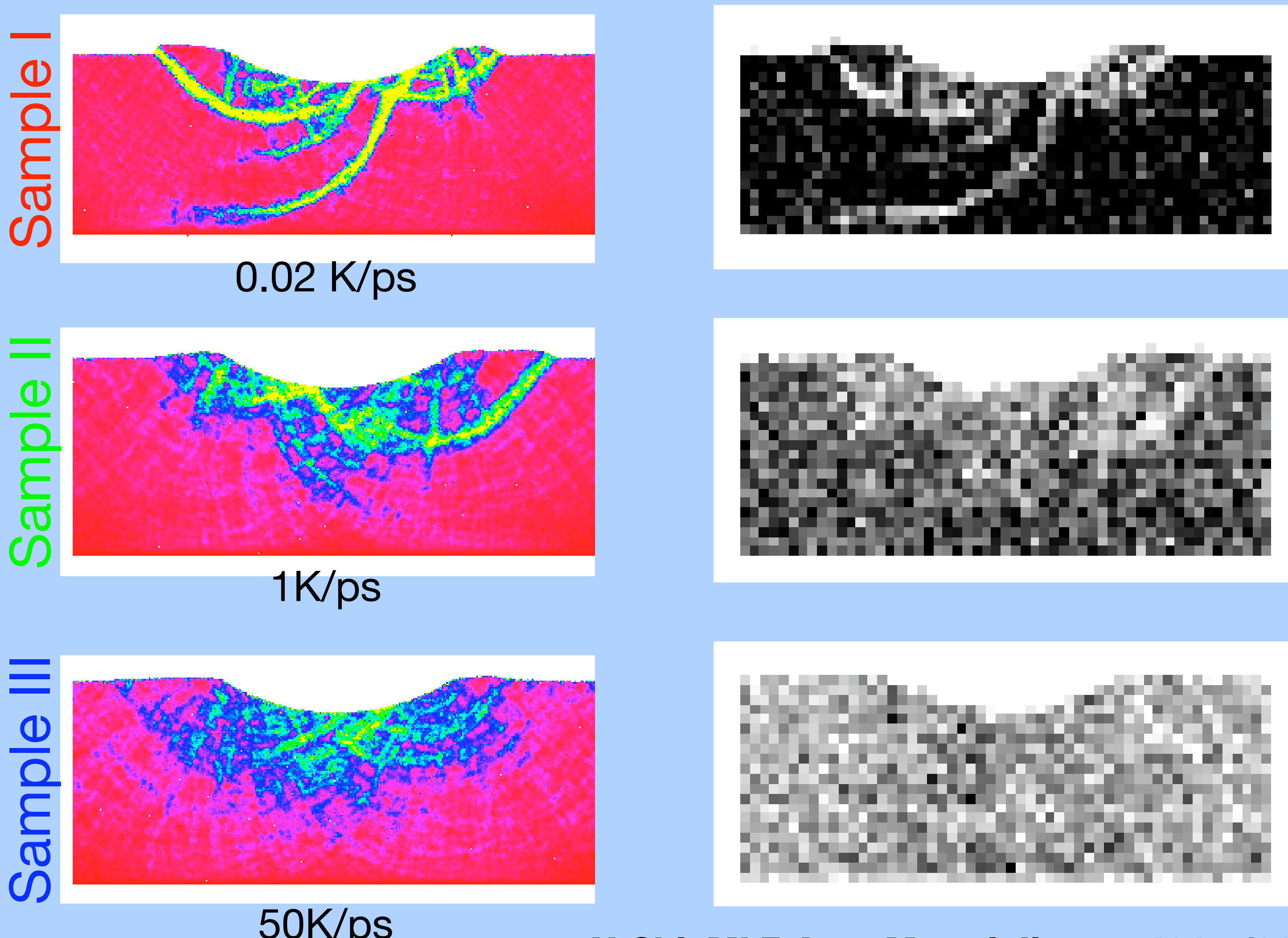

Y. Shi, MLF, Acta Materialia, 55, 4317 (2007)

2D Simulation System

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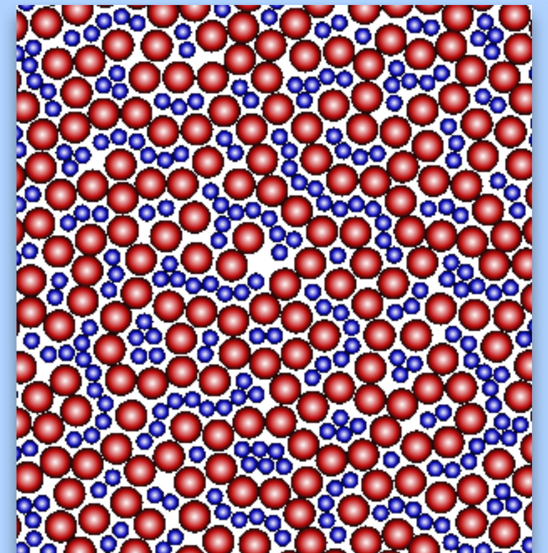
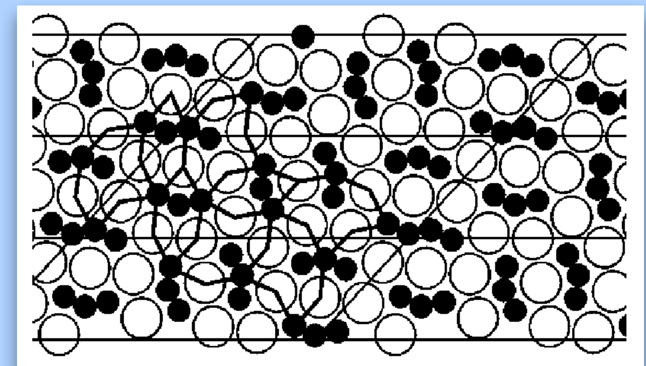
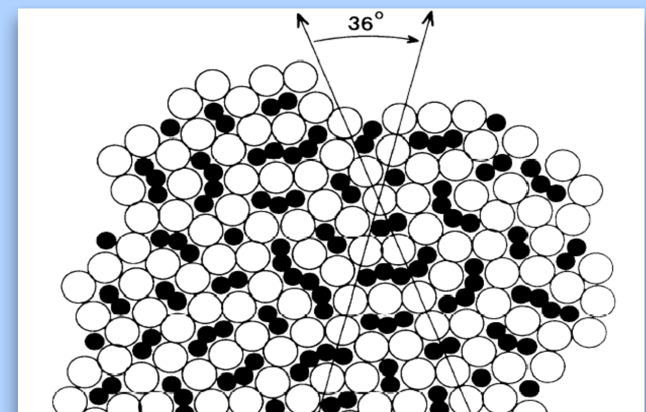


(Lancon et al, Europhys. Lett, 1986)



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
- $T_{MCT} \approx 0.325$

Quantifying the Dependence of Localization on Quench Rate (2D)

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- Performed 756 individual 2D uniaxial tensile test simulations at 0.1 T_g
- 10 different quench schedules starting from equilibrium liquids
- 6-10 samples at each quench schedule
- Each of these 84 specimens was tested at 9 different strain rates spanning 2 orders of magnitude

Quantification of Shear Localization

Deformation Participation Ratio

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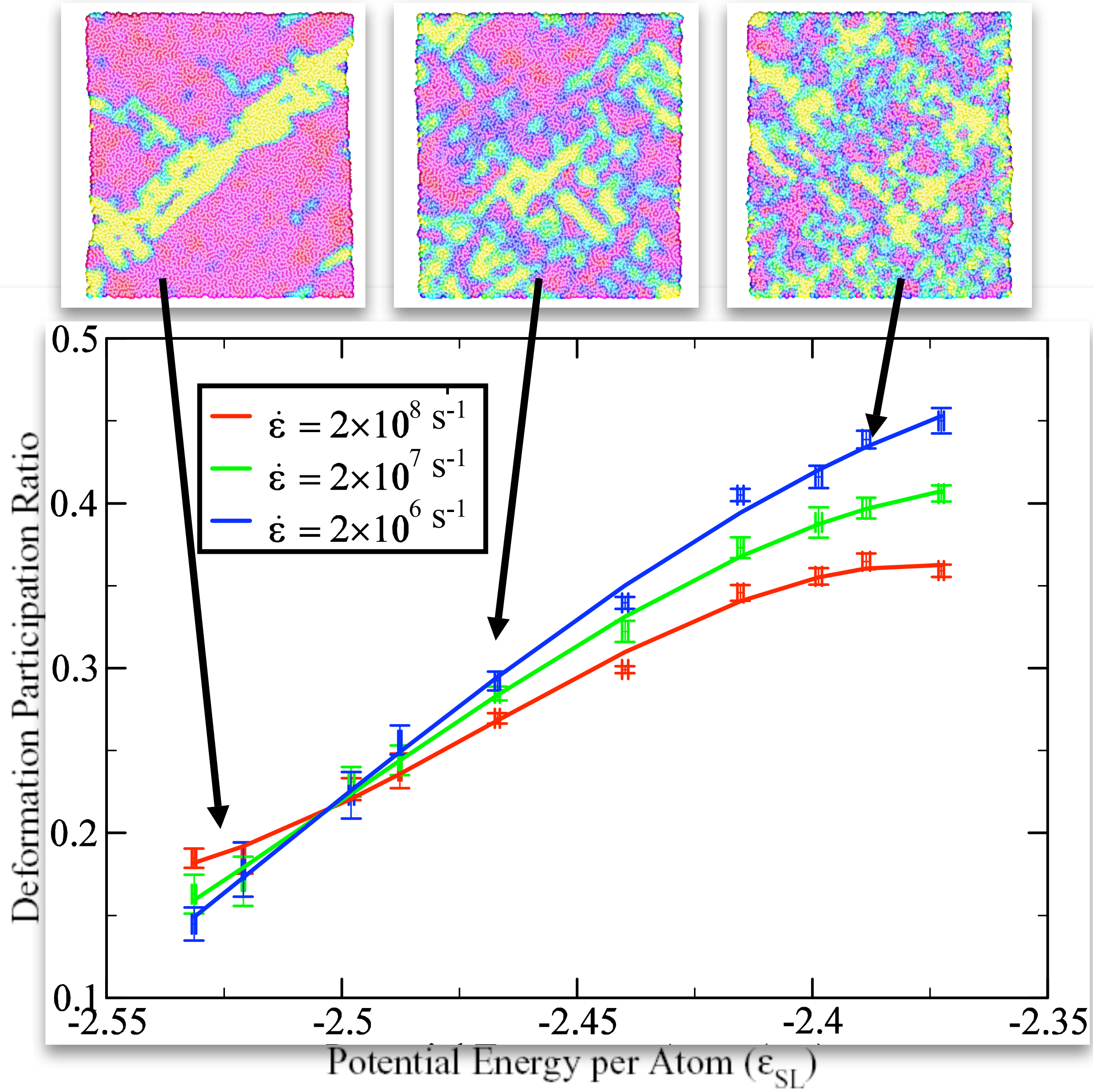
- Participation Ratio: Percentage of material with a local shear strain larger than the nominal strain
- Low strain rate favors homogenous deformation in instantaneously quenched samples
- Low strain rate favors inhomogeneous deformation in gradually quenched samples.

Shi and Falk, PRL (2005)



Strain-rate sensitivity of DPR

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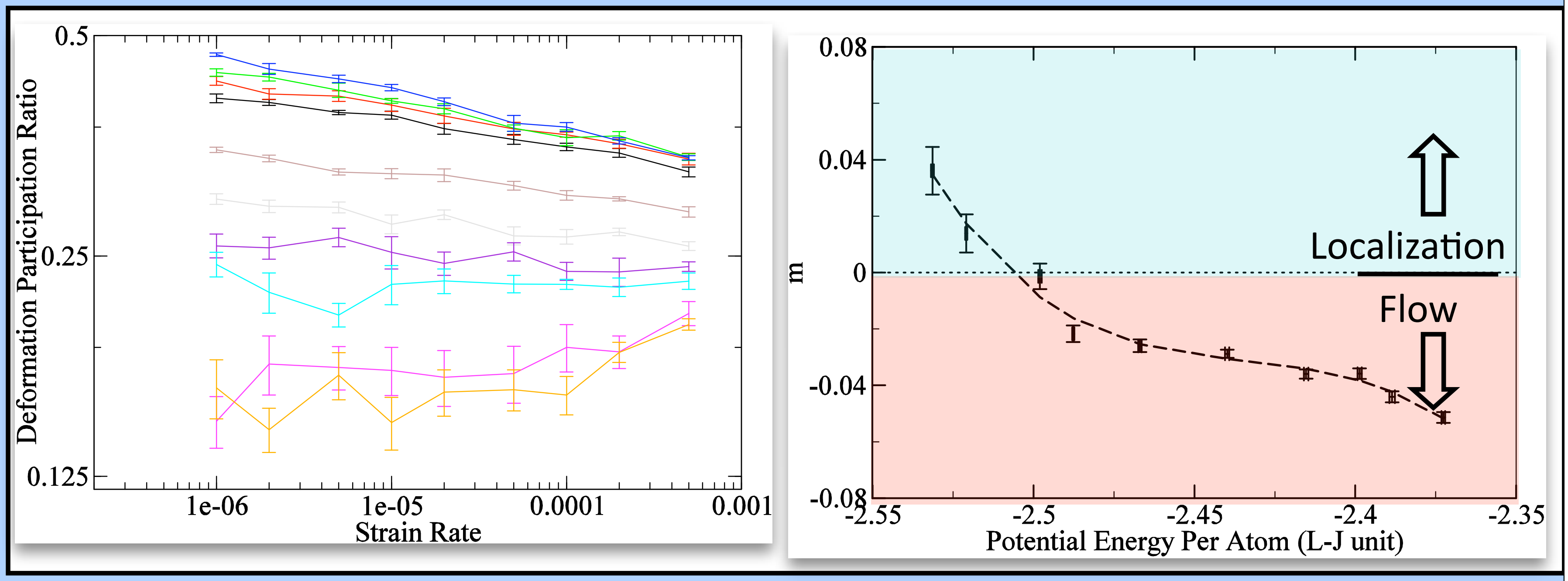

$$DPR \approx A\dot{\varepsilon}^{m}$$

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

$m < 0$: homogenous deformation

$m >= 0$: localized deformation

Shi and Falk, Scripta Mat (2005)

Local Structural Analysis

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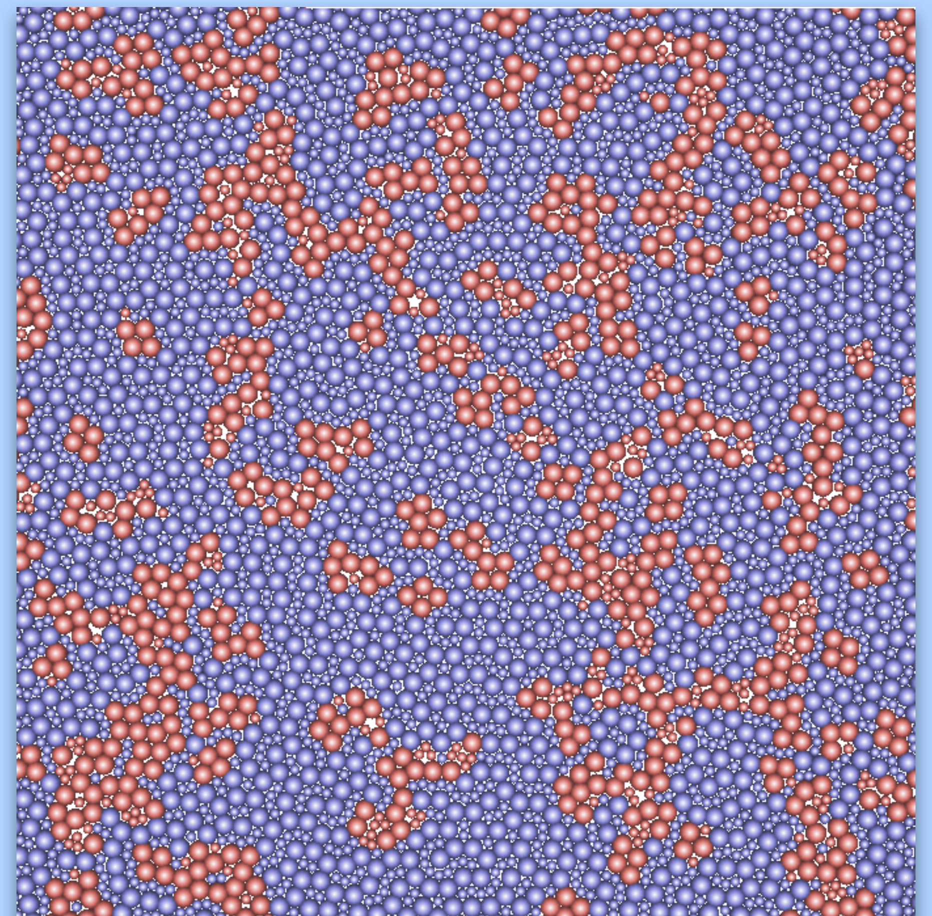
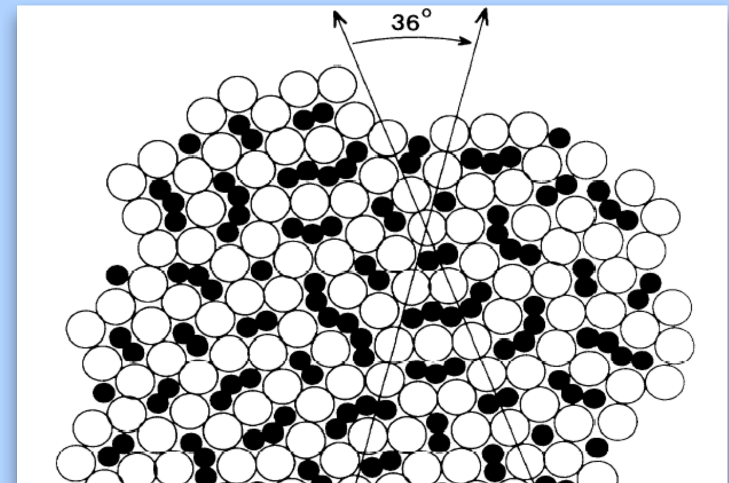
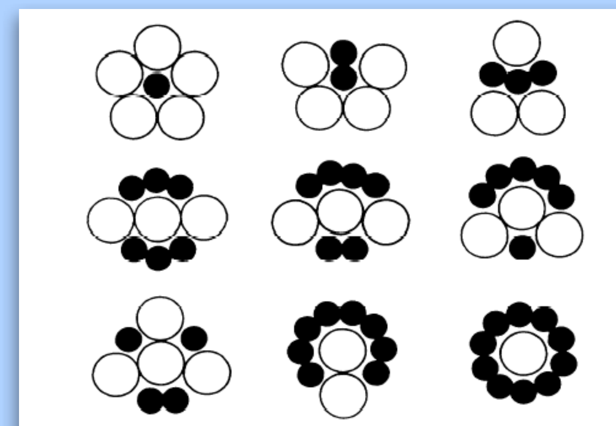




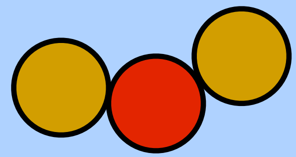
Widom, Strandburg, Swendsen (1987)



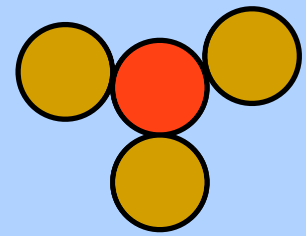
Complete set of low-energy local environments (Widom, 1987)

K-core Percolation of SRO

Serves as a simple approximation of rigidity percolation



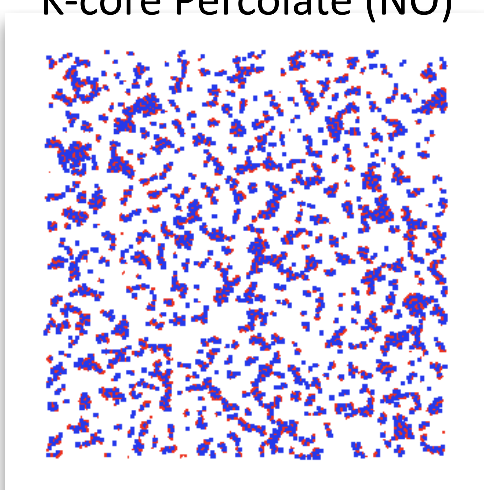
Mechanically unstable



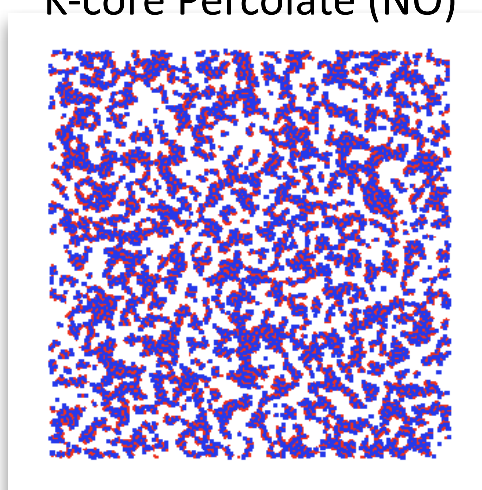
Mechanically stable

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

Percolate (NO)
K-core Percolate (NO)



Percolate (Yes)
K-core Percolate (NO)



Percolate (Yes)
K-core Percolate (Yes)

K-Core percolation and

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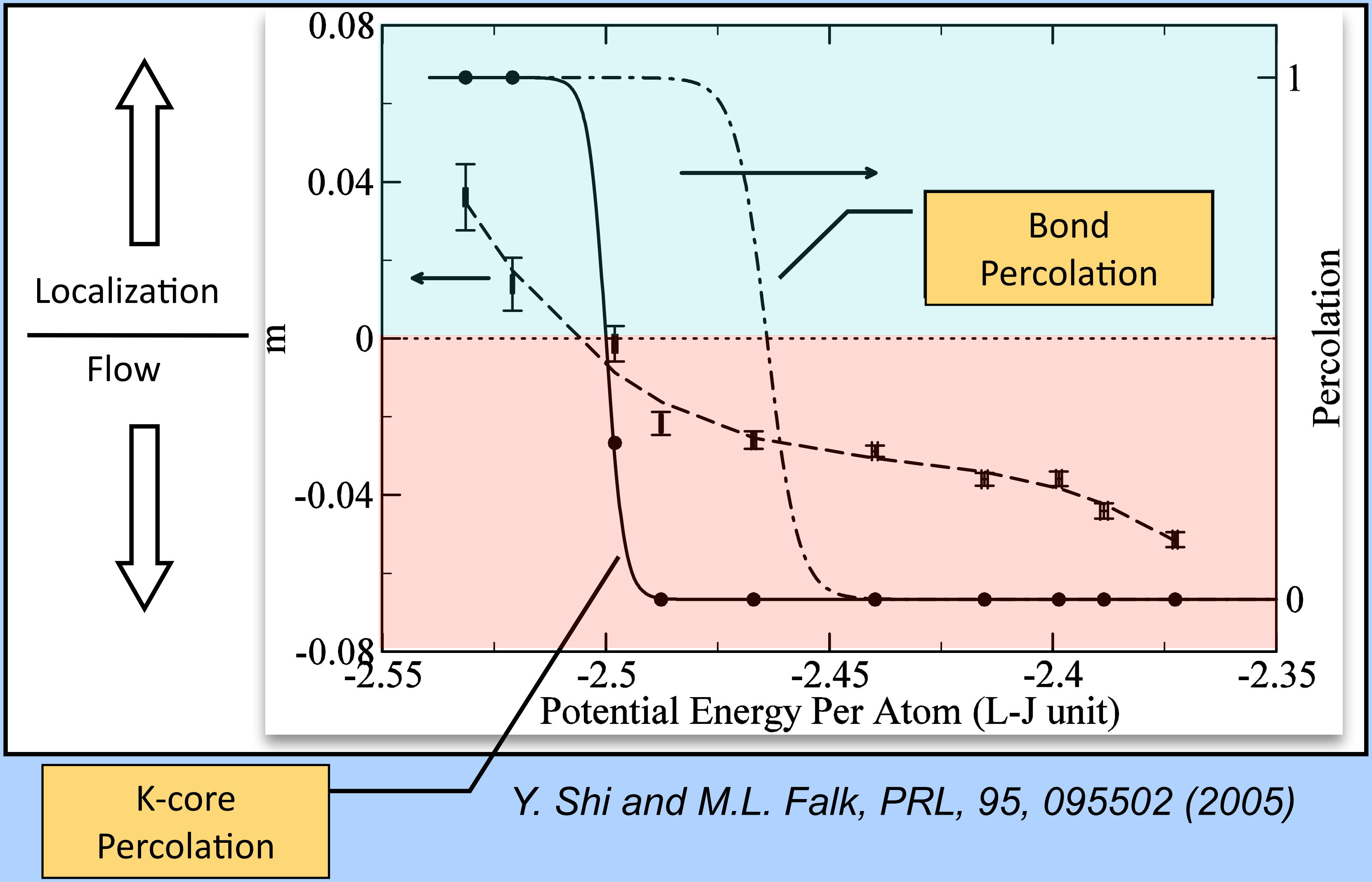

Y. Shi and M.L. Falk, PRL, 95, 095502 (2005)

3D Simulation Potentials

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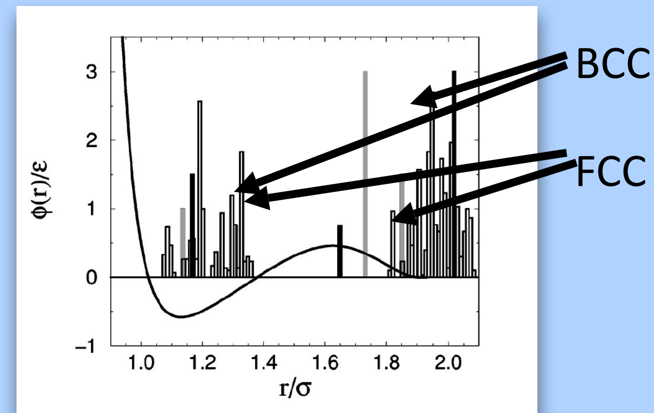
Dzugutov Potential

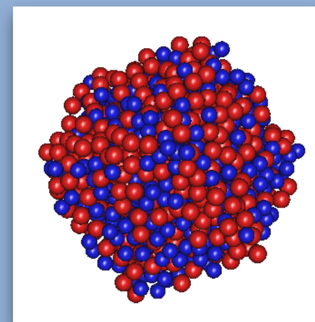


Roth and Denton, PRE (2000)

- 3D Monoatomic
- Energy penalties for crystalline phases
- Dodecagonal quasicrystal
- T_{MCT} @ 0.4

Zetterling et al., JNCS (2001)

Wahnstrom LJ Binary



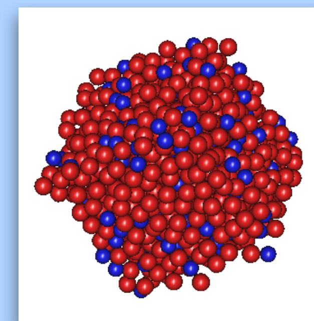
Bond length	Bond strength
AA 1.000	AA 1.0
AB 0.917	AB 1.0
BB 0.833	BB 1.0

- 3D binary LJ 12-6 potential
- 50:50 composition, 144,000 atoms
- T_{MCT} @ 0.57

Wahnstrom, PRA, 1991

Lacevic et al., PRB, 2002

Kob-Andersen LJ Binary



Bond length	Bond strength
AA 1.00	AA 1.0
AB 0.80	AB 1.5
BB 0.88	BB 1.0

- 3D binary LJ 12-6 potential
- 80:20 composition, 144,000 atoms
- T_{MCT} @ 0.435

Kob and Andersen, PRE 1995

3D Uniaxial Compression Test

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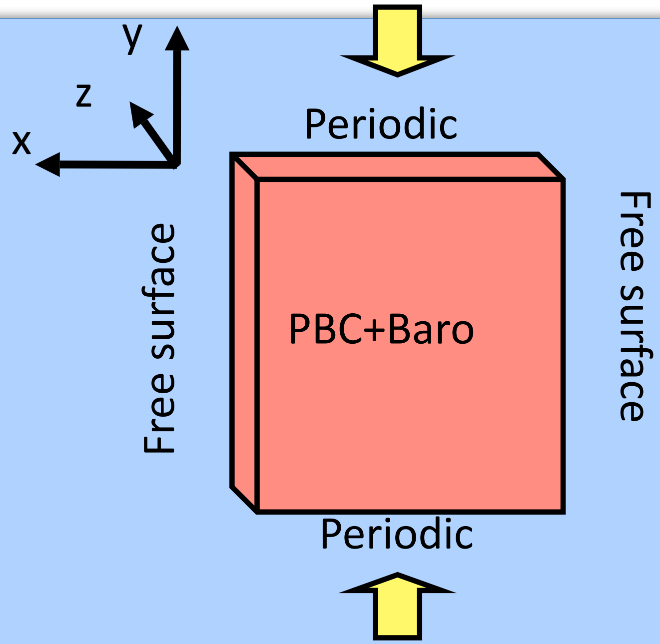
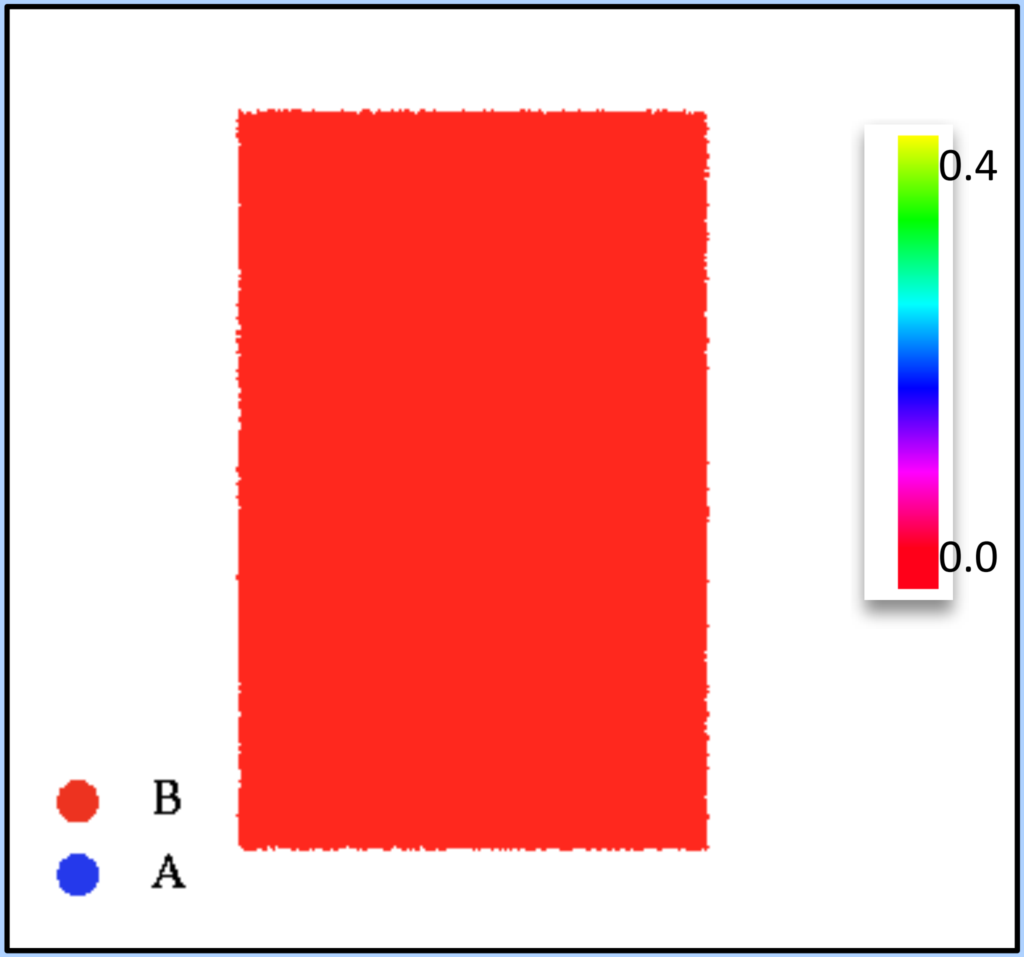


- Thin slab geometry to maximize in-plane spatial dimension 75×110 ×15: 140,000 atoms
- Free surfaces in Y-Z
- PBC in X-Y and Y-Z
- Plane Strain: Average σ_{zz} zero



3D Uniaxial Compression
Various Quench Times

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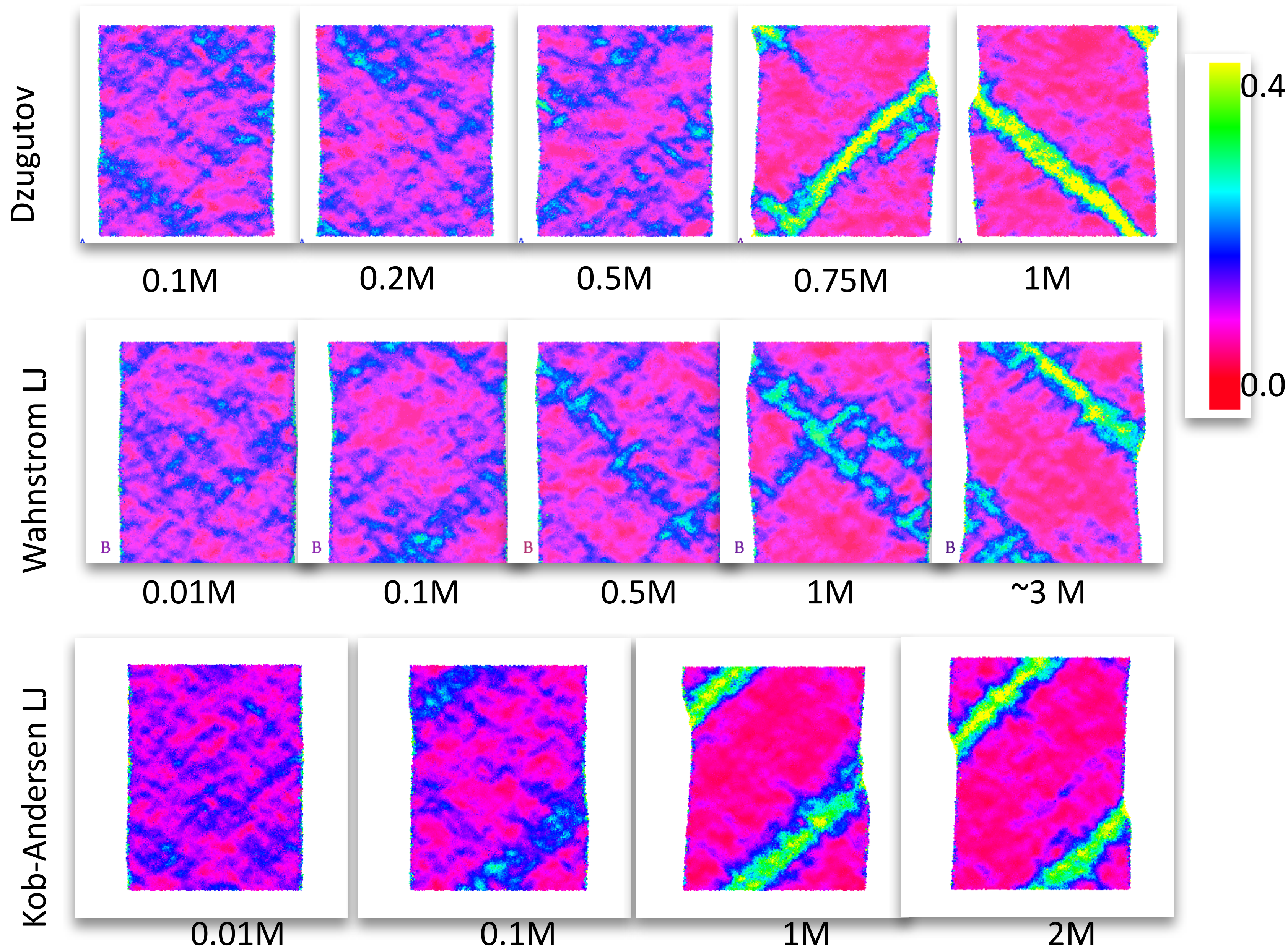

DPR and Strain Rate Sensitivity

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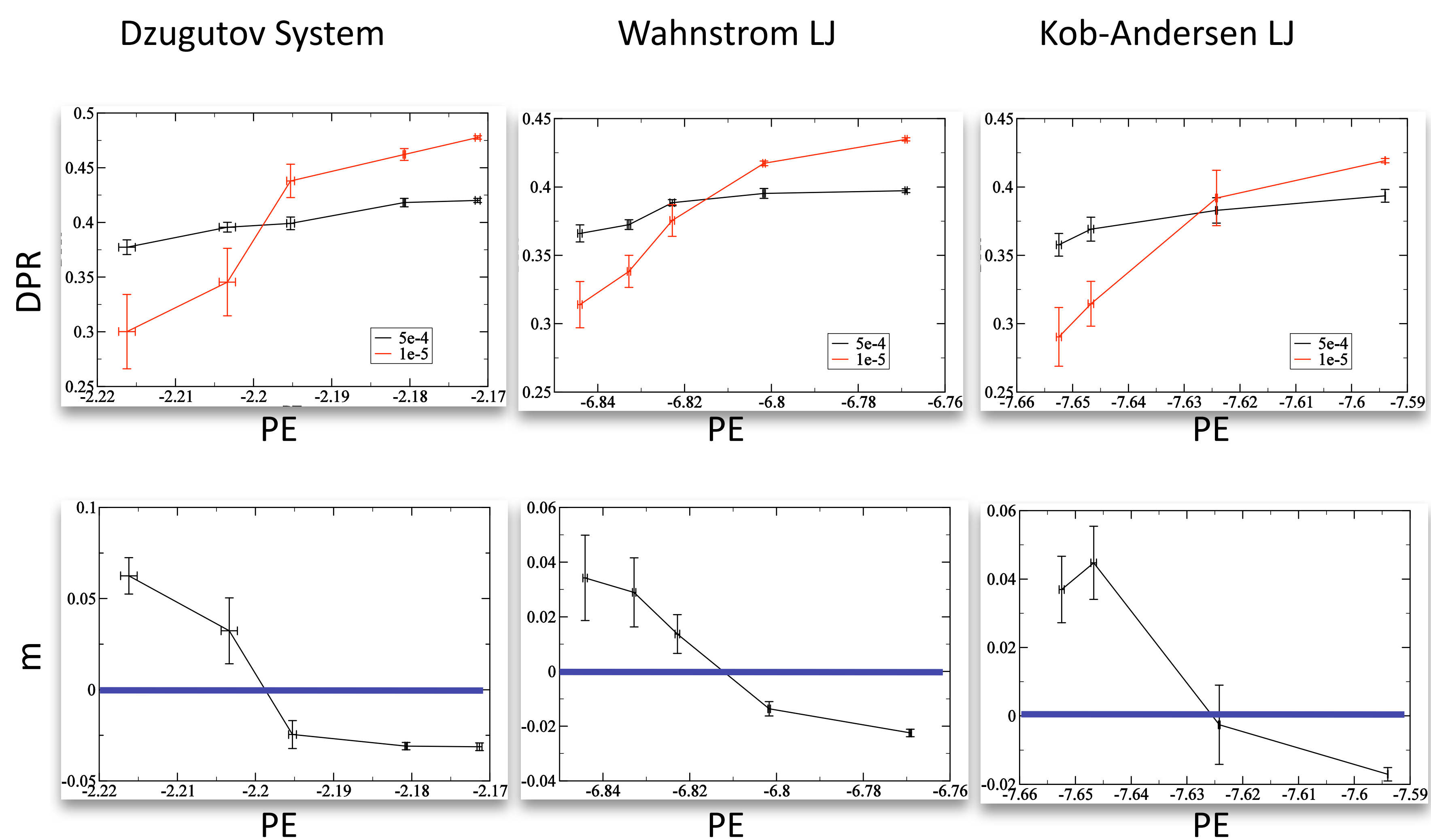

Triangulated Coordination Shell Analysis of SRO

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Triangulated Coordination Shells: Bonds by atoms within the coordination shell form only triangles. The center atom and the triangle has to form a space dividing tetrahedral.

Criterion: (From Euler's formula)

$$\sum_q (6-q)v_q = 12$$

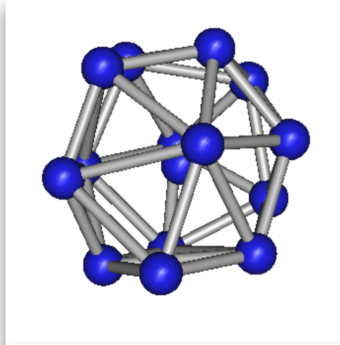
q is the surface coordination number (from 3 to 8 for now)

v_q is the count of neighbors has surface coordination number q

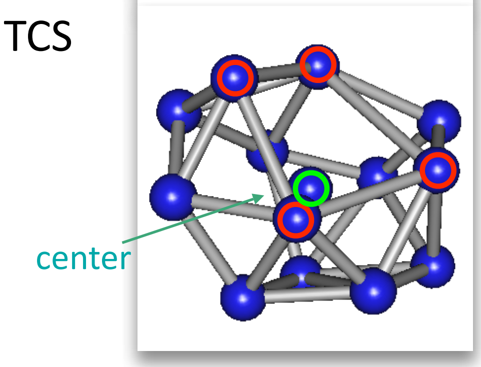
Glassy samples with lowest quenching rate

	TCS	Icosahedra
Dzugutov	25%	12%
Wahnstrom	13%	10%
K-A	3%	0.1%

TCS

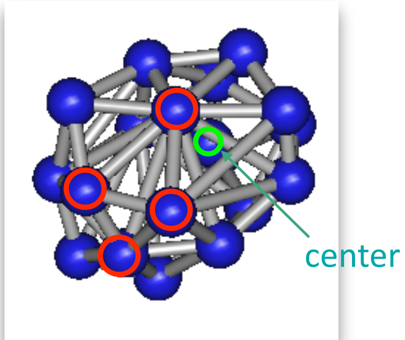


NOT TCS



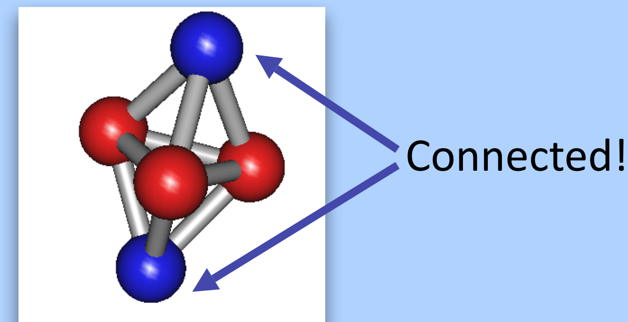
The four red atoms are forming a non-planar quadrilateral not a triangle

NOT TCS



The tetrahedra formed by 4 red atoms does not include the center atom (green)

3D Percolation Analysis



Two atoms sharing at least three atoms are “connected”

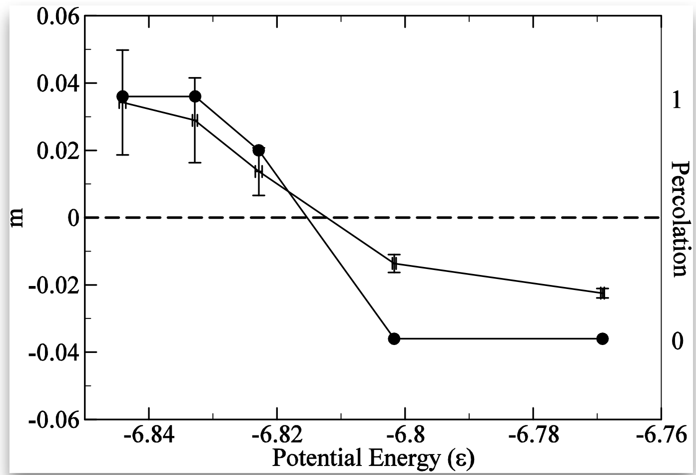
The cage of two atoms have to interpenetrate or sharing faces

Similar to Zettering, et al, JNCS, 2001

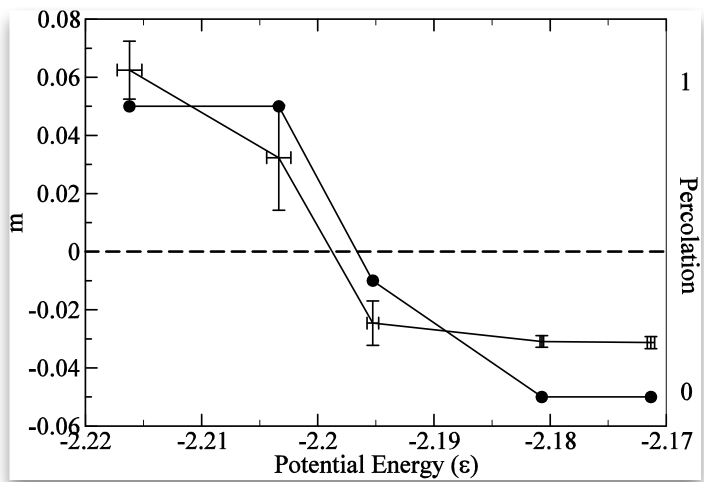
DZ: (all percolate)

KA: (none percolate)

WA system (TCS SRO)



DZ system (Icosahedral SRO)



Short Range Order and Shear Bands

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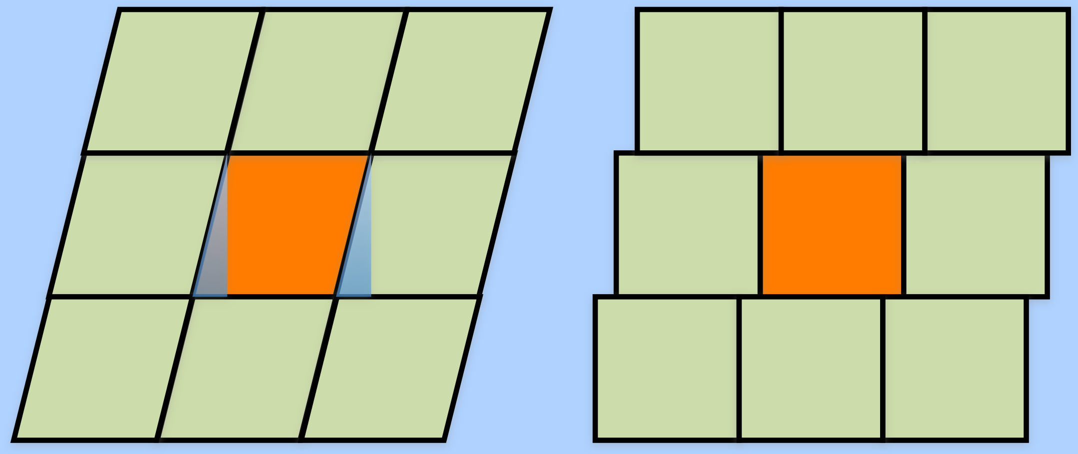
- Simulated glasses with higher degrees of topological SRO demonstrate a stronger tendency to localize strain.
- In more rapidly quenched samples localization **decreases** at lower strain rates.
- In more slowly quenched samples localization **increases** at lower strain rates.
- The transition from homogeneous to localized deformation in the quasi-static limit appears to correspond to the **percolation of a backbone of SRO**.
- How to unambiguously define the appropriate measure of SRO or MRO for a given system **remains an open question**.

Y. Shi and M.L. Falk,
Physical Review Letters, 95, 095502 (2005)
Physical Review B, 73, 214201 (2006)
Acta Materialia, 55, 4317 (2007)

MD with Periodicity

- Simple shear is imposed maintaining periodicity using Lees-Edwards boundary conditions



- Simultaneously couple to a heat bath throughout so T is always much less than T_g.

Simulations in Simple Shear (2D)

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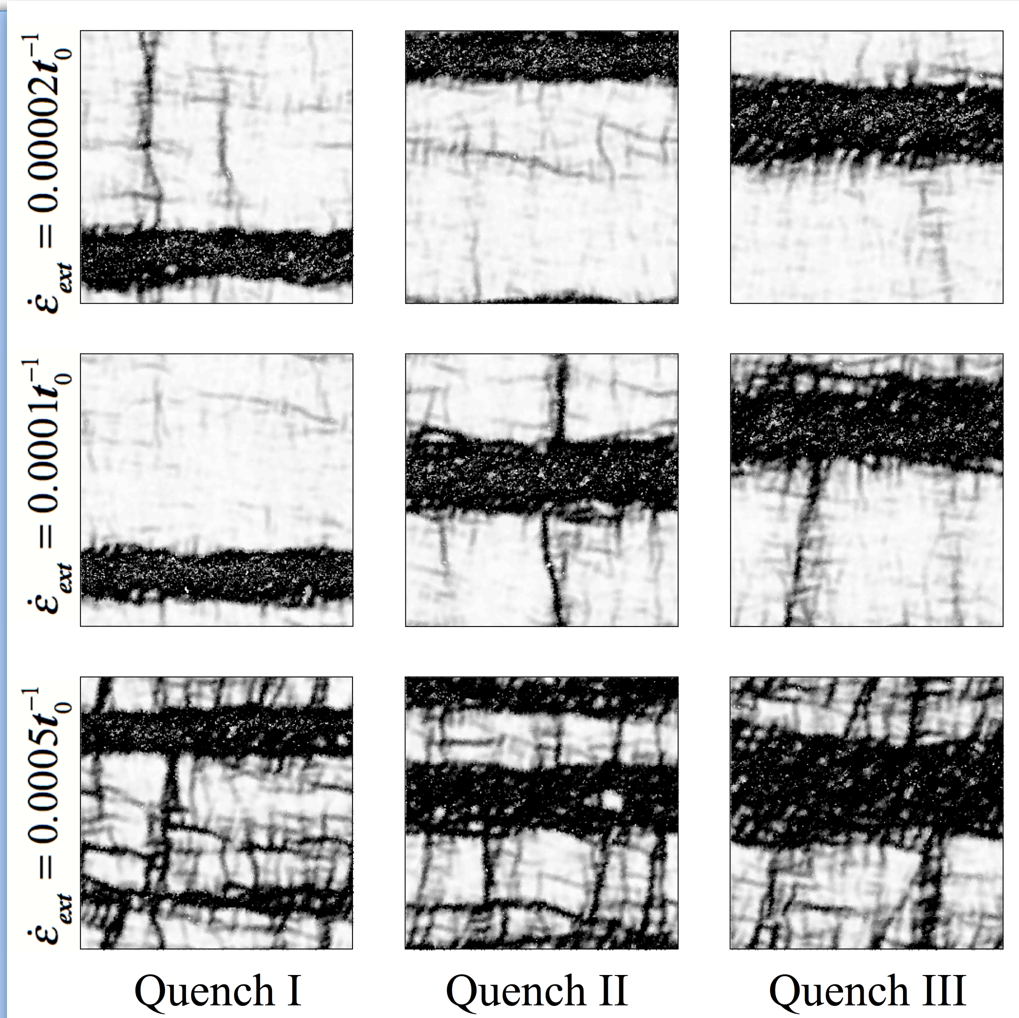

Cumulative strain up to 50% macroscopic shear

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

2D Simple Shear: Broadening

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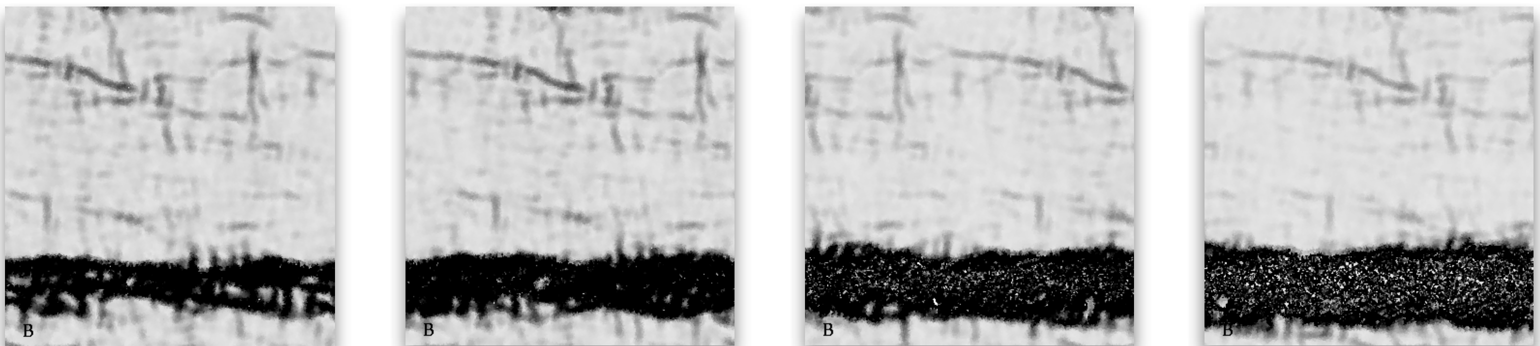
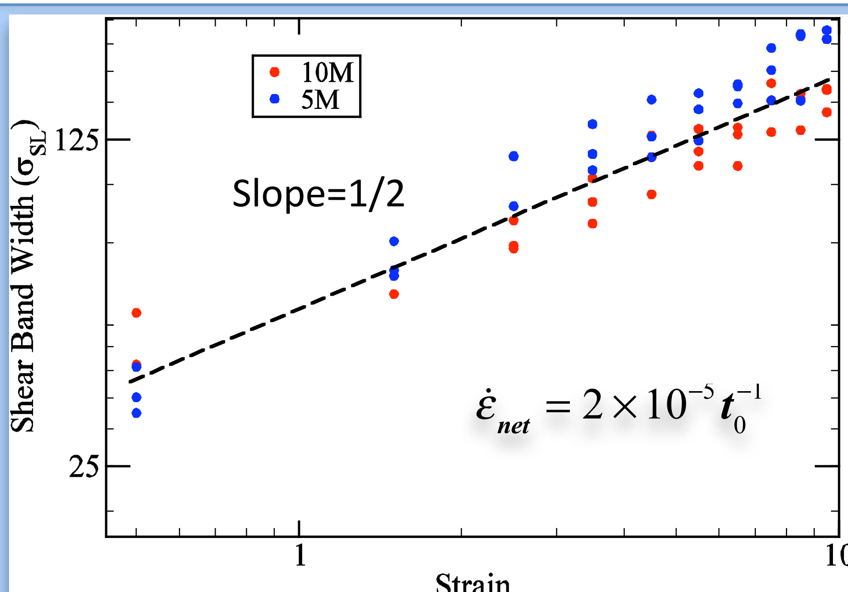


10% 20% 50% 100%



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

Development of a Shear Band

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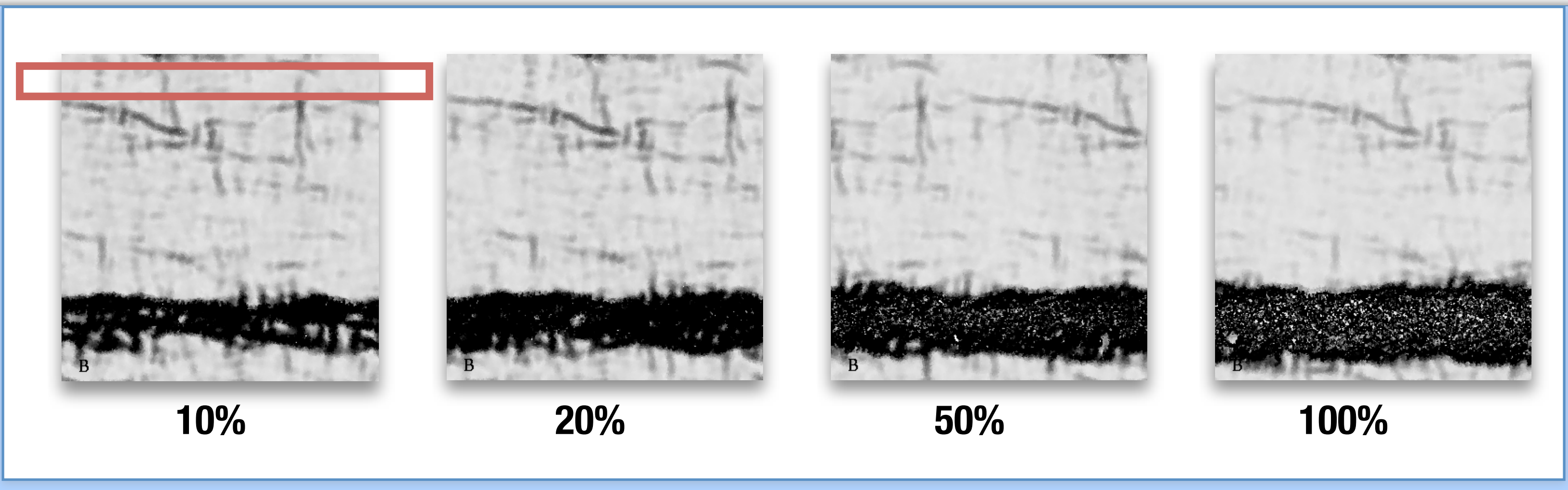

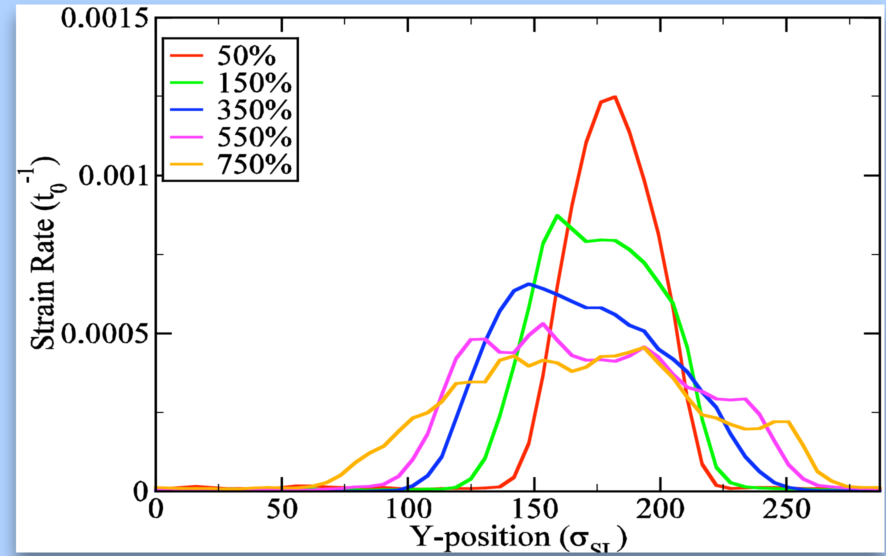

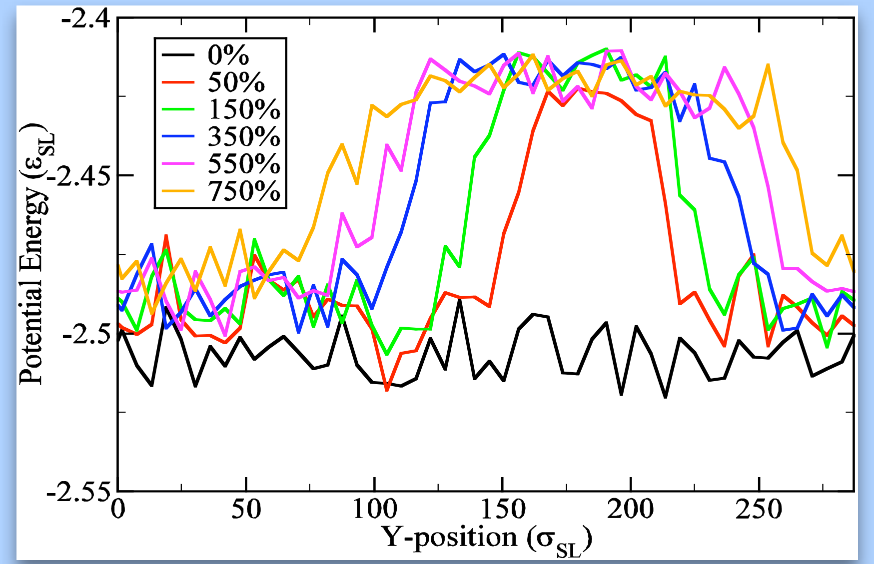

Y Shi, MB Katz, H Li, MLF, PRL, 98, 185505 (2007)

The STZ Model

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Recall the STZ Equations

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

We had derived an expression for Γ

$$\Gamma = \frac{\mathcal{C}(s) \left[s - \xi(m) \right] \left[\mathcal{T}(s) - m \right] + \Gamma^T}{1 - m\xi(m)}$$

Where $\psi'(m) = \xi(m) = \mathcal{T}^{-1}(m)$

Let's now recall where χ comes from.

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**

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

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

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

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**

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

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)

Effective Temperature In STZ

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- While Λ and m relax relatively quickly to equilibrium values that depend on the applied stress, we know that there exist longer time scales at work in glasses.
- Langer proposed that this ratio between annihilation and creation, $e^{-1/\chi}$, is controlled by the present structure of the glass.
- χ represents an "effective temperature", which evolves with the structure of the glass.

Effective Temperature In STZ

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- In equilibrium, the number of STZs would have to be set by the bath temperature and $\chi = k_B T / E_Z$.
- When the glass is quenched slow relaxation may result in a value of χ above the thermal equilibrium value.
- Dissipation, due to shearing, may raise χ to some upper, strain rate dependent value.
- Here we used a simplified χ dynamics, but an improved form has been proposed by Haxton and Liu (PRL 99, 195701 (2007)) and further developed by Manning and Langer (Phys. Rev. E 76, 056107 (2007)).

Testing Theories of Plastic Deformation

(Falk and Langer (1998), Falk, Langer and Pechenik (2004), Heggen, Spaepen, Feuerbacher (2005), Langer (2004), Lemaitre and Carlson (2004))

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- Is there an intensive thermodynamic property (called χ here) that controls the number density of deformable regions (STZs)?

$$n_{STZ} \propto e^{-1/\chi}$$

- This would be an "disorder temperature" that characterizes structural degrees of freedom quenched into the glass.

$$\dot{\epsilon}_{ij}^{pl} = e^{-1/\chi} f_{ij}\left(s_{kl}\right)$$

$$c_0 \dot{\chi} = 2 s_{ij} \dot{\epsilon}_{ij}^{pl} \left(\chi_{\infty} - \chi\right) - \kappa(T) e^{-\beta/\chi}$$

mechanical disordering

thermal annealing

Disorder Temperature T_d

$$\chi \equiv \frac{kT_d}{E_Z}$$

Free Volume v_f

$$\chi \equiv \frac{v_f}{V^*}$$

Relating χ to the microstructure

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

$$C_1\chi = PE - PE_0$$

$$\dot{\varepsilon}_{pl} = e^{-1/\chi} f(s)$$

$$c_0\dot{\chi} = 2s\dot{\varepsilon}_{pl}(\chi_\infty - \chi) - \kappa e^{-\beta/\chi}$$

- Is there an underlying scaling?

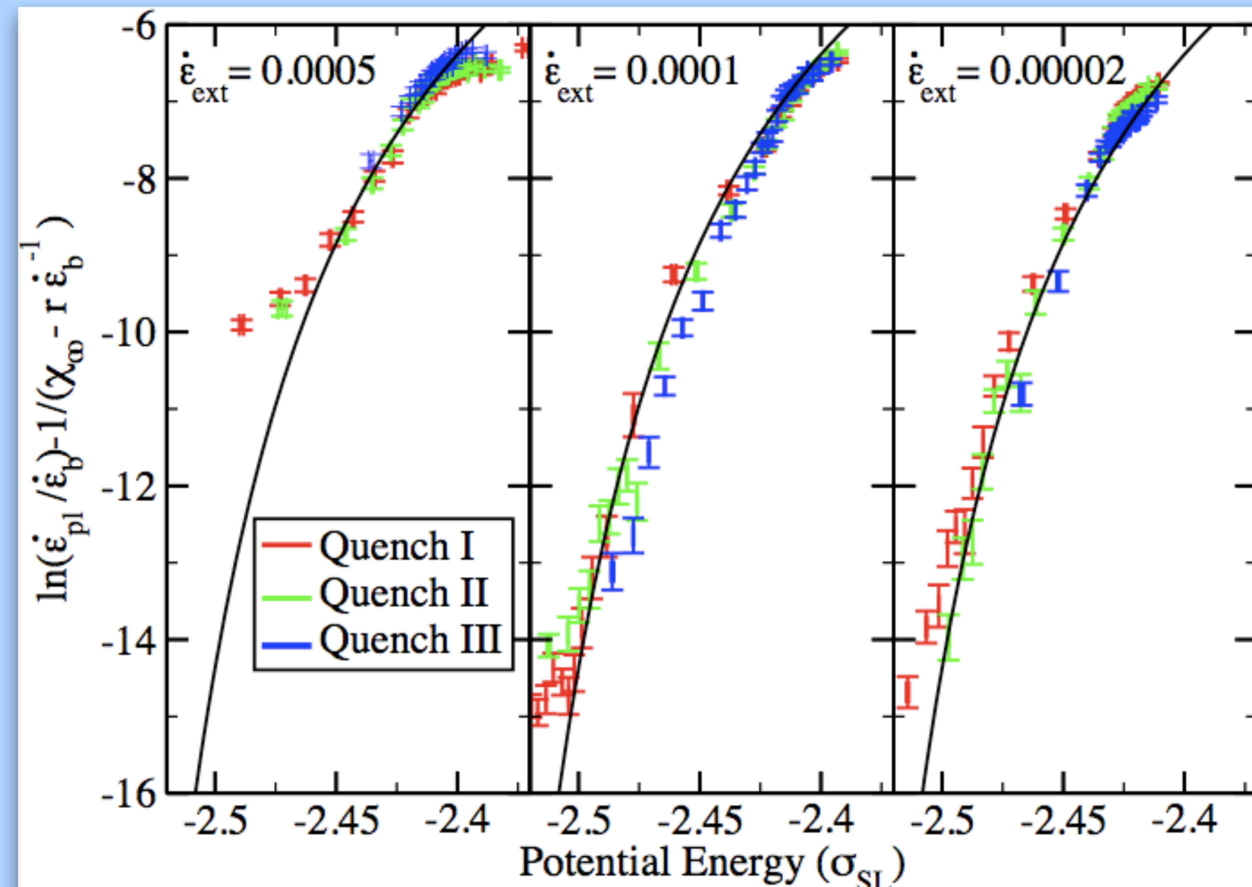
$$\frac{\dot{\varepsilon}_{pl}(y)}{\dot{\varepsilon}_b} = e^{1/\chi_b - 1/\chi(y)}$$

$$ln\left[\frac{\dot{\varepsilon}_{pl}(y)}{\dot{\varepsilon}_b}\right] = \frac{1}{\chi_b} - \frac{C_1}{PE - PE_0}$$

$$2s\dot{\varepsilon}_b(\chi_\infty - \chi_b) = \kappa e^{-\beta/\chi_b}$$

$$ln\left[\frac{\dot{\varepsilon}_{pl}(y)}{\dot{\varepsilon}_b}\right] - \frac{1}{\chi_\infty - r\dot{\varepsilon}_b^{-1}} = -\frac{C_1}{PE - PE_0}$$

Scaling verifies the hypothesis



- **Assuming,** $\chi_\infty = \frac{kT_g}{E_Z}$, E_Z=1.9ε

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

Implications for Constitutive Models

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- To model the band a length scale must enter the constitutive relations

$$\partial_t \chi = \frac{2s\dot{\varepsilon}_{pl}}{c_0}\left(\chi_\infty - \chi\right) \quad \Longrightarrow \quad \partial_t \chi - D\partial_x^2 \chi = \frac{2s\dot{\varepsilon}_{pl}}{c_0}\left(\chi_\infty - \chi\right)$$

Numerical Results

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

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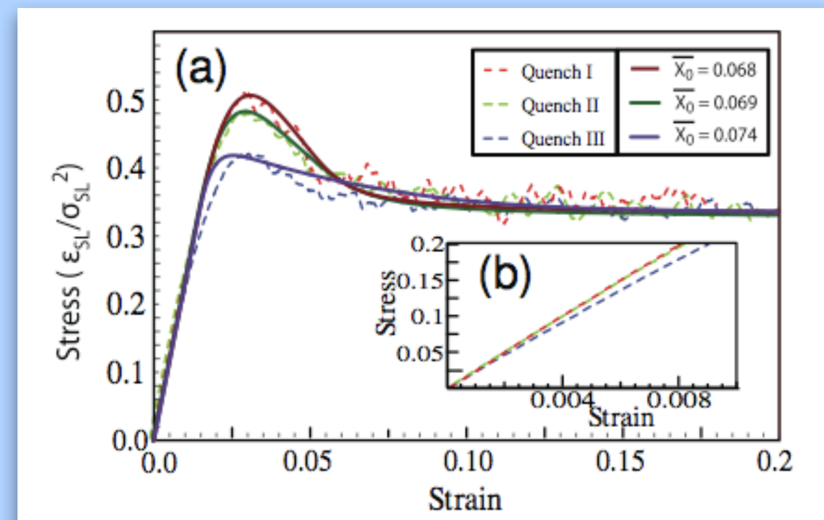
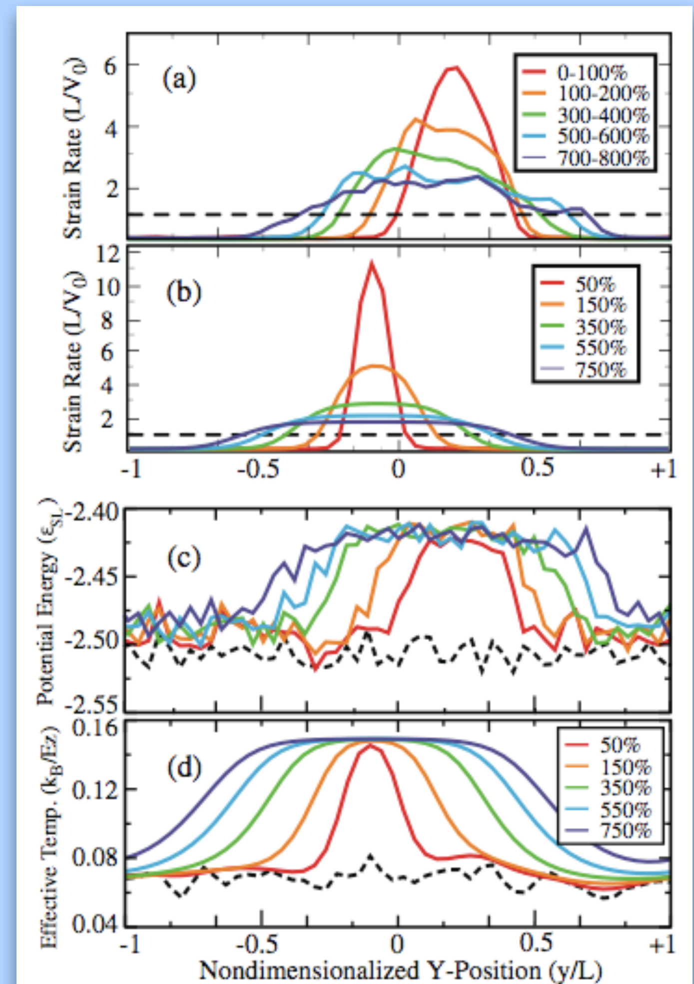
- **These equations closely reproduce the details of the strain rate and structural profiles during band formation**





More Analysis by Manning, et al.

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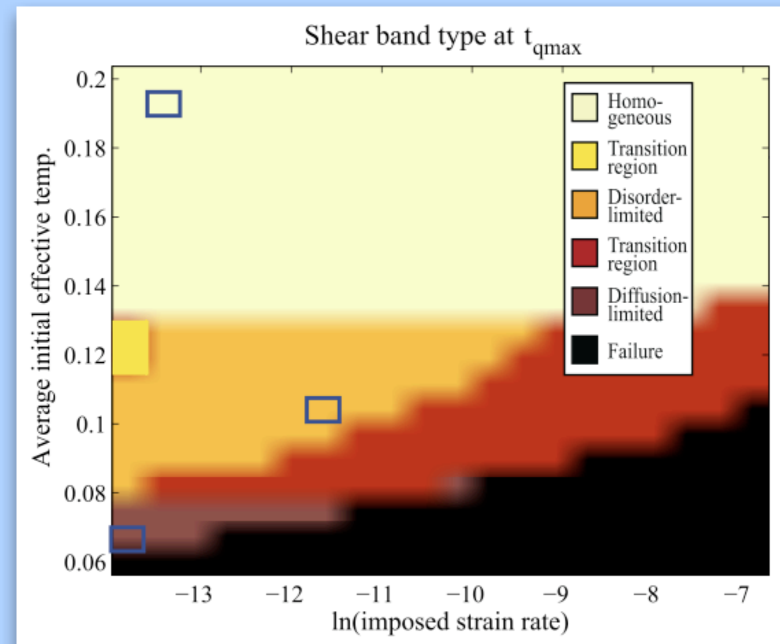
Manning, Daub, Langer, Carlson, Phys. Rev. E 79, 016110 (2009)

- **Incorporates the Haxton-Liu effective temperature dynamics and shear rate dependent diffusivity.**
- **Identifies 3 failure modes:**
  - Diffusion limited bands
  - Disorder limited bands
  - Failure/Fracture/Melting



Summary

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- Shear bands in metallic glasses arise due to **mechanical softening** caused by disordering.
- A **percolating backbone of short range order** appears to be necessary for localization to dominate at low shear rates.
- No unique means exists for characterizing the geometric character of this short range order for a known alloy description.
- Analysis of the transition from flow to jammed material in a shear band reveals that **potential energy per atom may be a good measure of "effective temperature"**.
- The **proportionality of strain rate to** $\exp(-1/\chi)$ has been tested and appears to hold.
- The data also indicates that the **energy to create an STZ** is about 2 bonds per STZ.