WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

Plastic Deformation in Amorphous Materials

Michael L. Falk
Materials Science and Engineering
Whiting School of Engineering
Johns Hopkins University

My Thread This Week

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

Mon
Intro to Mechanics of Materials

Tues
Intro to Molecular Dynamics

Wed
Plasticity in Amorphous Materials

Thurs
STZ Constitutive Theory

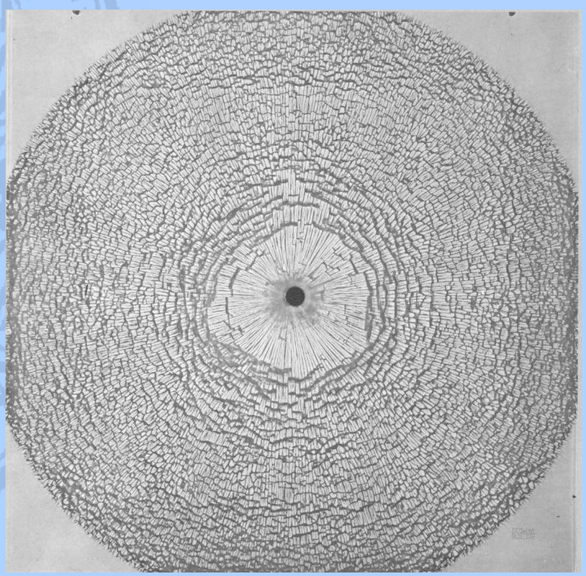
Amorphous Materials (Glass)

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

- **Represent a broad class of useful metal, ceramic and polymer materials in current application and in development.**

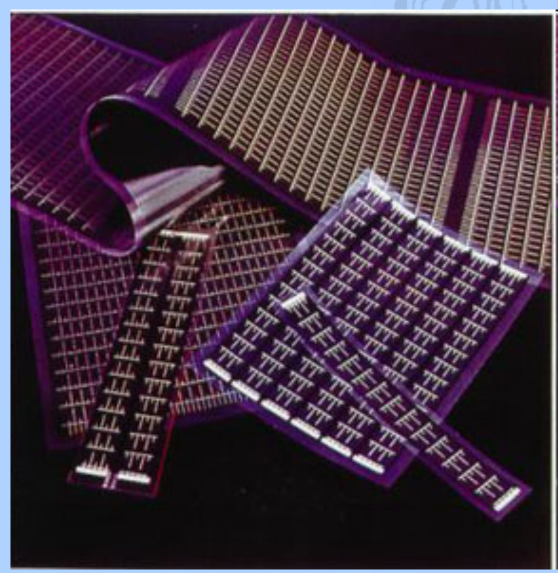
  Their common characteristic is a lack of crystalline order.

PMMA house wares



Safety Glass Cracking, Harold Edgerton, 1938

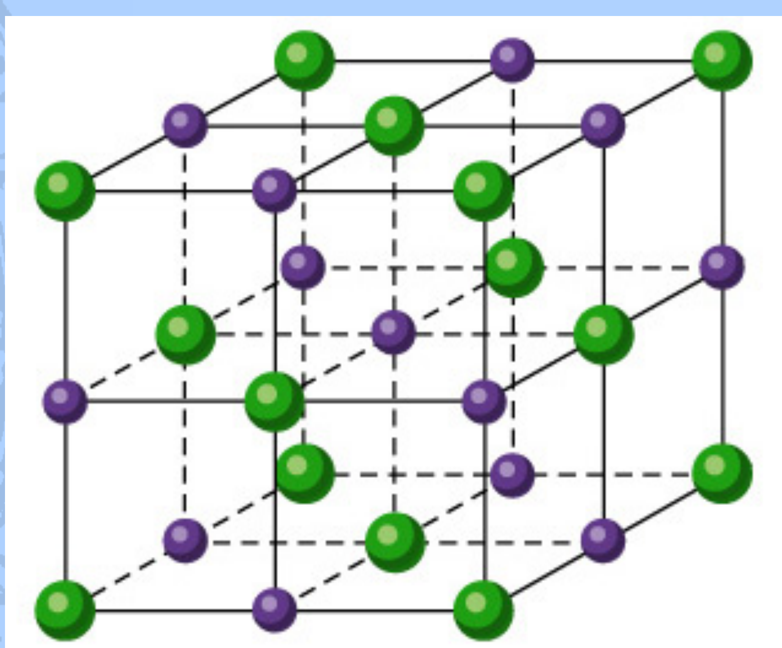
Metallic Glass Golf Club Head, Liquidmetal Tech.

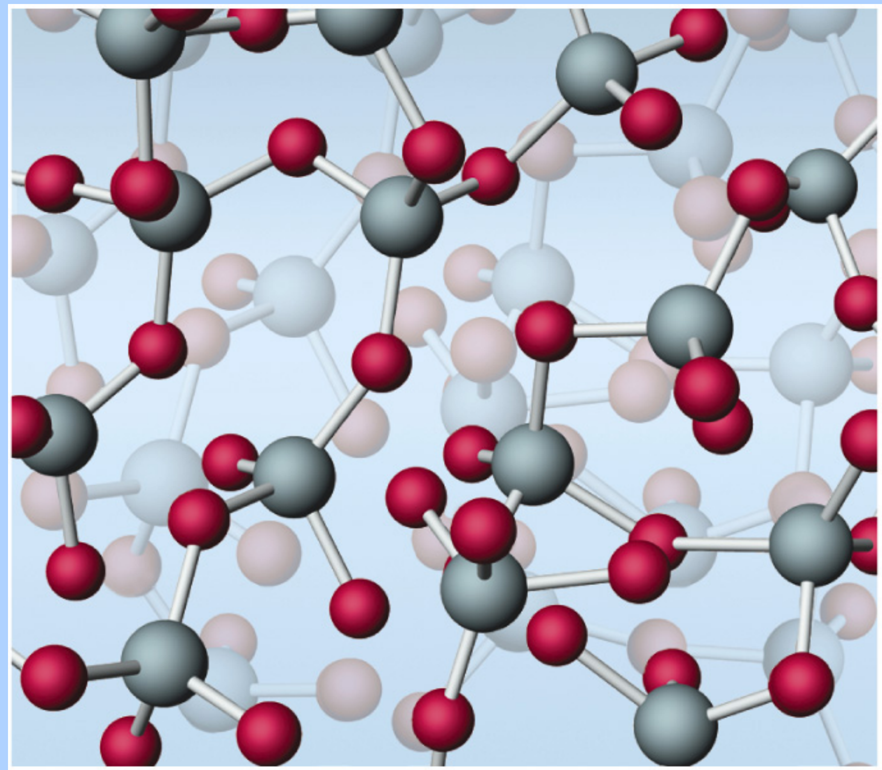


Flexible Si Solar Cells, Iowa Thin Film Tech.

Orderly Crystals vs. Disorderly Glass

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

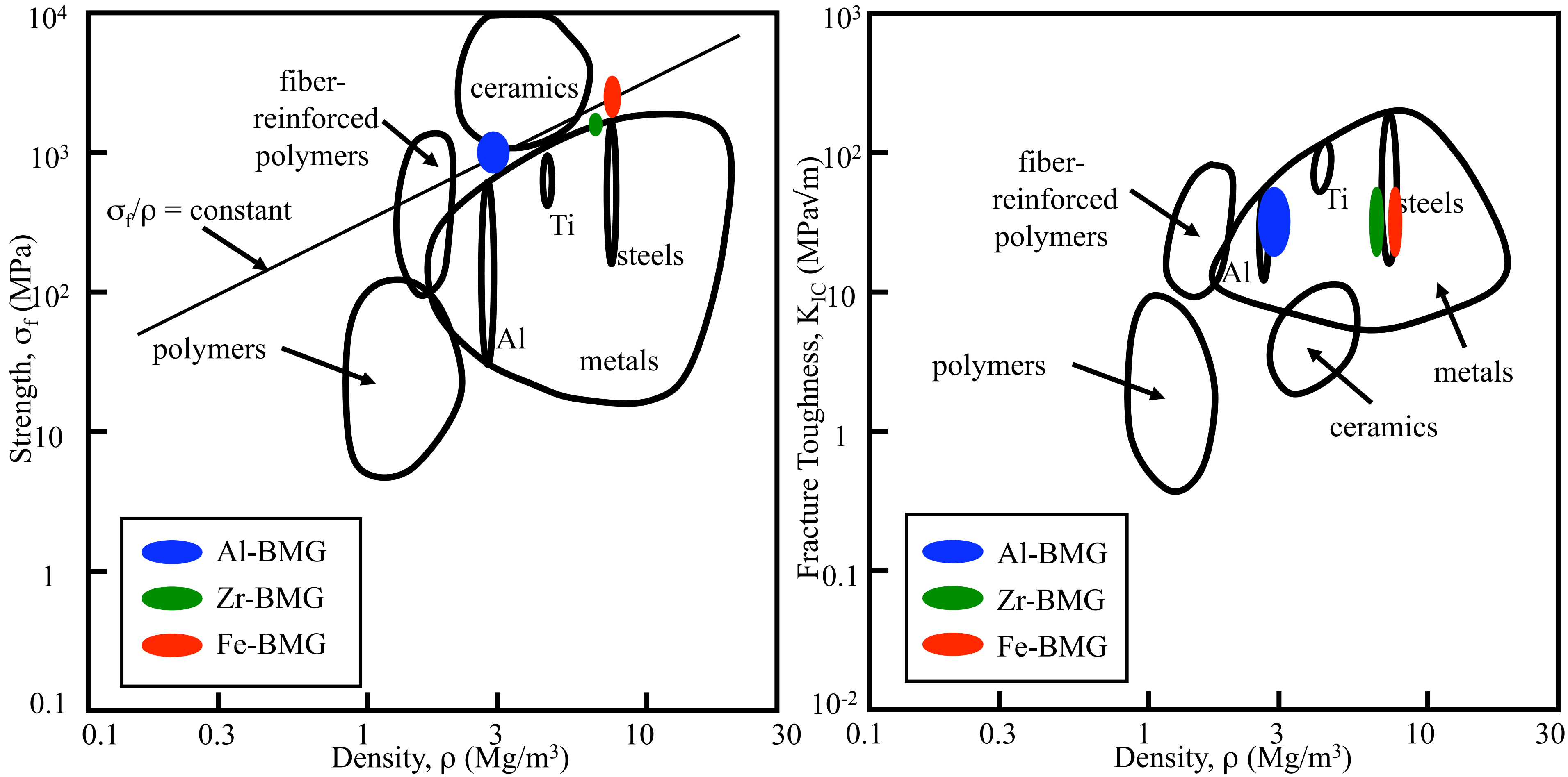




Metallic Glass

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

graphs courtesy of Katherine Flores, OSU



Applications of Bulk Metallic Glasses

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY



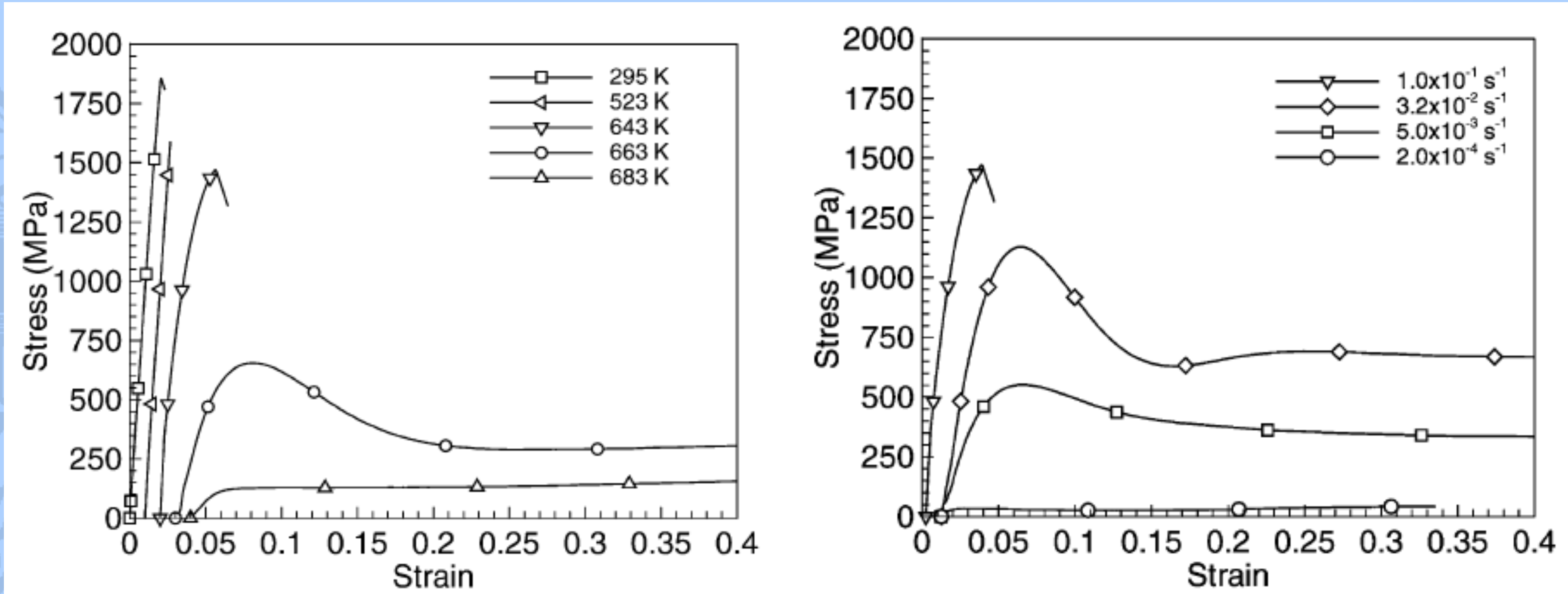






http://www.liquidmetal.com

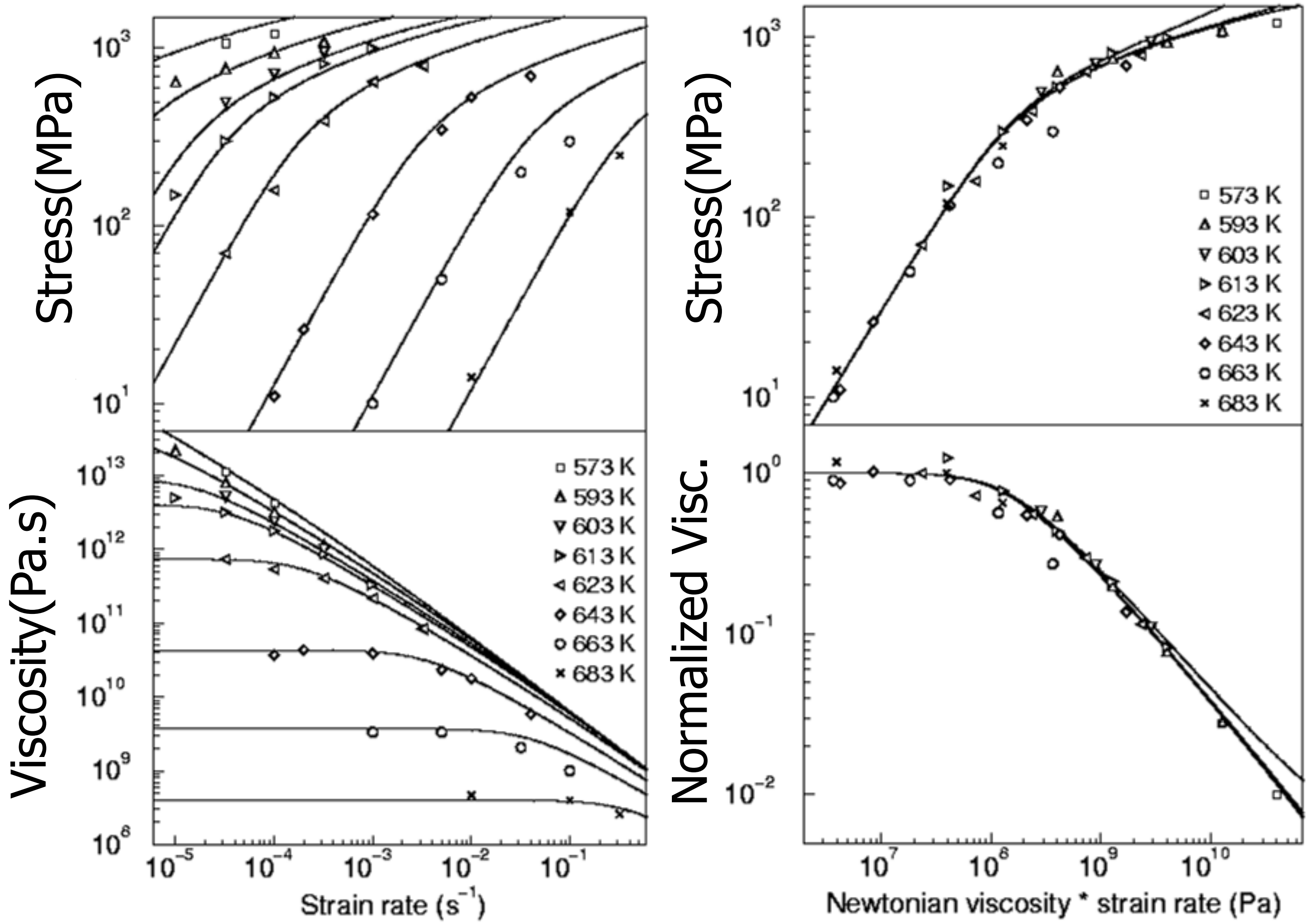
Mechanical Response Near T_g



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

Rheology Near T_g

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

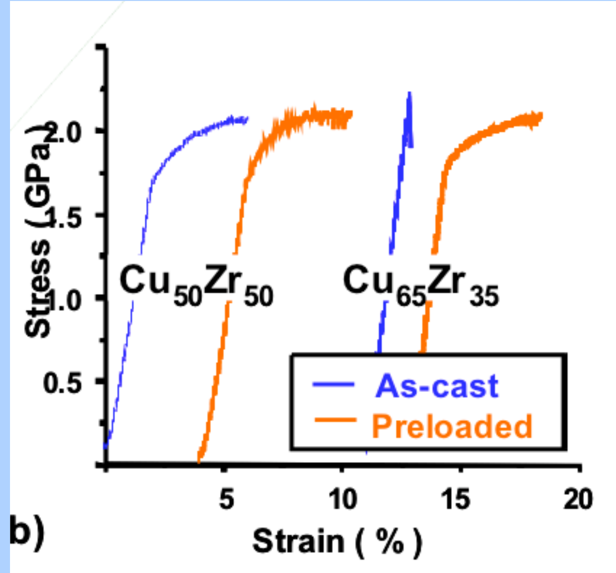


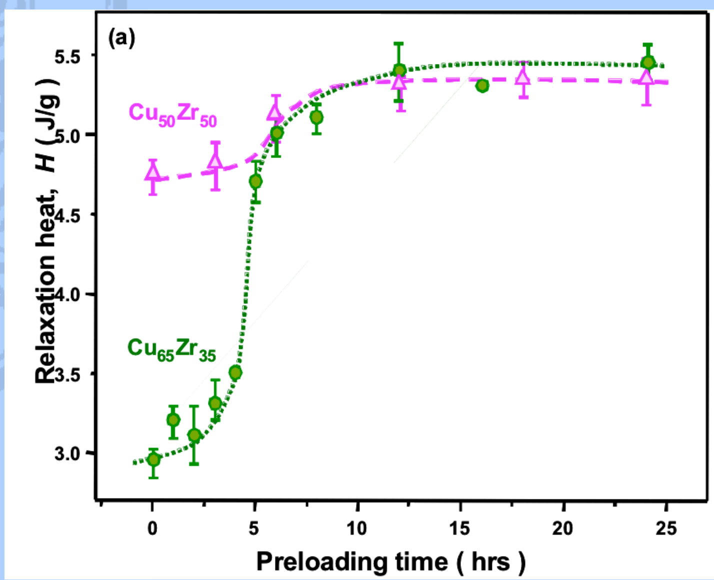
Lu, Ravichandran, Johnson Acta Mat. 51, 3429 (2003)

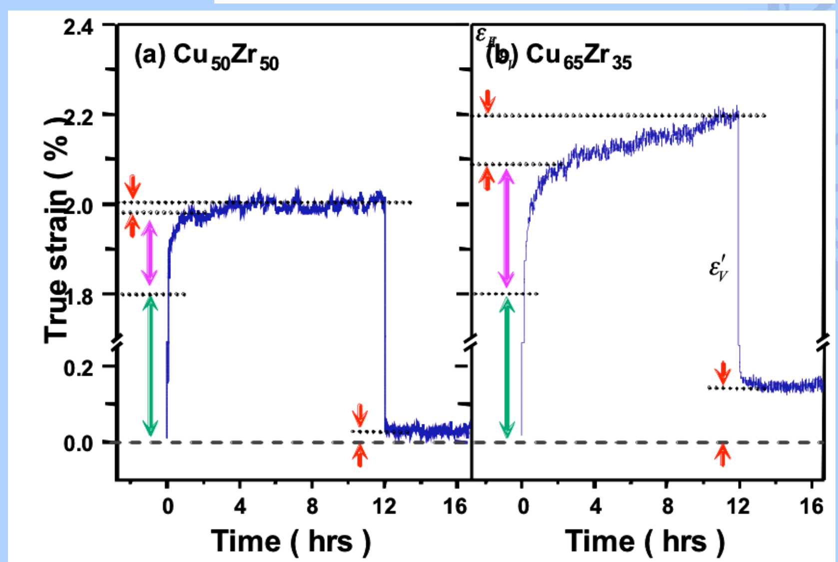
Behavior at Room Temperature

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

- Recent work in collaboration with Jae-Chul Lee at Korea University shows apparent contradiction
- Alloys that exhibit a large degree of plasticity when loaded at constant stress, show low ductility loaded at constant strain rate
- This appears to be related to structural changes during shear

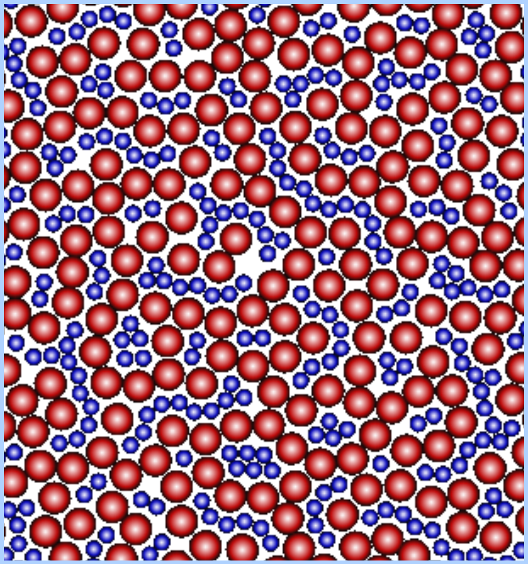




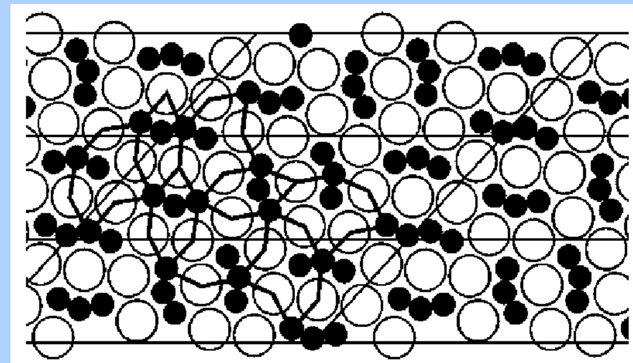


2D Simulation System

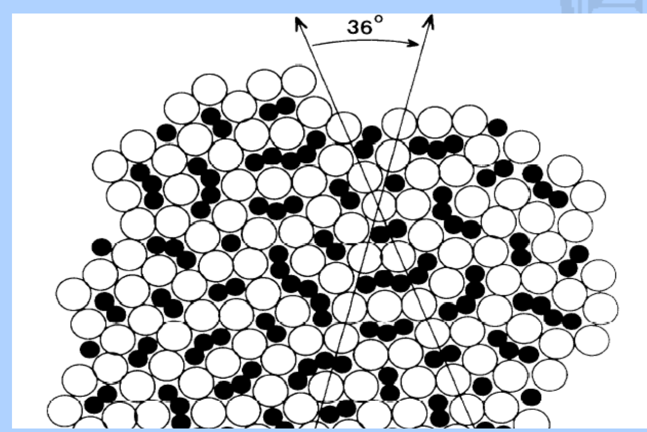
WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY



(Lancon et al, Europhys. Lett, 1986)



Lee, Swendsen, Widom (2001)



Widom, Strandburg, Swendsen (1987)

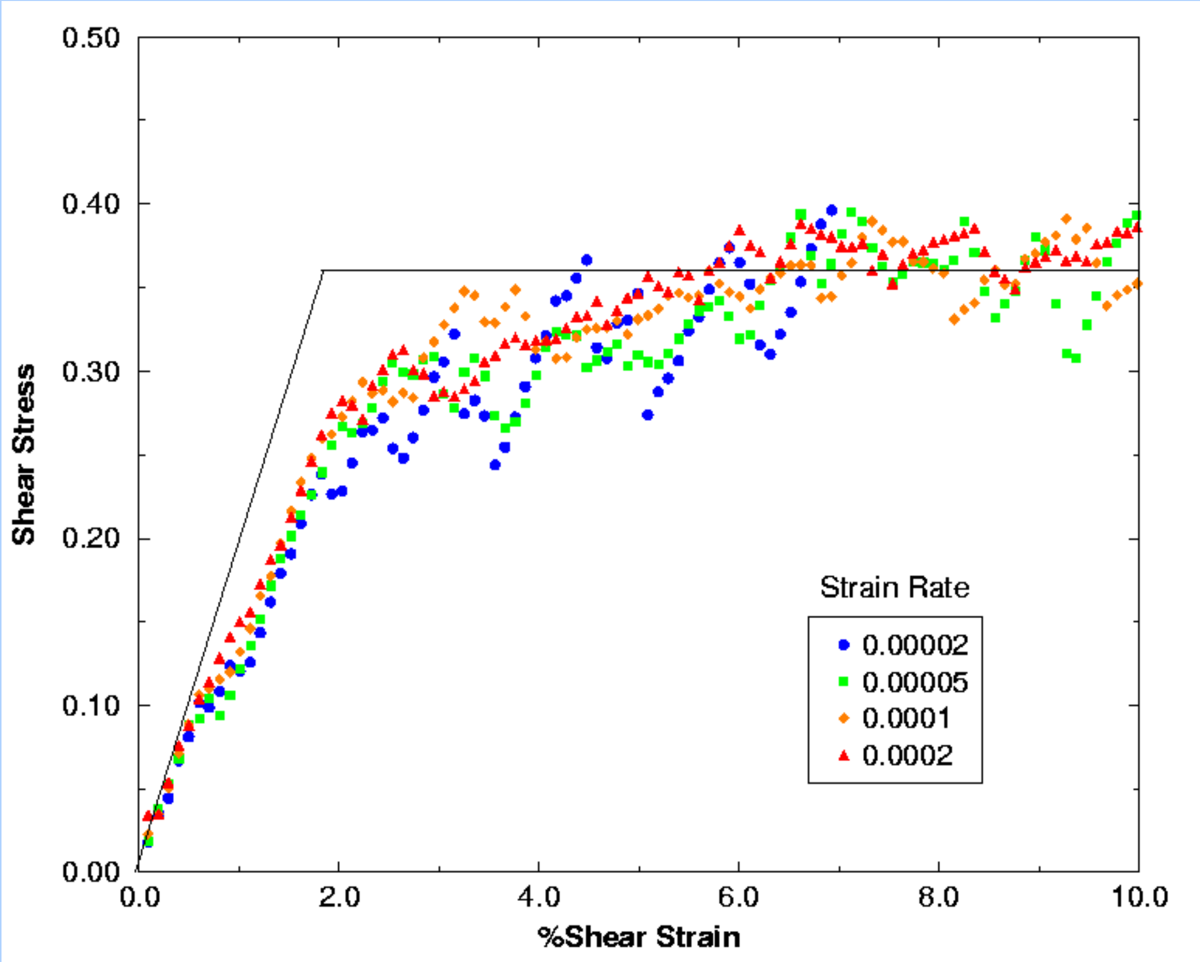
- 2D binary Lennard-Jones 12-6 potential
- Binary system with quasi-crystalline packing

45:55 composition, 20,000-80,000 atoms

- $T_{MCT} \approx 0.325$

Homogeneous MD Simulations

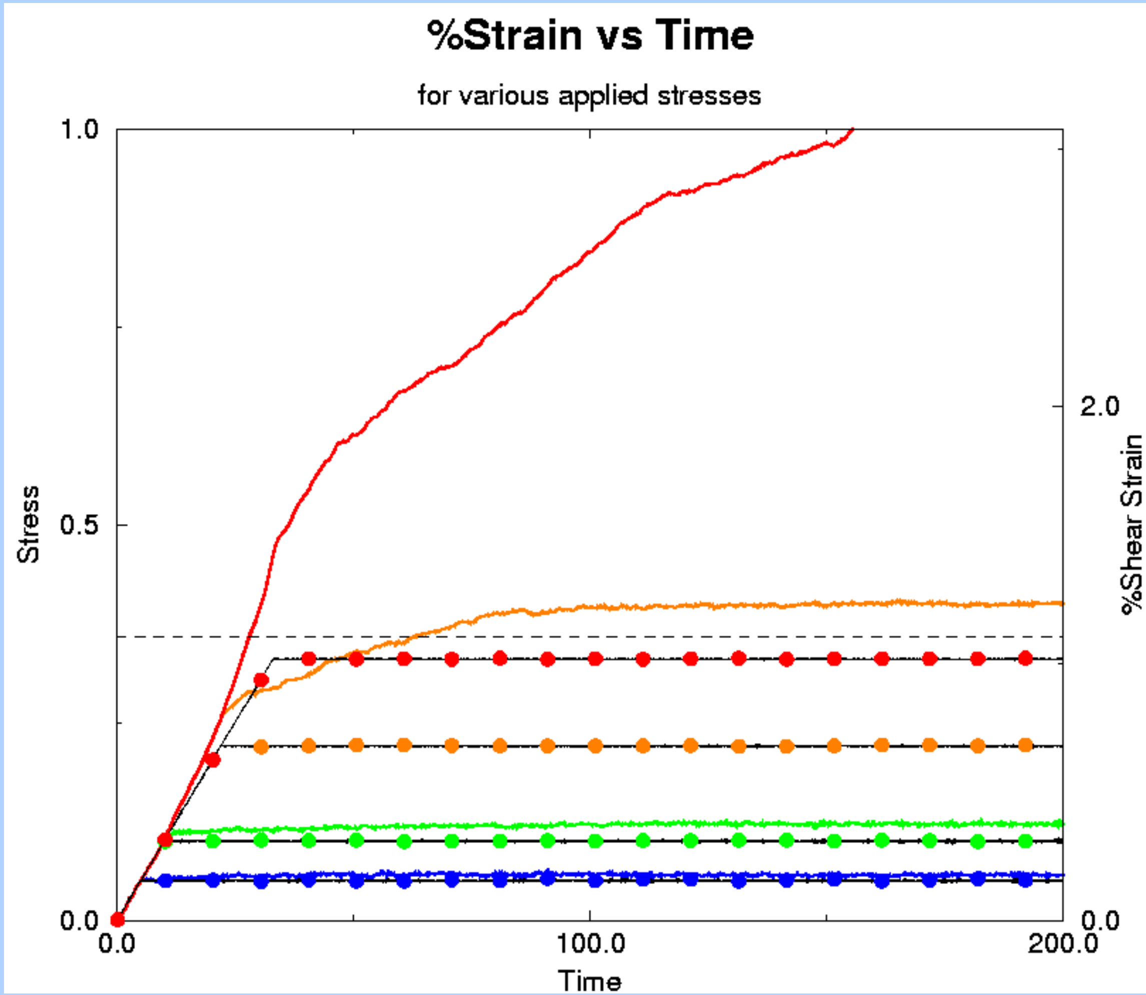
WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY



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

Homogeneous MD Simulations

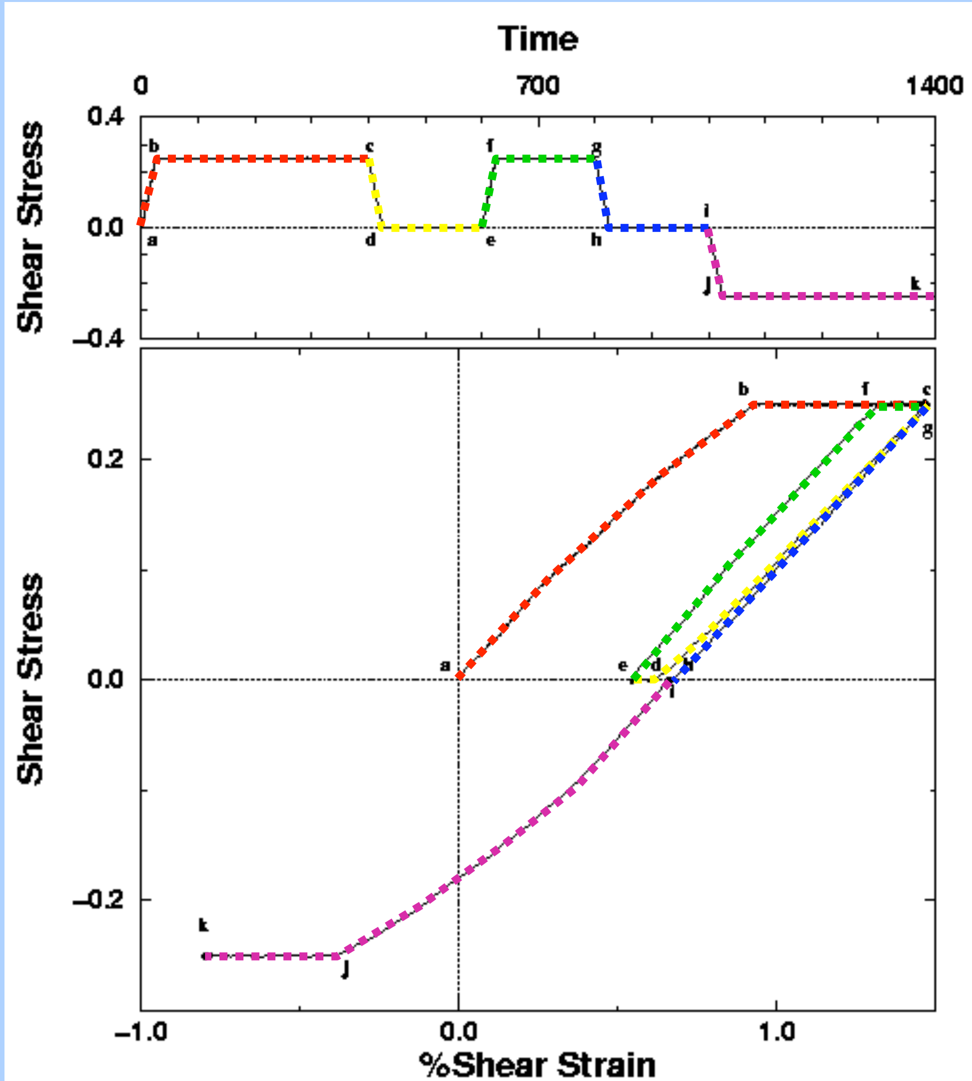
WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY



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

Homogeneous MD Simulations

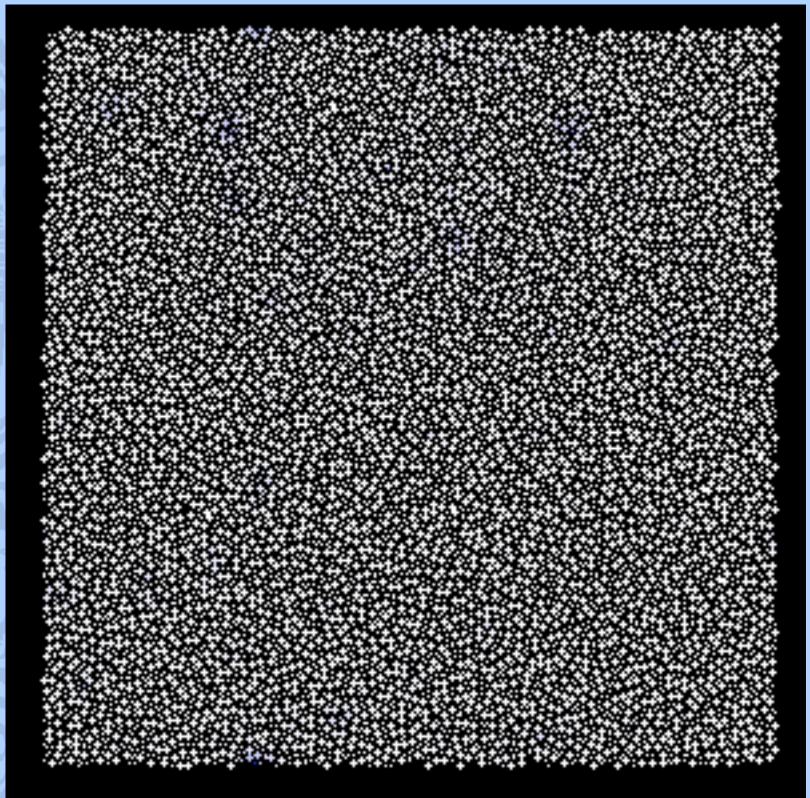
WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

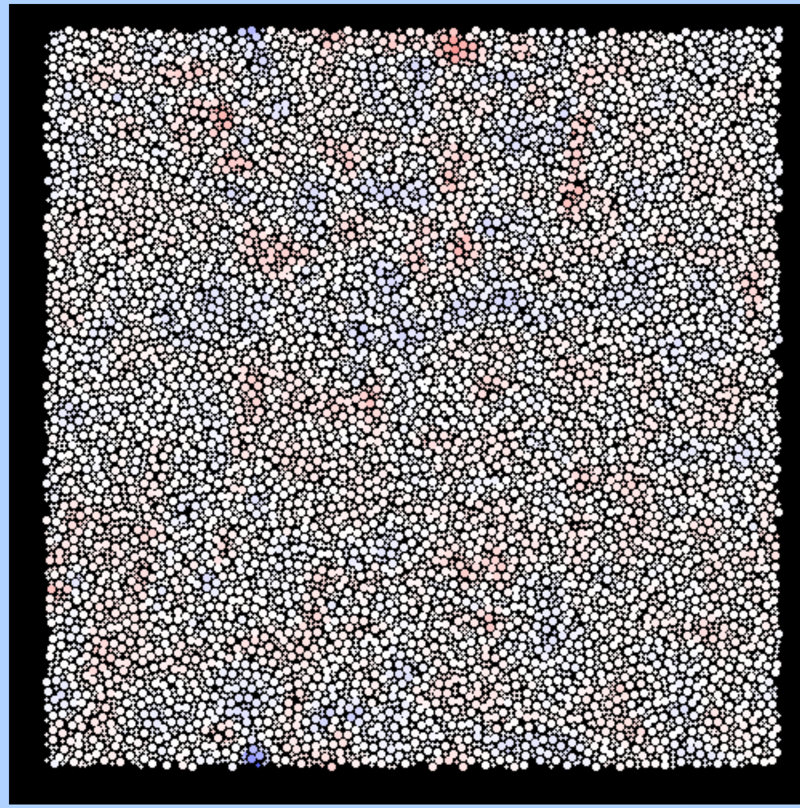


MLF and JS Langer, PRE, Vol. 57, pp. 7192-7205 (1998)

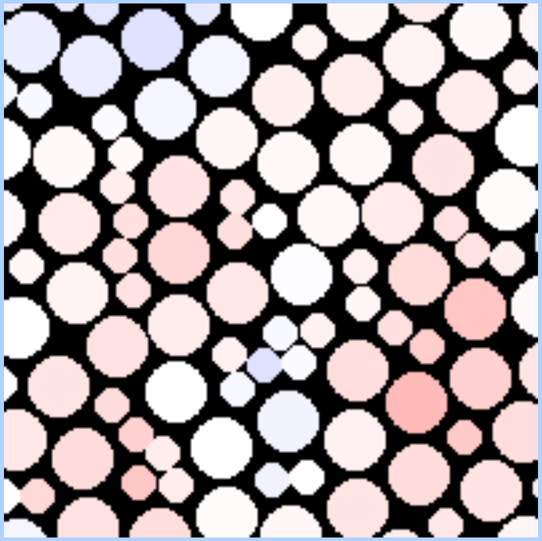
STZ Picture

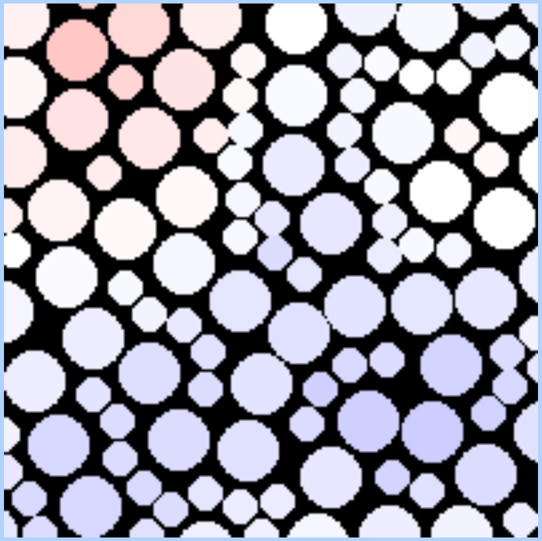
WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY





STZ Picture



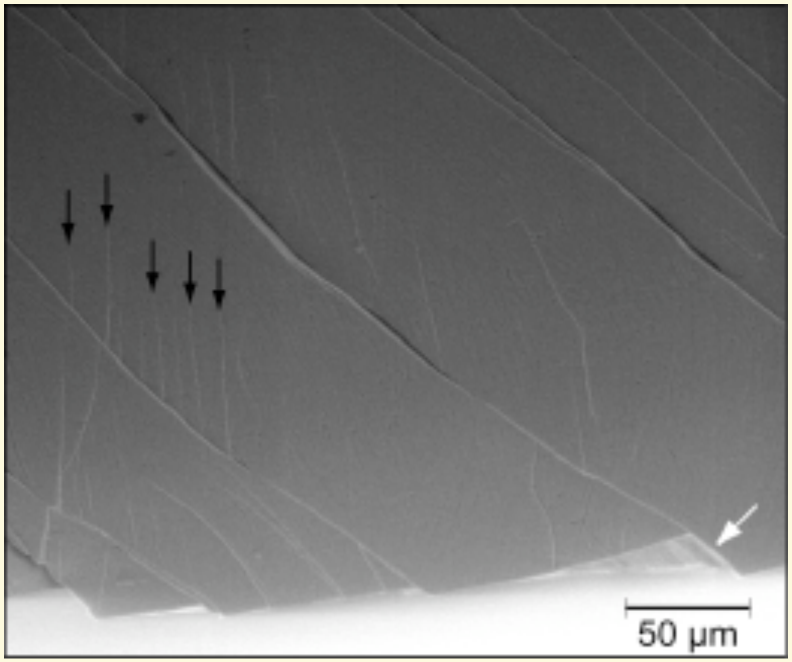


- STZs have a particular orientation. They are susceptible to shear to the extent that the shear is along this direction.
- STZs are reversible until their environment rearranges. They behave as 2-state systems.
- STZs are transient. They can be created and destroyed by neighboring plastic activity.

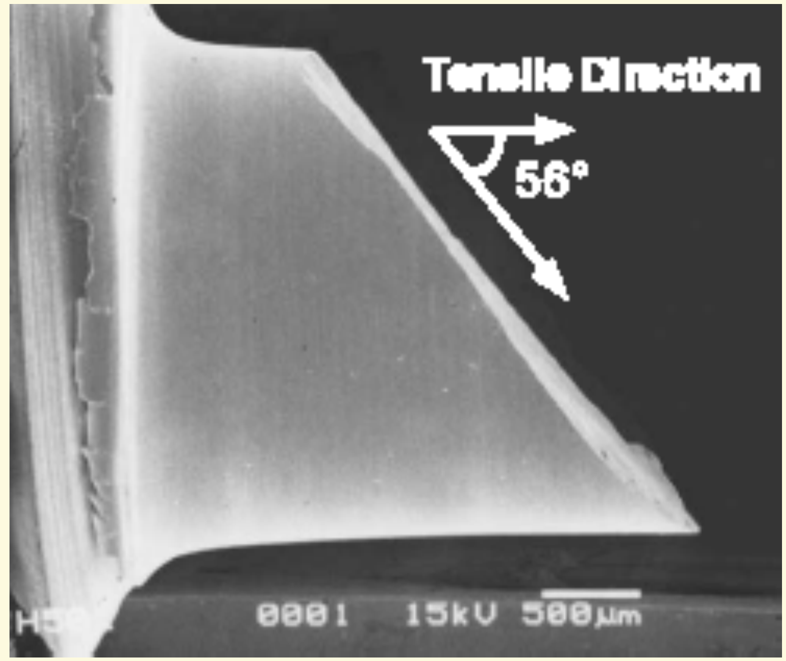
Metallic Glass Failure

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

strain localization (shear banding) is the primary failure mode



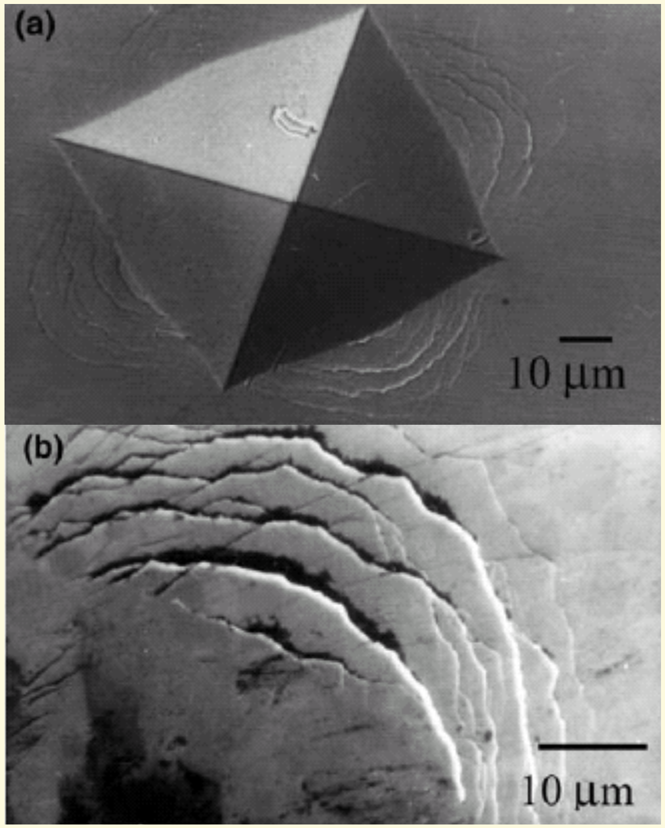
Electron Micrograph of Shear Bands Formed in Bending Metallic Glass
Hufnagel, El-Deiry, Vinci (2000)



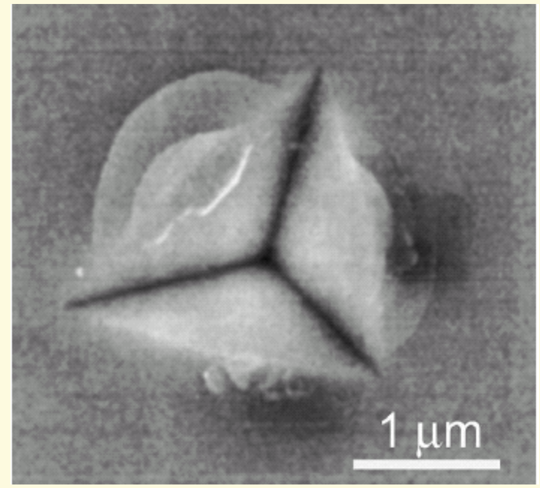
Quasistatic Fracture Specimen
Mukai, Nieh, Kawamura, Inoue, Higashi (2002)

Indentation Testing of Metallic Glass

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY



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

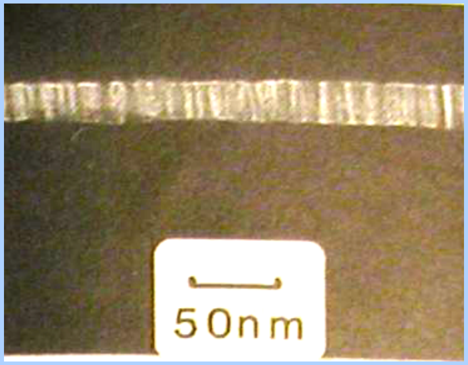


"Nanoindentation studies of shear banding in fully amorphous and partially devitrified metallic alloys"
Mat. Sci. Eng. A (2005)
A.L. Greer., A. Castellero, S.V. Madge, I.T. Walker, J.R. Wilde

Shear Bands

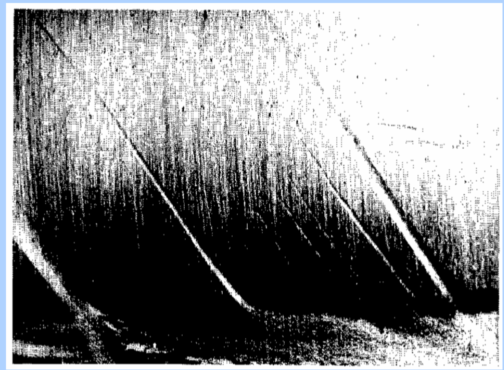
WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

Polymer Crazing



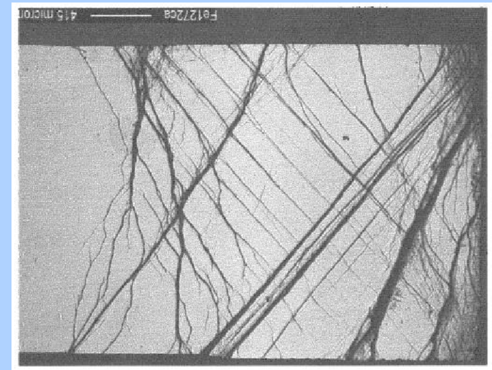
Young and Lovell (1991)

Mild Steel



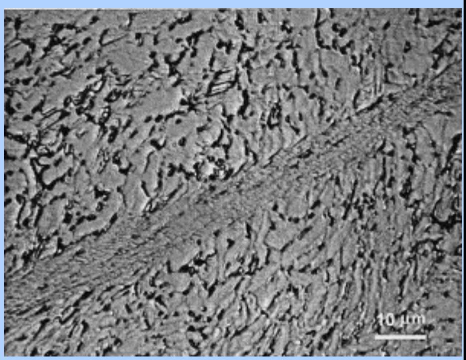
Van Rooyen (1970)

Nanograined Metal



Wei, Jia, Ramesh and Ma (2002)

Steel @ High Rate

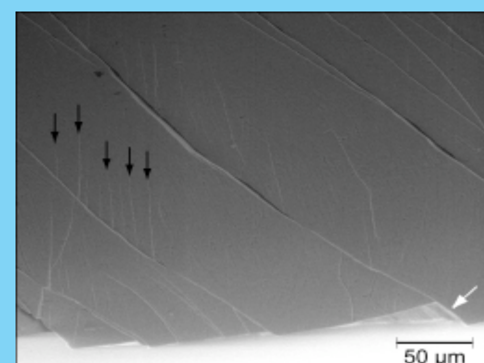


Xue, Meyers and Nesterenko (1991)

Granular Materials

Mueth, Debregeas and et. al. (2000)

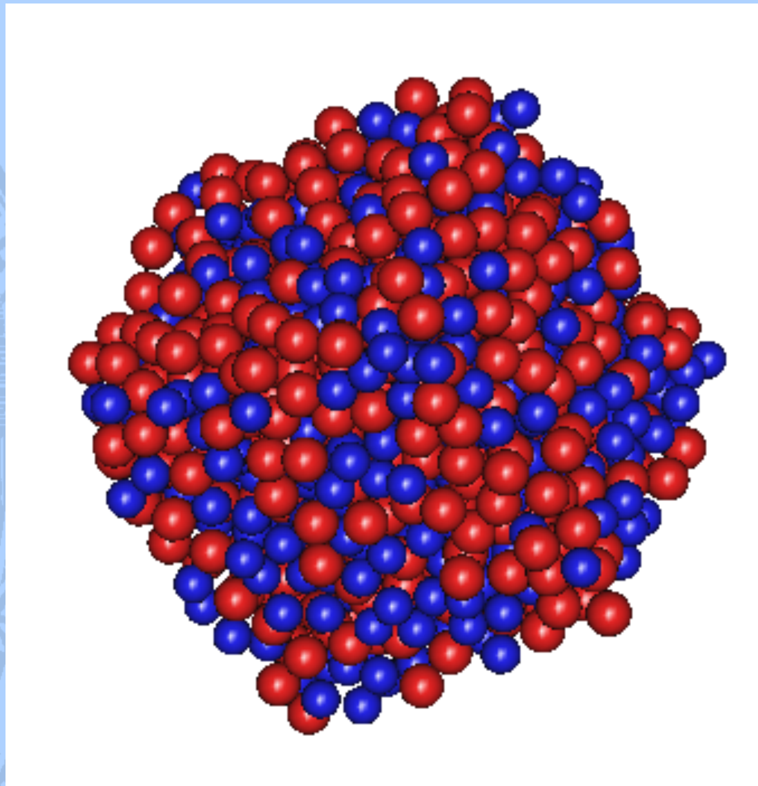
Bulk Metallic Glasses



Hufnagel, El-Deiry and Vinci (2000)

Simulated System: 3D Binary Alloy

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY



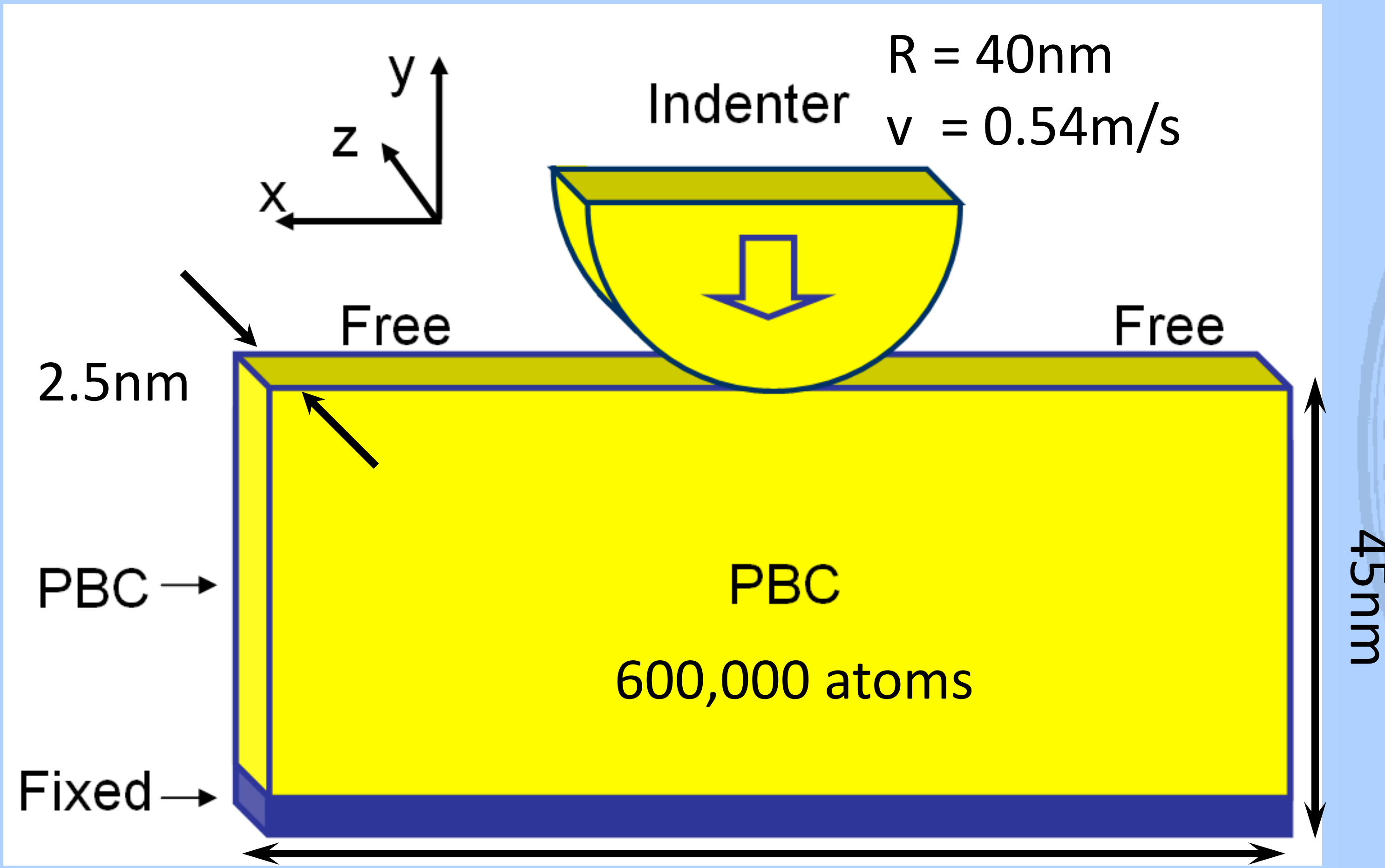
- Wahnstrom Potential (PRA, 1991)
- Rough Approximation of $Nb_{50}Ni_{50}$
- Lennard-Jones Interactions
- Equal Interaction Energies
- Bond Length Ratios:
  - $a_{NiNi} \sim {}^{5}/_{6}\, a_{NbNb}$
  - $a_{NiNb} \sim {}^{11}/_{12}\, a_{NbNb}$
- $T_g \sim 1000K$
- Studied previously in the context of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

- **Unlike the simulation of 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

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

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



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

100nm

Metallic Glass Nanoindentation

color = deviatoric strain

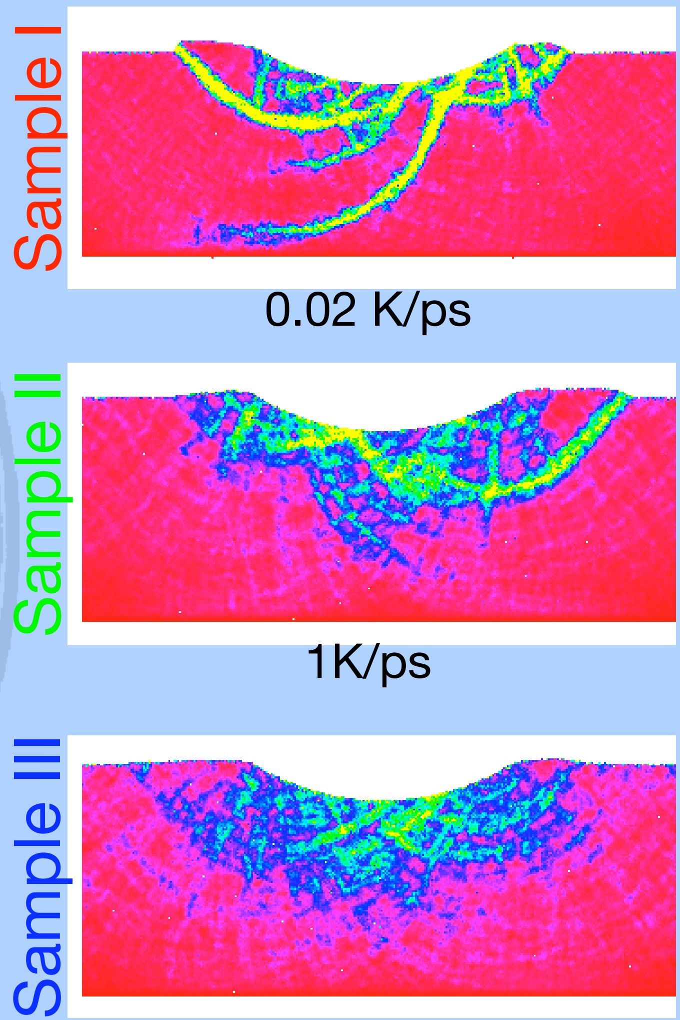
0%

40%

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

Metallic Glass Nanoindentation

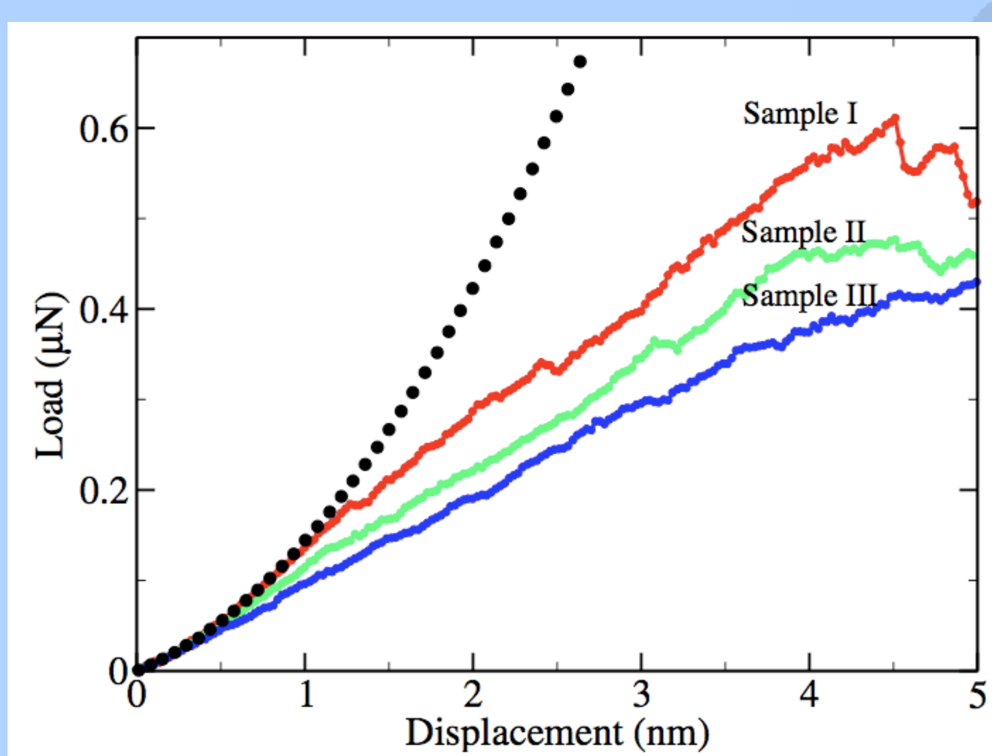
WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY



0.02 K/ps

1K/ps

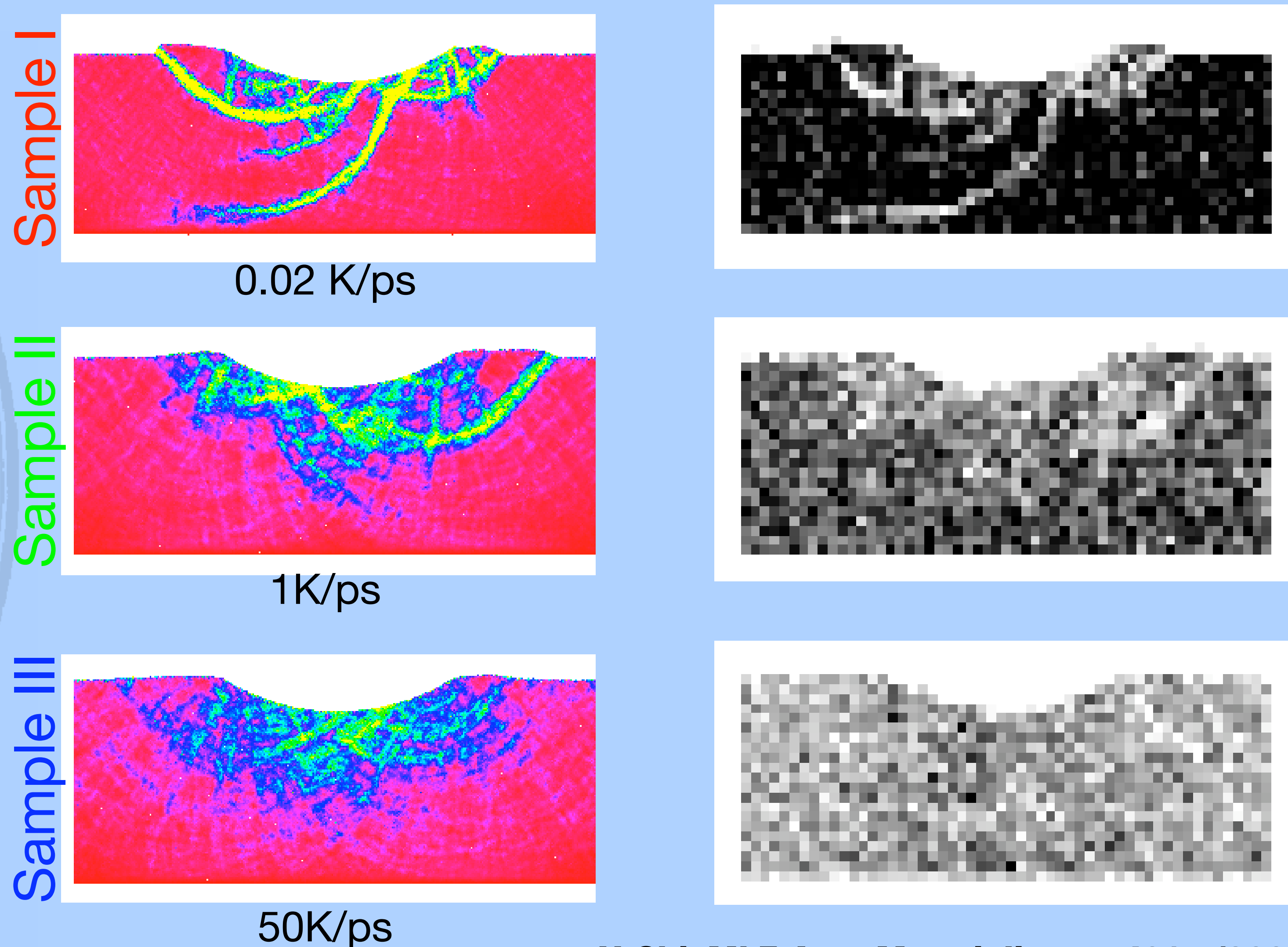
50K/ps



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

Metallic Glass Nanoindentation

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY



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

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

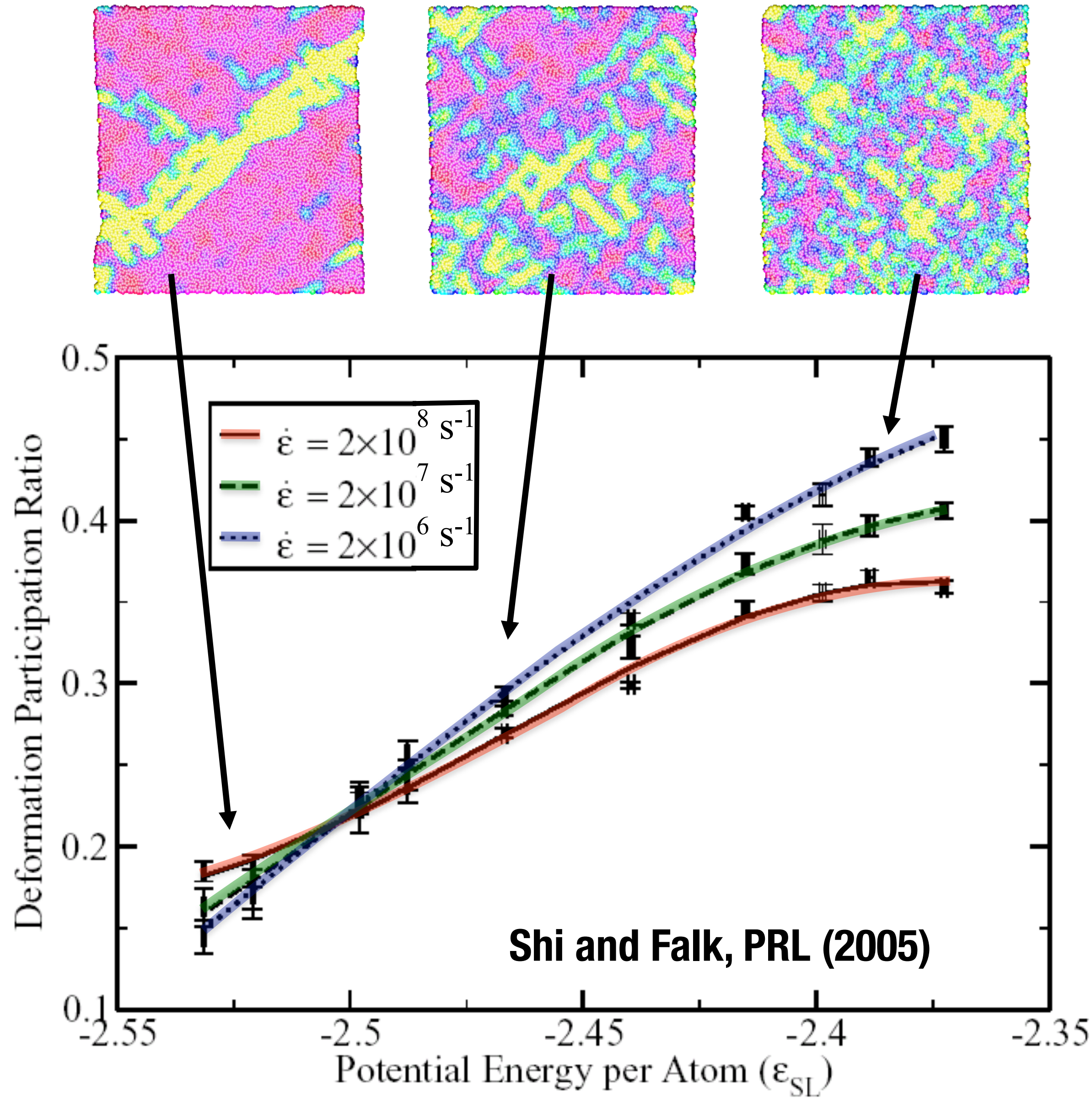
WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

- 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

Shear Localization (DPR) vs. PE

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

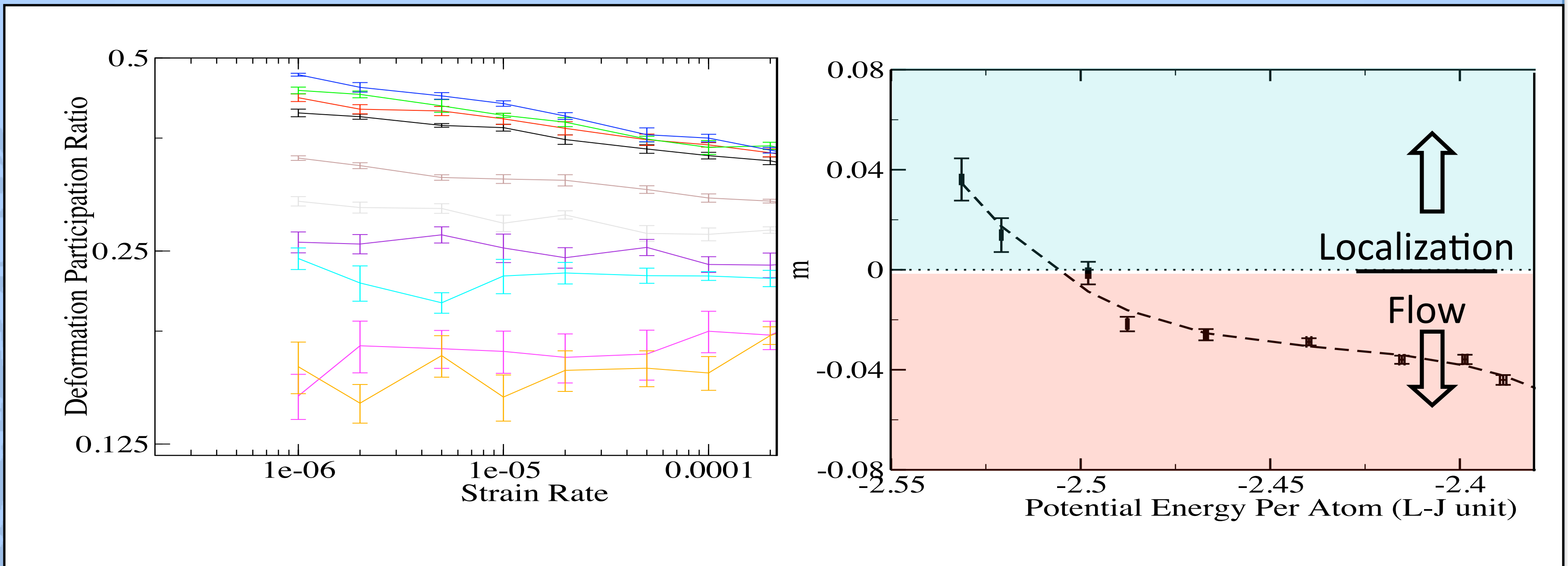
- **Deformation Participation Ratio**: Percentage of material with a local shear strain larger than the nominal strain
- Low strain rate favors homogenous deformation in instantaneously quenched samples
- Low strain rate favors inhomogeneous deformation in gradually quenched samples.



Shi and Falk, PRL (2005)

Strain-rate sensitivity of DPR

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY



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

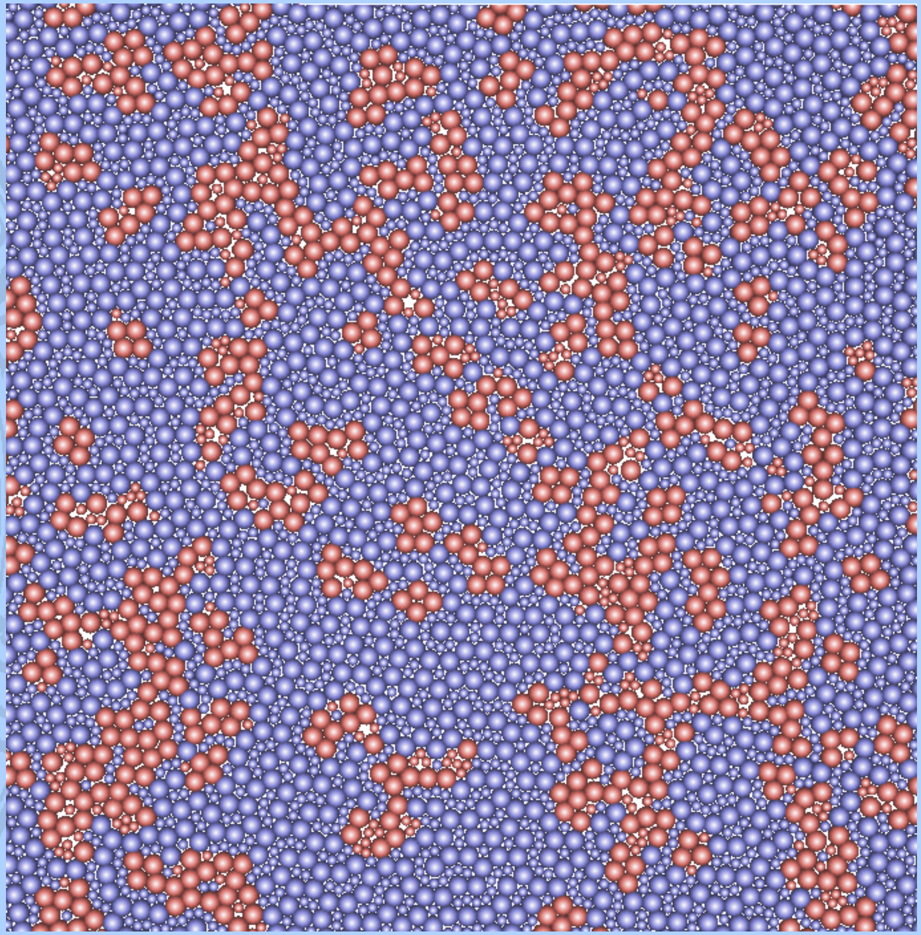
For $\dot{\varepsilon} \rightarrow 0$ and system size $\rightarrow \infty$

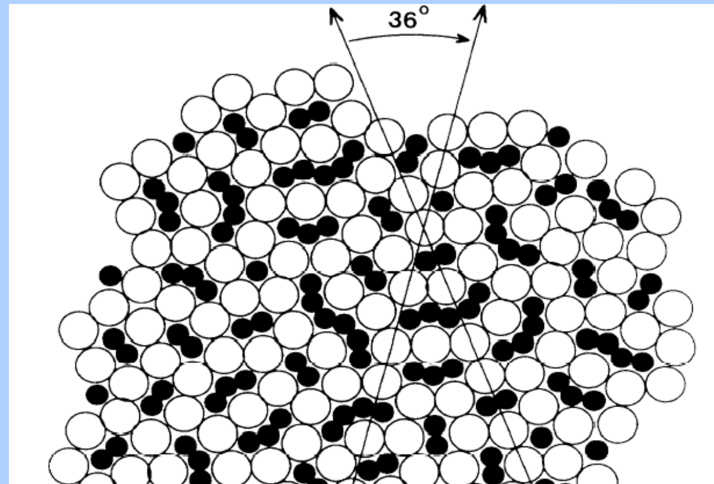
m < 0: homogenous deformation

m >= 0: localized deformation

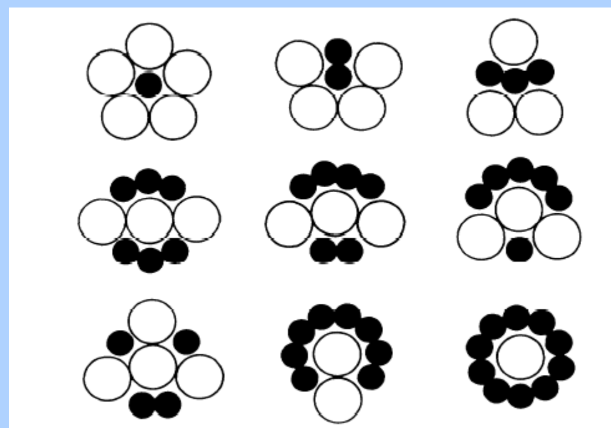
Shi and Falk, Scripta Mat (2005)

Local Structural Analysis



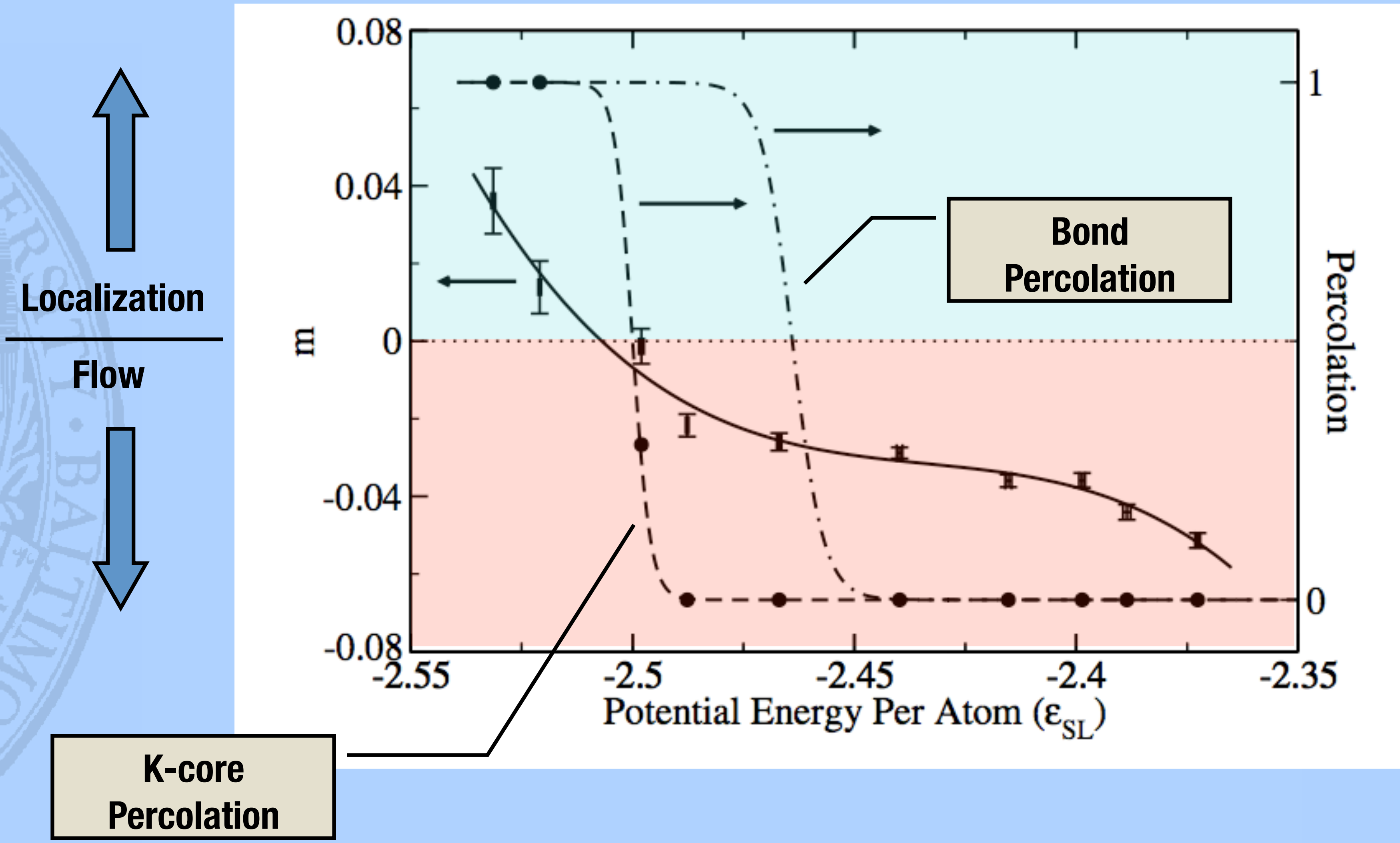


Widom, Strandburg, Swendsen (1987)



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

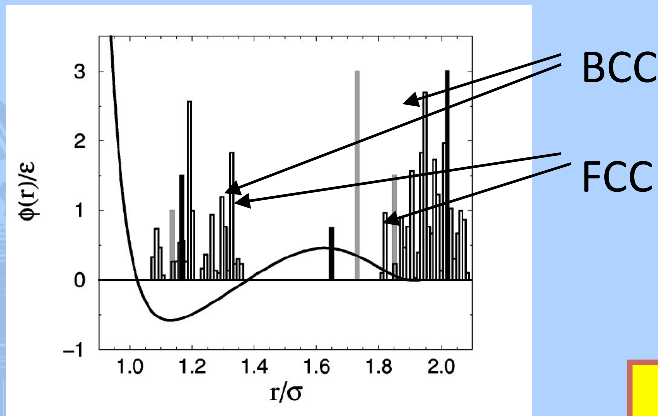
Percolation and Localization



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

3D Simulation Potentials

Dzugutov Potential

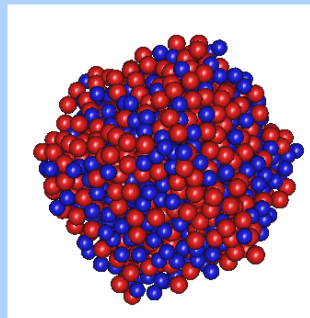


Roth and Denton, PRE (2000)

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

Zetterling et al., JNCS (2001)

Wahnstrom LJ Binary



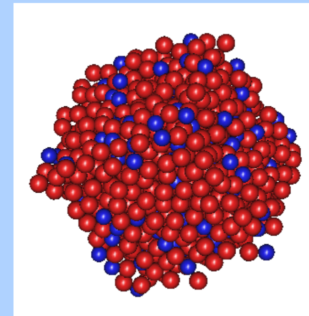
Bond length	Bond strength
AA 1.000	AA 1.0
AB 0.917	AB 1.0
BB 0.833	BB 1.0

- 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



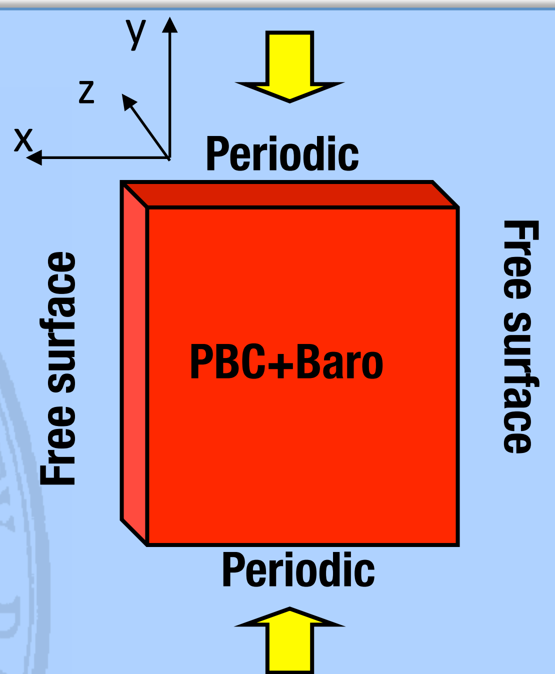
Bond length	Bond strength
AA 1.00	AA 1.0
AB 0.80	AB 1.5
BB 0.88	BB 1.0

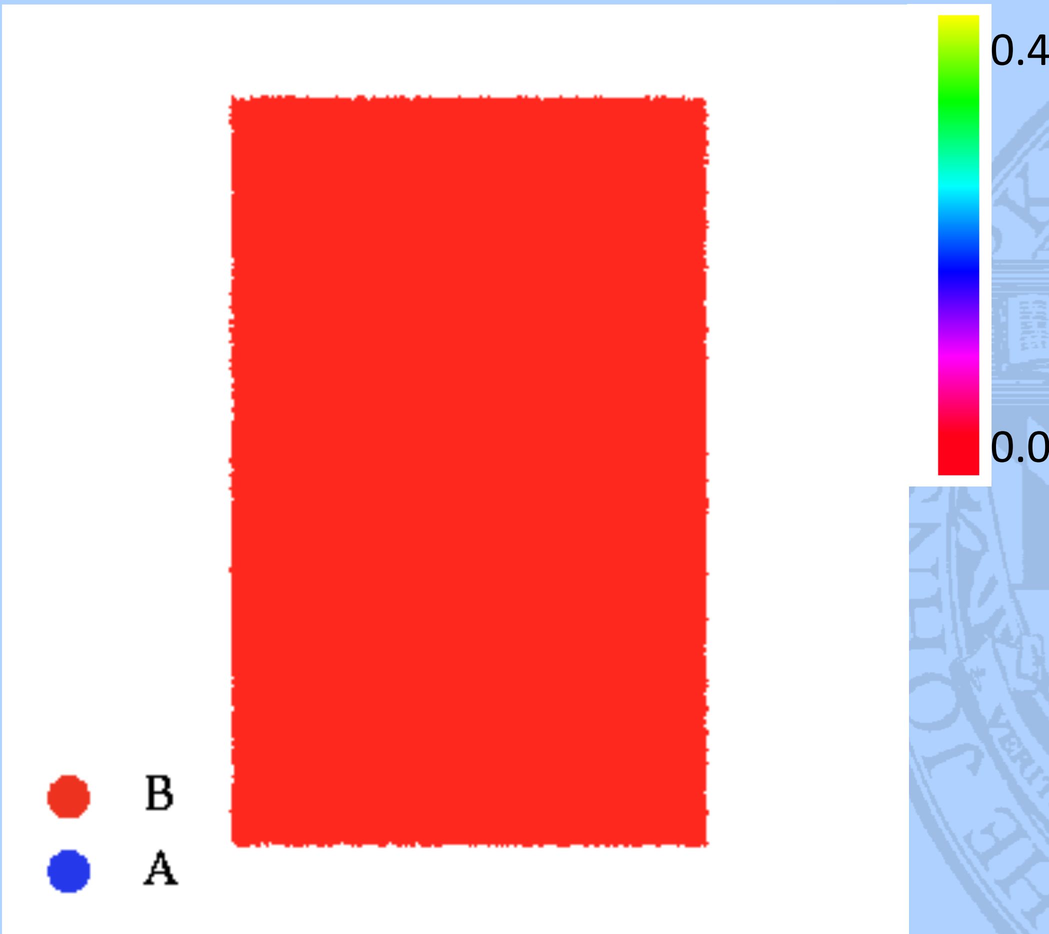
- 3D binary LJ 12-6 potential
- 80:20 composition, 144,000 atoms
- $T_{MCT} = 0.435$

Kob and Andersen, PRE 1995

3D Uniaxial Compression Test

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

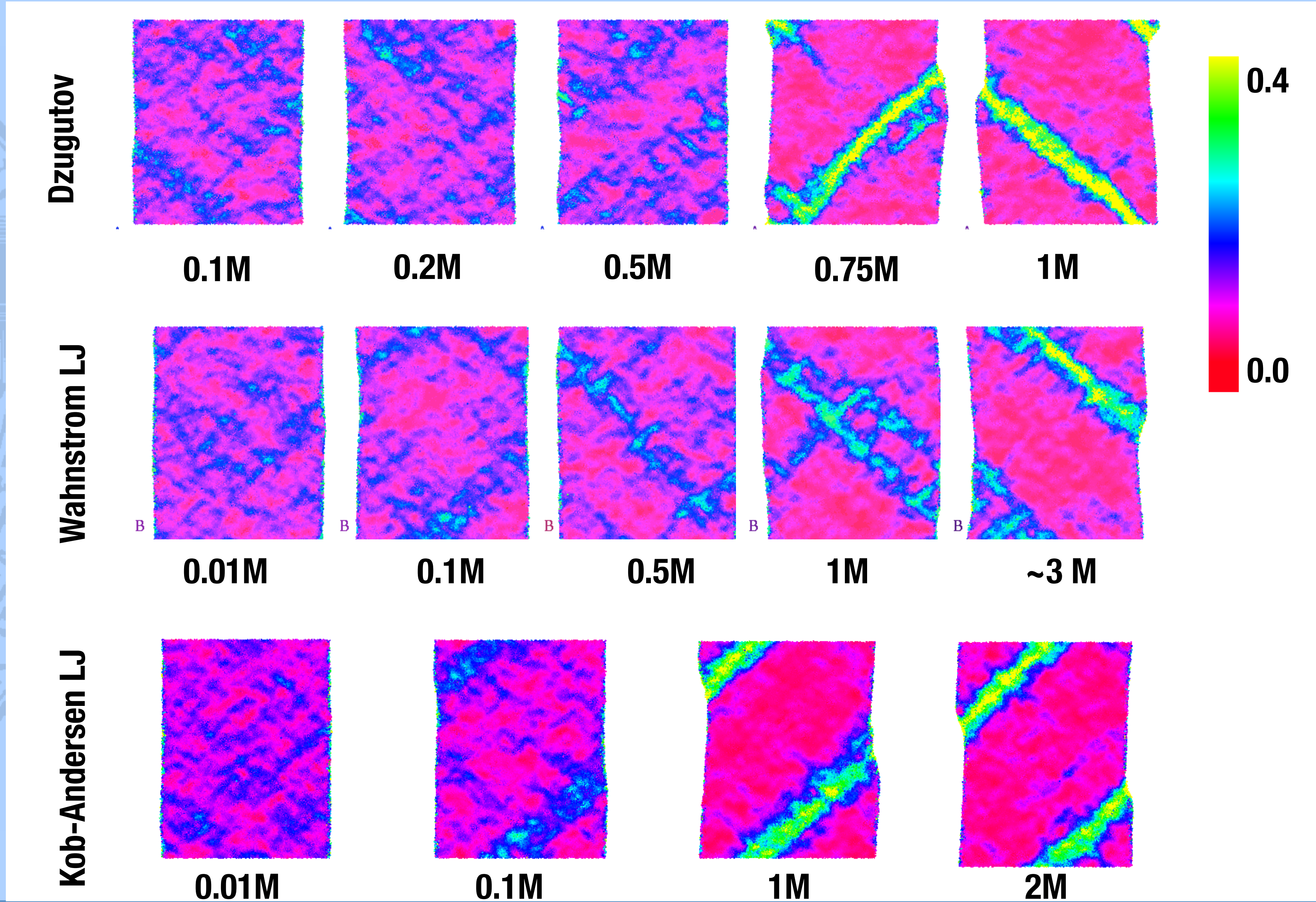




- Thin slab geometry to maximize in-plane spatial dimension
  75×110 ×15: 140,000 atoms
- Free surfaces in Y-Z
- PBC in X-Y and Y-Z
- Plane Strain: Average σ_{zz} zero

Compression: Various Quenches

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

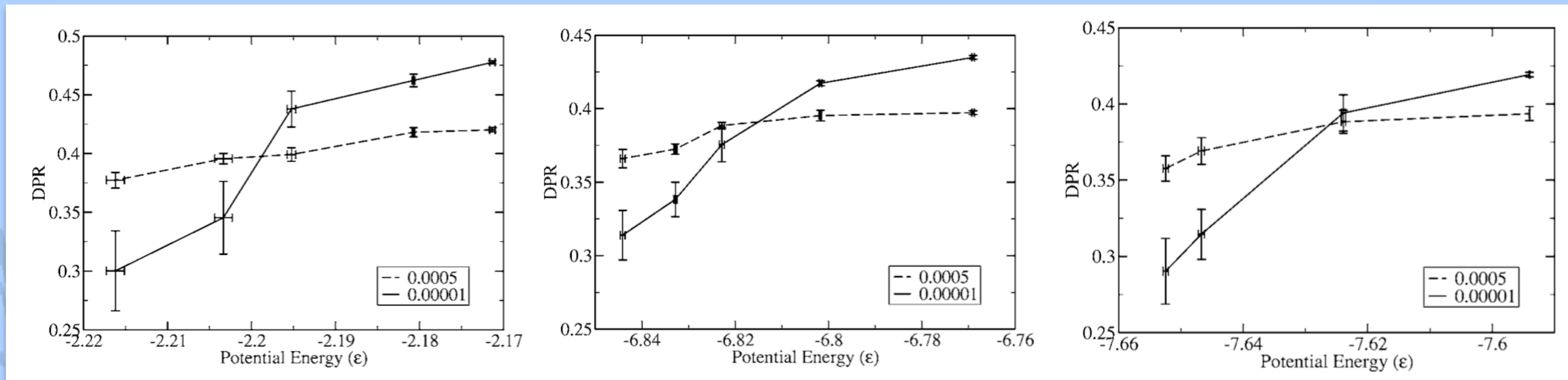


DPR and Strain Rate Sensitivity

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

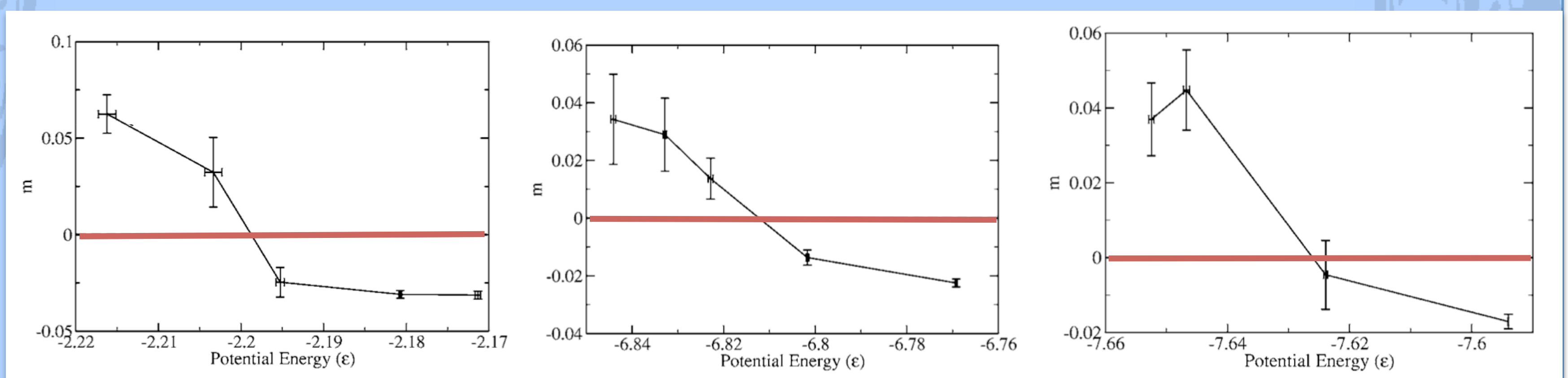
Dzugutov System	Wahnstrom LJ	Kob-Andersen LJ

DPR



PE PE PE

m



PE PE PE

Triangulated Coordination Shell Analysis

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

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)

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

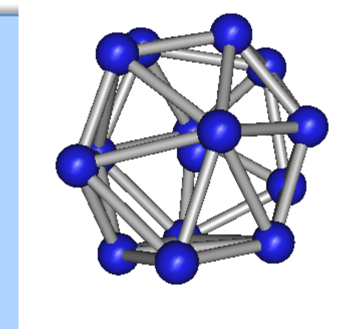
q is the surface coordination number (from 3 to 8 for now)

v_q is the count of neighbors has surface coordination number q

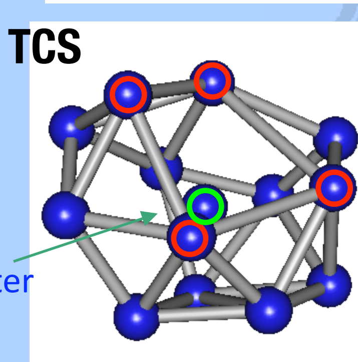
Glassy samples with lowest quenching rate

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

TCS



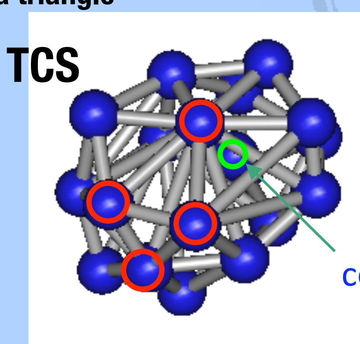
NOT TCS



center

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

NOT TCS

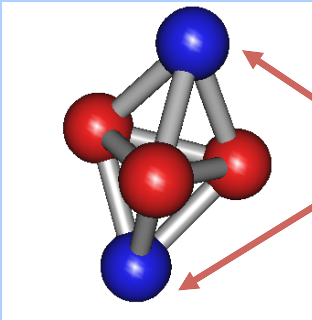


center

The tetrahedral formed by 4 red atoms are space dividing but not consisting the center atom (green)

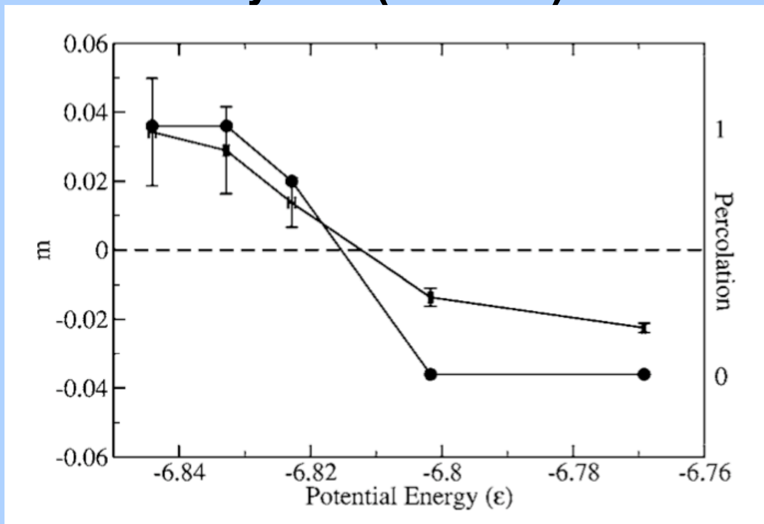
3D Percolation Analysis

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

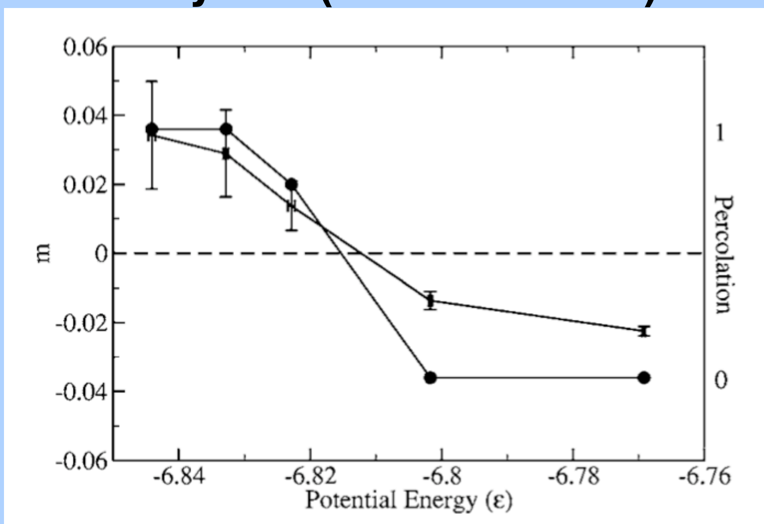


Connected!

WA system (TCS SRO)



DZ system (Icosahedral SRO)



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)

Observations

WHITING SCHOOL OF ENGINEERING
JOHNS HOPKINS UNIVERSITY

- **Experimental investigations of metallic glass reveal interesting behavior:**
  - Shear softening
  - Nonlinear Rheology
  - Systematic changes in ductility and creep dependent on alloy composition and sample history
  - Strong tendency to localization
- **Simulations confirm these and also reveal**
  - Plastic Hysteresis (Bauschinger effects)
  - Existence of a yield stress
  - Local nature of rearrangements
- **Recent investigations of shear banding show**
  - Slowly quenched samples more susceptible to localization
  - Samples that exhibit localization contain percolated short range order
  - CAVEAT: there is no universal method for defining short range order
- **Tomorrow: building a theory of plasticity**