Deformation of Metallic Glasses: Experimental Puzzles and Theoretical Needs

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With special contributions from:

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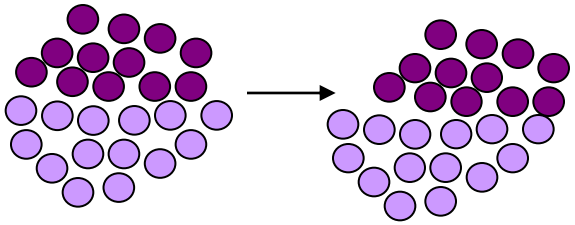
The prevailing mechanistic view



Shear Transformation Zone (STZ)

Interacting STZs

???

Independent STZs

$$\dot{\gamma} = \alpha_0 \nu_0 \gamma_0 \cdot \exp\left(-\frac{Q}{kT}\right) \sinh\left(\frac{\tau V}{kT}\right)$$

Spaepen, Acta Metall 1977

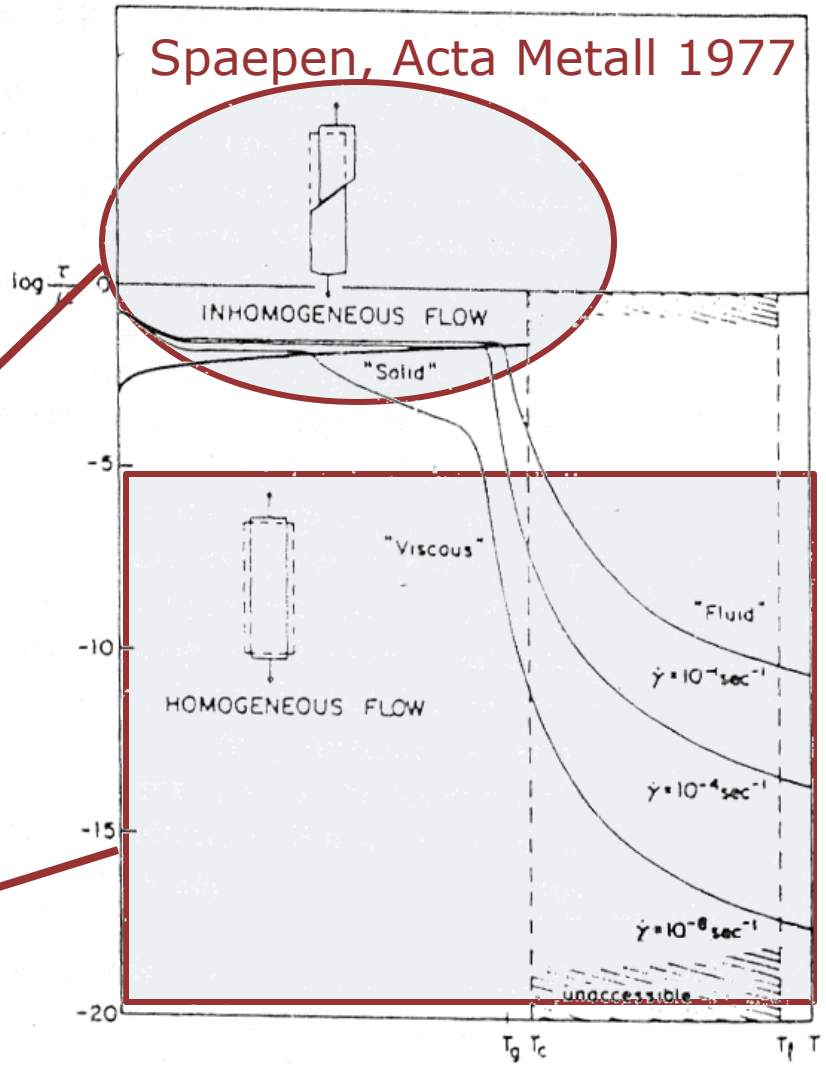
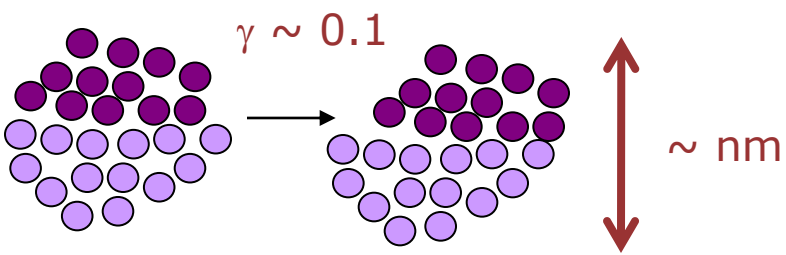


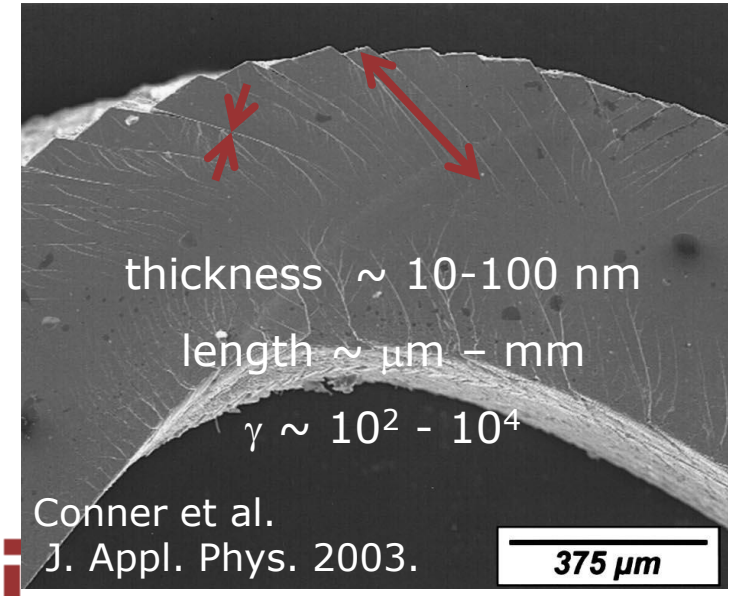
Fig. 2. Schematic deformation map of a metallic glass. The various modes of deformation are indicated.

Puzzles: the gap between atomic motion and shear bands



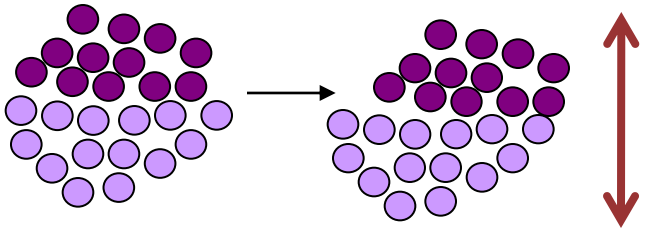
after Argon. Acta Metall. 1979.

???



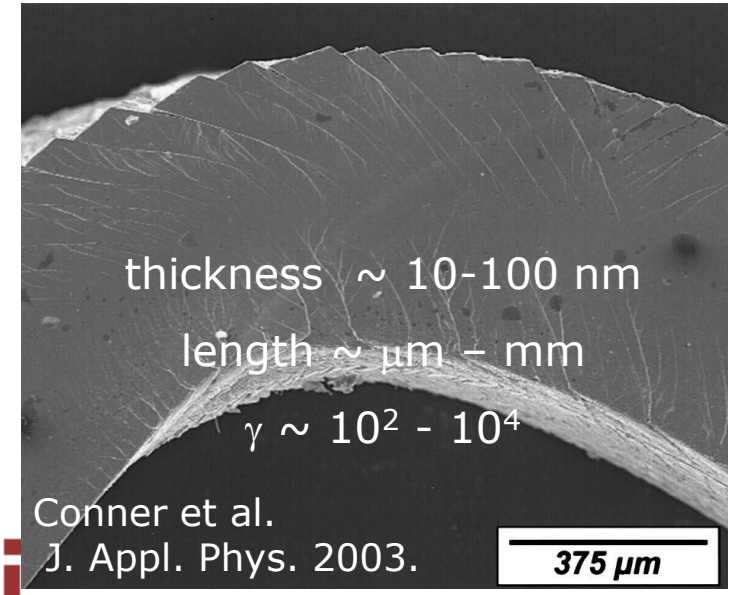
- Kinetics
- Behavior in gradients of stress
- Event spectrum

Kinetics



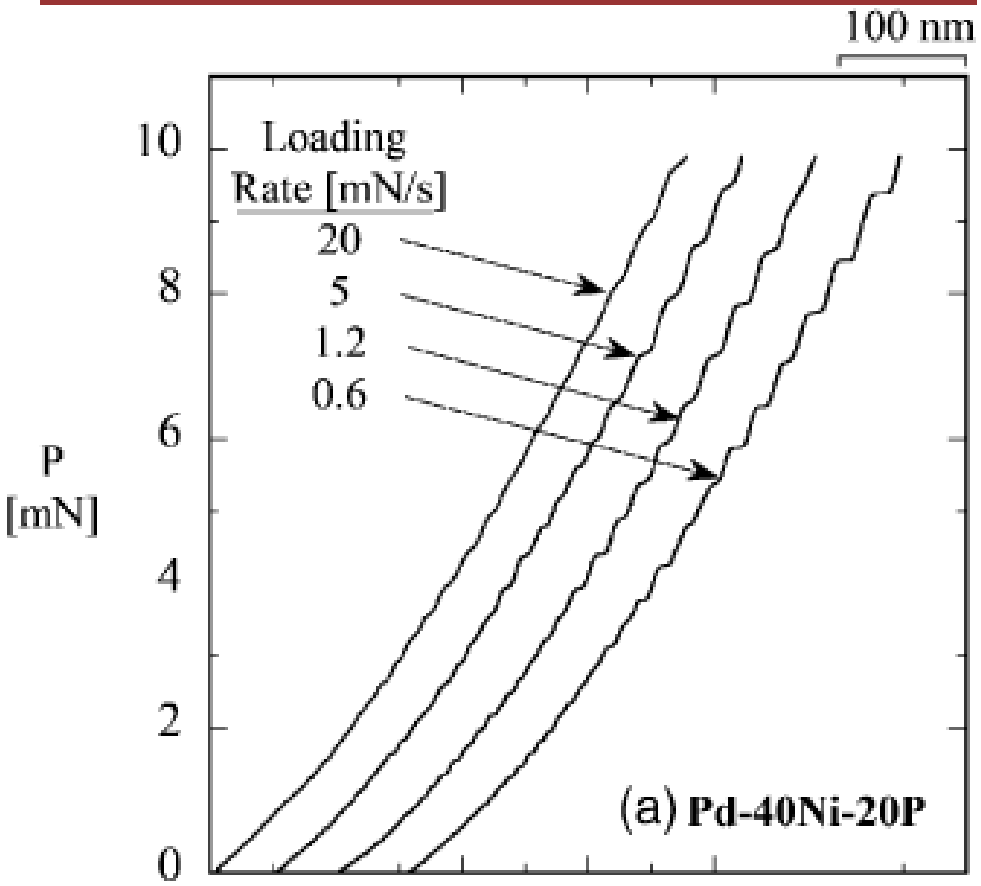
after Argon. Acta Metall. 1979.

~ nm **$t \sim 10^{-(10-12)}$ s**



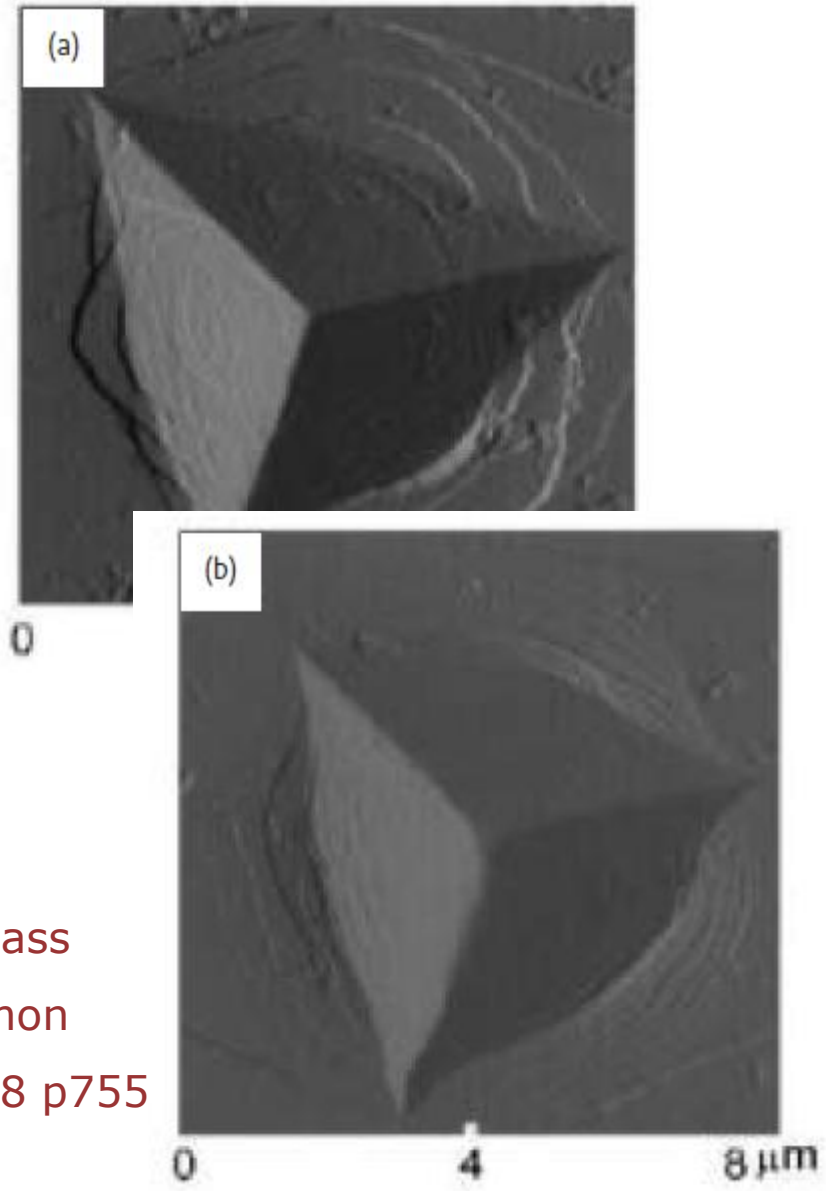
t ~ ???

Timescale for shear bands



Schuh, Nieh

Acta Mater (2003) v51 p87



Al based glass

Jiang, Atzmon

JMR (2003) v18 p755

Timescale for shear bands

Critical strain rates:

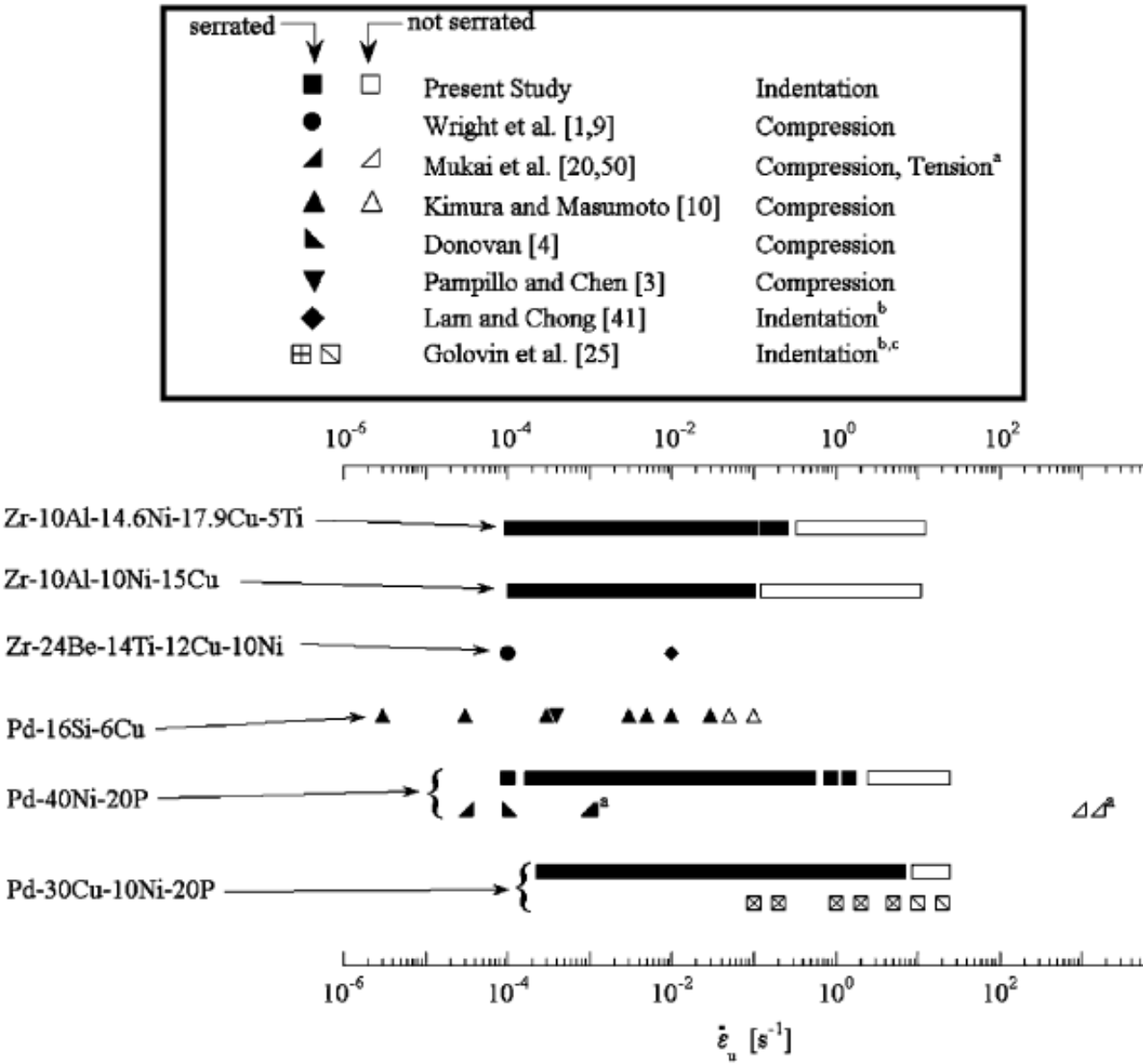
10^{-1} to 10^{1} s^{-1}

Strain accommodated:

.05

Critical time:

0.4 to 40 ms

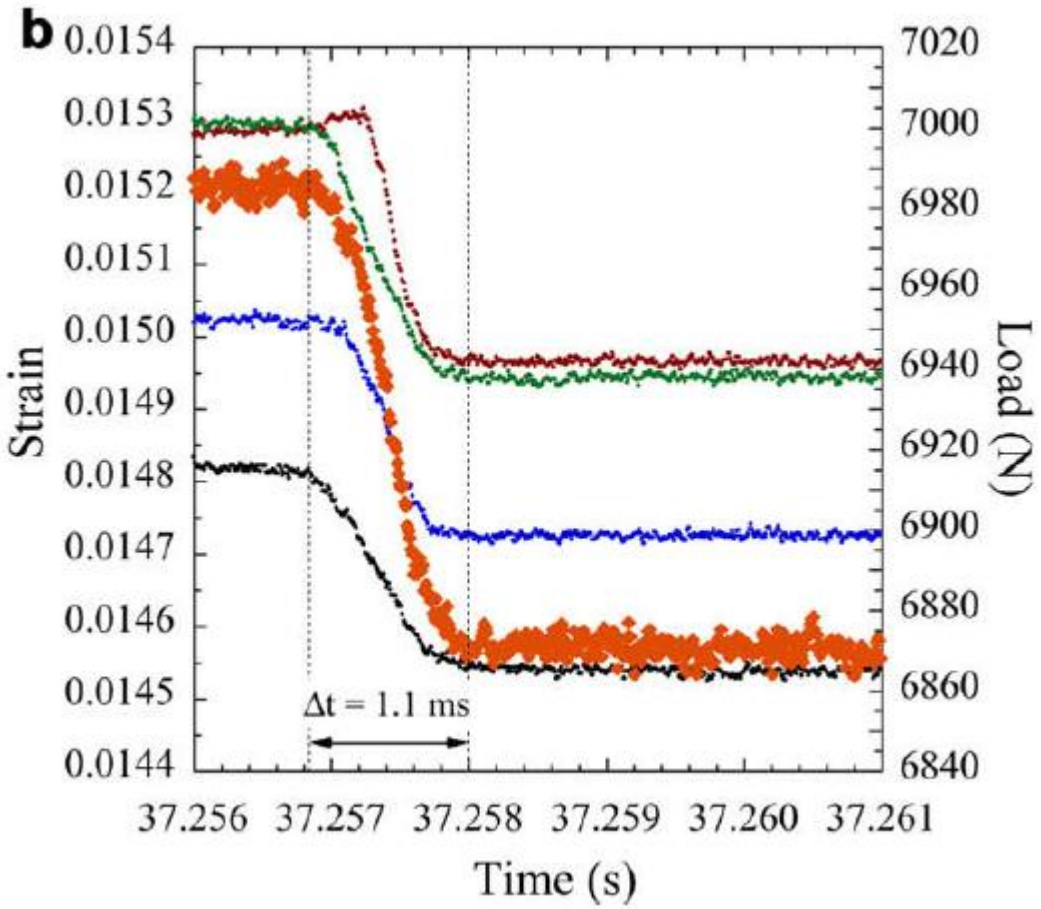


Schuh, Nieh

Acta Mater (2003) v51 p87

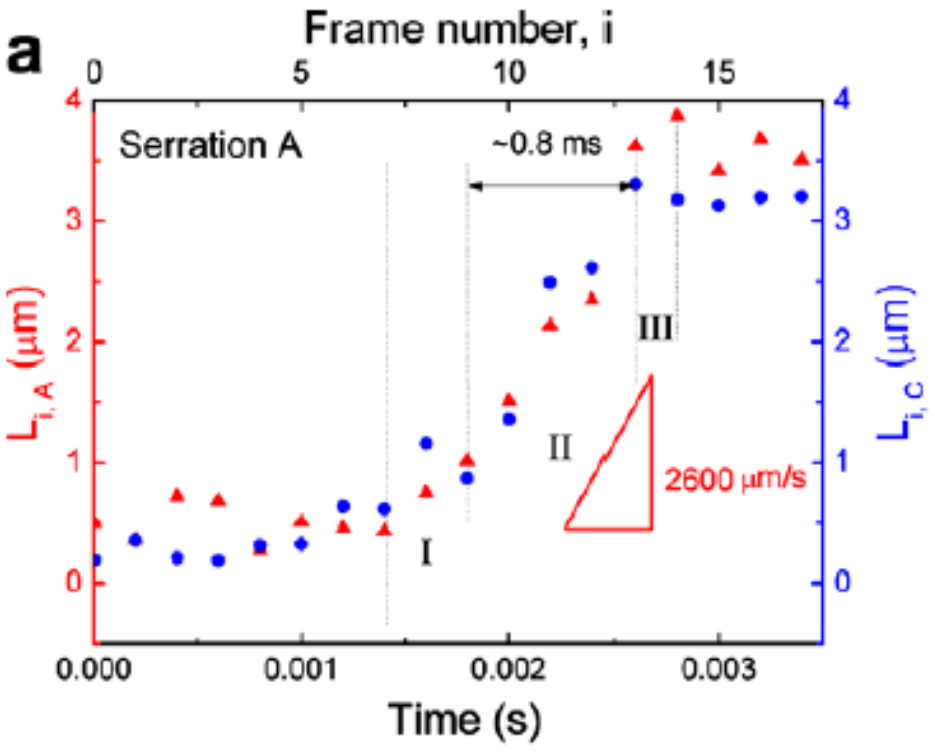
Strain gauge measurements

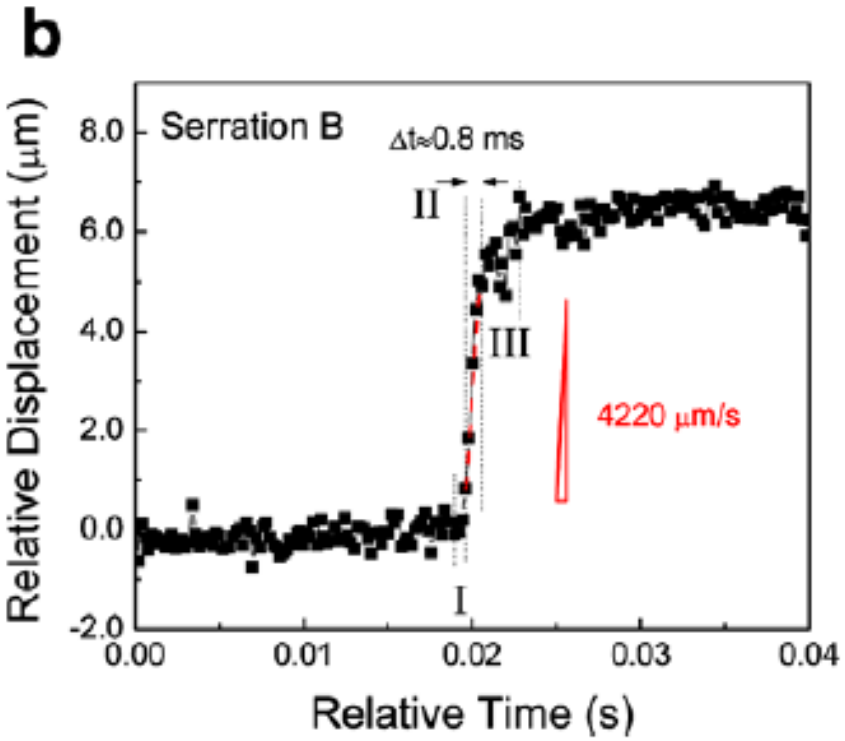
Wright et al. Acta Mater (2009) v57 4639



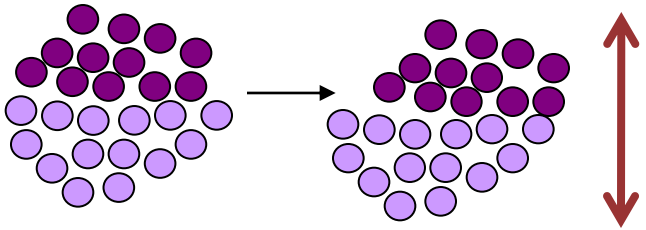
High speed videography

Song and Nieh (2010) Scripta Mater v62 847





Kinetics

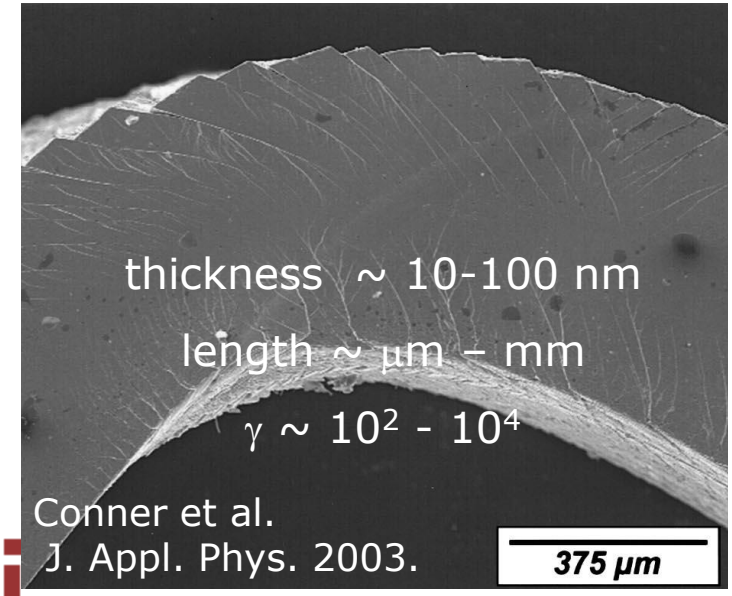


after Argon. Acta Metall. 1979.

~ nm

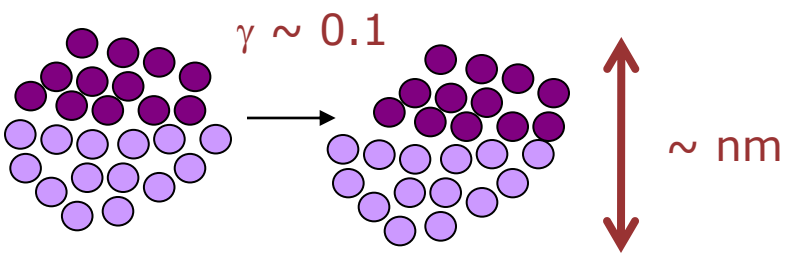
t ~ 10^{-11} s

What controls the shear band timescale?



t ~ 10^{-3} s

Puzzles: the gap between atomic motion and shear bands



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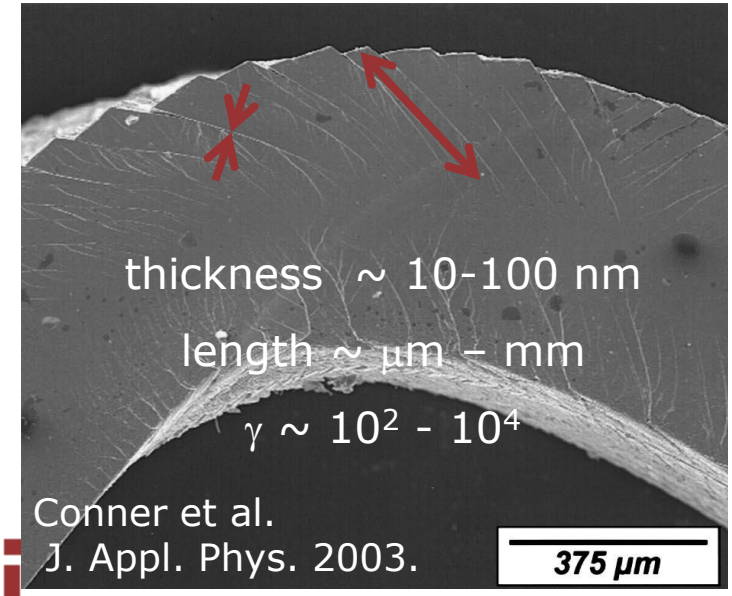
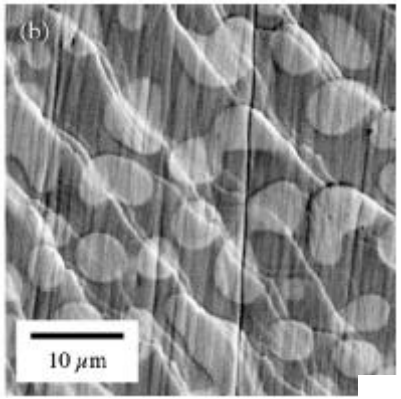
???



- Kinetics
- Behavior in gradients of stress
- Event spectrum

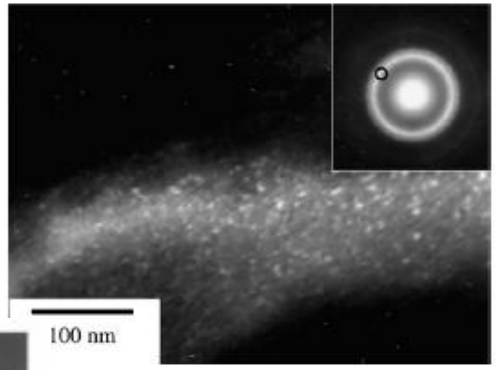
Shear localization around stress concentrators

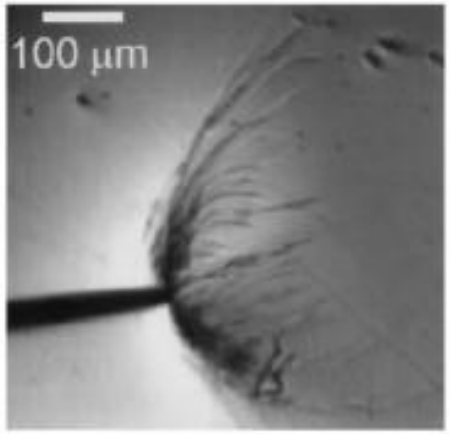
- Glass-matrix composites
- Phase transformations during deformation
- Fracture mechanics



Hays et al.
PRL (2000)
v84, 2901

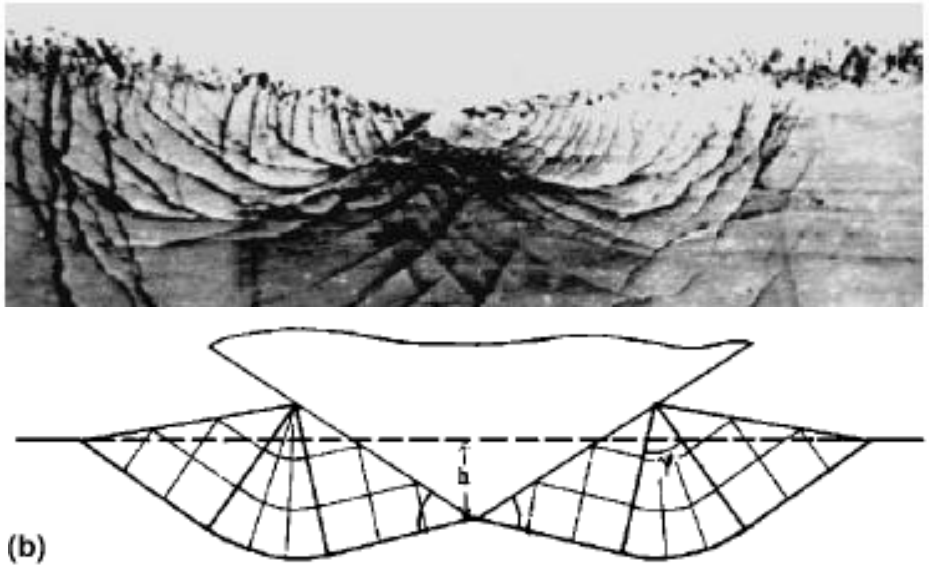
Jiang, Atzmon,
Acta Mater (2003)
v51, p4095





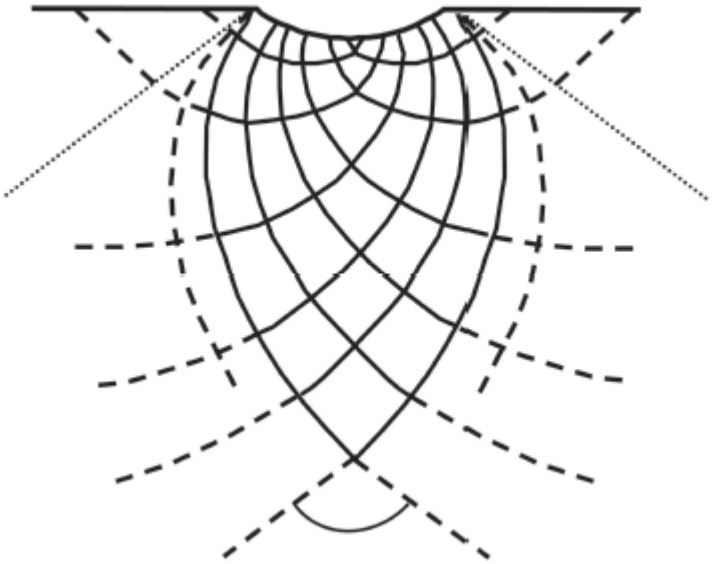
Flores, Dauskardt
Scripta Mater (1999)
v41, p937

Slip line fields

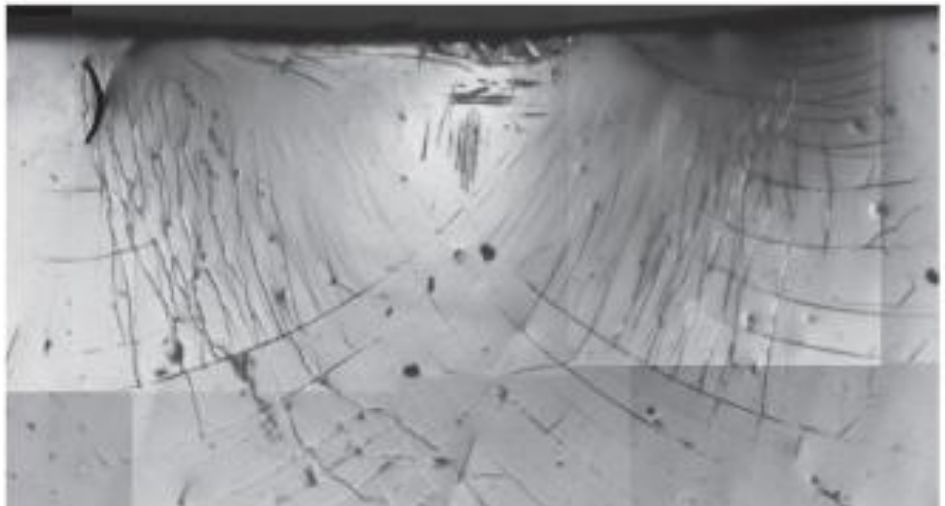


Schuh, Nieh

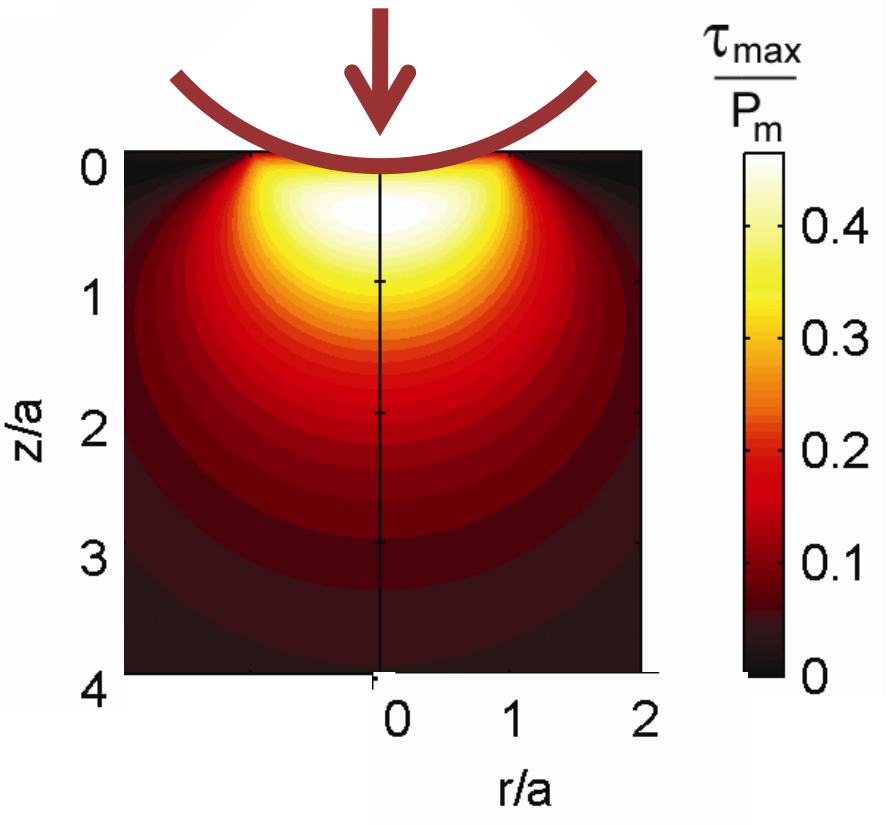
JMR (2004) v19 46

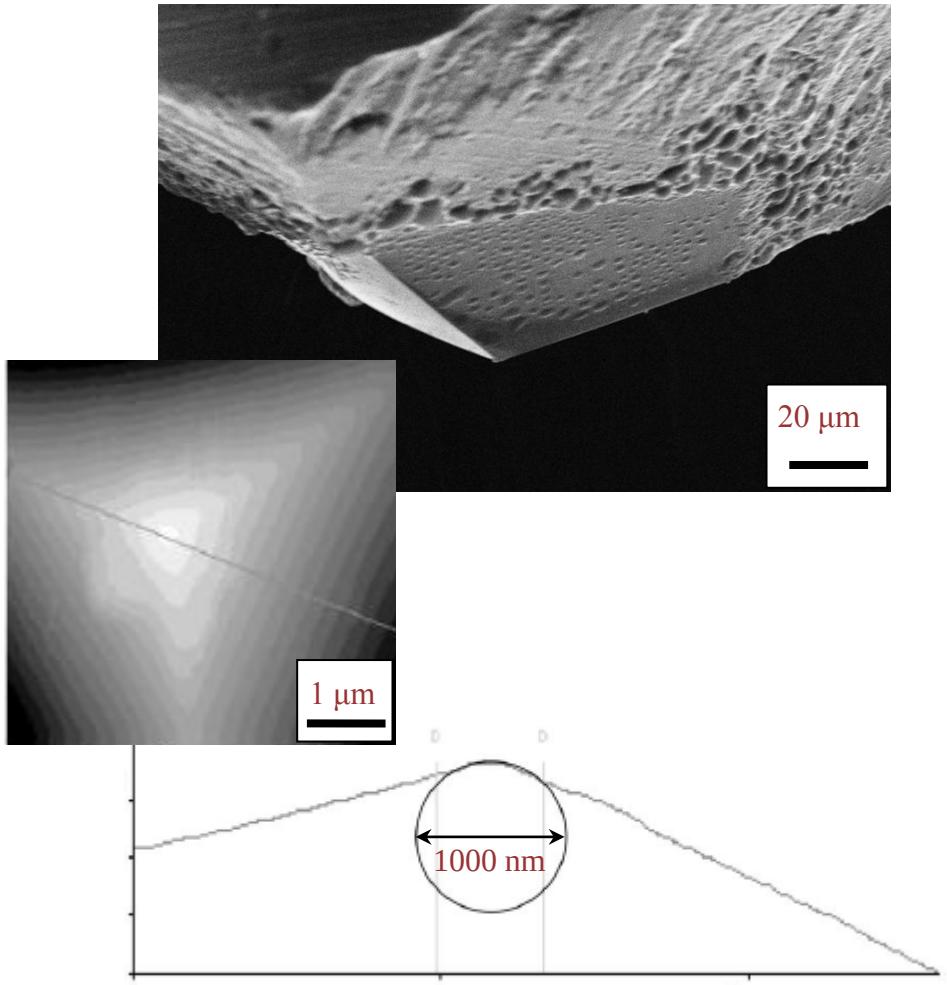


Antoniou, JMR (2007) v22 514



Nanoindentation measurements

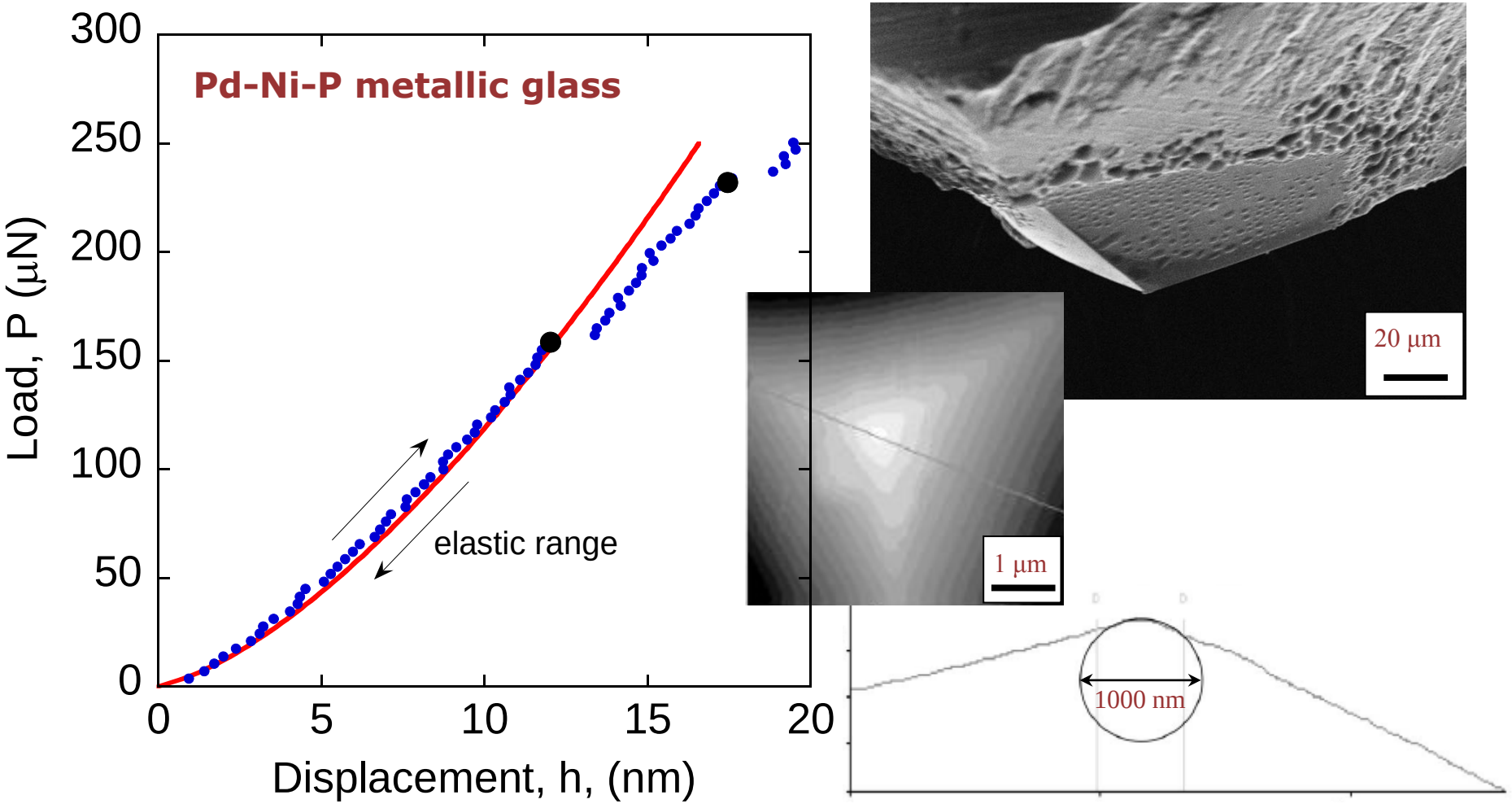




Images from Trelewicz, Packard (MIT)

as well as Chiu and Ngan, Acta Mater, 2002

Nanoindentation measurements



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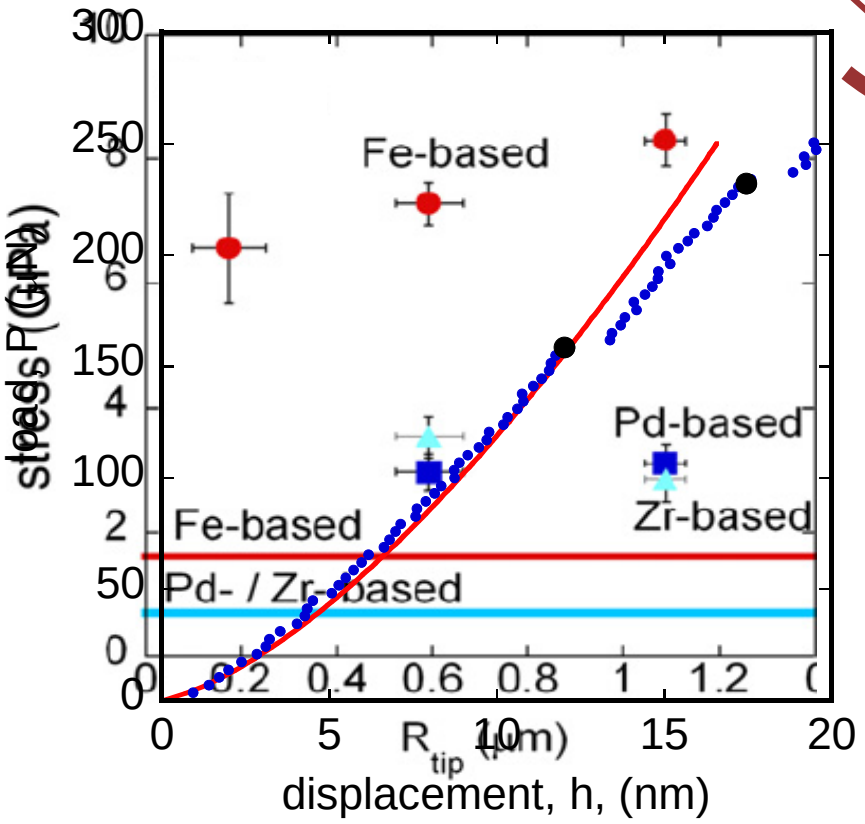
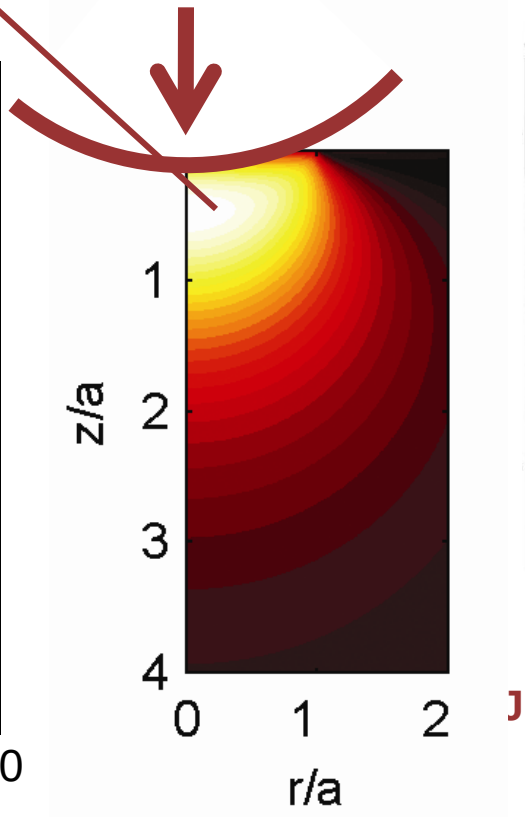
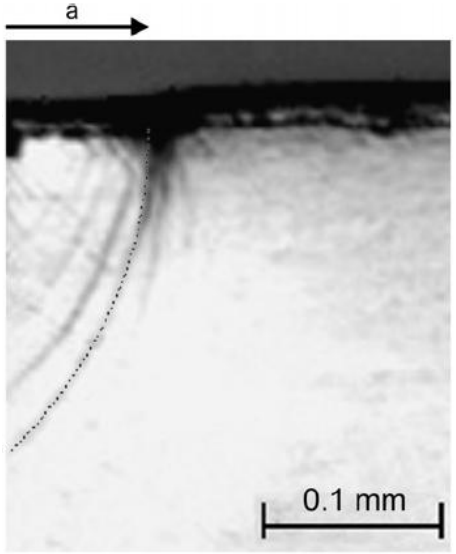
Metallic glass: yield avoids τ_{max}

$$\tau_{\max} = \frac{0.47}{\pi} \cdot \left(\frac{4E_R}{3R_{tip}} \right)^{2/3} P^{1/3}$$



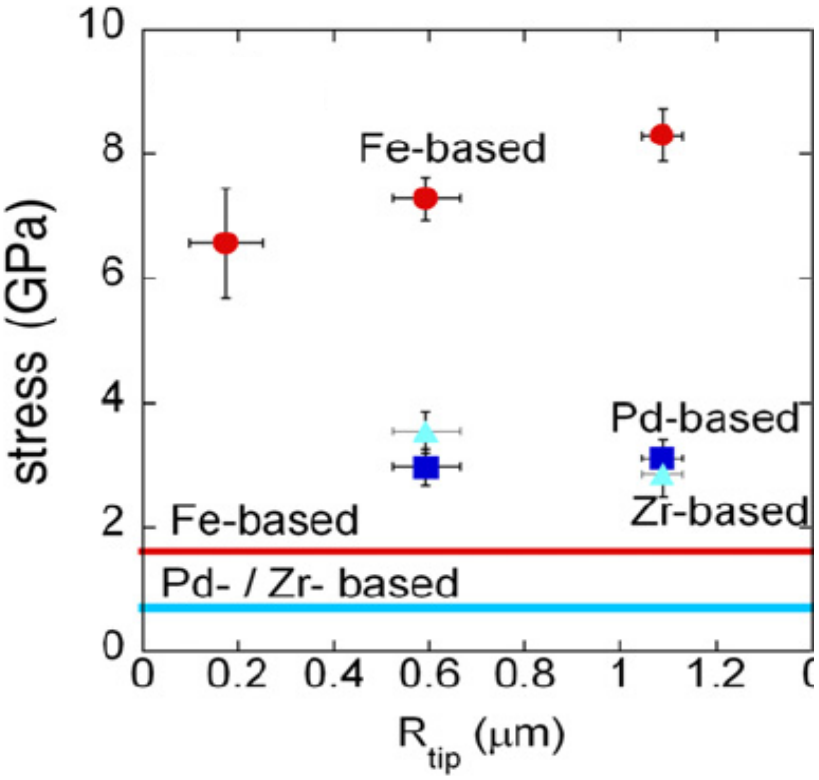


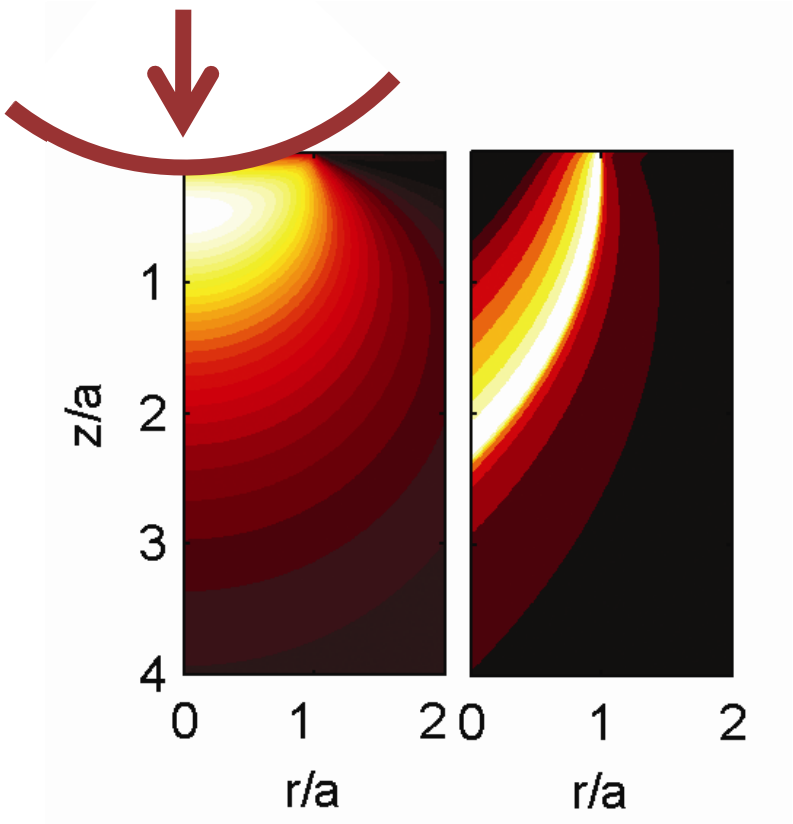


Adapted from L. Anand

J.Mech.Phys.Solids 2005

Metallic glass: yield avoids τ_{max}

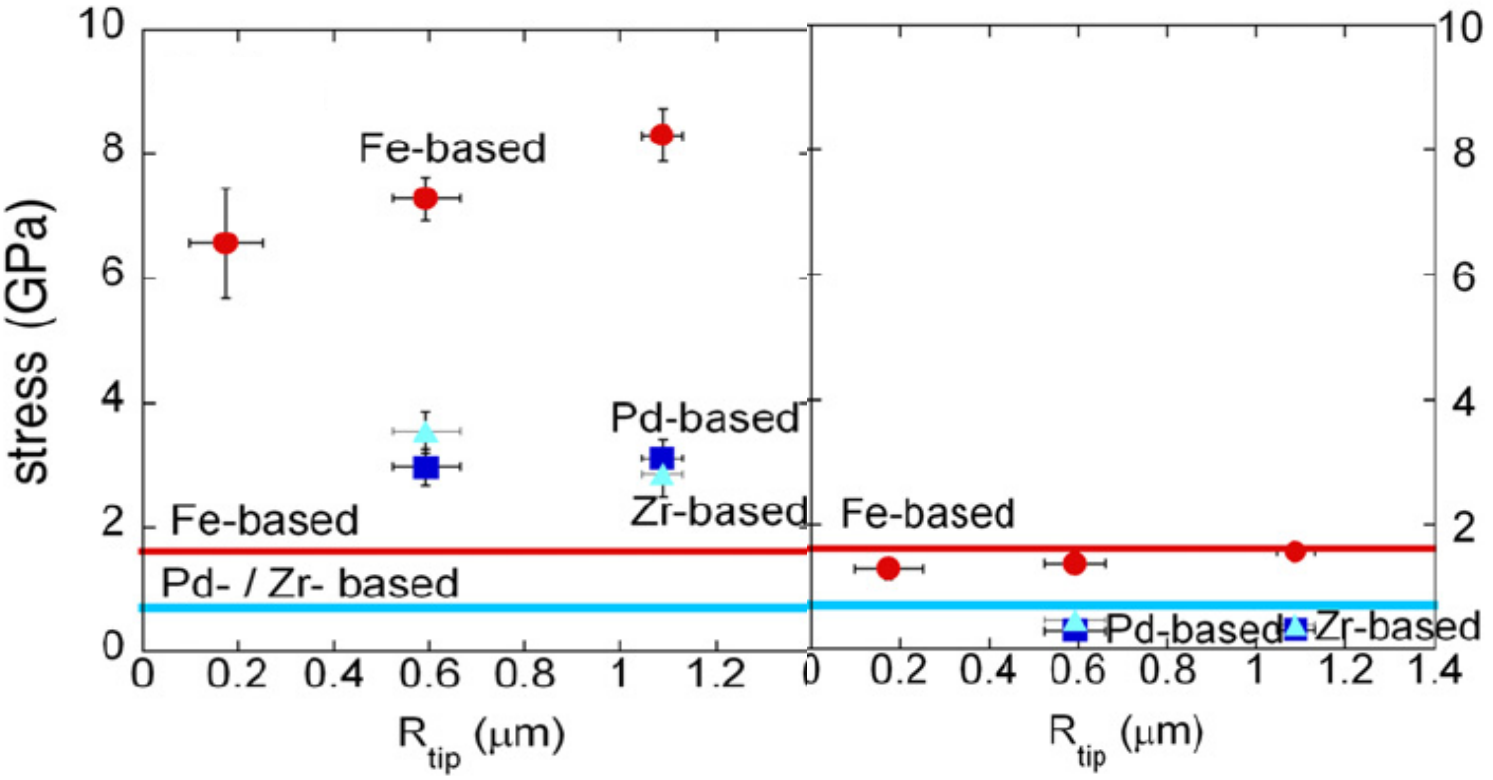




Metallic glass: yield avoids τ_{max}

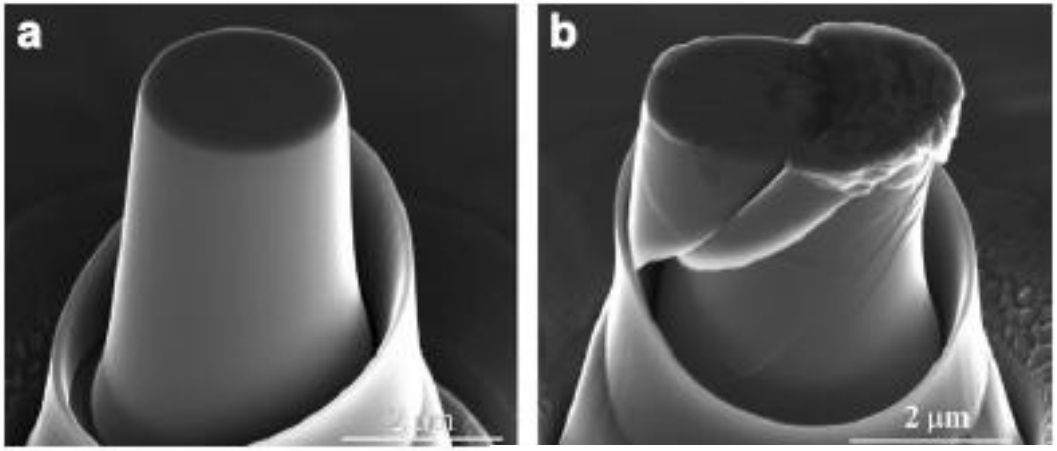
Packard and Schuh

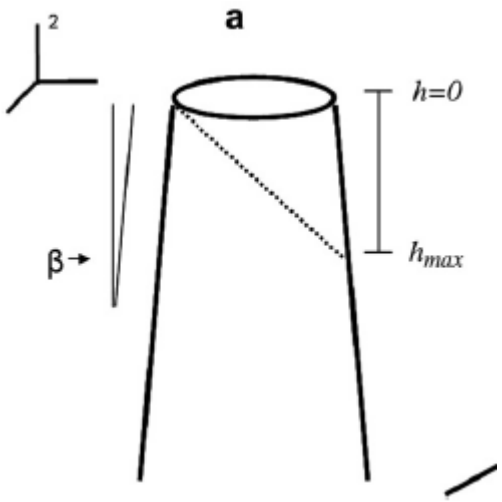
Acta mater. 2007, v55 p5348

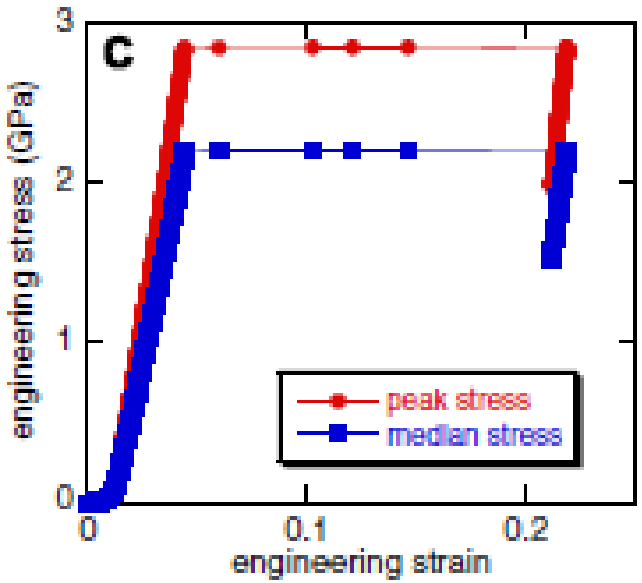


Tapered microcompression

Schuster et al., Acta Mater (2008) v56, 5091







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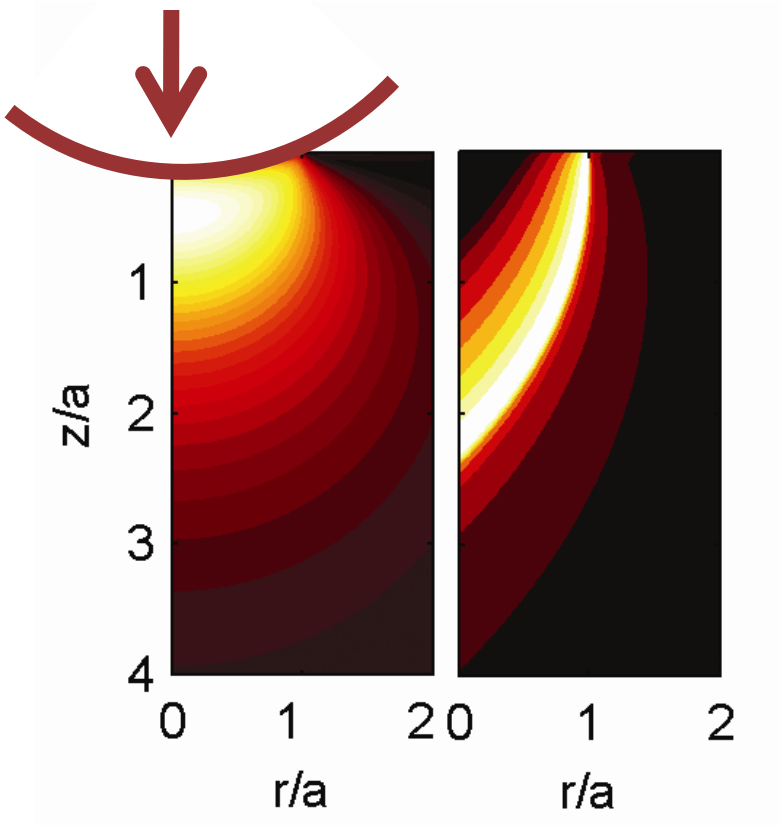
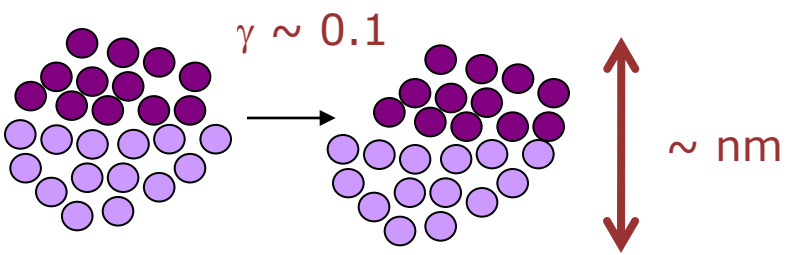


Yield is controlled by the *lowest stress* point on the *highest stress* shear path!

What is the process of STZ assembly that governs the development of the shear plane in a complex stress field?

Puzzles: the gap between atomic motion and shear bands



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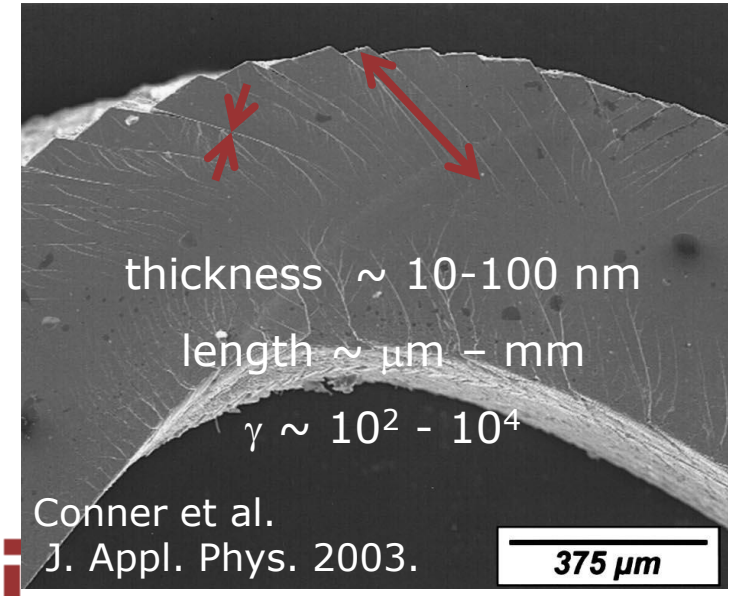
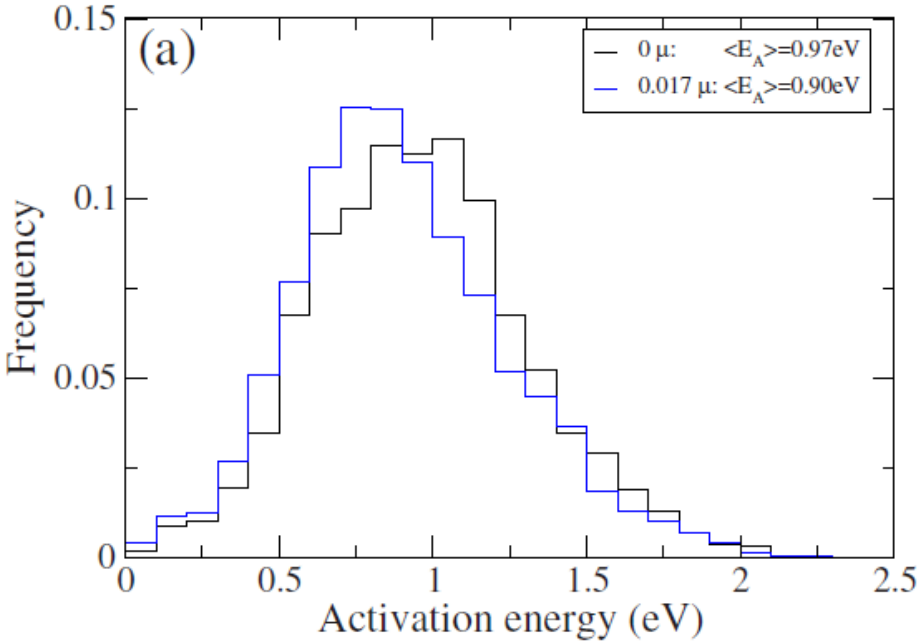
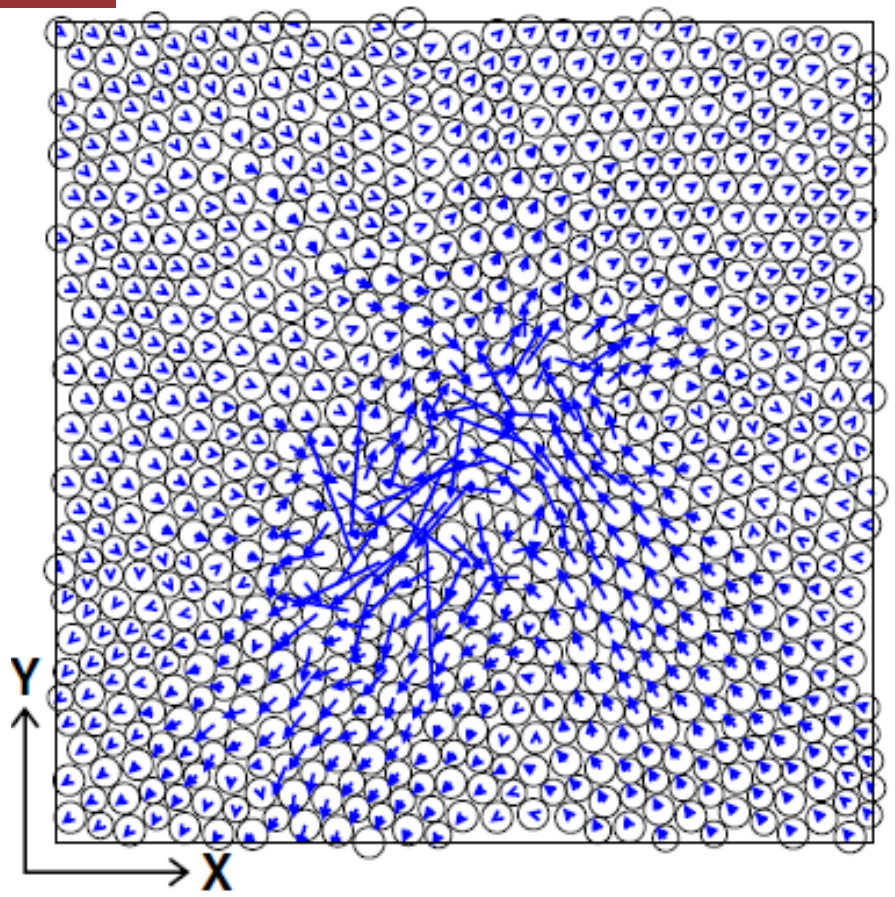
???



- Kinetics
- Behavior in gradients of stress
- Event spectrum

Event spectrum



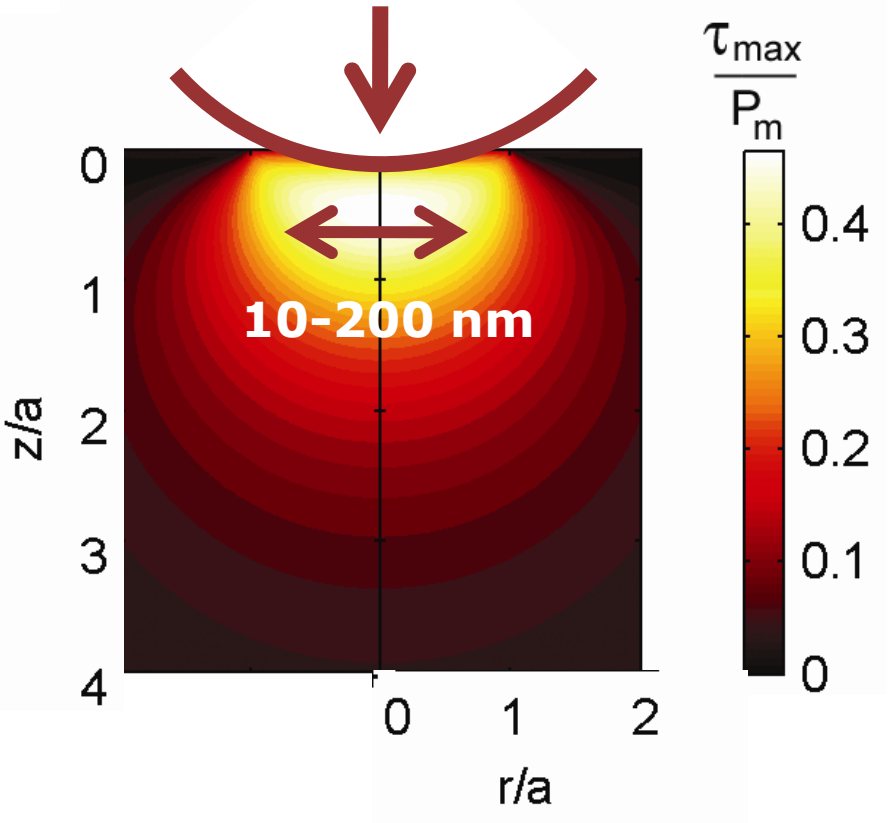


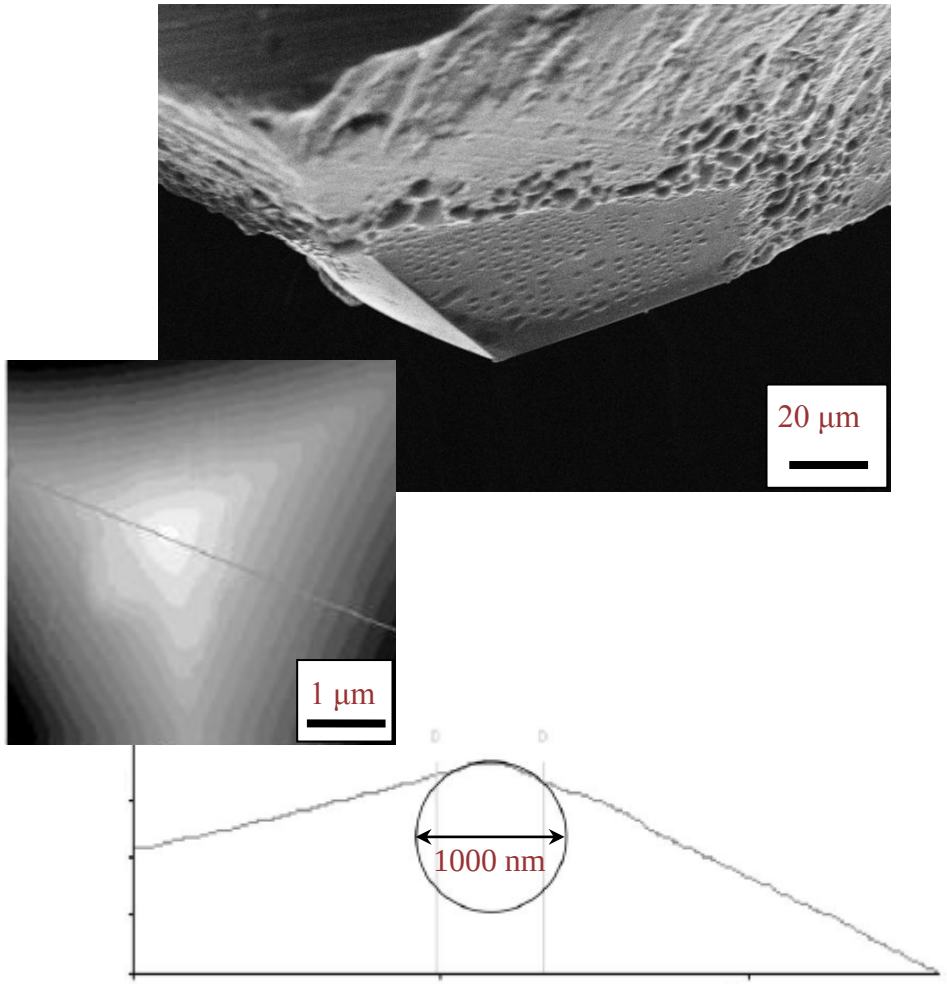
In 'jammed' configuration at T = 0 K

D. Rodney: PRL (2009) v102 235503

PRB (2009) v80 184203

Nanoindentation measurements





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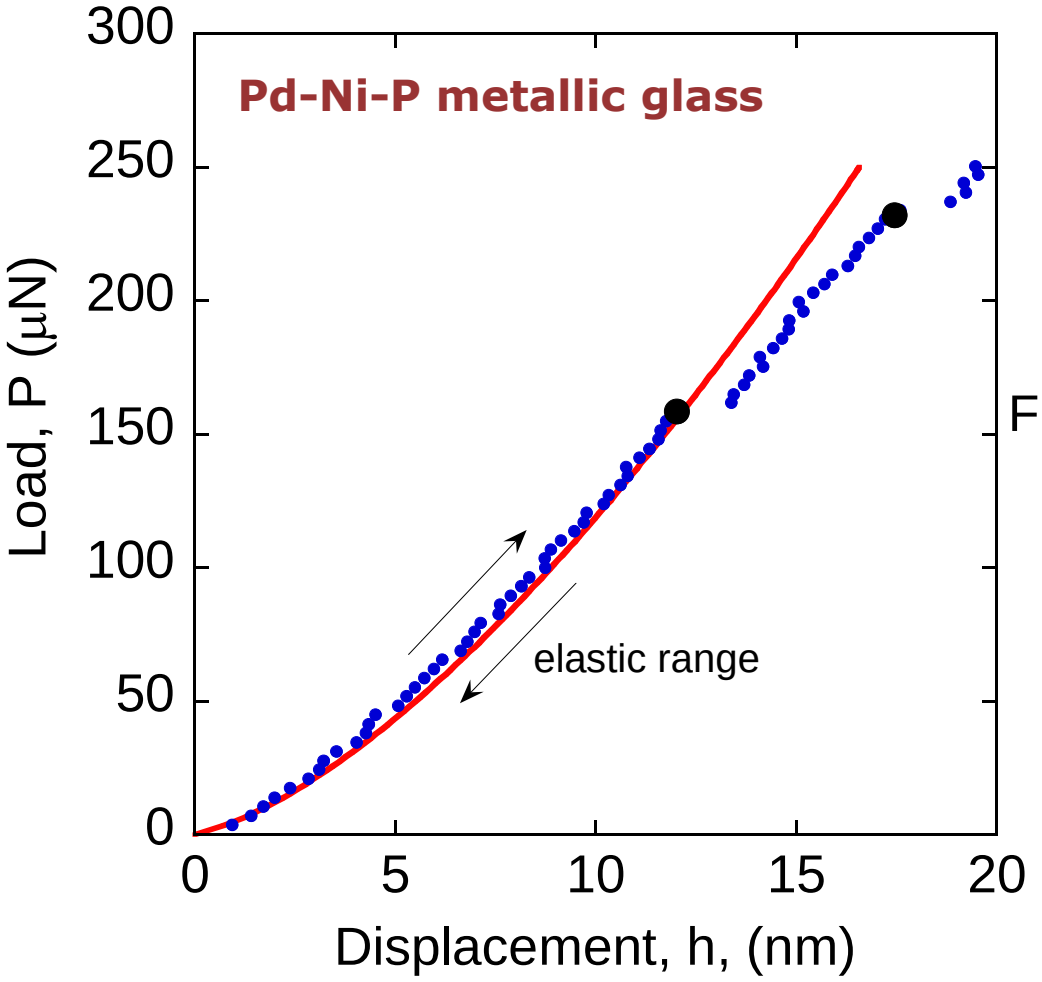
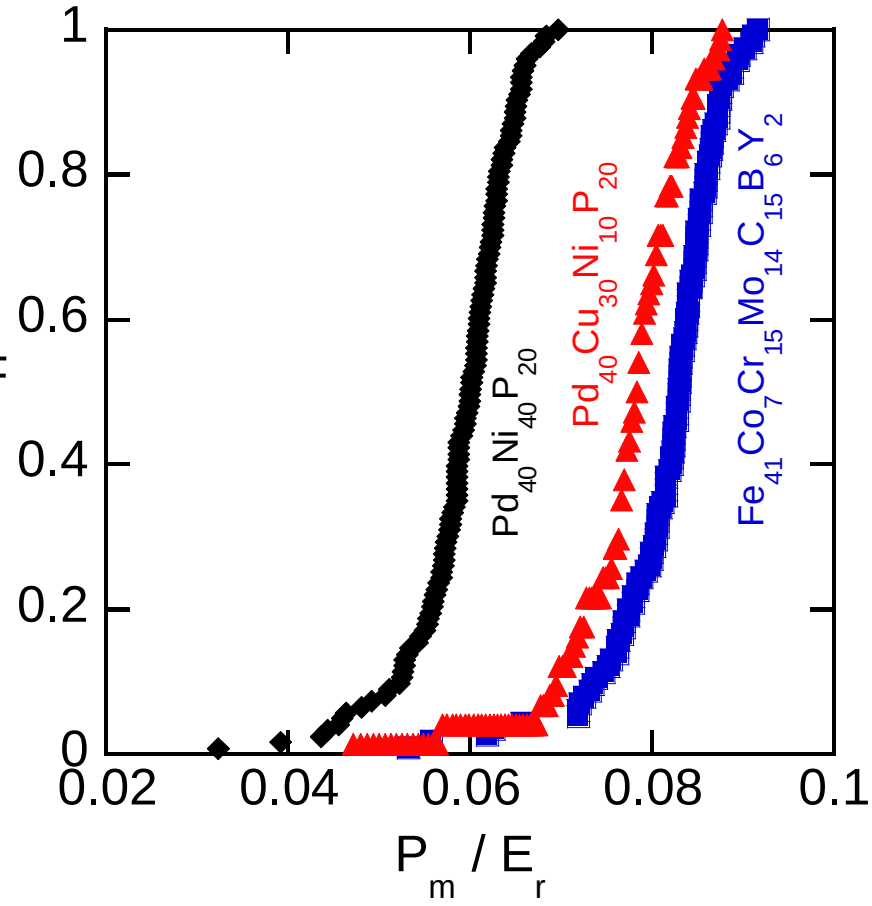
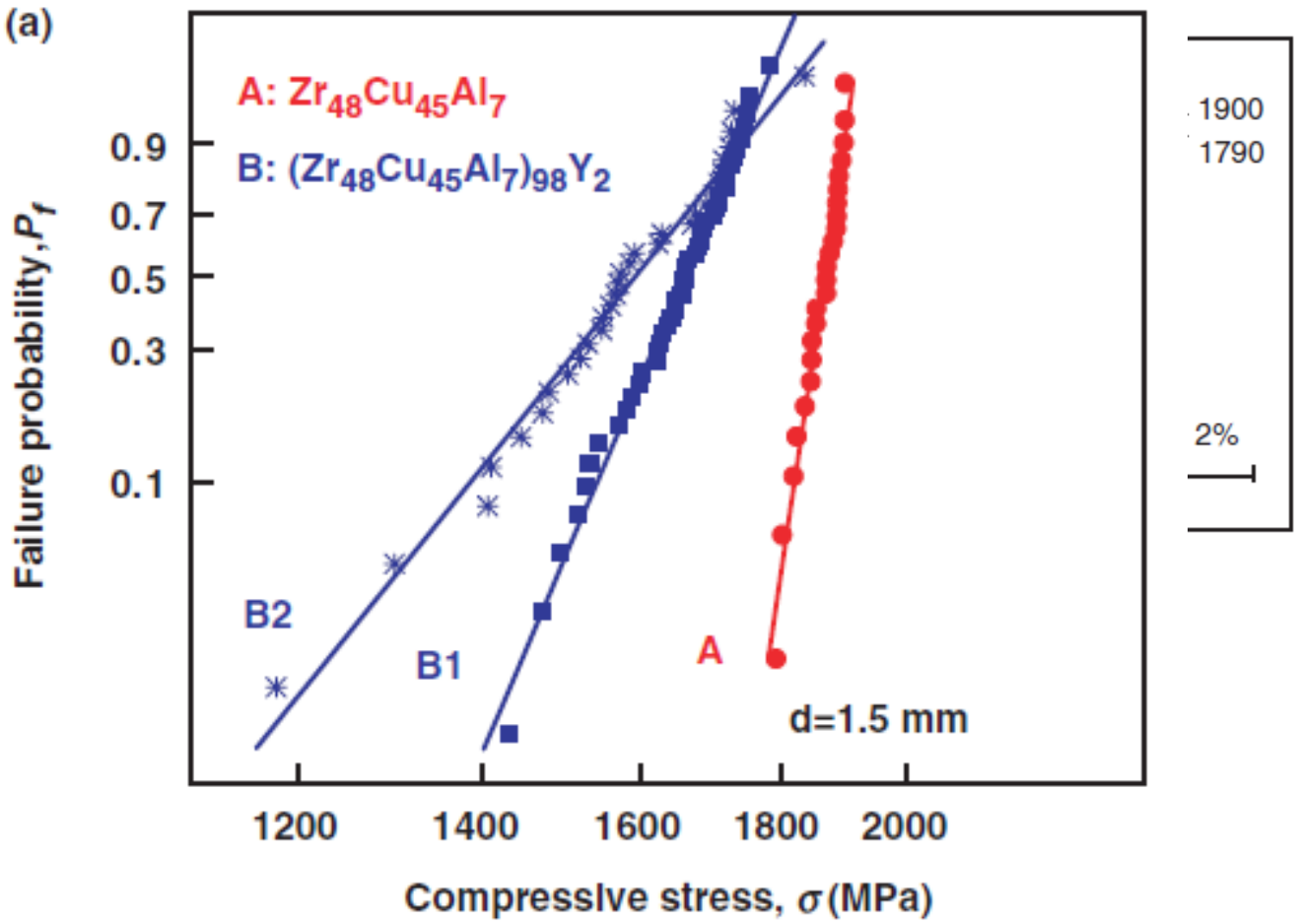




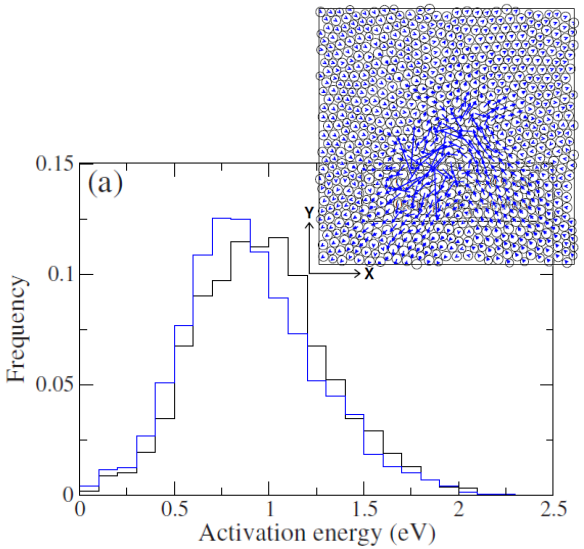
Event spectrum

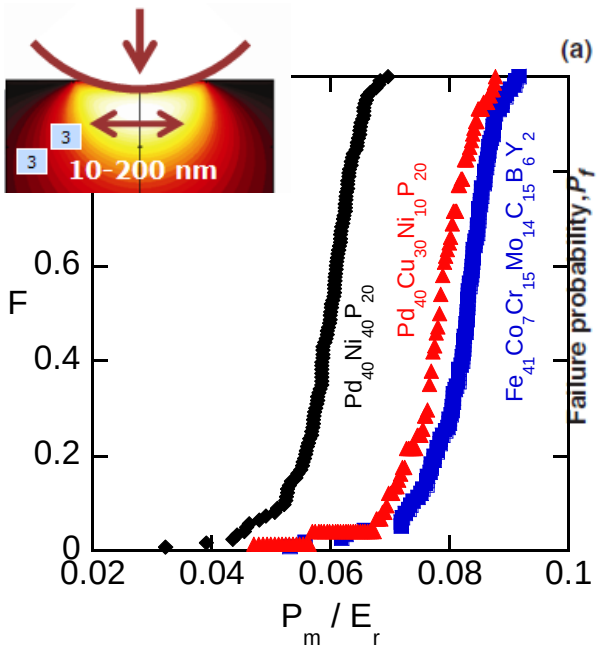


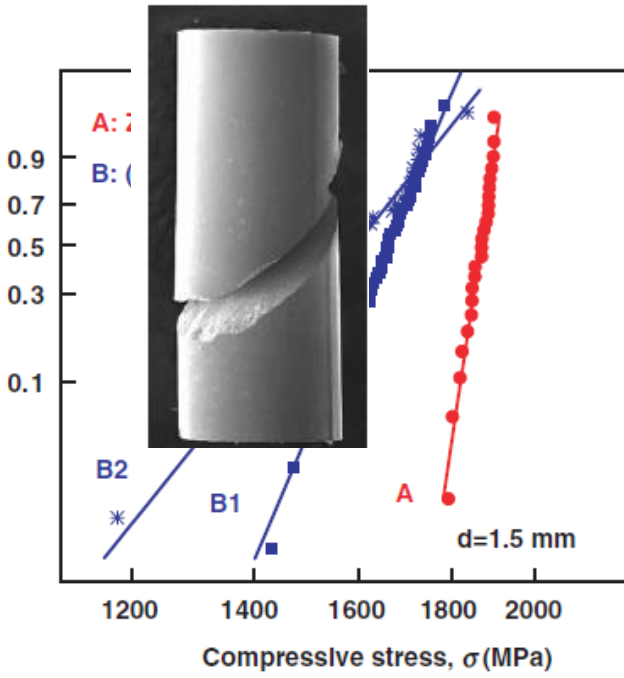
W.F. Wu, Y. Li, and C.A. Schuh

Phil Mag (2008) v88 p71

Spectra at all scales

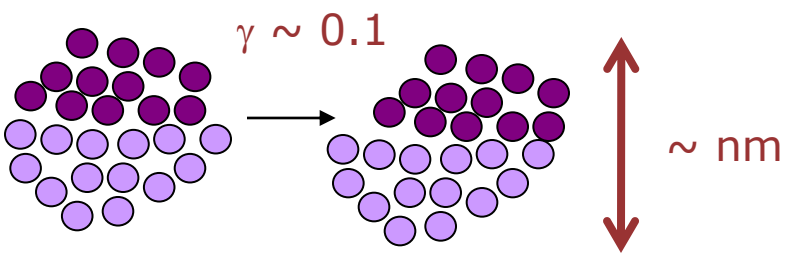






What is the STZ assembly process that governs strength at larger scales?

Puzzles: the gap between atomic motion and shear bands



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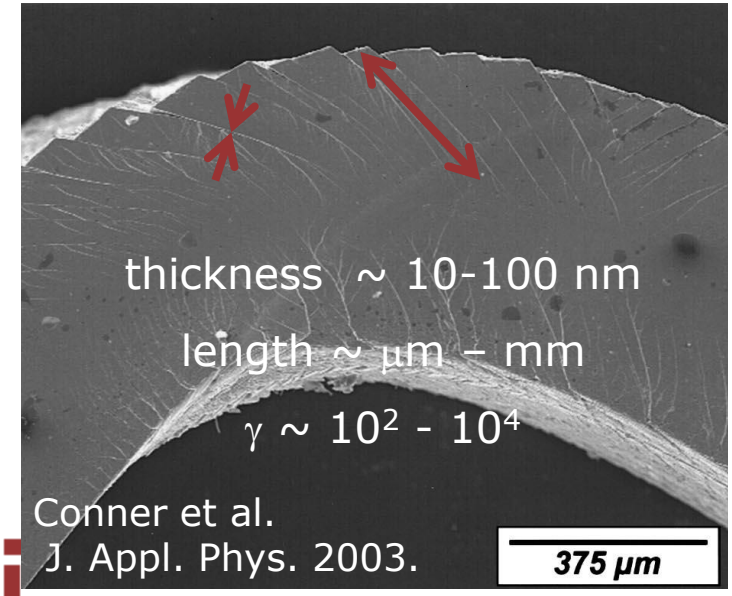


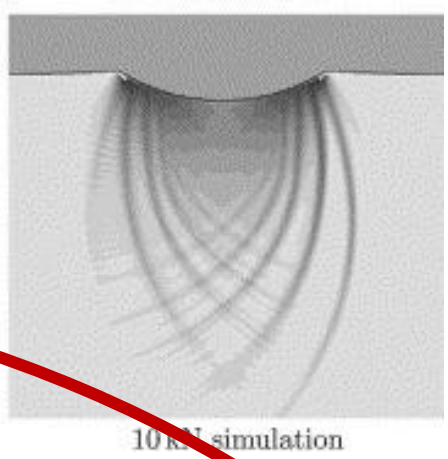
- Kinetics
- Behavior in gradients of stress
- Event spectrum

STZ Dynamics

- Shear Transformation Zone (STZ)
  - Stochastic stress-biased thermally activated event

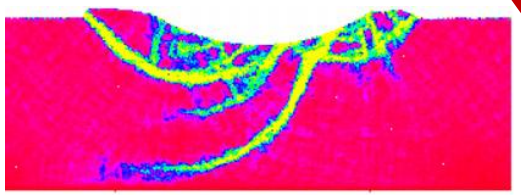
$$\dot{s} = \nu_o \exp\left(-\frac{\Delta F_o - \tau V^*}{k_B T}\right)$$

Continuum Simulations

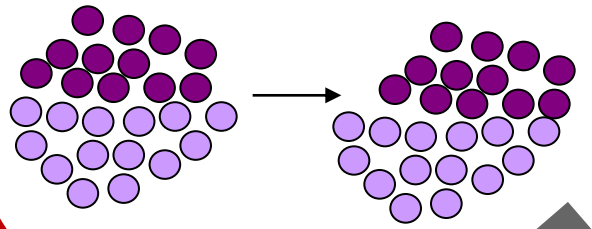


Su, Anand. Acta Mat 2006.

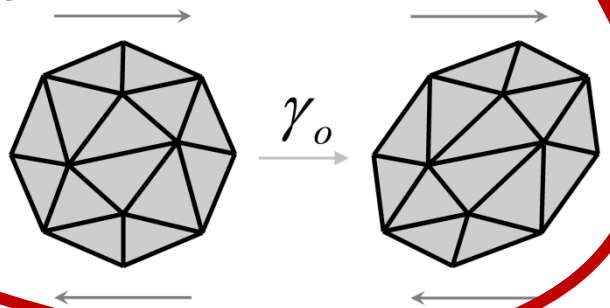
Atomistic Simulations



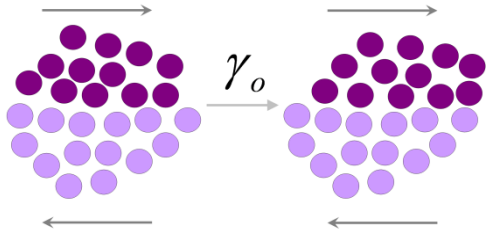
Shi, Falk. Acta Mat 2007.



STZ Dynamics

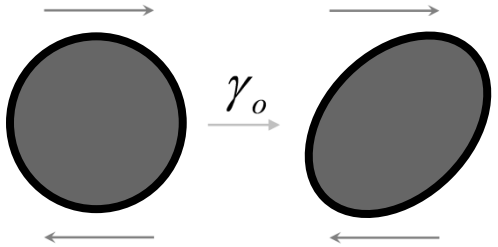


Coarse-graining the shear transformation zone

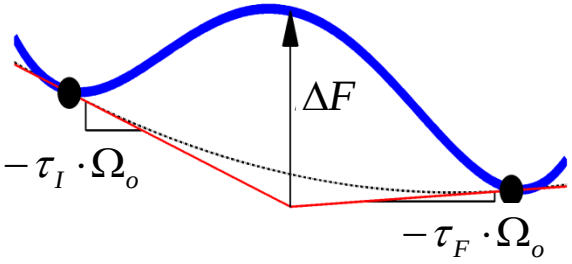


Argon. Acta Metall. 1979.

Coarse-Grain



Potential Energy Landscape

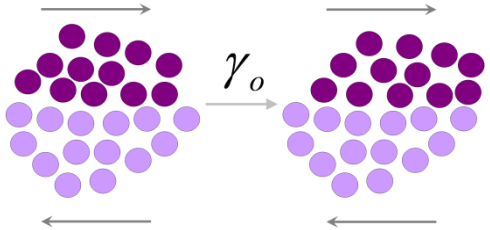
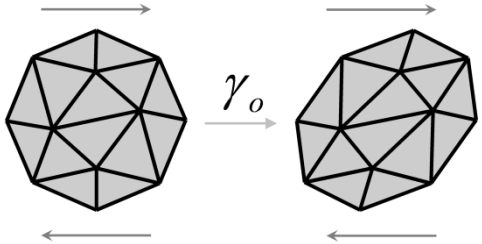
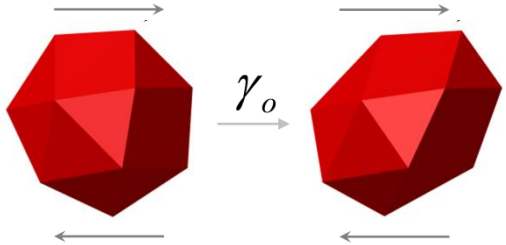


Bulatov, Argon. Model. Simul. Mater. Sci. Eng. 1994.

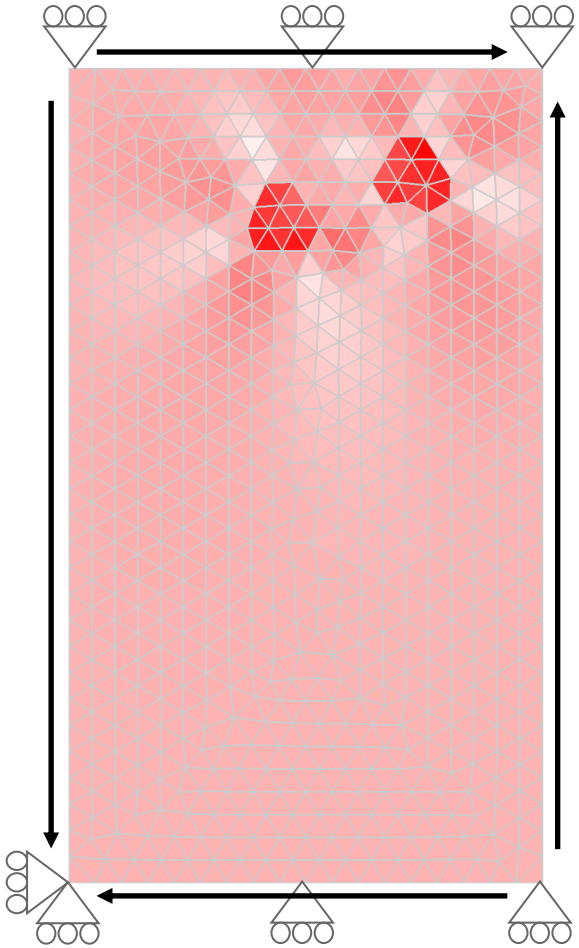
Characteristic Attempt Frequency

$$\dot{s} = \nu_o \cdot \exp\left(-\frac{\Delta F - \frac{1}{2}\tau \cdot \gamma_o \cdot \Omega_o}{kT}\right)$$

Key elements for a mesoscale model

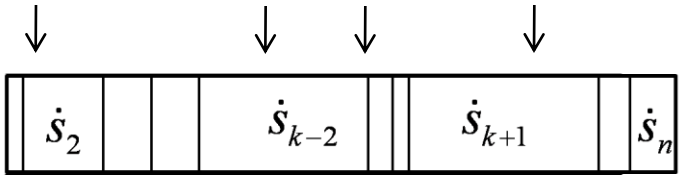
	Coarse-Grain	STZ Activation Rate
STZ		$\dot{s} = \nu_o \cdot \exp\left(-\frac{\Delta F - \frac{1}{2}\tau \cdot \gamma_o \cdot \Omega_o}{kT} \right)$
2D		$\dot{s} = \nu_o \cdot \exp\left(-\frac{\Delta F}{kT} \right) I_o\left(\frac{\tau_{\max} \cdot \gamma_o \cdot \Omega_o}{2kT} \right)$
3D		$\dot{s} = \nu_o \cdot \exp\left(-\frac{\Delta F}{kT} \right) \iiint_{g \in G} \exp\left(-\frac{\tau(\sigma, g) \cdot \gamma_o \cdot \Omega_o}{2kT} \right) dg$

KMC plus FEM



Kinetic Monte Carlo

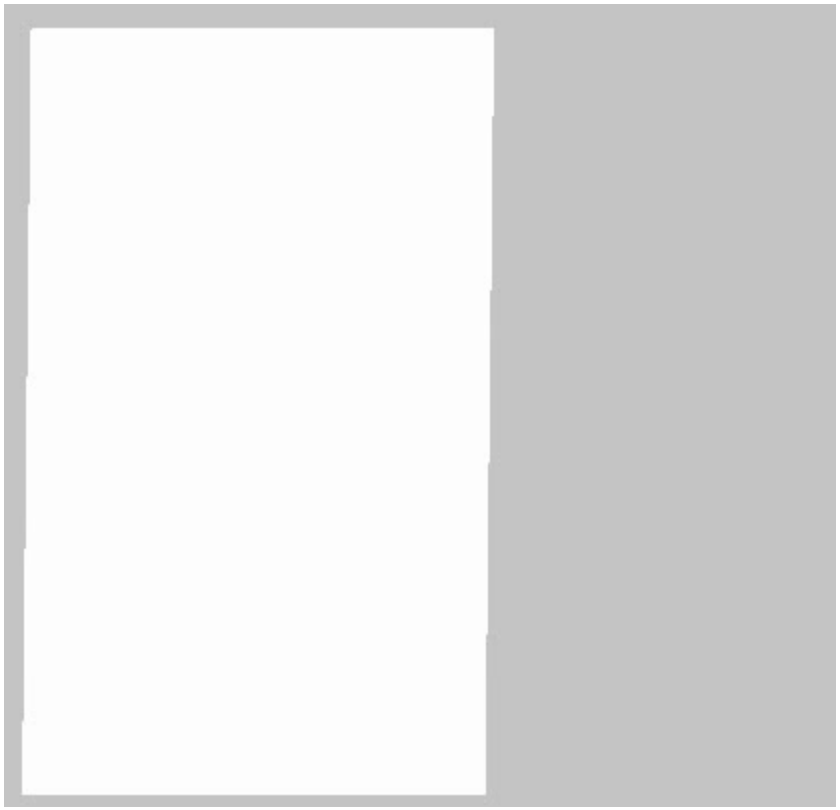
$$\dot{s} = \nu_o \cdot \exp\left(-\frac{\Delta F}{kT}\right) I_o\left(\frac{\tau_{\max} \cdot \gamma_o \cdot \Omega_o}{2kT}\right)$$



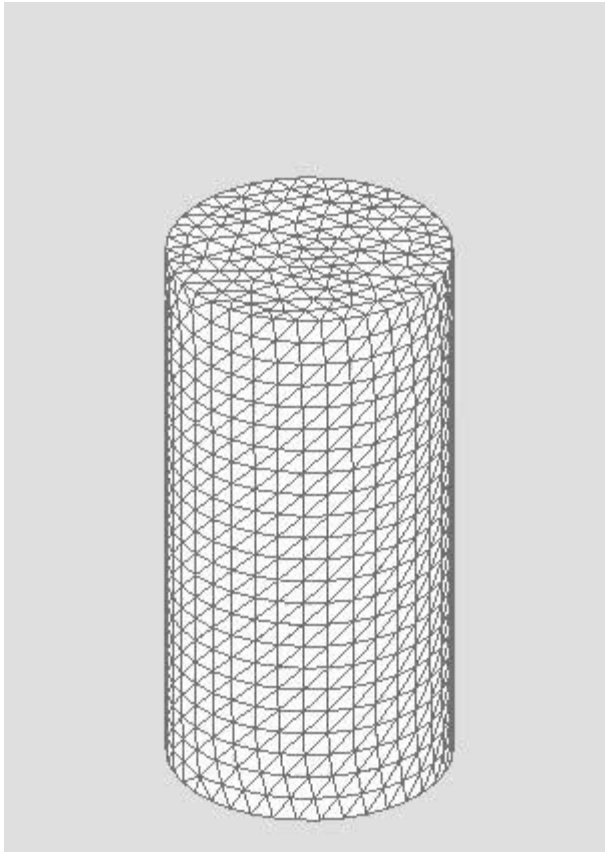
ABAQUS

High temperature

2D



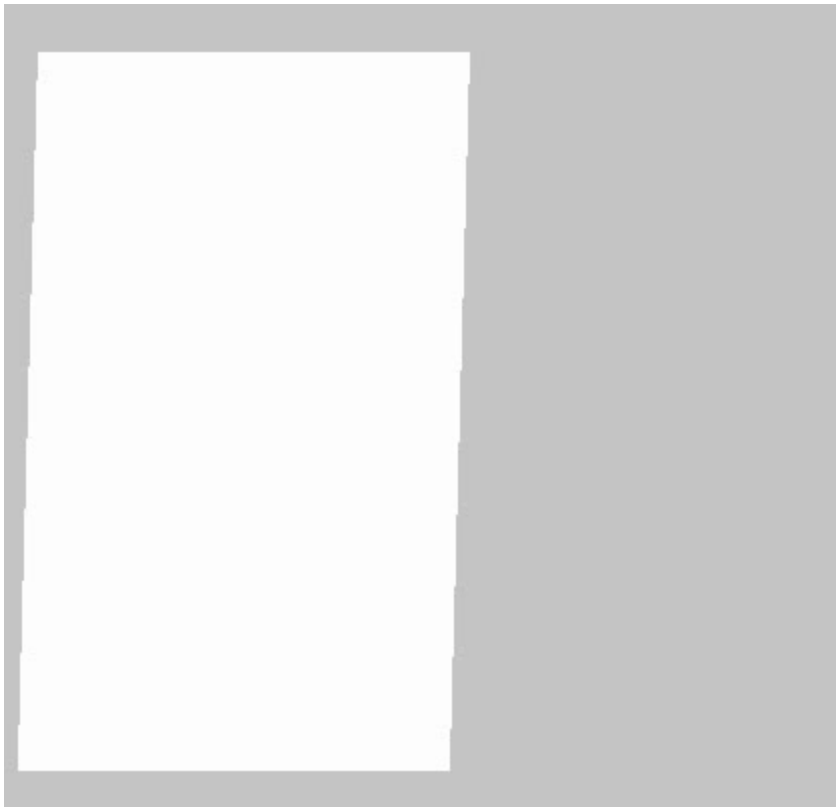
3D



Homer, Schuh. Acta Mat. 2009.

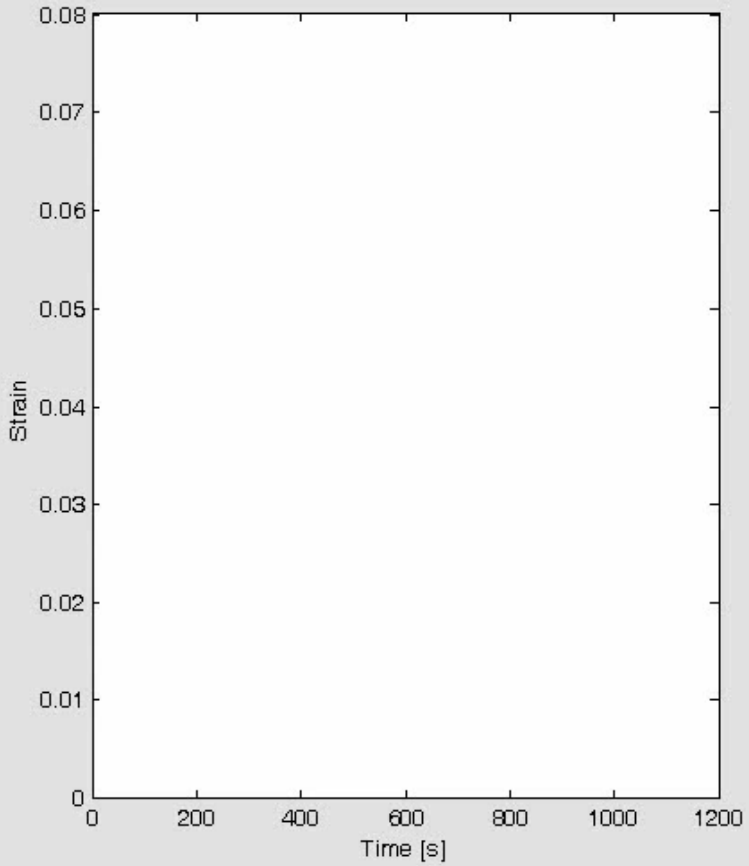
Low temperature

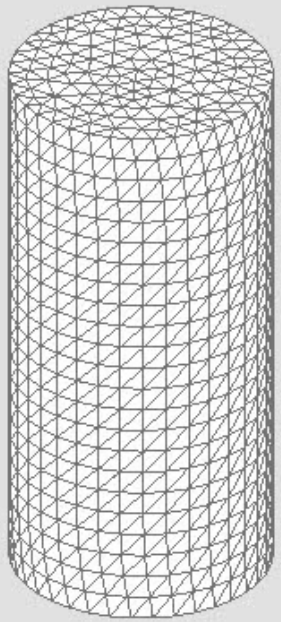
2D

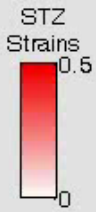


Low temperature

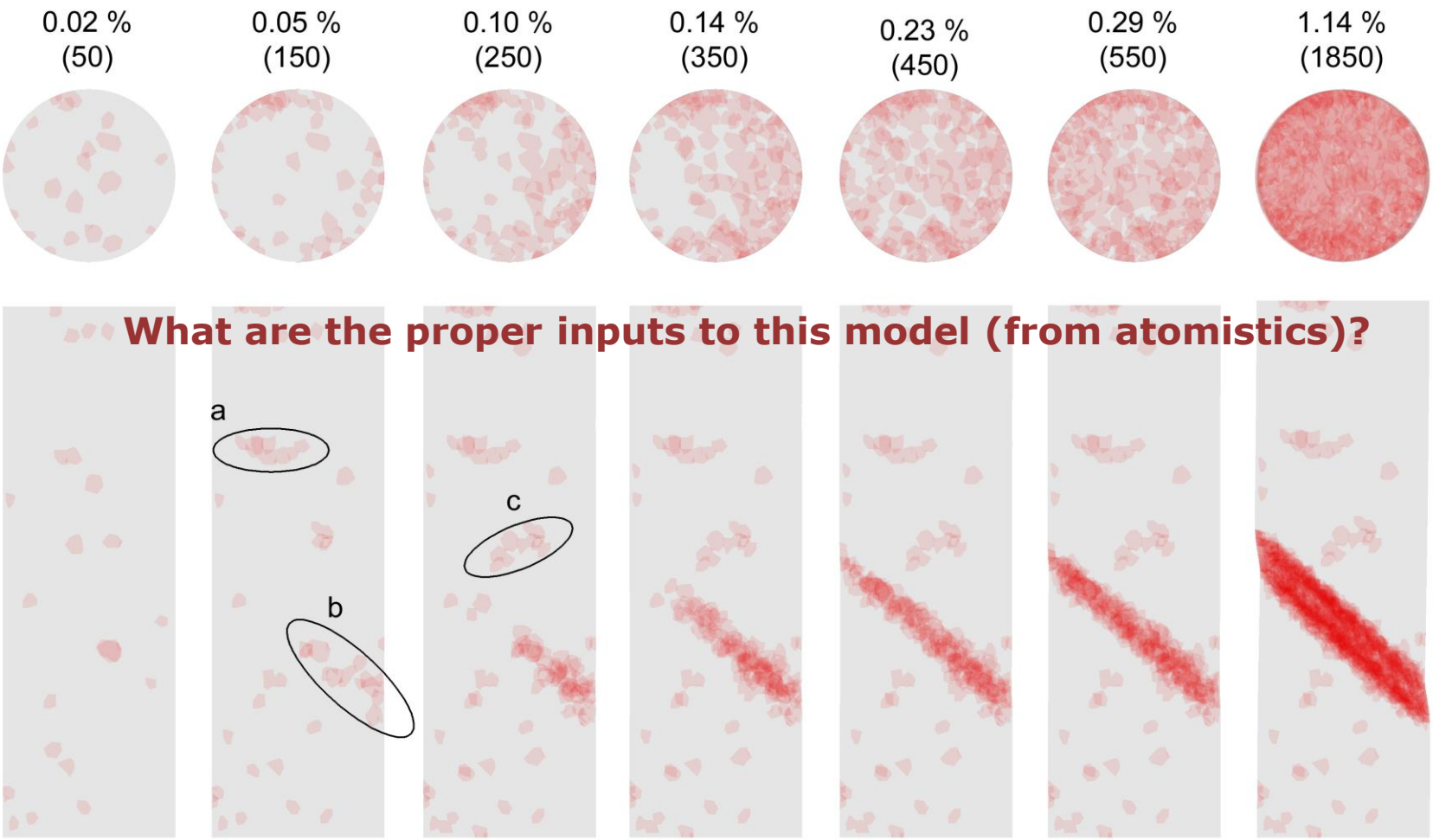
3D





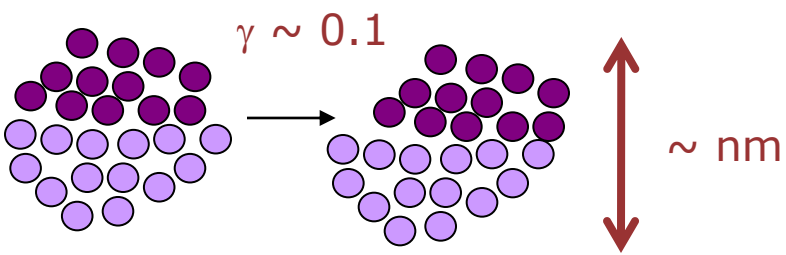


Shear band formation



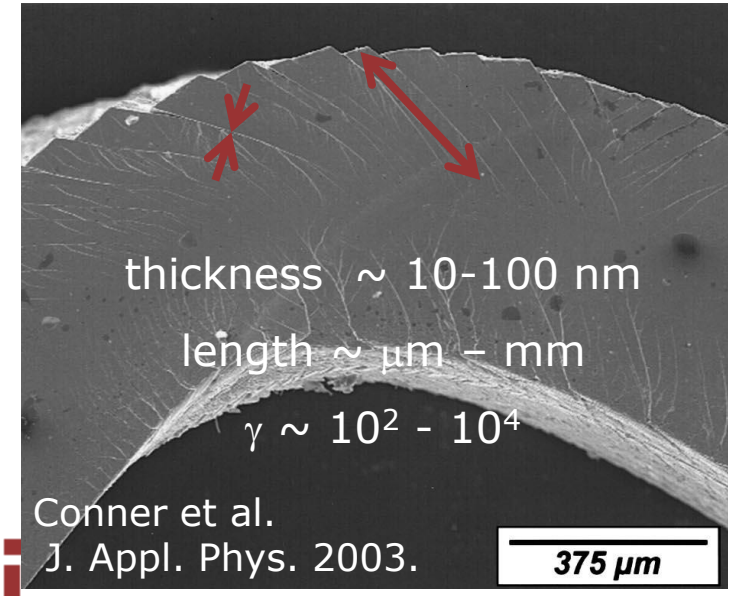
What are the proper inputs to this model (from atomistics)?

Puzzles: the gap between atomic motion and shear bands



after Argon. Acta Metall. 1979.

???



- Kinetics
- Behavior in gradients of stress
- Event spectrum