Continuum aspects of plastic deformation in amorphous alloys - pressure sensitivity

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Overview No. 144

Mechanical behavior of amorphous alloys

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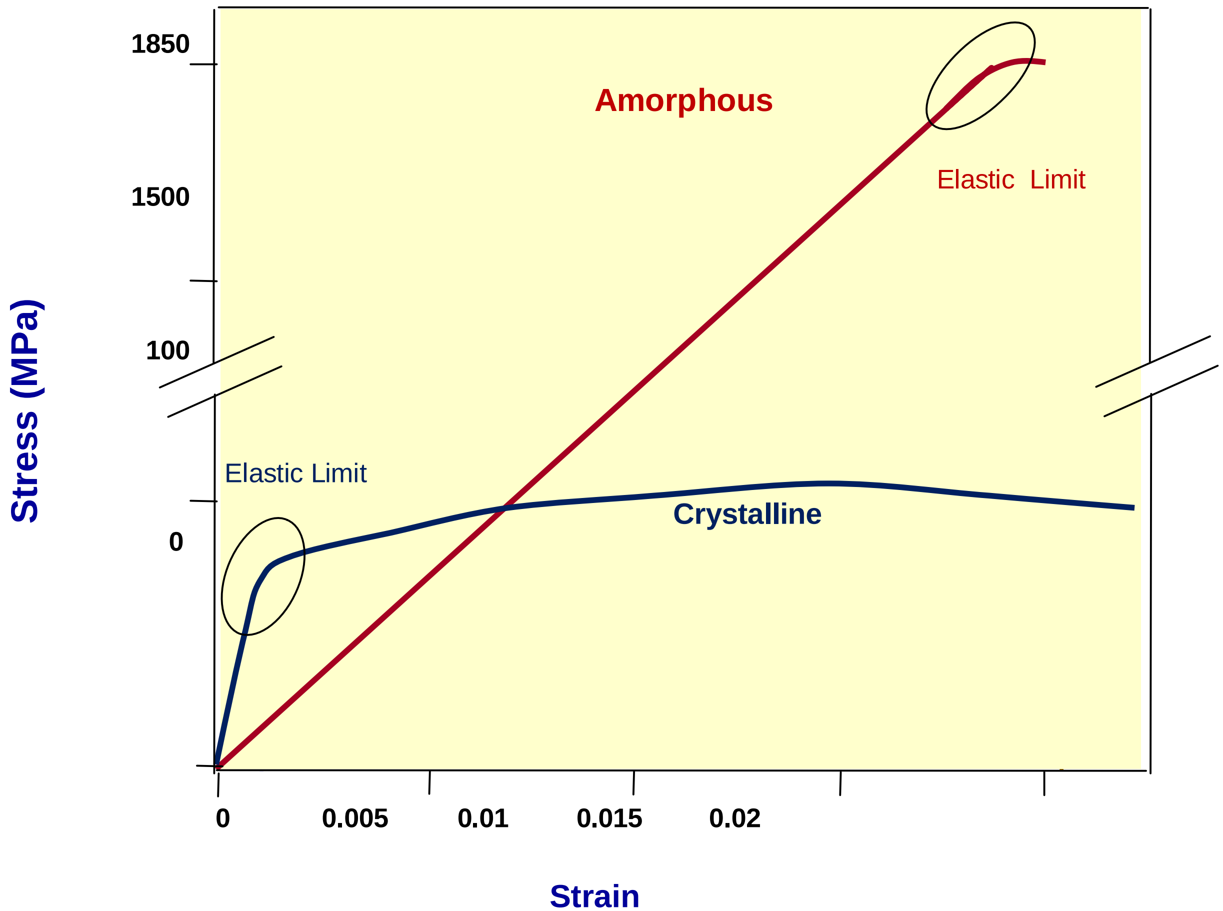
Fundamental issues

- Which compositions show good GFA and why?
- Plasticity – STZ to shear band connection?
- Fracture – what really happens in fracture process zone? (physics of fracture)
- Fatigue – what causes the kinematic irreversibility?

Why is the deformation behavior in amorphous alloys is interesting?



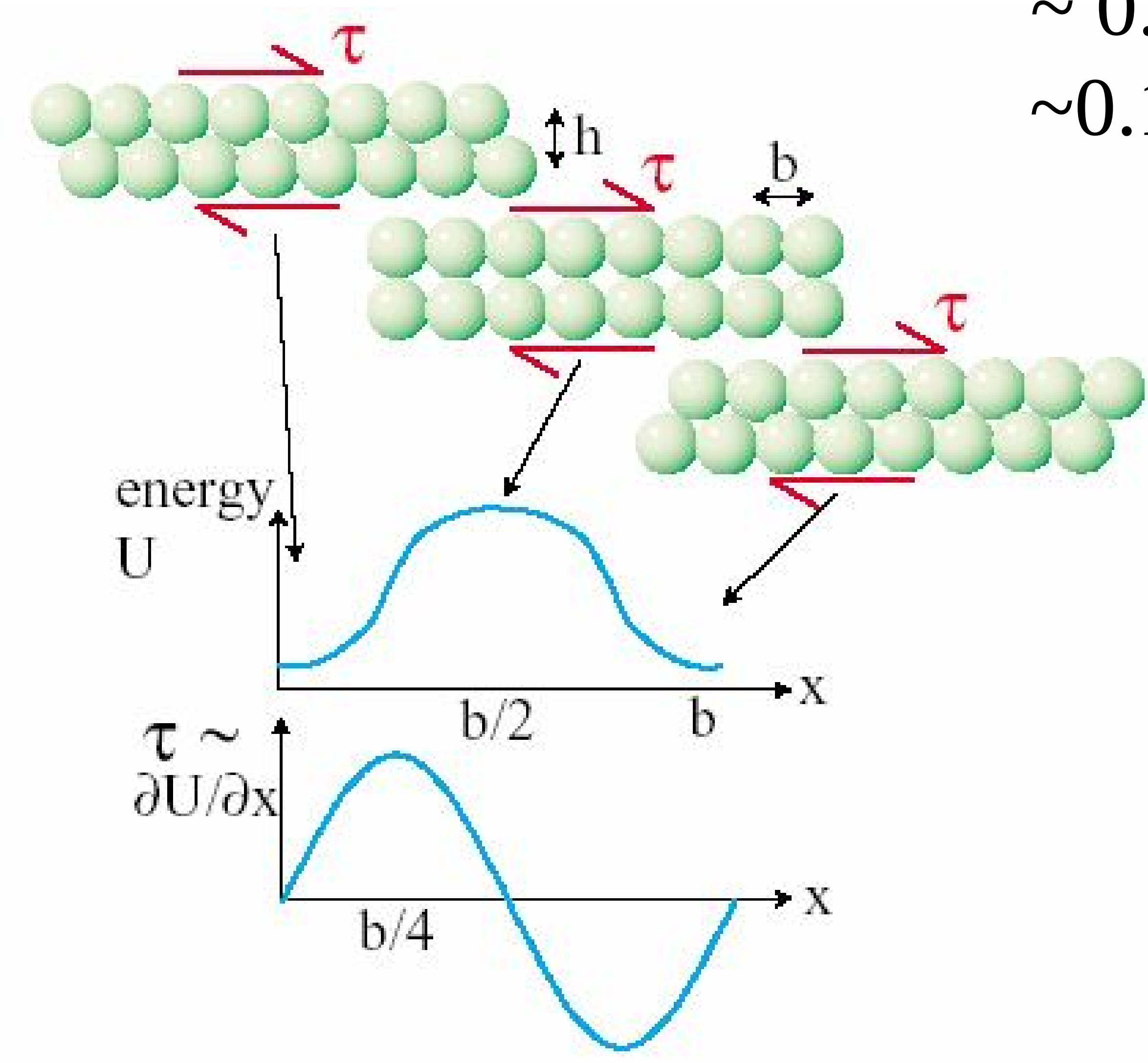
amorphous alloys exhibit High yield strengths, large yield strains and show little or no plasticity

Yield strains

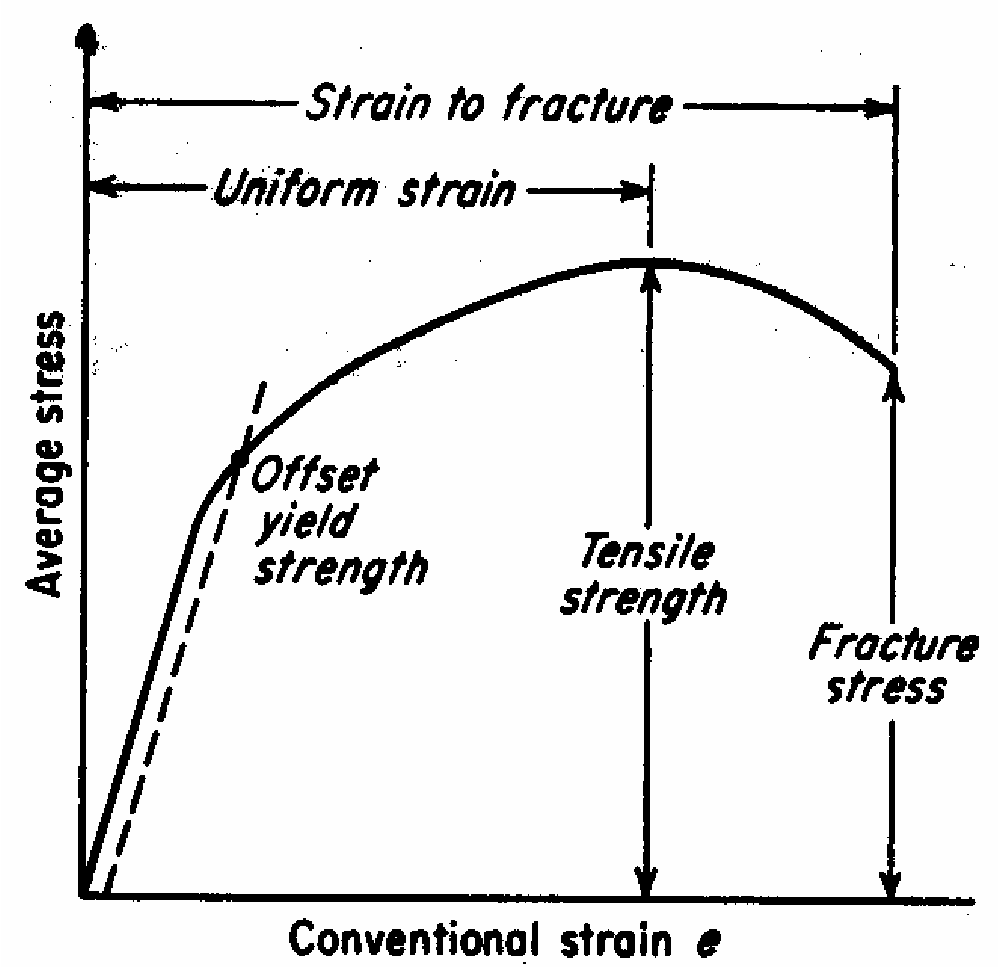
$\sigma_y/E \sim 10^{-3}$ crystalline metals

~ 0.02 metallic glasses

~ 0.1 perfect crystals



Stress-strain response of crystalline metals and alloys



Yield criteria

In uniaxial loading, plastic flow begins when $\sigma = \sigma_0$, the tensile yield stress

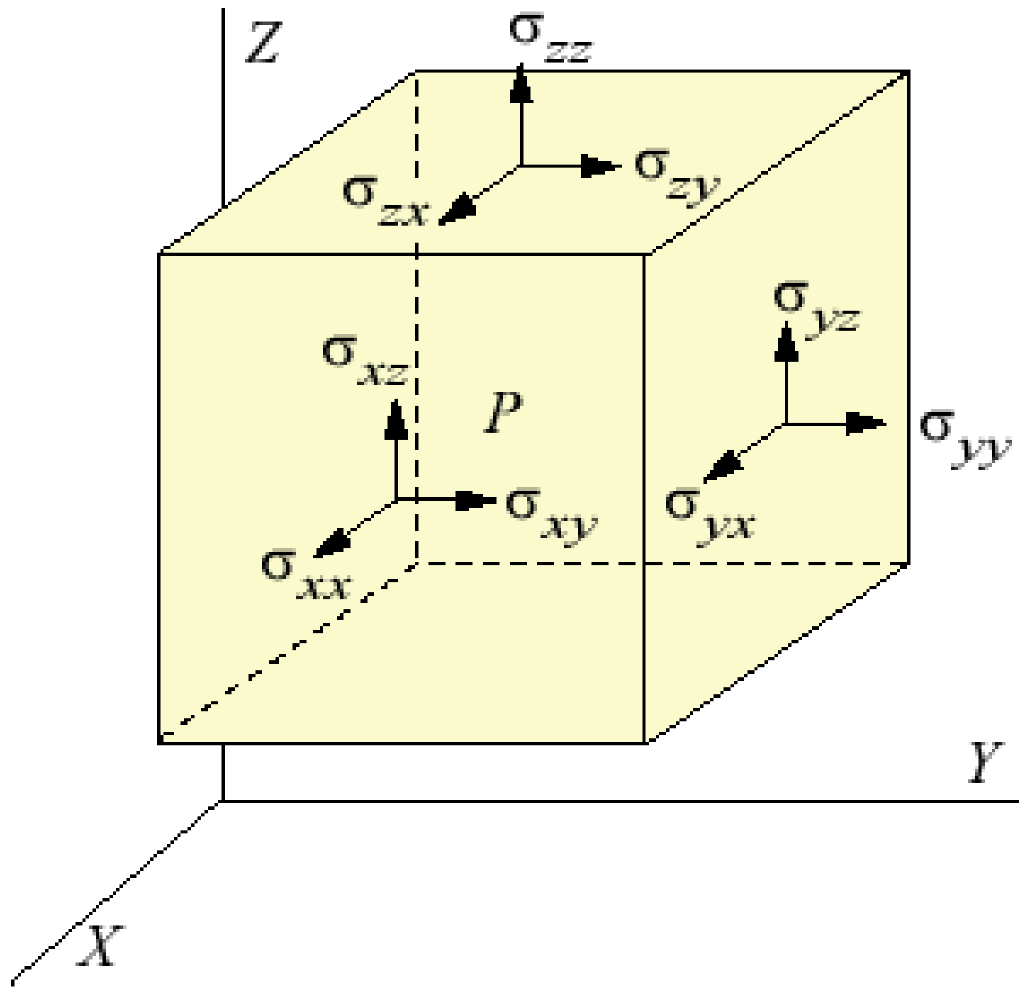
When does yielding begin when a material is subjected to an arbitrary state stress?

Some basics

Stress

$$\begin{bmatrix} \sigma_x & \tau_{xy} & \tau_{zx} \\ \tau_{xy} & \sigma_y & \tau_{yz} \\ \tau_{zx} & \tau_{yz} & \sigma_z \end{bmatrix}$$

$$\begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \end{bmatrix}$$



Convention, $\sigma 1 > \sigma 2 > \sigma 3$

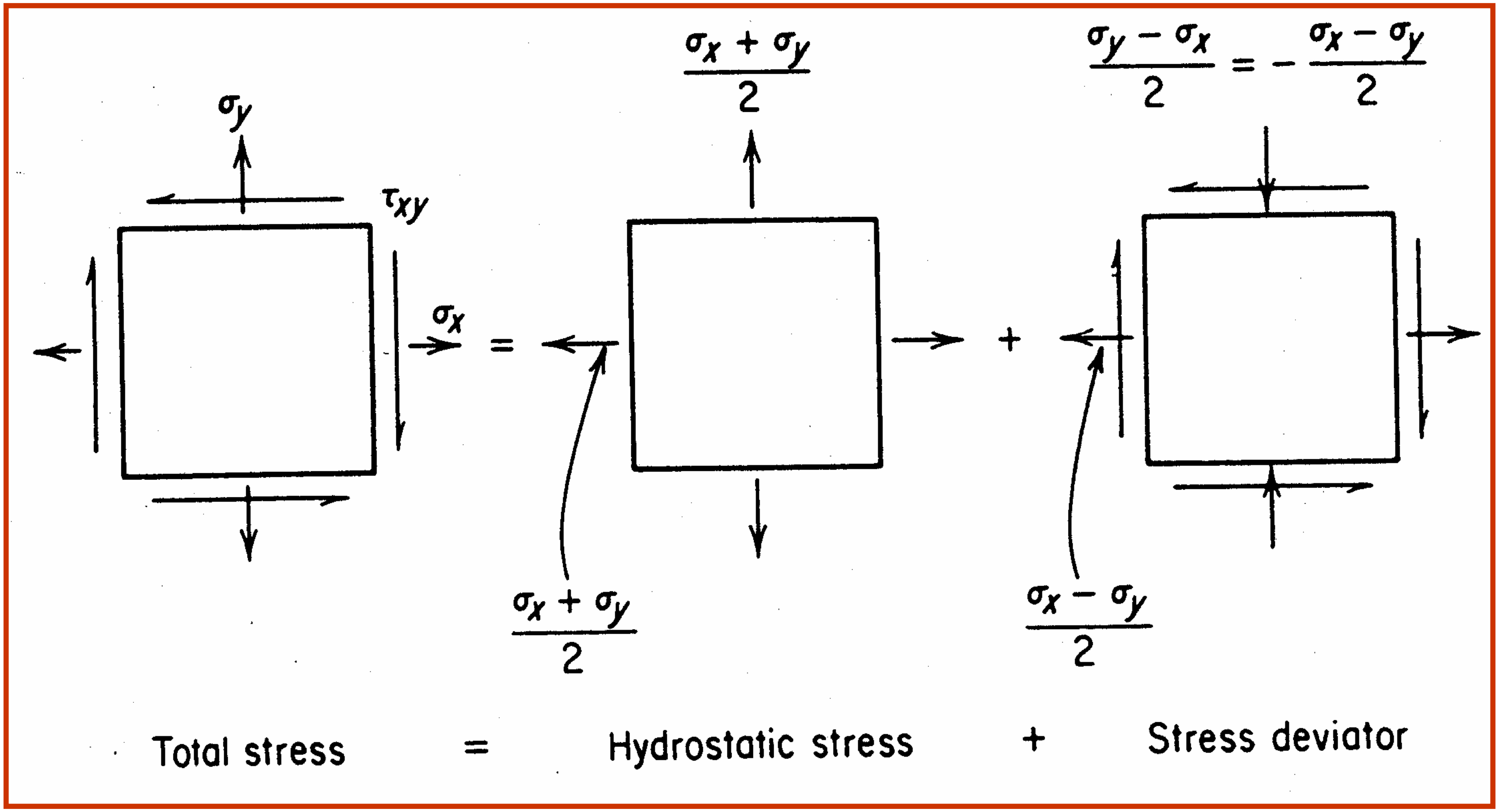
Invariants

$$\mathbf{I}_1 = \sigma_x + \sigma_y + \sigma_z$$

$$\mathbf{I}_2 = \sigma_x\sigma_y + \sigma_y\sigma_z + \sigma_z\sigma_x - \tau_{xy}^2 - \tau_{yz}^2 - \tau_{zx}^2$$

$$\mathbf{I}_3 = \sigma_x\sigma_y\sigma_z + 2\tau_{xy}\tau_{yz}\tau_{zx} - \sigma_x\tau_{yz}^2 - \sigma_y\tau_{zx}^2 - \sigma_z\tau_{xy}^2$$

The sum of normal stresses for any orientation in the coordinate system is equal to the sum of the normal stresses for any other orientation



$$\begin{bmatrix} \sigma_x & \tau_{xy} \\ \tau_{xy} & \sigma_y \end{bmatrix} = \begin{bmatrix} \dfrac{\sigma_x + \sigma_y}{2} & 0 \\ 0 & \dfrac{\sigma_x + \sigma_y}{2} \end{bmatrix} + \begin{bmatrix} \dfrac{\sigma_x - \sigma_y}{2} & \tau_{xy} \\ \tau_{xy} & -\dfrac{\sigma_x - \sigma_y}{2} \end{bmatrix}$$

- Hydrostatic stress is given by

$$\boxed{\sigma_m = \frac{\sigma_{kk}}{3} = \frac{\sigma_x + \sigma_y + \sigma_z}{3} = \frac{\sigma_1 + \sigma_2 + \sigma_3}{3}}$$

- Decomposition of the stress tensor:

$$\sigma_{ij} = \sigma'_{ij} + \tfrac{1}{3}\delta_{ij}\sigma_{kk}$$

$$\sigma'_{ij} = \sigma_{ij} - \sigma_m\delta_{ij}$$

$$\sigma'_{ij} = \begin{vmatrix} \dfrac{2\sigma_x - \sigma_y - \sigma_z}{3} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \dfrac{2\sigma_y - \sigma_z - \sigma_x}{3} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \dfrac{2\sigma_z - \sigma_x - \sigma_y}{3} \end{vmatrix}$$

- J_1, J_2, and J_3 are the principal values of the deviatoric stress tensor.
- J_1 is the sum of the diagonal terms:

$$\boxed{J_1 = (\sigma_x - \sigma_m) + (\sigma_y - \sigma_m) + (\sigma_z - \sigma_m) = 0}$$

- J_2 is the sum of the principal minors:

$$\boxed{J_2 = \frac{1}{6}\begin{bmatrix} (\sigma_y - \sigma_z)^2 + (\sigma_z - \sigma_x)^2 + (\sigma_x - \sigma_y)^2 \\ + 6(\tau_{xy}^2 + \tau_{yz}^2 + \tau_{xz}^2) \end{bmatrix}}$$

- J_3 is the determinant of the deviatoric stress matrix.

Yield Criteria for Metals

- Pure hydrostatic pressure or mean stress tensor, σ_m, doesn't affect yielding in metals.
- Only the deviatoric stress, σ'_{ij}, which represents the shear stresses causes plastic flow.
- For an isotropic solid, the yield criterion must be independent of the choice of the axes, i.e., *it must be an invariant function*.

$\therefore$ Yield criterion must be some function of the J's.

Von Mises' Yield Criterion

- "Yielding would occur when J_2 exceeds some critical value" $J_2 = k^2$
- Yielding in uniaxial tension: $\sigma_1 = \sigma_0$, $\sigma_2 = \sigma_3 = 0$

$$J_2 = \frac{1}{6}\left[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2\right]$$

$$\sigma_0/\sqrt{3} = k$$

$$\boxed{\sigma_0 = \frac{1}{\sqrt{2}}\left[(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2\right]^{1/2}}$$

Tresca Criterion

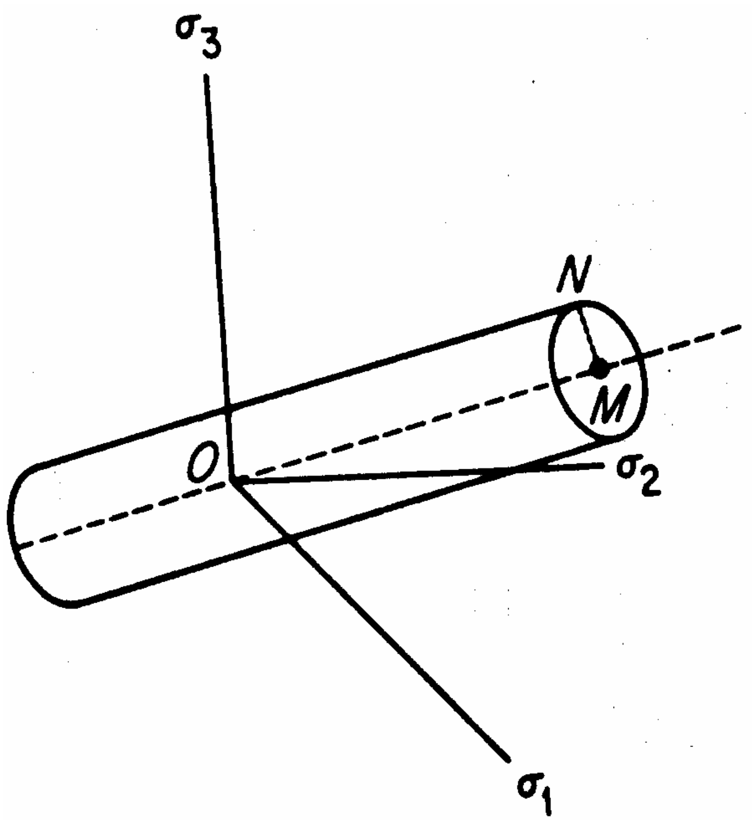
"Yielding occurs when the max. shear stress reaches the value of shear yield stress in the uniaxial tension test."

- Max shear stress, $\tau_{\max} = (\sigma_1 - \sigma_3)/2$
- In uniaxial tension, $\tau_0 = \sigma_0 /2$
- Tresca criterion: $\boxed{(\sigma_1 - \sigma_3) = \sigma_0}$
- Pure shear: $\sigma_1 = -\sigma_3 = k;\ \sigma_2 = 0$

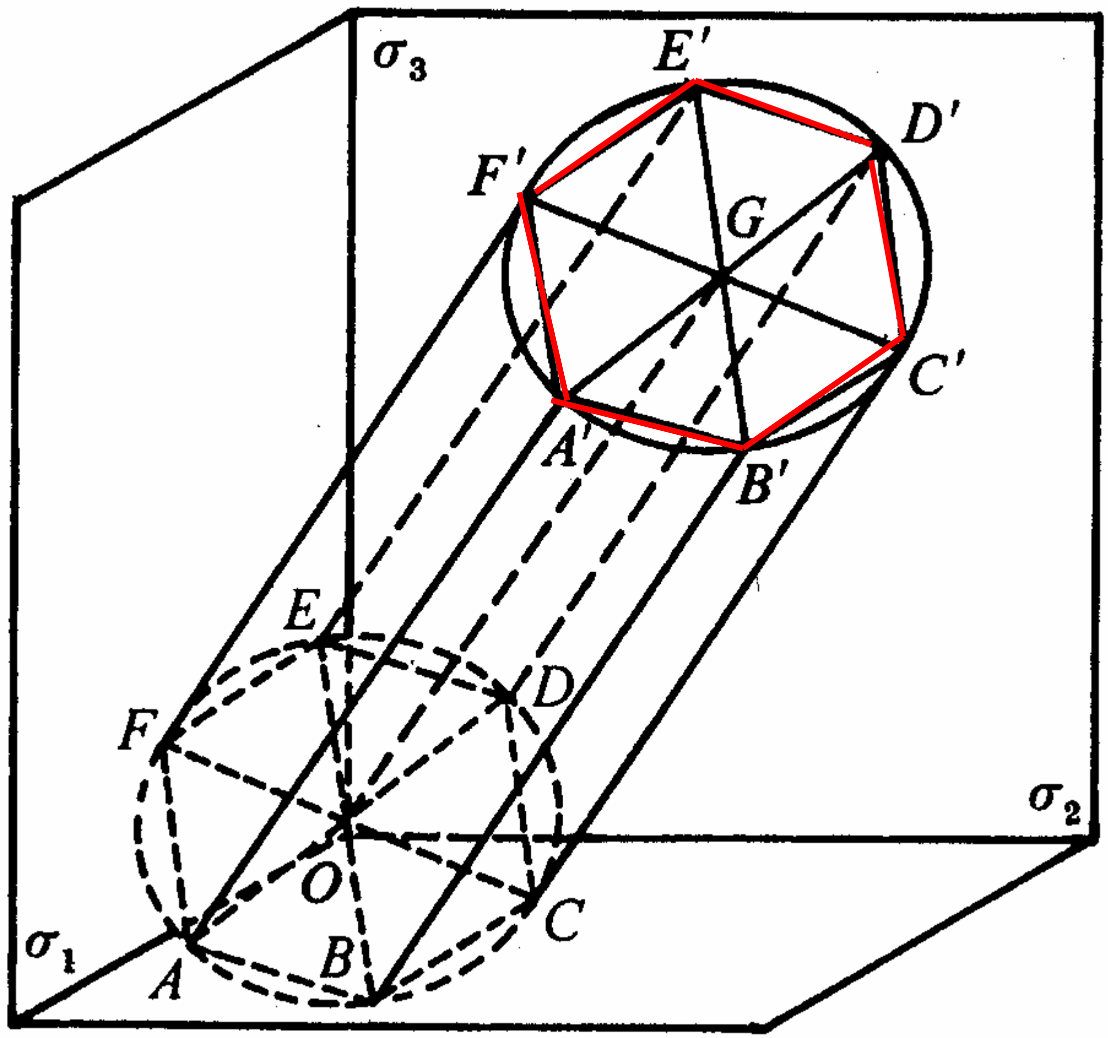
$$(\sigma_1 - \sigma_3) = 2k = \sigma_0 \Rightarrow k = \sigma_0 /2$$

Yield Surface

The yield criteria can be represented geometrically by a cylinder oriented at equal angles to the σ_1, σ_2, & σ_3 axes.

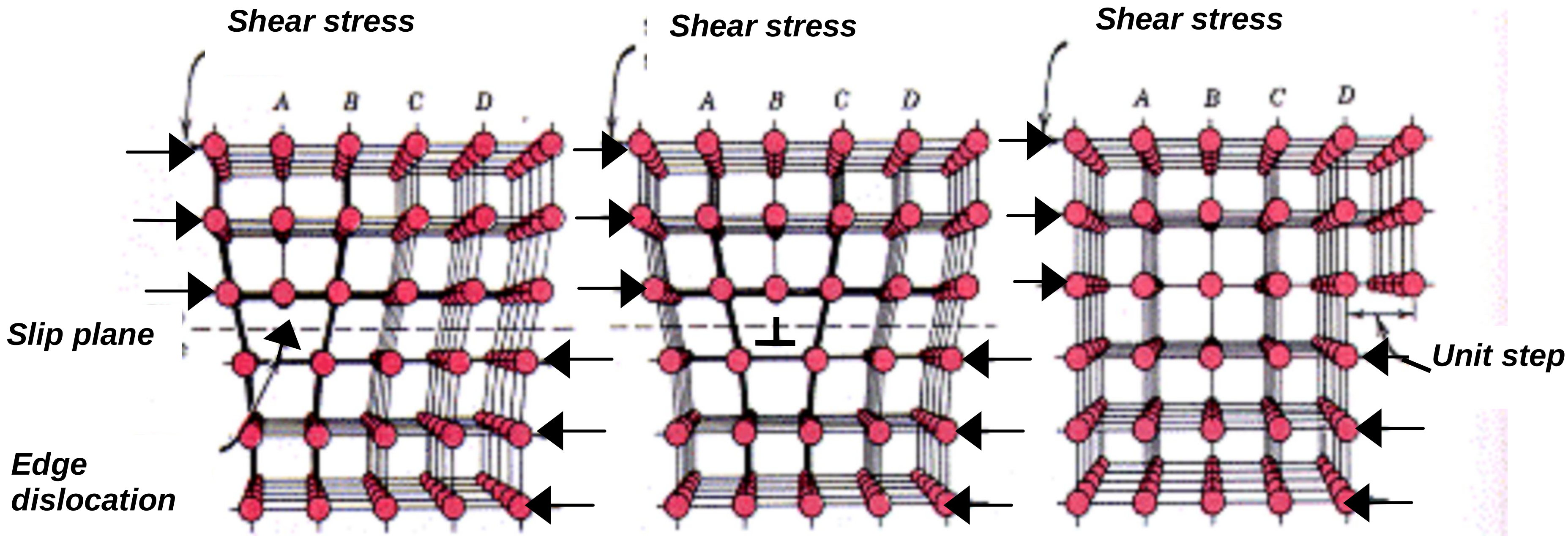


- A state of stress which gives a point inside the cylinder represents elastic behavior.
- Yielding begins when the state of stress reaches the surface of the cylinder.
- MN, the cylinder radius is the deviatoric stress.

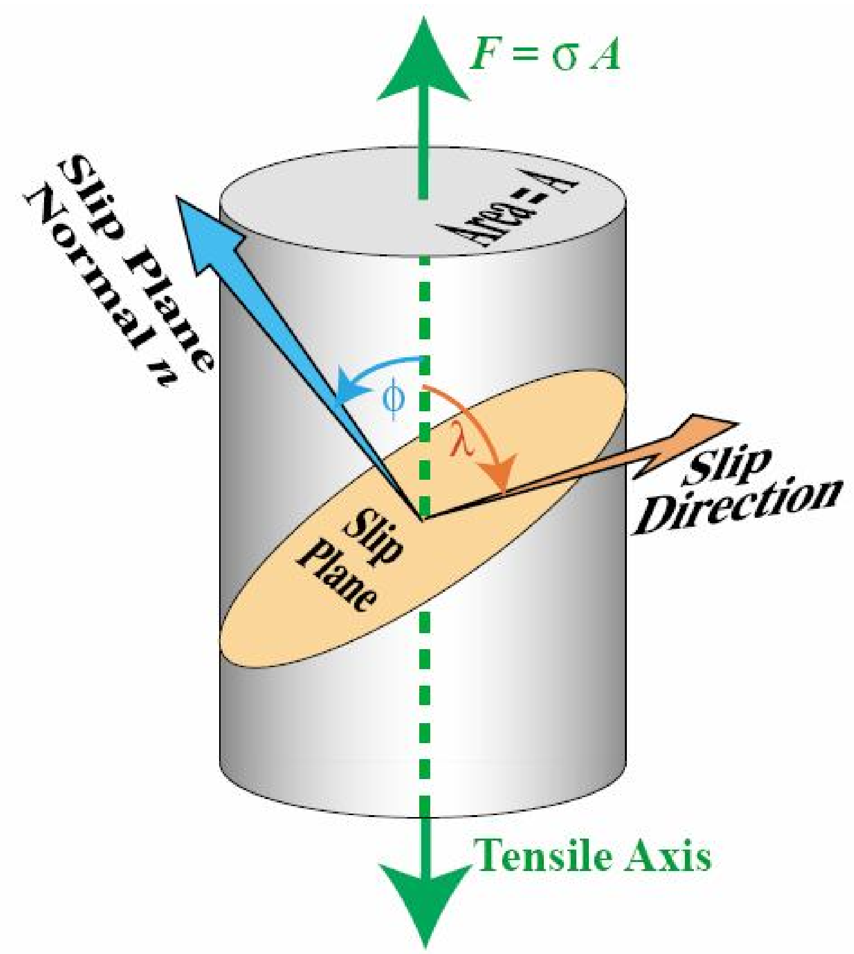


σ_3
E'
D'
F'
G
C'
A'
B'
E
D
F
σ_2
O
C
σ_1
B
A

Plastic deformation in crystalline materials



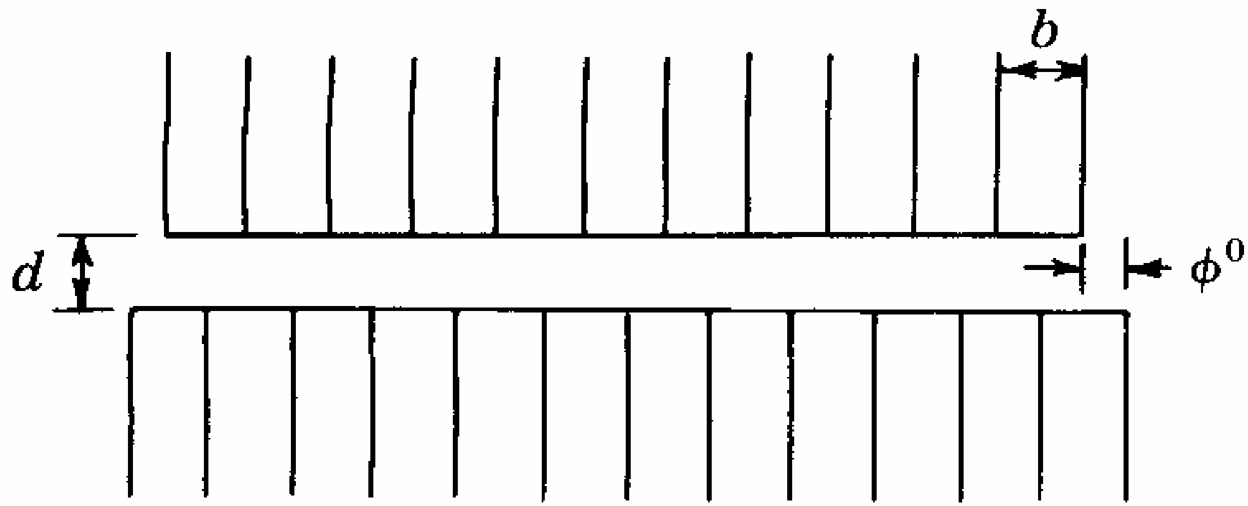
Geometry of Slip



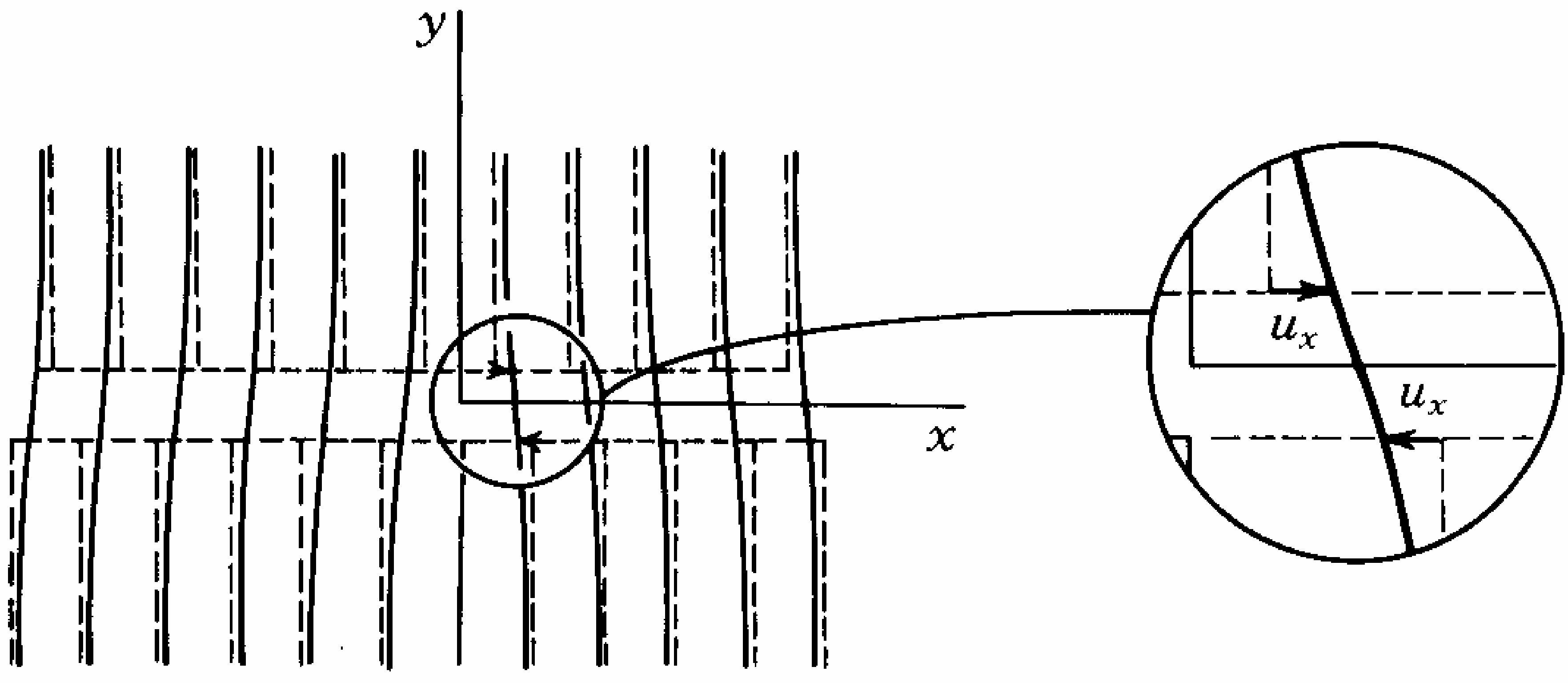
- Single crystal subjected to stress.
- $A_{slip\text{-}plane} = A_0/\cos\phi$
- $P_{resolved} = P\cos\lambda$
- Resolved shear stress,

  $\tau_{rss} = (P/A_0)\cos\phi\cos\lambda$
- Plastic deformation starts when slip gets activated, i.e.,

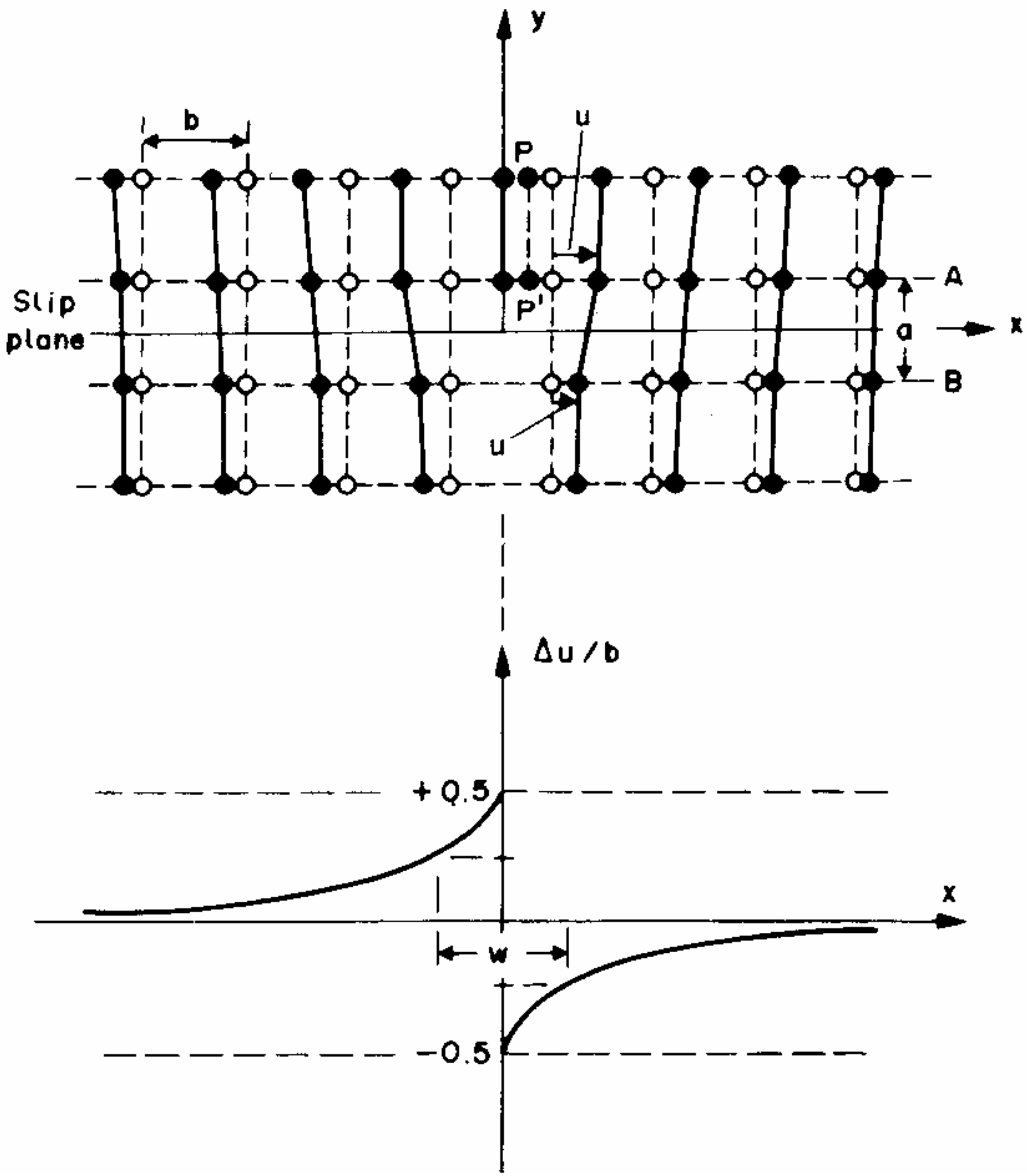
  $\tau_{rss} = \tau_{crss}$ Critical RSS
- The product "$\cos\phi\cos\lambda$" is known as **Schmid factor**



$$\phi_x^0 = \begin{cases} \dfrac{b}{2} & x > 0 \\ -\dfrac{b}{2} & x < 0 \end{cases}$$



Disregistry of atoms

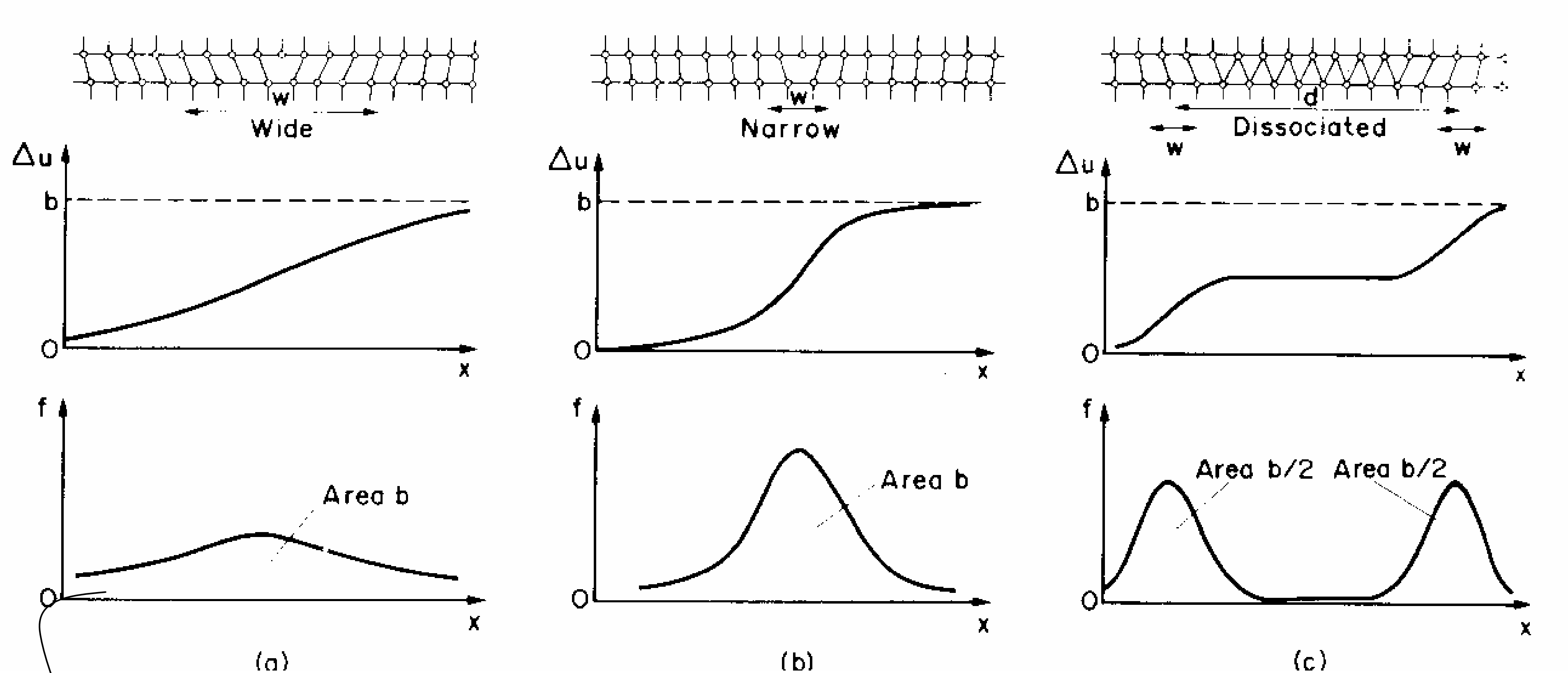


Defined as displacement difference Δu between two atoms on adjacent sites above and below the slip plane

$$\Delta u = u(B) - u(A)$$

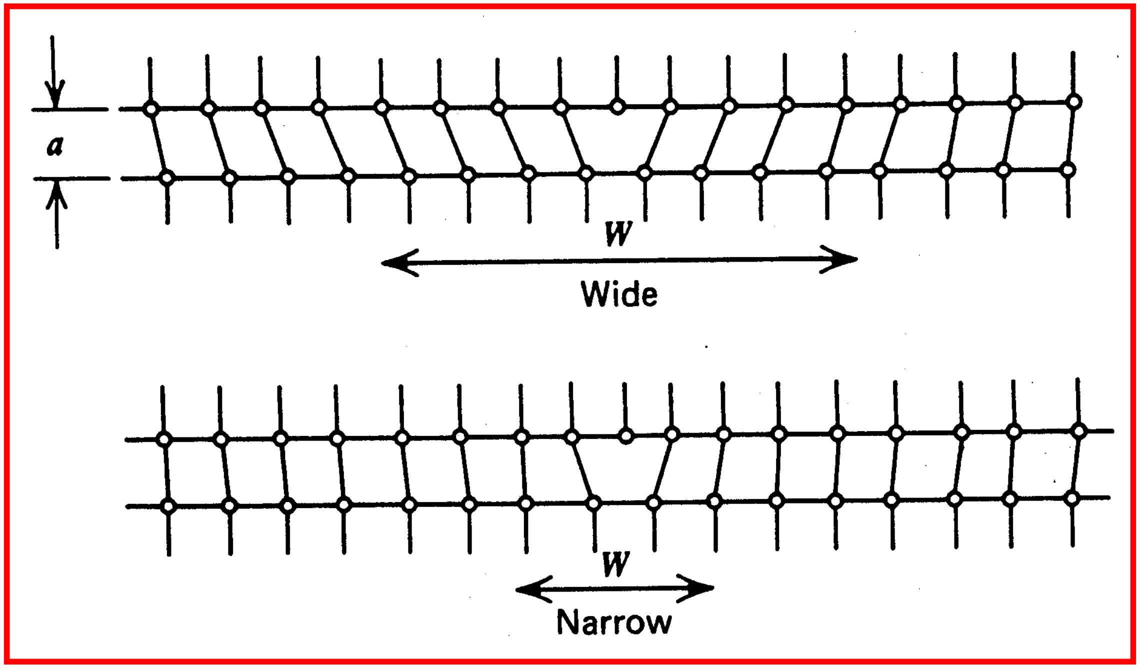
Width, w, of a dislocation is defined as the distance over which Δu is one half of its max value, i.e. $-b/4 \leq \Delta u \leq b/4$

A measure of the size of the dislocation core wherein the elasticity theory fails



$f(x) = d(\Delta u)/dx$ Distribution of Burgers Vector

Core width, b-5b, depends on interatomic potential
and crystal structure



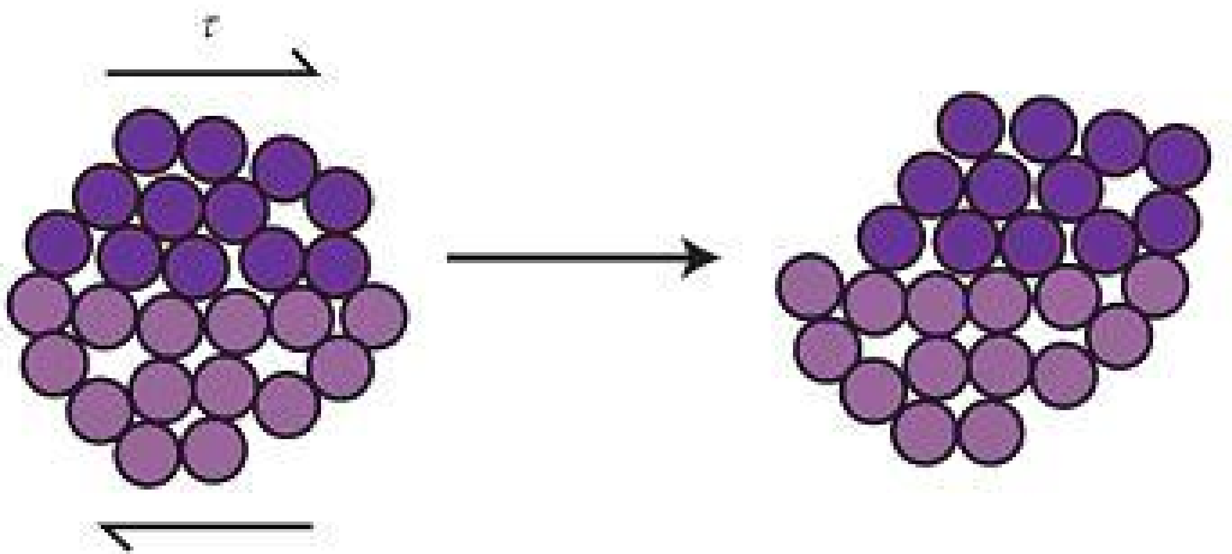
$$\tau_{P\text{-}N} \propto \mu \exp(-2\pi W/b)$$
$$W = a/(1-\nu)$$

$\tau_{P\text{-}N}$ decreases with increasing a.

$\Rightarrow$ *Close packed planes preferred*.

Amorphous alloys

Shear Transformation Zones



Fundamental carriers of plasticity in metallic glasses:

Shear Transformation Zones (STZs)

STZs are clusters of atoms which undergo small, cooperative rearrangements between two metastable states

(Argon, Acta Mater. 1981)

Large dilatational component

Yield criteria for amorphous materials

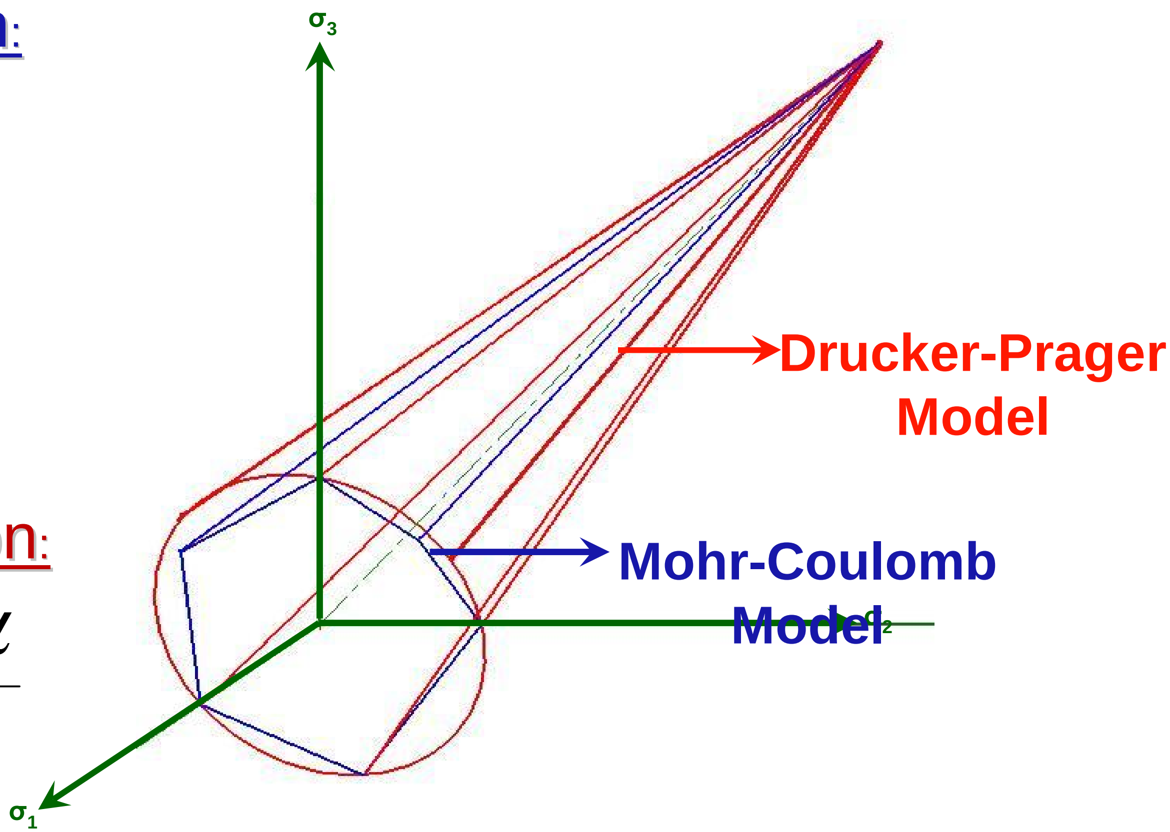
Mohr - Coulomb criterion:

$$\tau_c = k + \alpha\sigma_n$$

Drucker – Prager criterion:

$$\sigma_o^c = \frac{\sigma_e - \sigma_m \tan\alpha}{(1 - \frac{1}{3}\tan\alpha)}$$

$$\sigma_e = \sqrt{3J_2}\,;\ \ \sigma_m = \frac{1}{3}\sigma_{kk}$$



Consequences of pressure sensitivity

- Tension-Compression asymmetry
- Deviation in fracture angles from 45°

	$Zr_{41.25}Ti_{13.75}Cu_{12.5}Ni_{10}Be_{22.5}$	$Pd_{40}Ni_{40}P_{20}$
Tension (σ_T)	**1.89 GPa**	**1.45 GPa**
Compression (σ_C)	**1.93 GPa**	**1.78 GPa**
Fracture angle in tension (Φ_T)	**56^0**	**50^0**
Fracture angle in compression (Φ_C)	**45^0**	**41^0**

Donovan, Acta Metall (1989), Mukai etal., Scripta Mat. (2002)

Direct evidence for pressure sensitivity

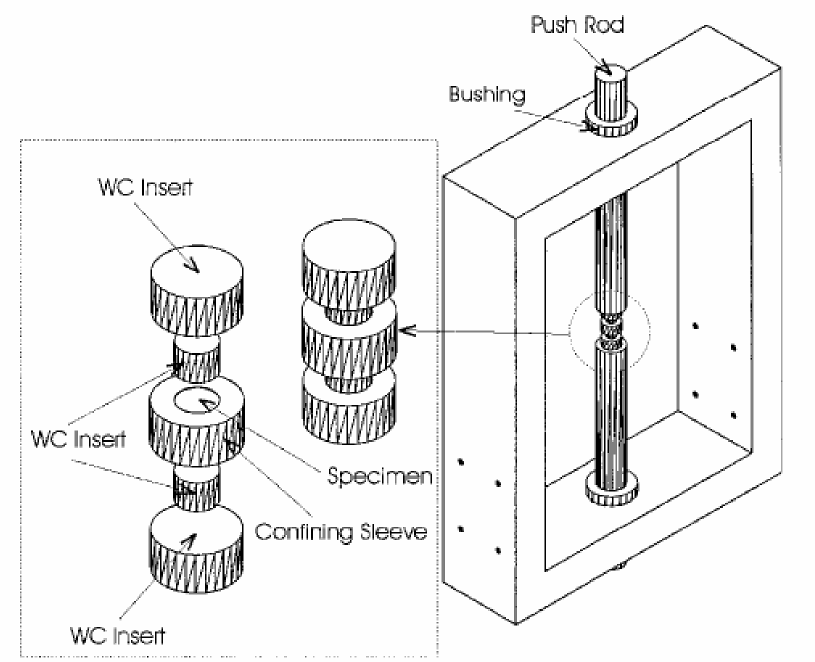
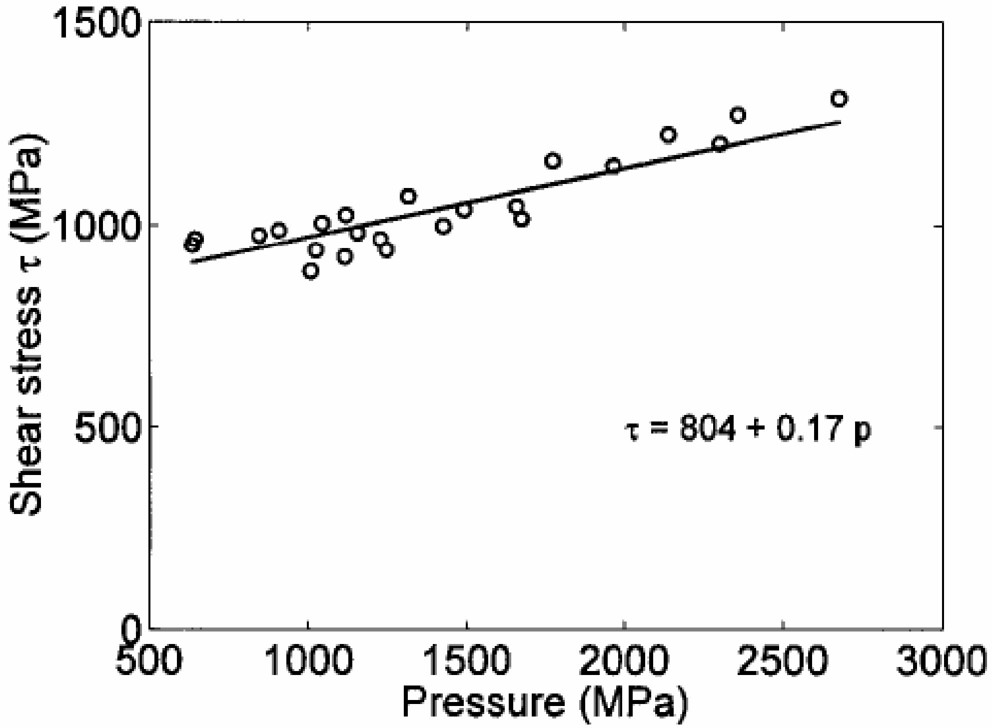


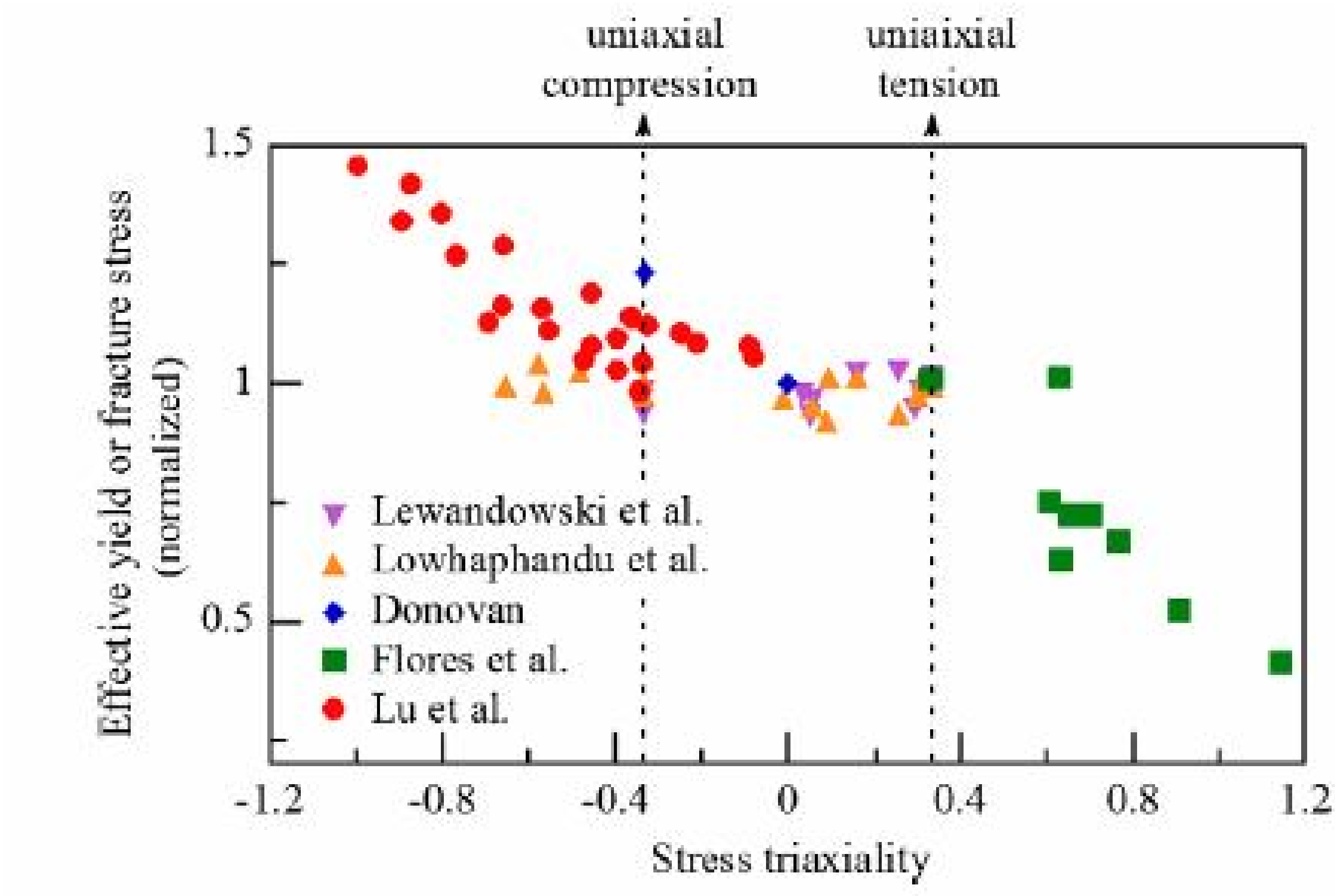
FIG. 1. Quasistatic compression fixture and the radial confinement apparatus.



Mohr-Coulomb criterion: $$\tau_c = \tau_o + \alpha\sigma_n$$

Confining sleeve experiments with pressures up to 2 GPa on Vit-1

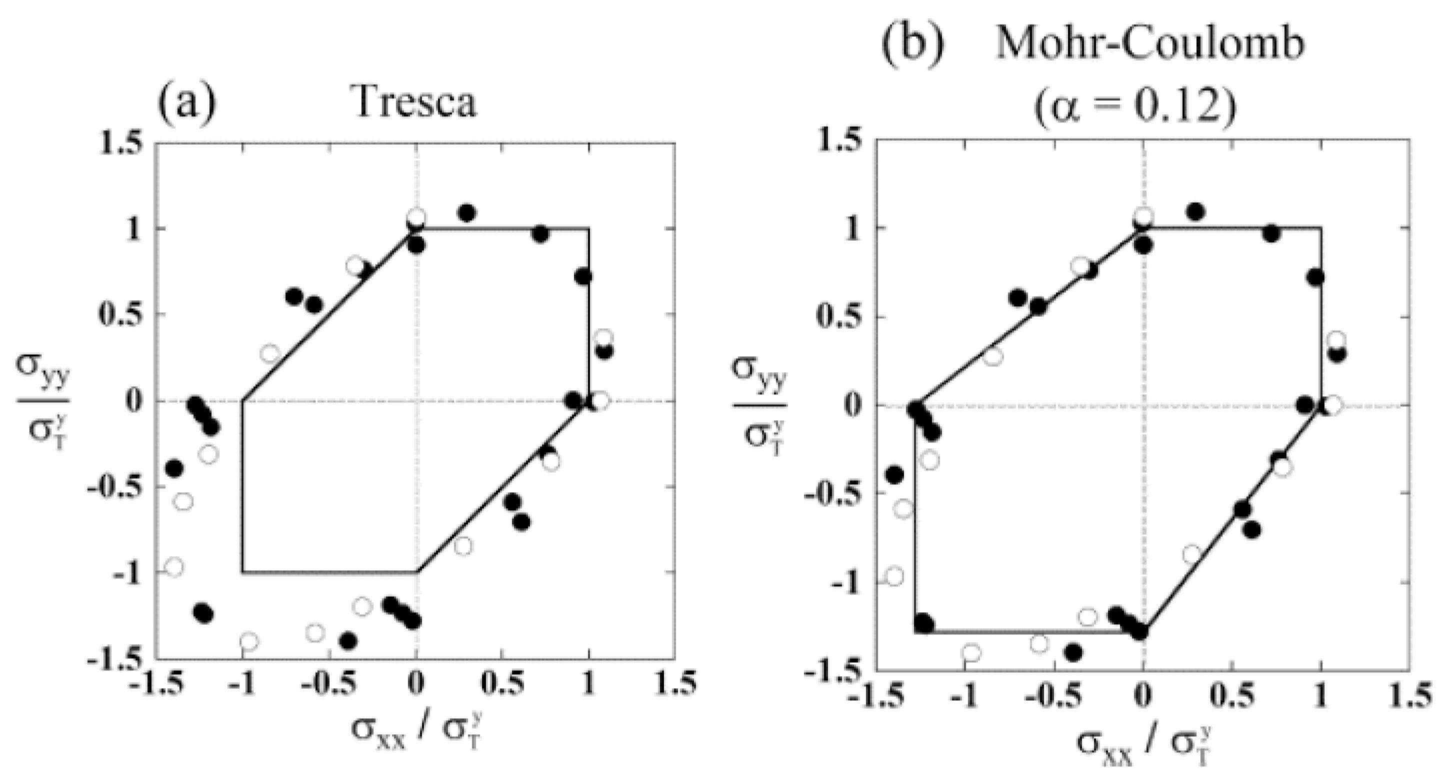
Lu and Ravichandran, J. Mater. Res. (2003)



C. Schuh, T. Hufnagel and U. Ramamurty, Acta Mat. (2007)

MD Simulations

$Cu_{50}Zr_{50}$ binary glass

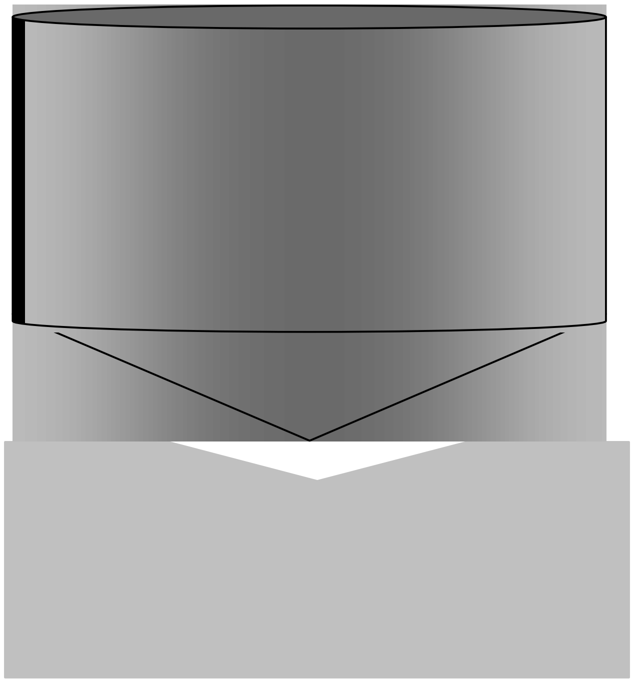


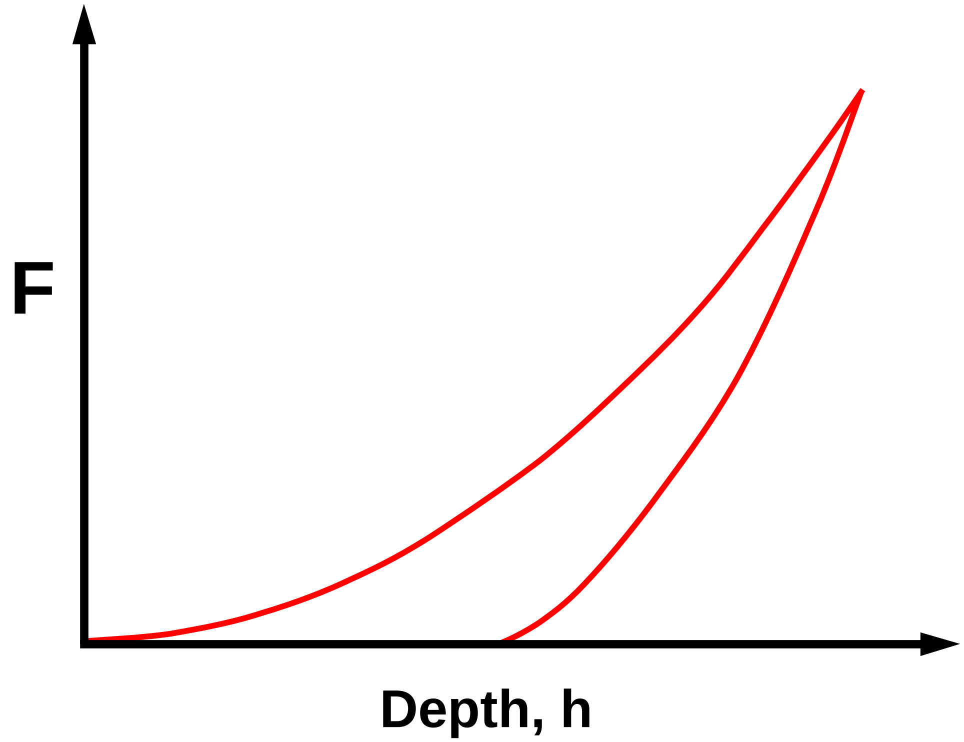
MD simulations show that Mohr-Coulomb criterion is suitable with a pressure sensitive index, α, of 0.12 to describe the yield behavior in these glasses

A.C. Lund and C.A. Schuh, Acta Mat. (2003)

Indentation experiments

The multiaxial stress state that exists under the indenter can be used to model the pressure sensitive behavior.

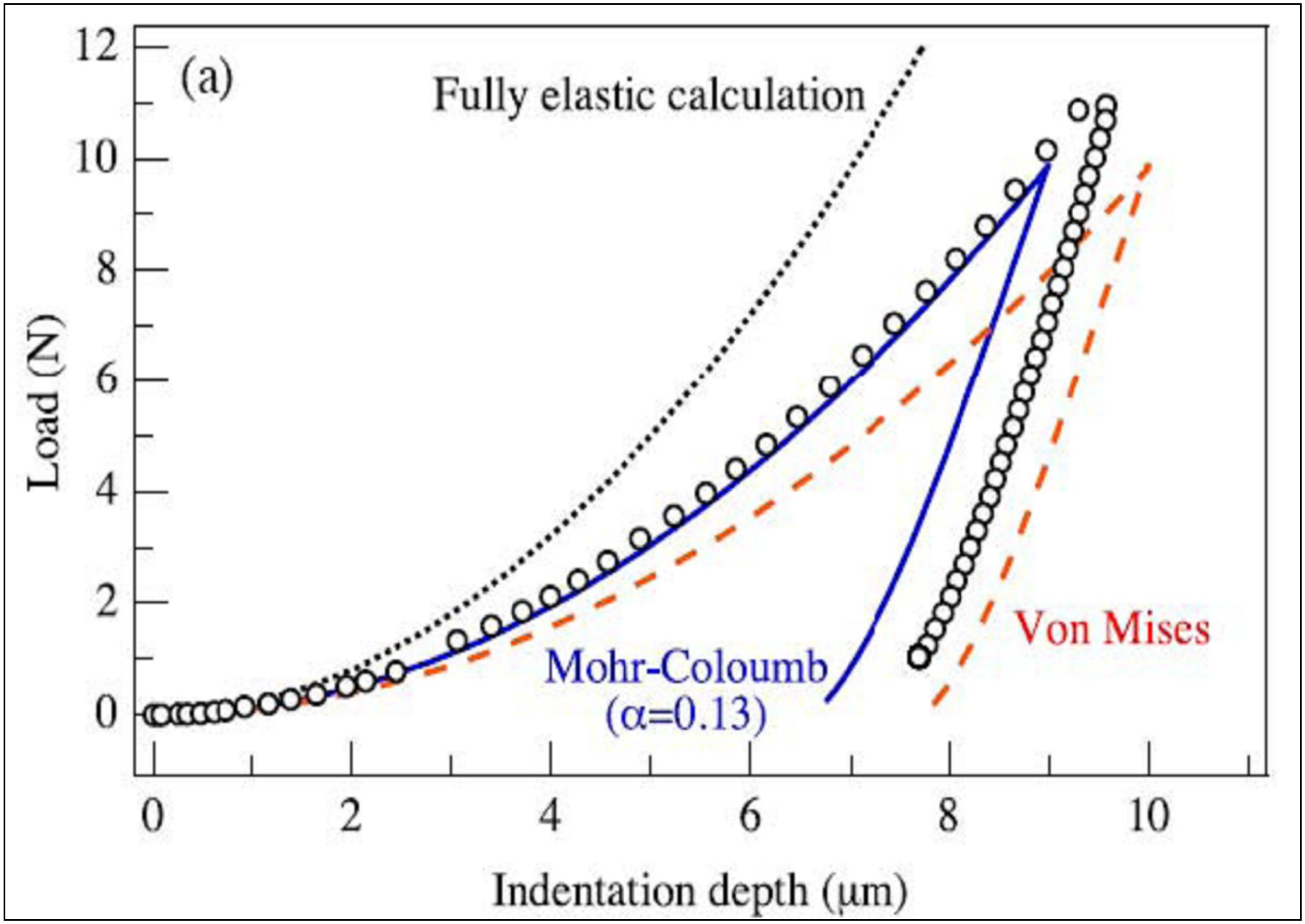




Pressure sensitive behavior effects the following during indentation

- P-h curve
- Plastic zone size
- Constraint factor

Indentation: P-h Curve

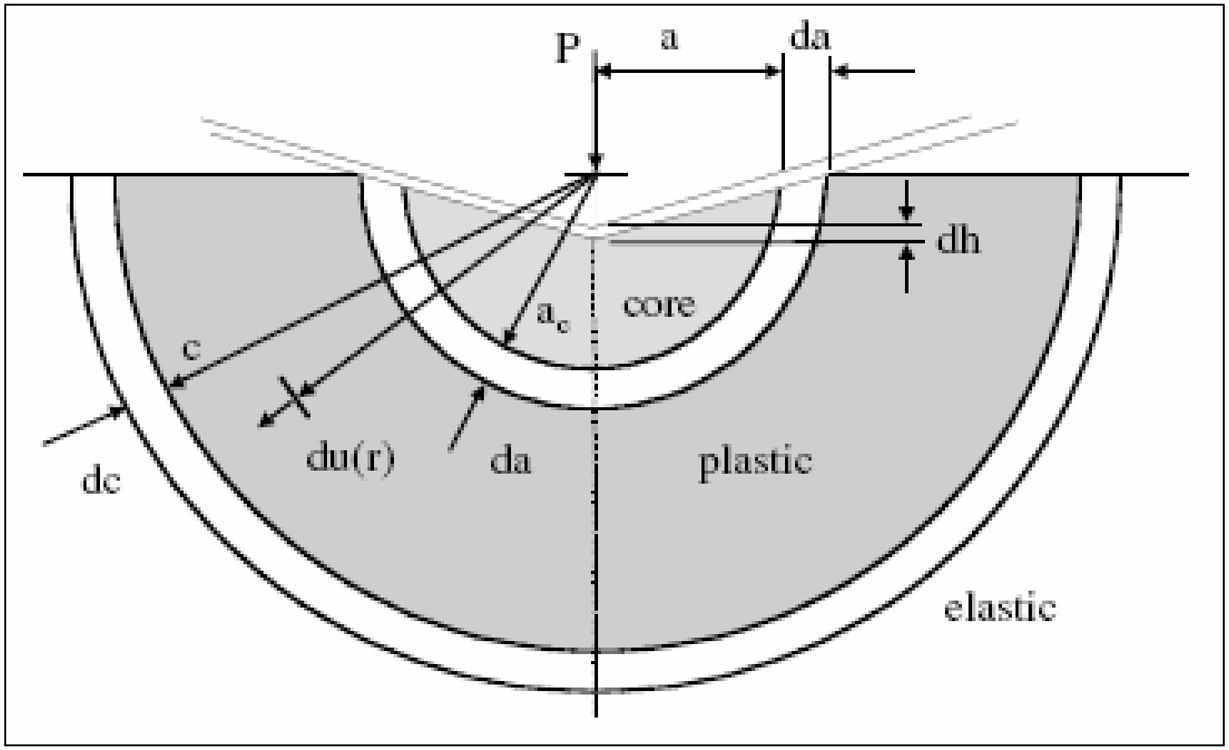


Vaidyanathan et al., Acta Mater (2001), Patnaik et al., Acta Mater (2004), Keryvin, Acta Mater (2007)

Hardness and constraint factor

Constraint factor, C, is defined as the ratio of hardness, H, to the yield strength, σ_y

$$C = \frac{H}{\sigma_y}$$

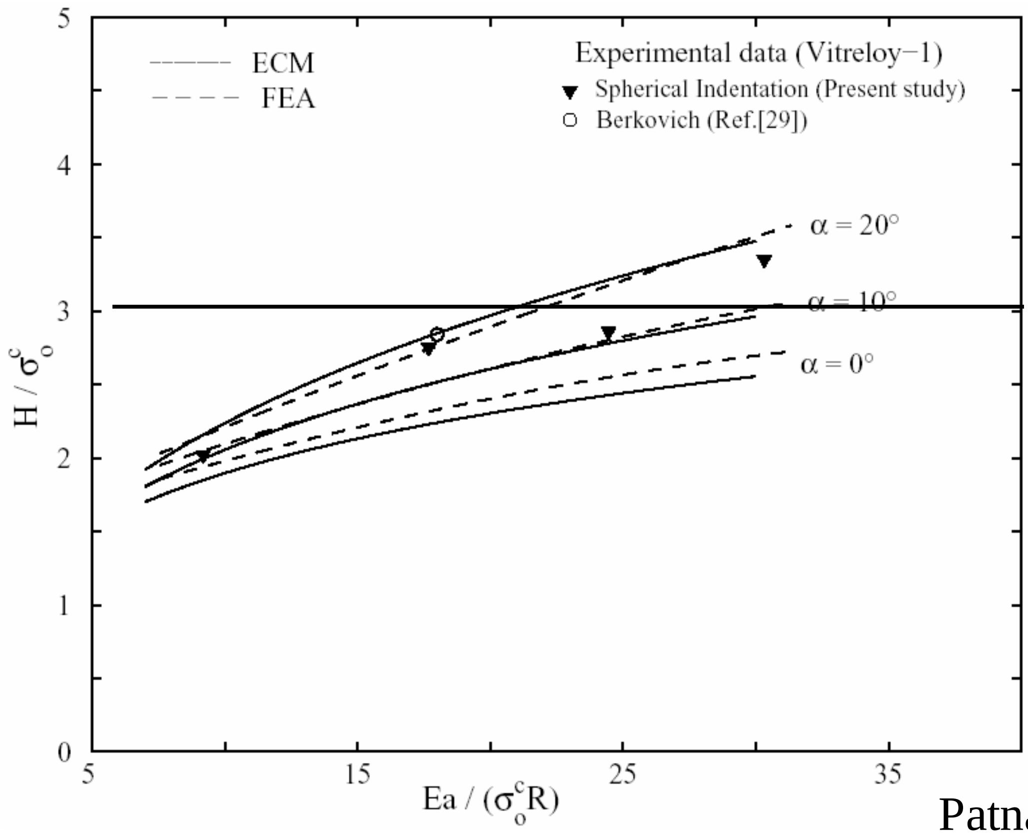


The elastic region surrounding the plastic zone offers high constraints for deformation resulting in high "*H*" values vis a vis large "*C*" values

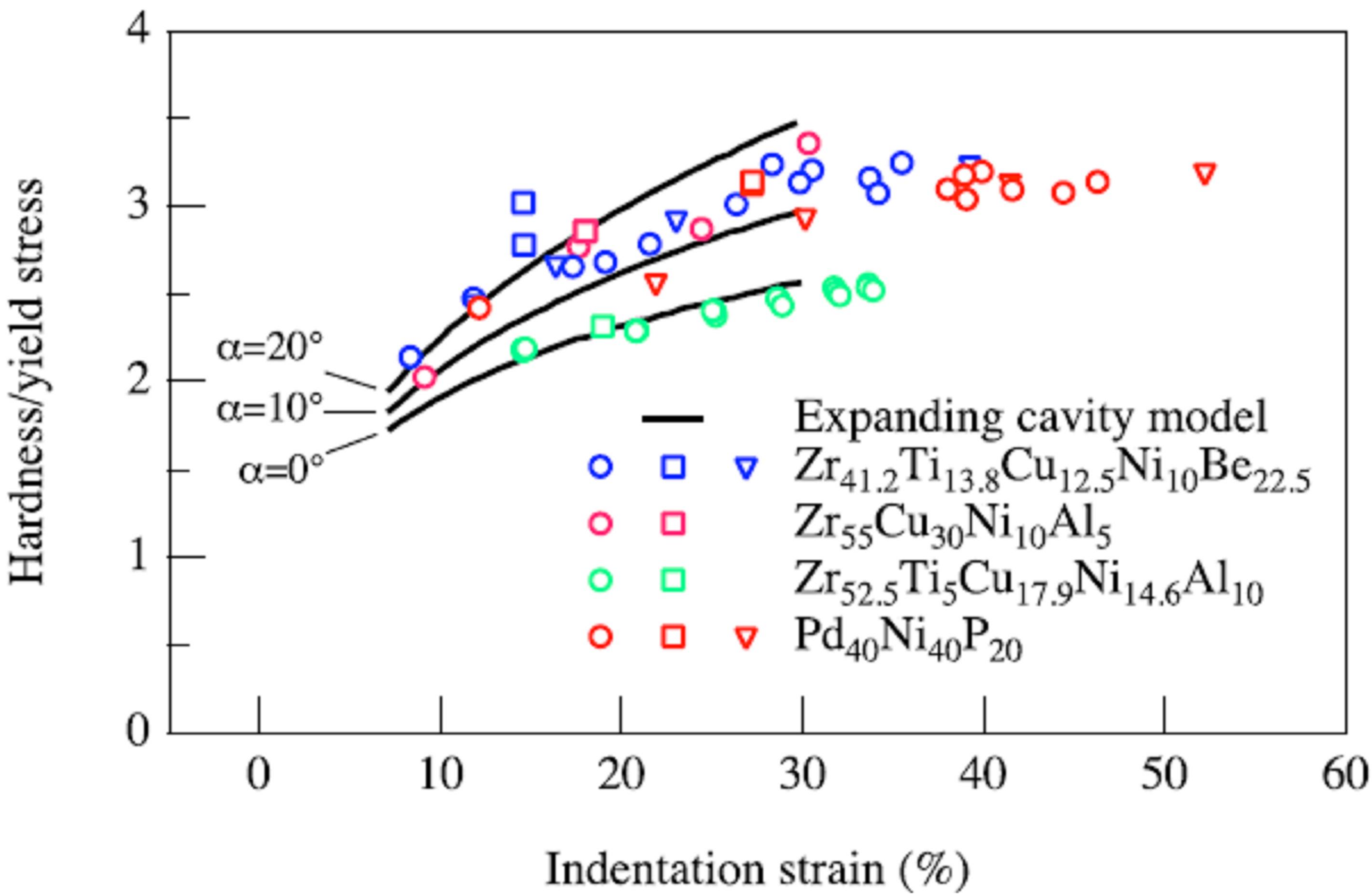
K.L. Johnson, JMPS (1970), Patnaik et al., Acta Mater (2004)

Pressure Sensitivity & Hardness

- High hardness values (i.e., $H/\sigma_Y > 3$)
- Numerical simulation of spherical indentation response using the Drucker-Prager constitutive theory with different levels of pressure sensitivity



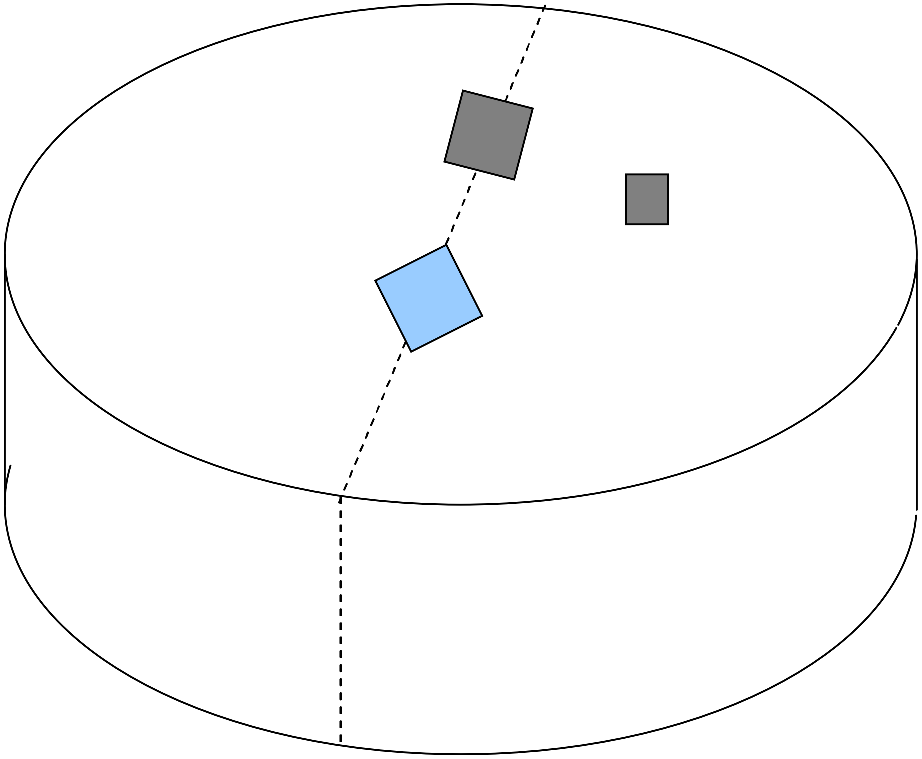
Patnaik, Narasimhan, Ramamurty, Acta Mat.2004



Keryvin, Acta Mat 2007

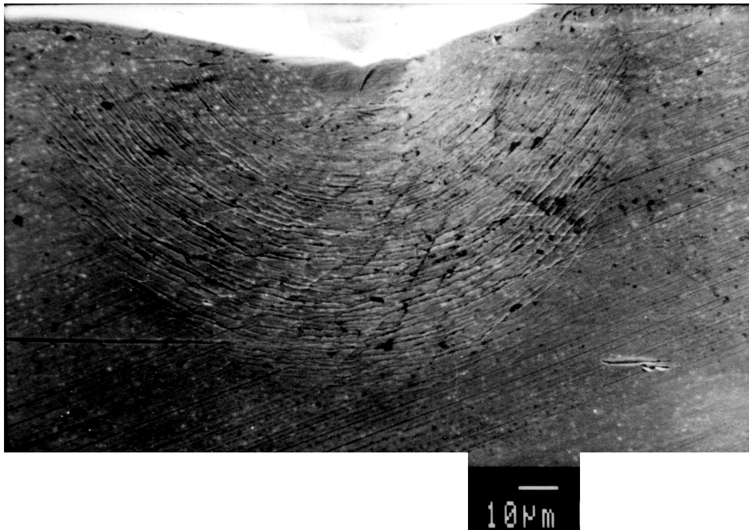
Imaging the Plastic Deformation thru the Bonded Interface Technique

1. Cut into two pieces
2. Polish cut surfaces to mirror polished
3. Join the polished faces using adhesive
4. Indent along cut line
5. Dissolve the adhesive
6. Examine using SEM

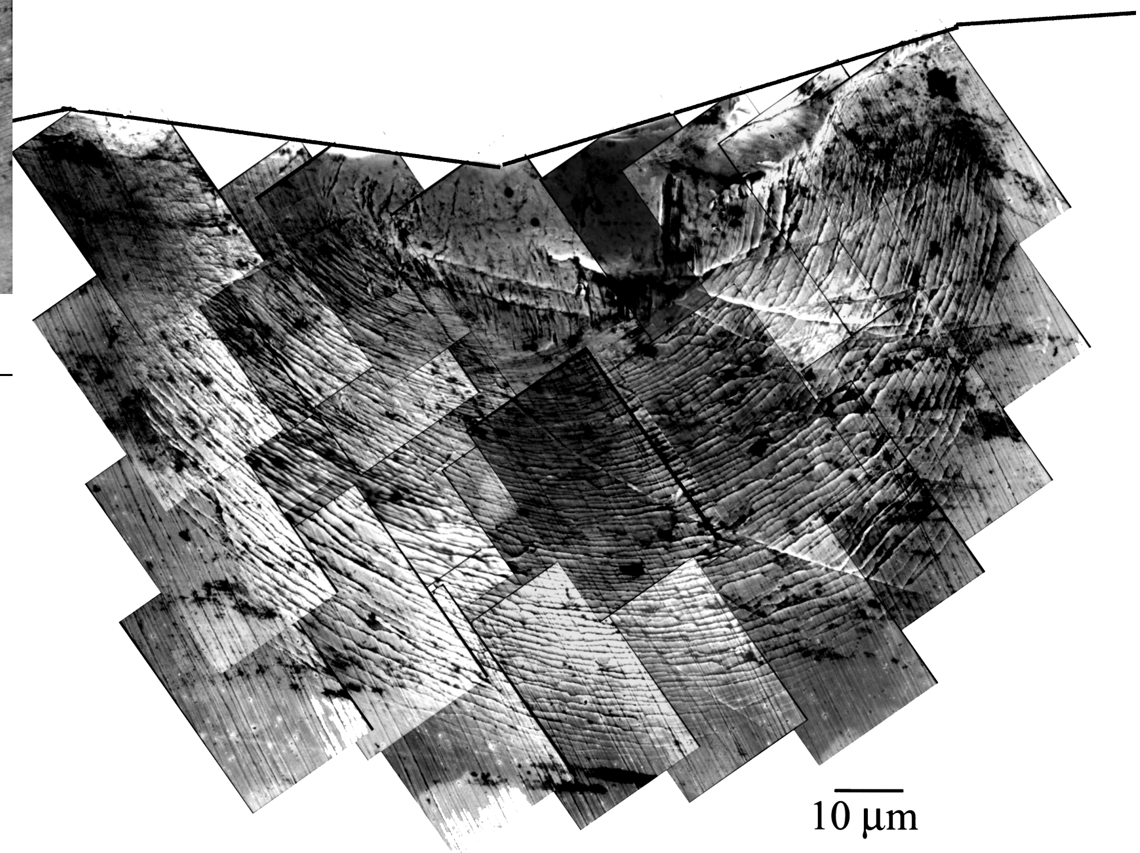


Jana et al. Mat. Sci. Eng. A, 2004

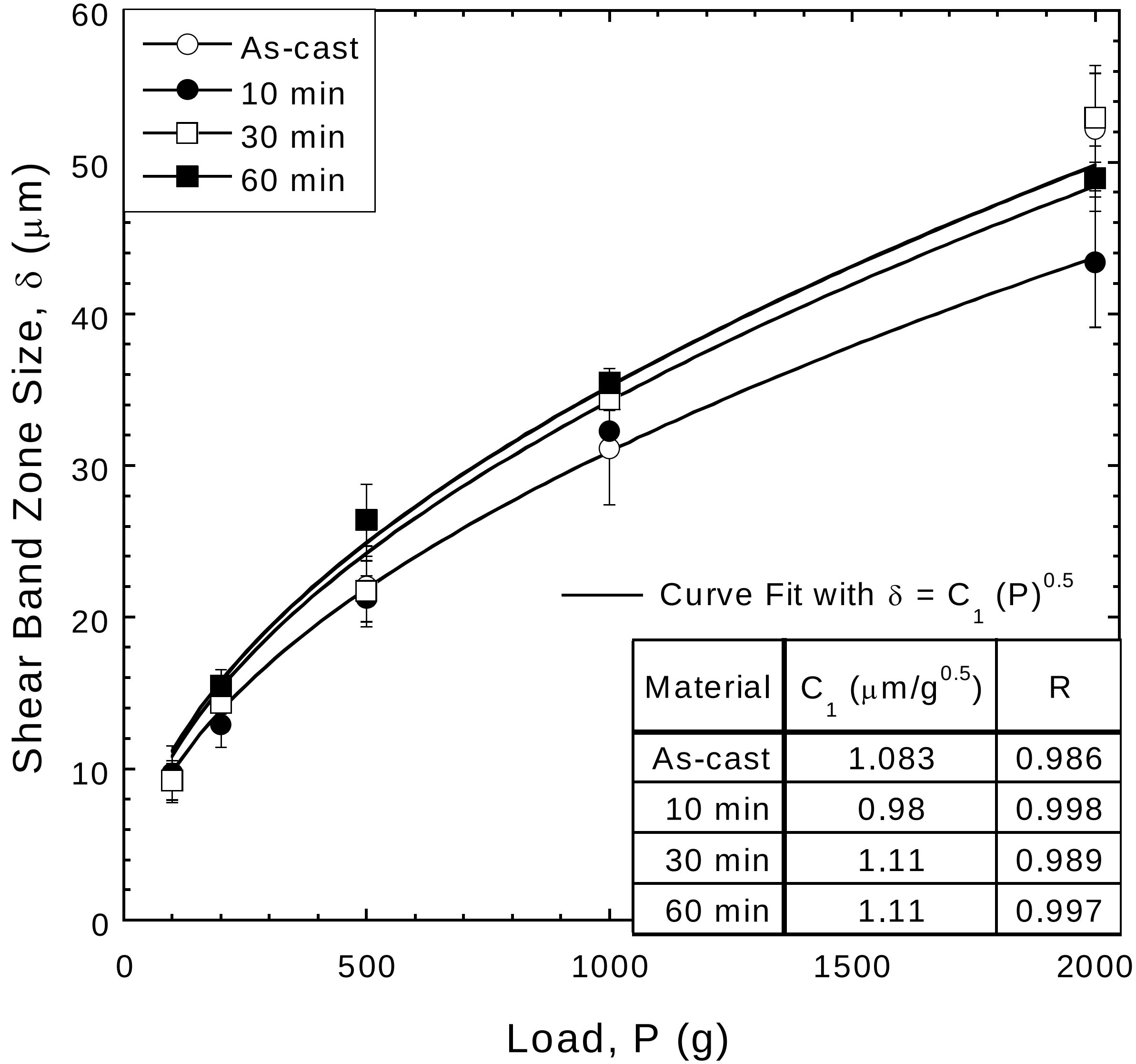
Plastic Flow Beneath the Indenter



Load: 5 kg



Ramamurty et al. Acta mat. 2005



Material	C_1 ($\mu m/g^{0.5}$)	R
As-cast	1.083	0.986
10 min	0.98	0.998
30 min	1.11	0.989
60 min	1.11	0.997

$$\delta = \left[\frac{3P}{2\pi\sigma_y}\right]^{0.5}$$

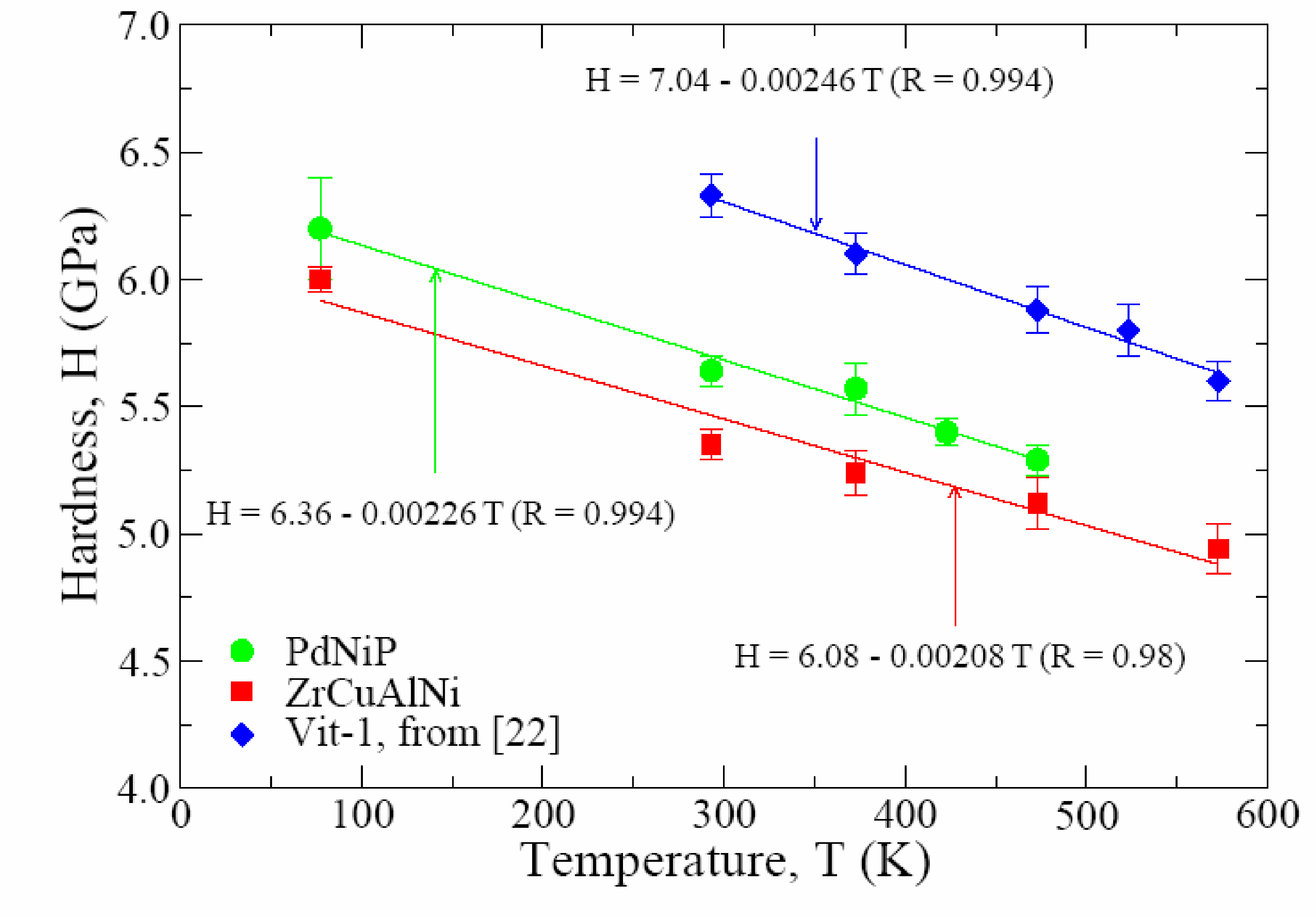
σ_y= 2.8 GPa

Expt. 1.8 GPa

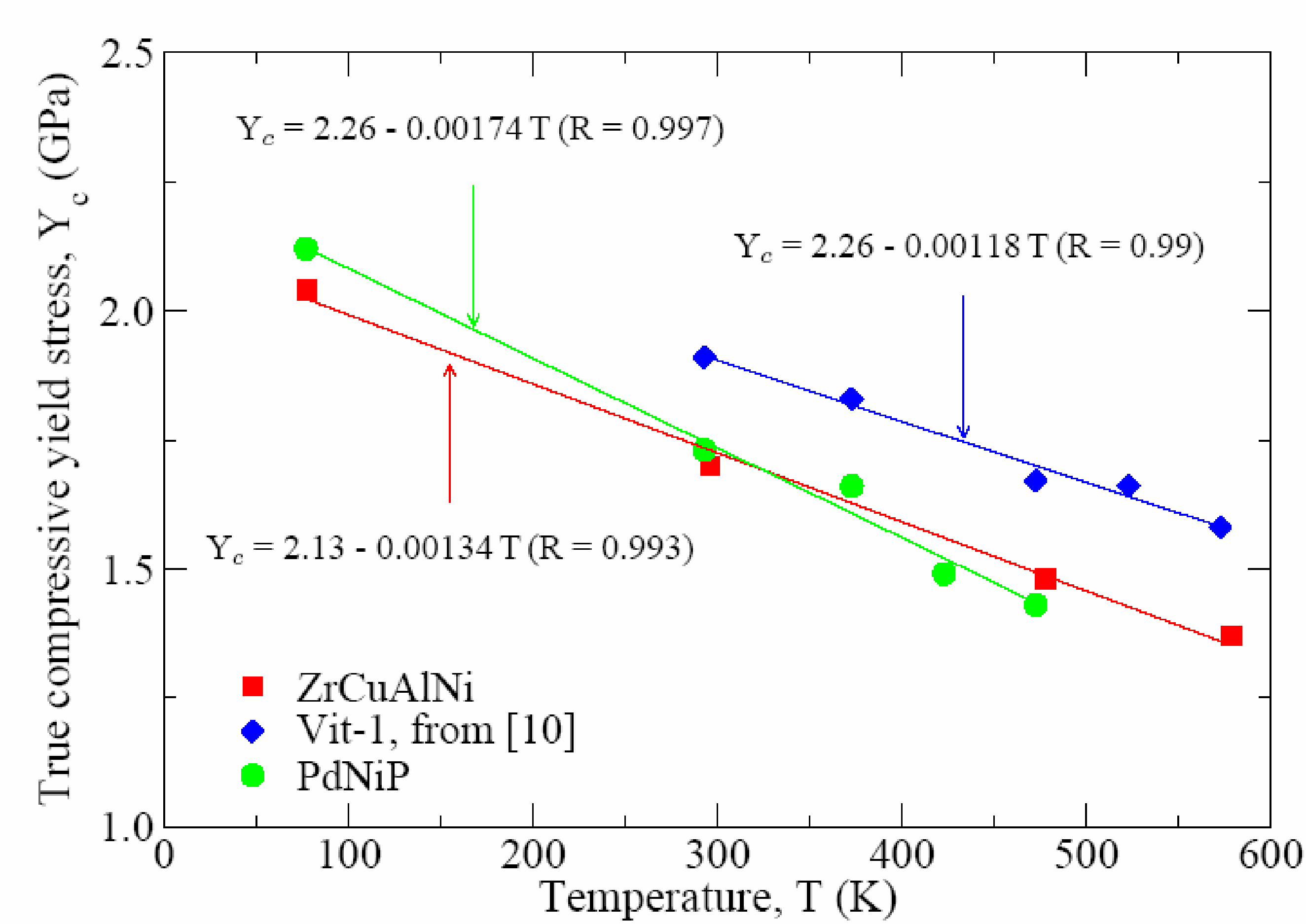
$$C_1 = [0.3/\sigma_y]^{0.5}$$

σ_y= 2.5 GPa

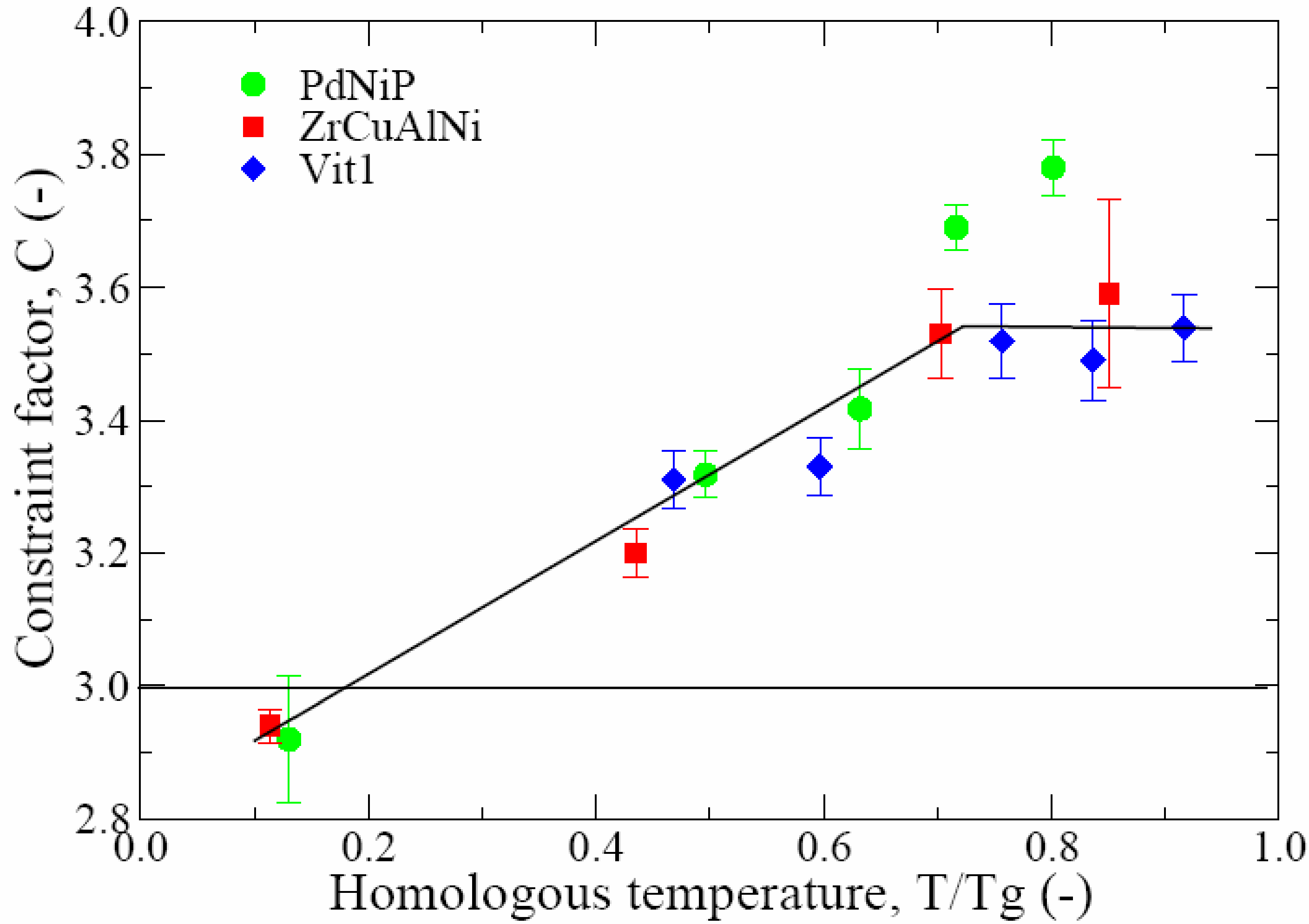
Pressure Sensitivity with T



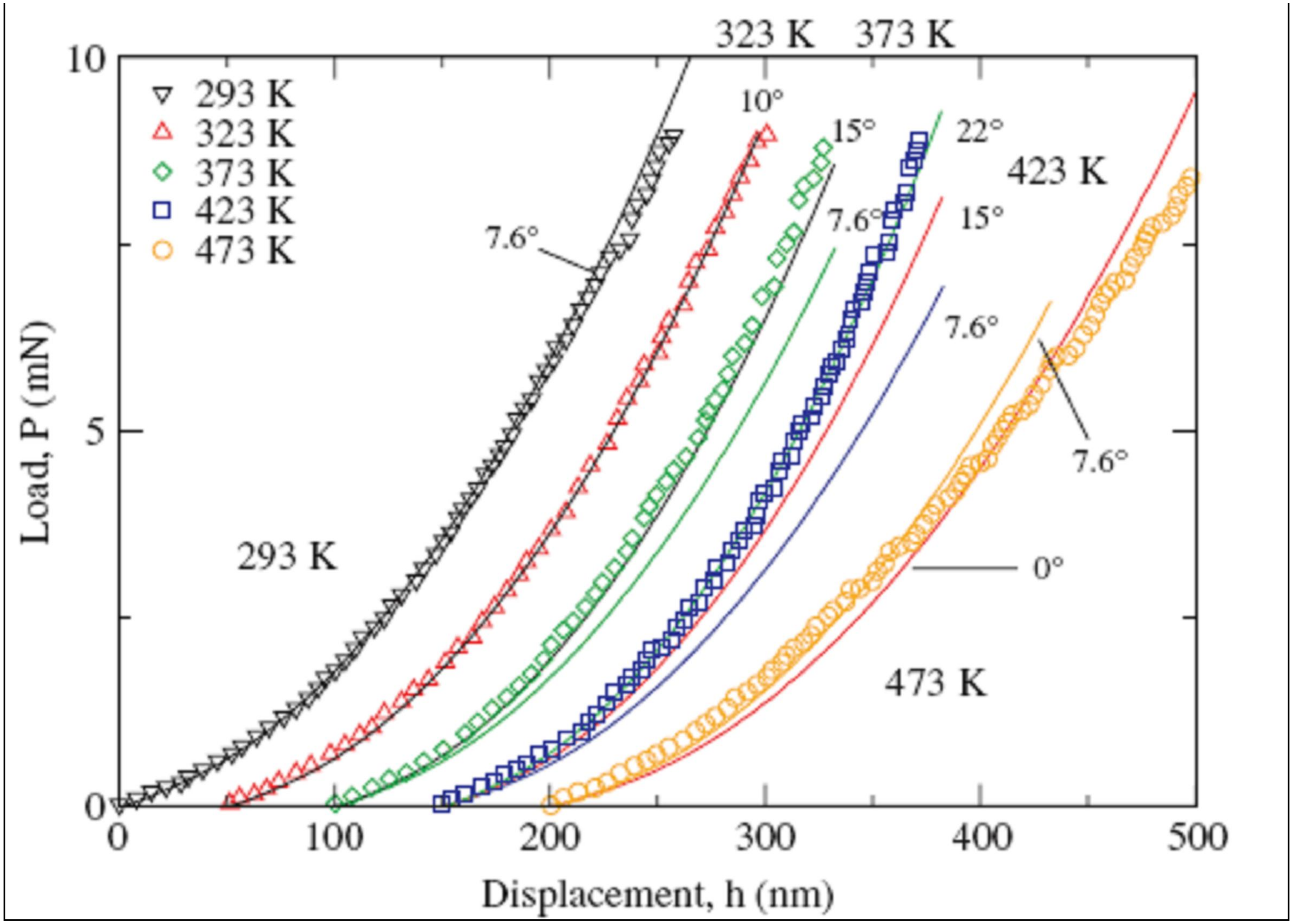
Eswar Prasad et al. Scripta Mat 2007, Keryvin et al. Phil Mag. 2008



Glass composition (at.%)	T_g (K)	Ref.
$Pd_{40}Ni_{40}P_{20}$	590	[4]
$Zr_{41.2}Ti_{13.75}Cu_{12.5}Ni_{10}Be_{22.5}$	625	[49]
$Zr_{55}Cu_{30}Al_{10}Ni_5$	680	[50]

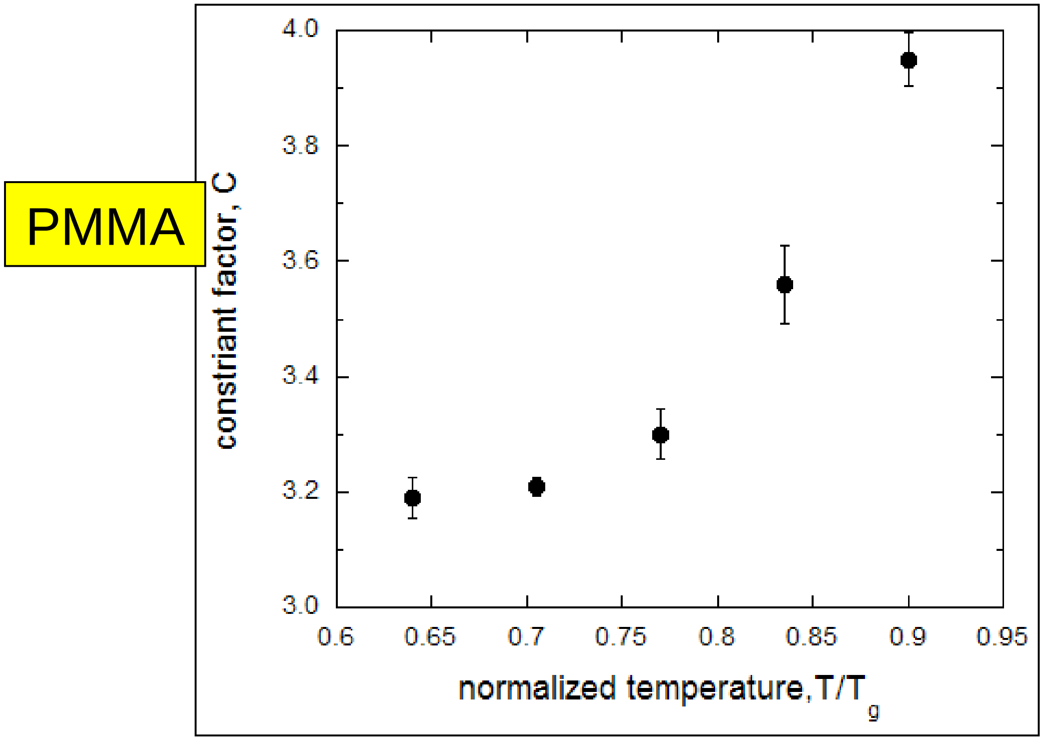


PdNiP
ZrCuAlNi
Vit1
Constraint factor, C (-)
Homologous temperature, T/Tg (-)
4.0
3.8
3.6
3.4
3.2
3.0
2.8
0.0
0.2
0.4
0.6
0.8
1.0



- P-h curves are simulated using FEM using Drucker-Prager model for different levels of pressure sensitivity.
- FEM simulations show that the pressure sensitivity increases with increasing temperature.

Eswar prasad etal, Scripta Mat. (2007), V. Kervyin, Phil Mag A (2008)



- For polymers the β-relaxation mechanisms that are active in this temperature regime.
- For MGs also the relaxation of the matrix surrounding an STZ could be a reason for increasing pressure sensitivity.

K. Eswar prasad, V. Keryvin and U. Ramamurty, JMR (2009)

Micropillar compression & in-situ indentation experiments – effect of structural state

$Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ (LM1)

- As-cast ($T_g \approx 625$ K) **Γ = 1.1 J**

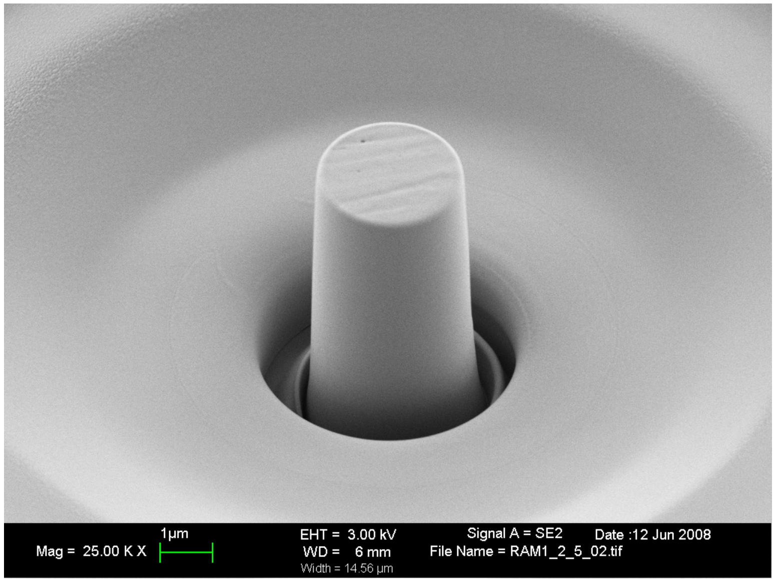
- Structurally relaxed (563 K for 12 h)

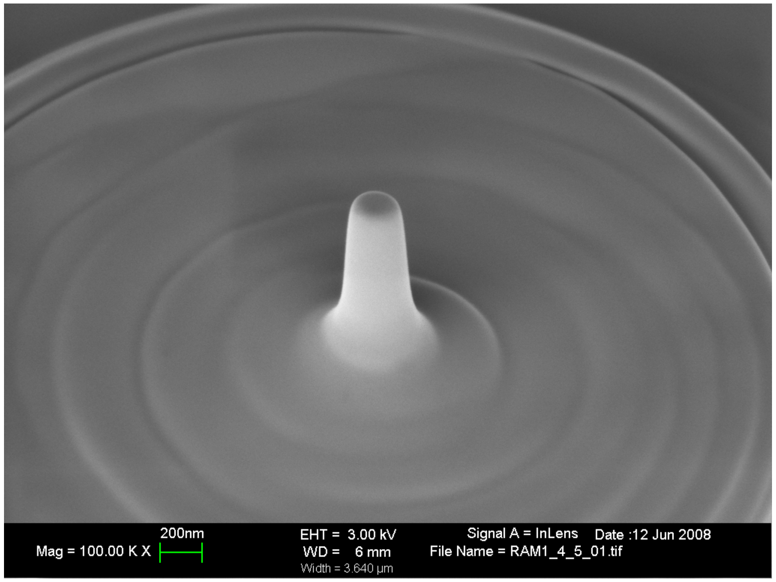
  Γ = 0.1-0.2 J

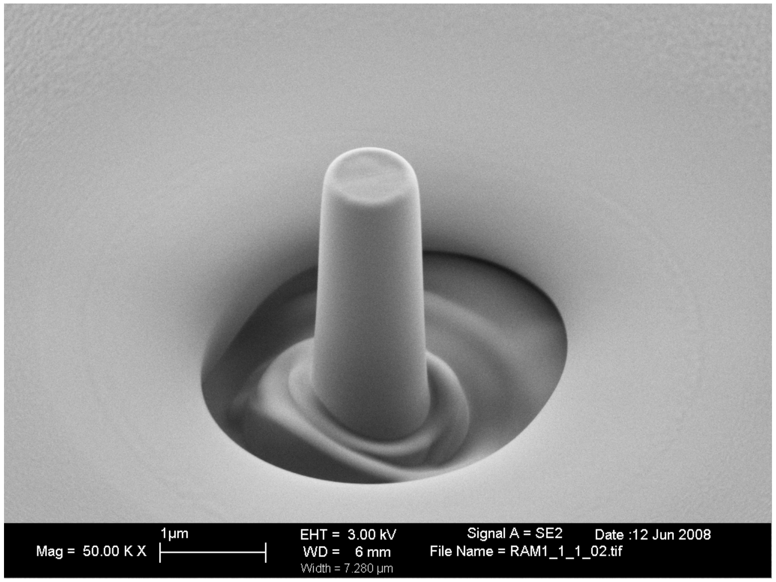
- Shot peened (layer thickness ≈ 40 μm)

  (see Raghavan et al. Scr. Mat 2008)

Dubach et al. Scripta mat, 2009

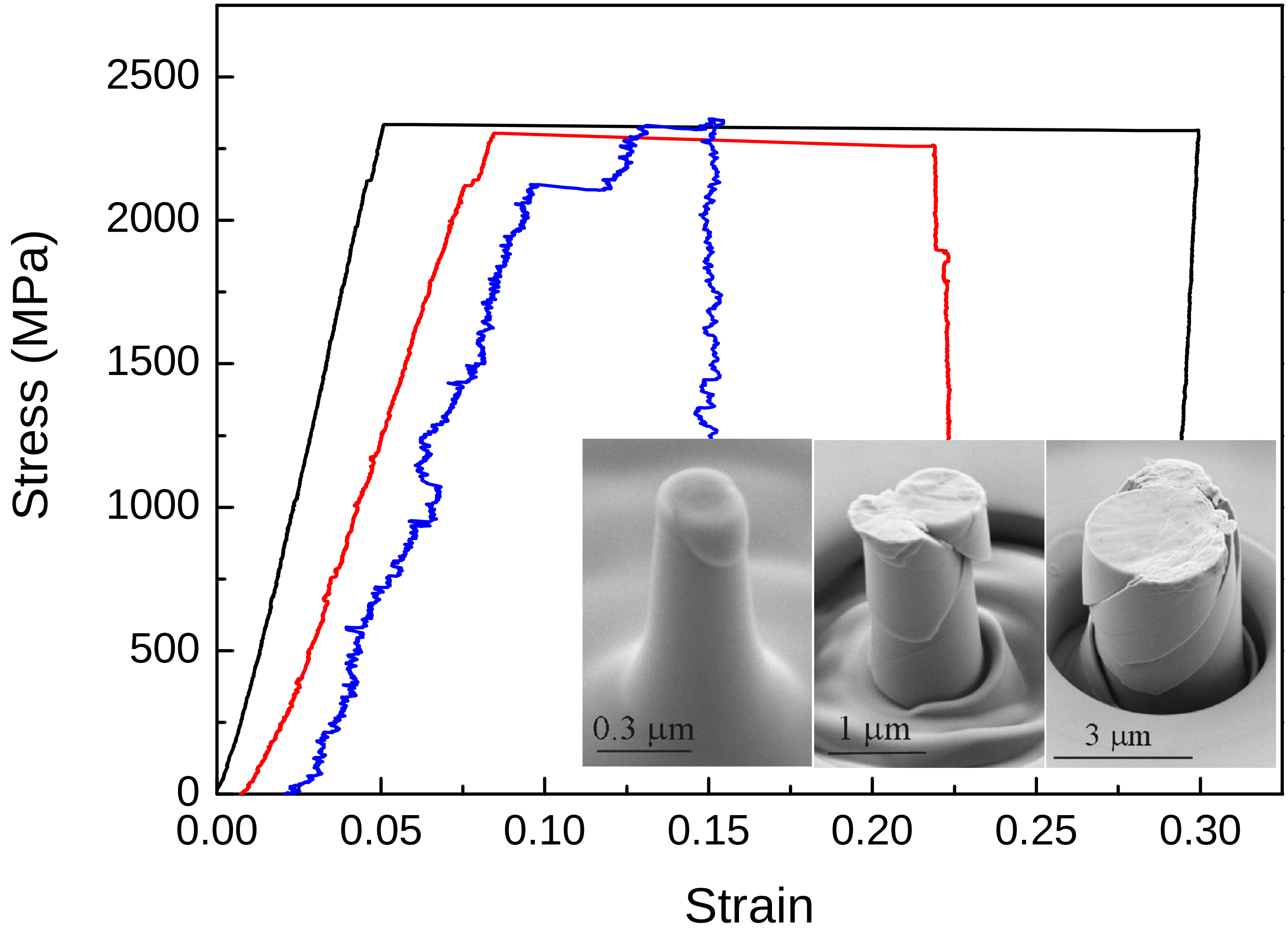






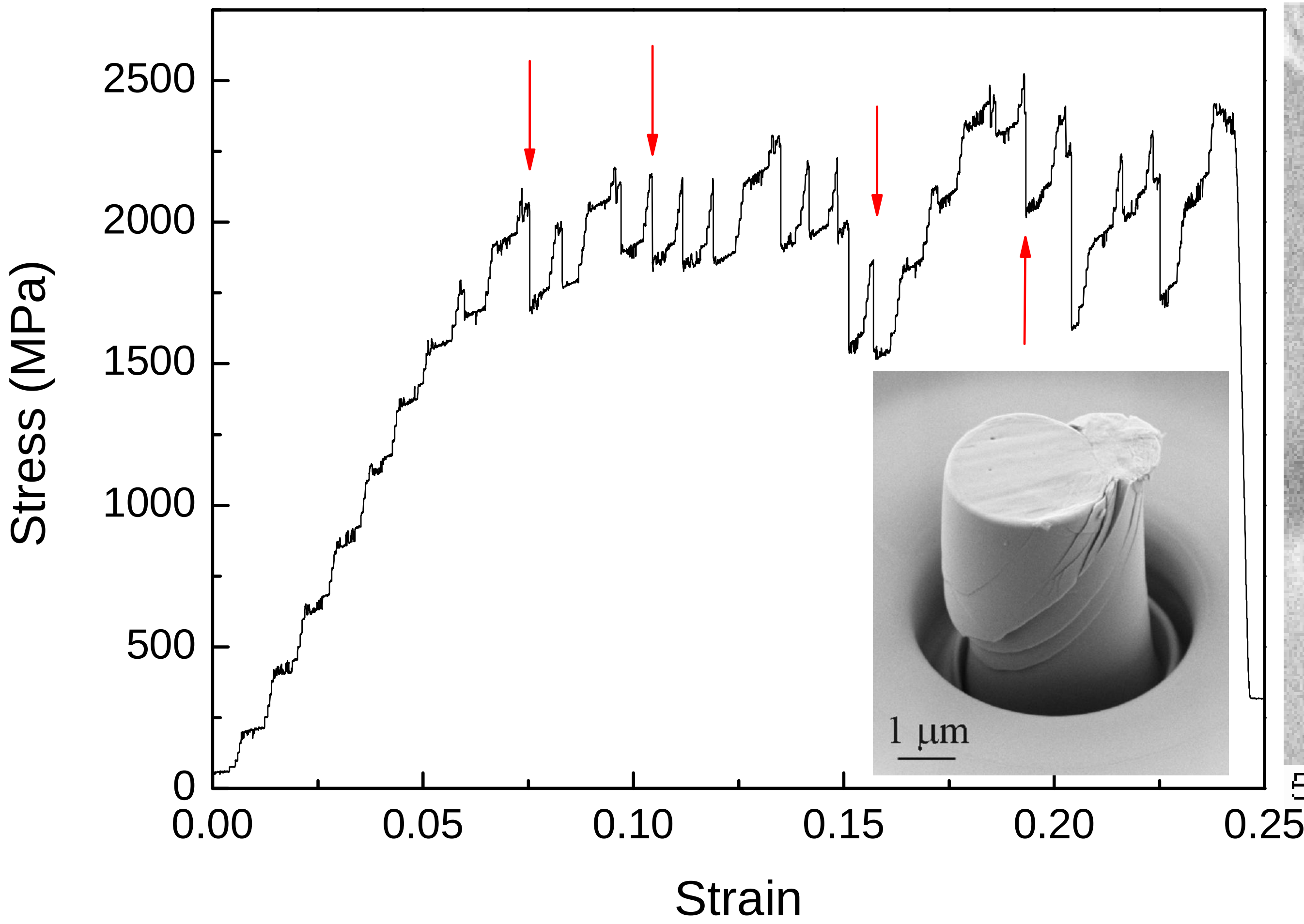
FIB 0.3, 1, and 3 μm pillars with 2 to 2.5 aspect ratio

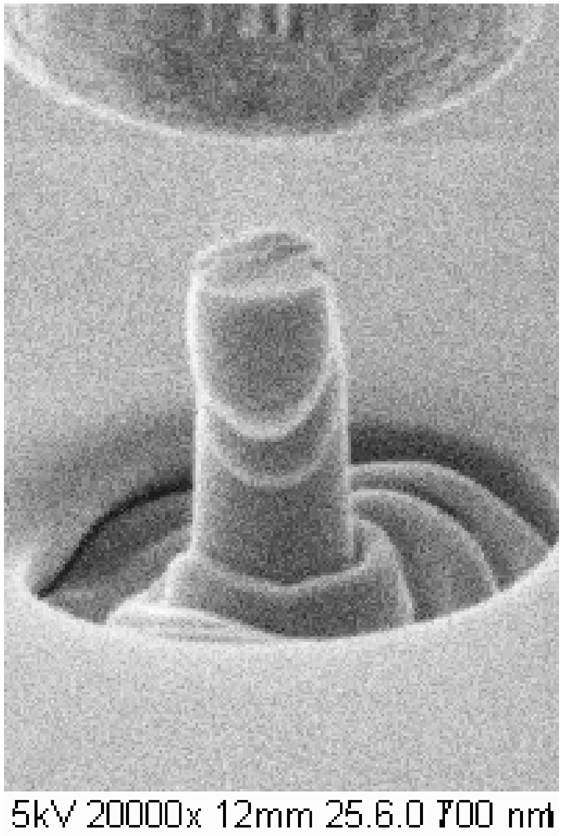
Ex-situ, load controlled test

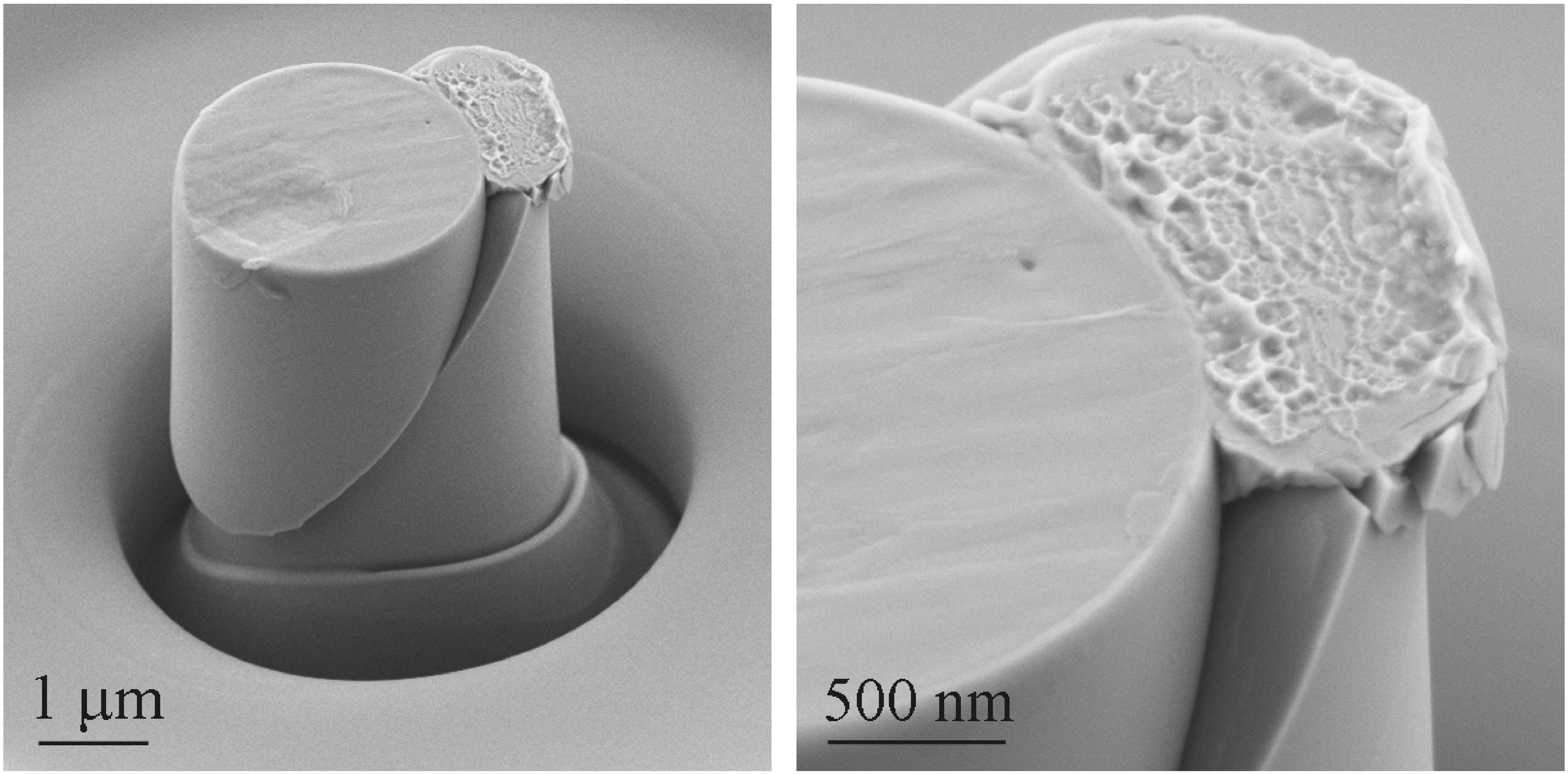


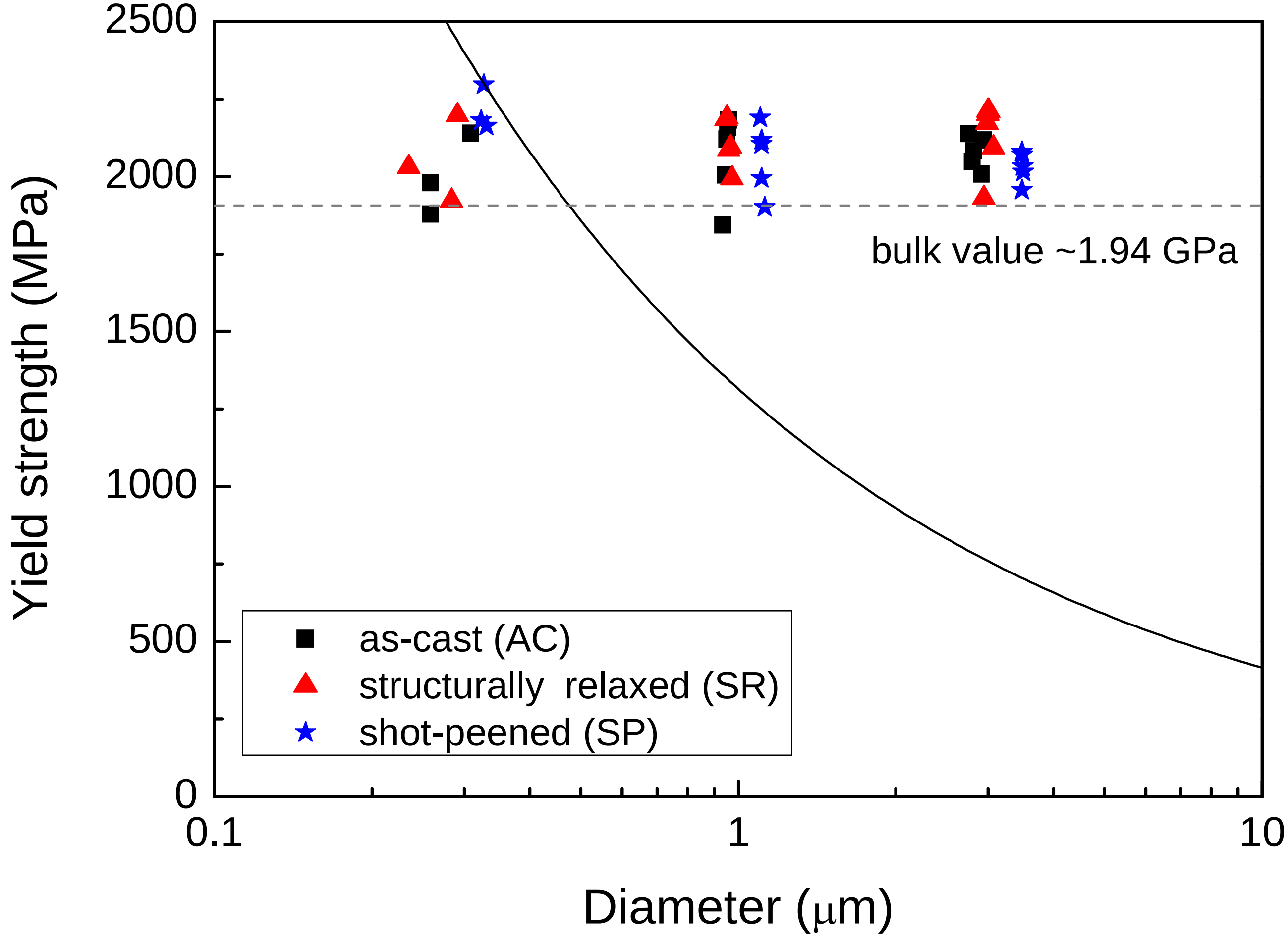
As-cast alloy

In situ, displacement control test

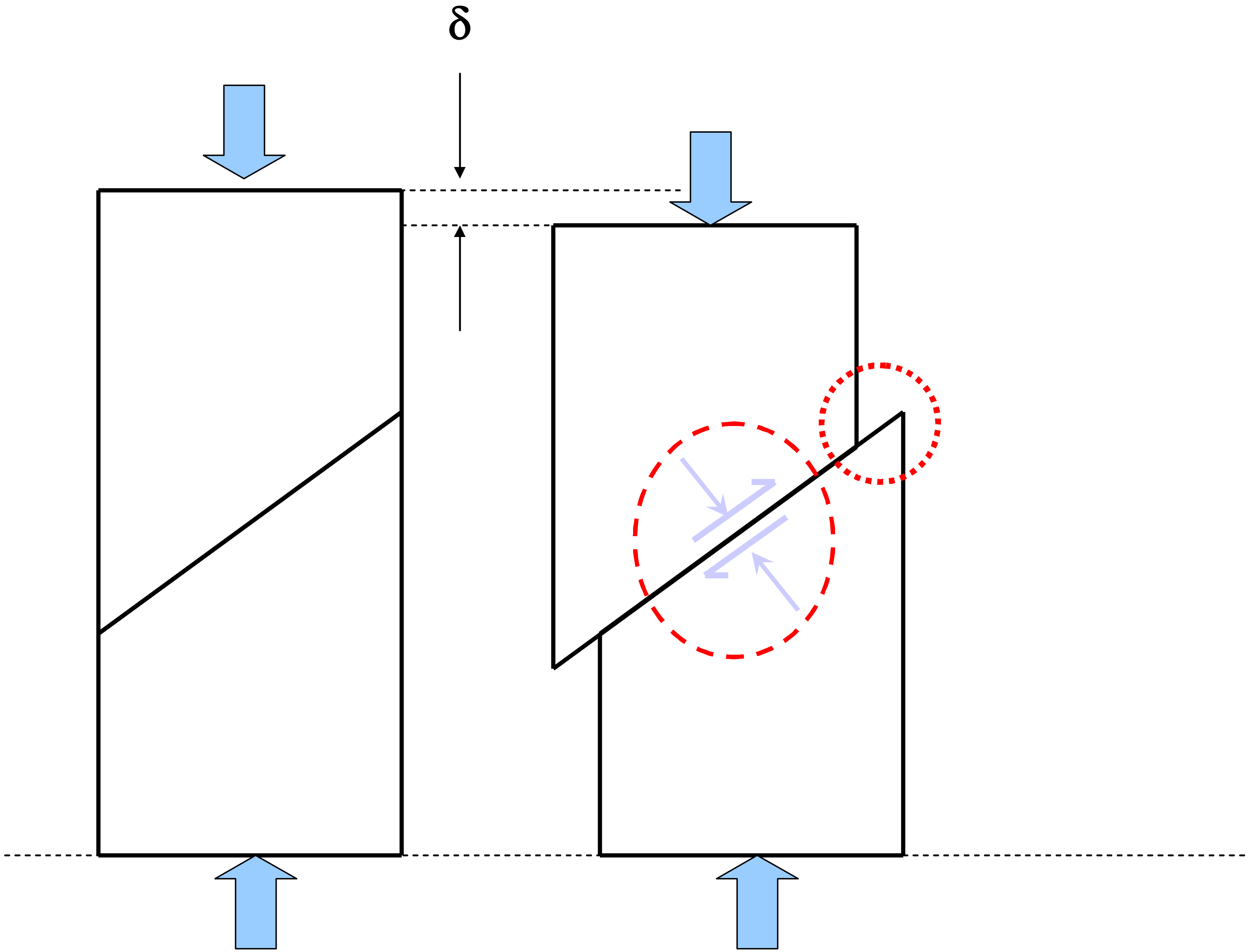





1 μm
500 nm



Yield strength (MPa)
2500
2000
1500
1000
500
0
0.1
1
10
Diameter (μm)
bulk value ~1.94 GPa
as-cast (AC)
structurally relaxed (SR)
shot-peened (SP)

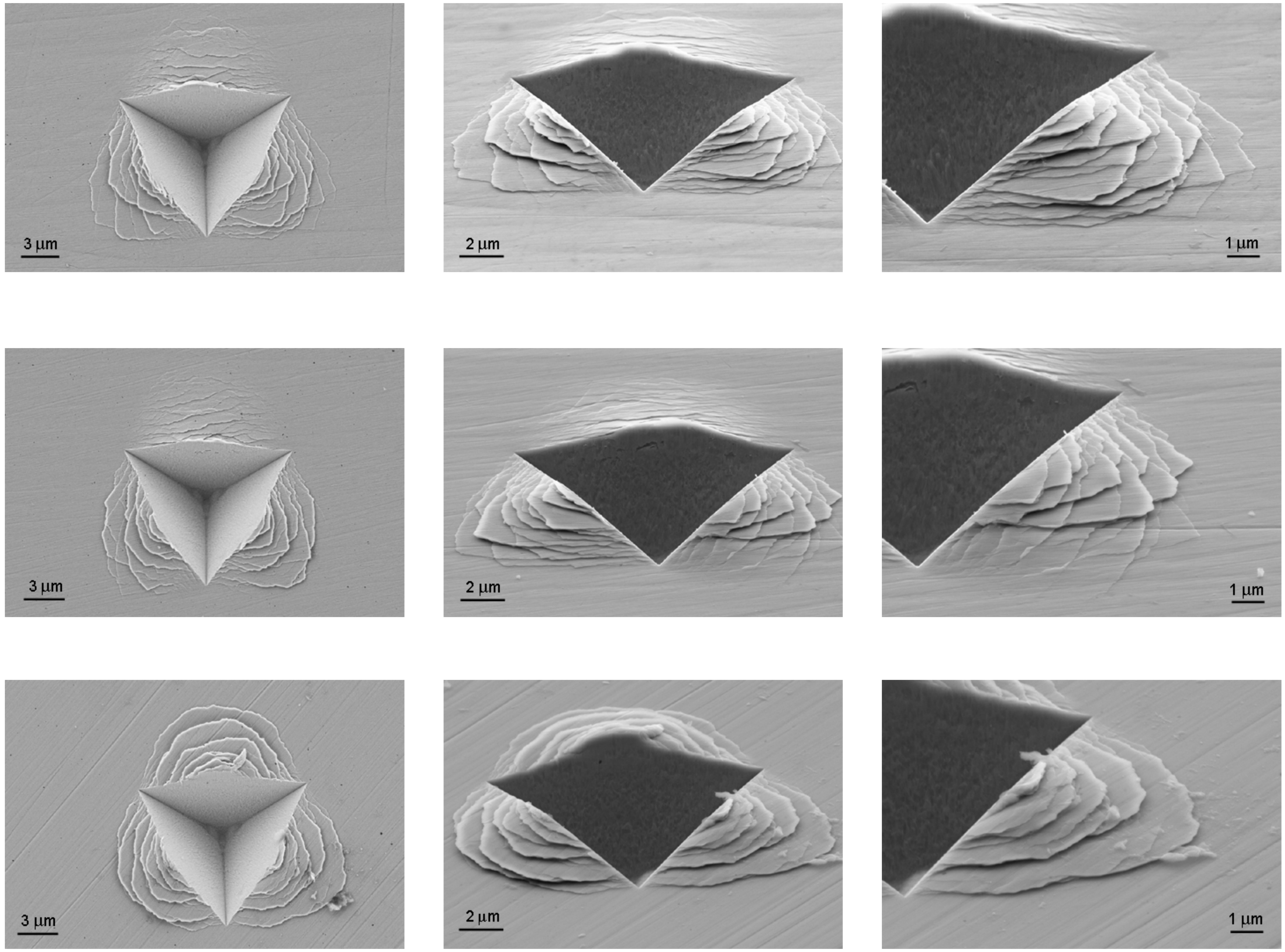

δ

SEM images

as-cast

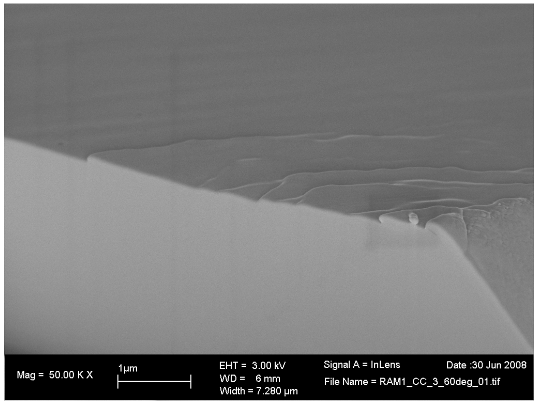
structurally-relaxed

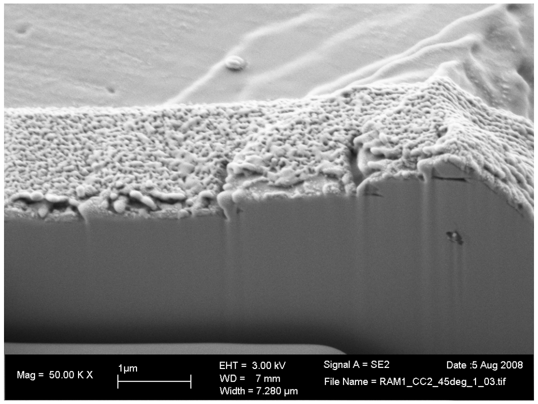
shot-peened



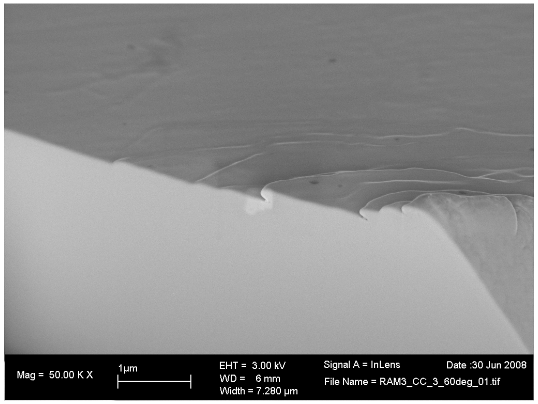
FIB-cut indent profiles

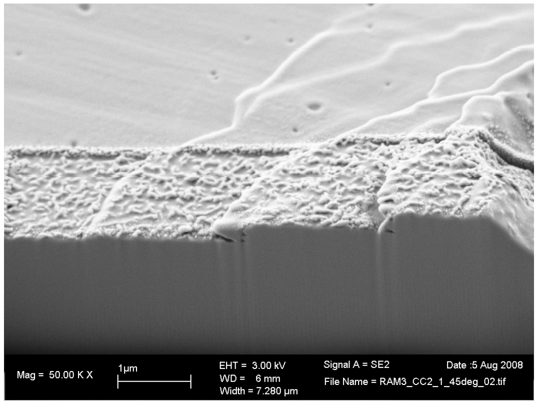
as-cast



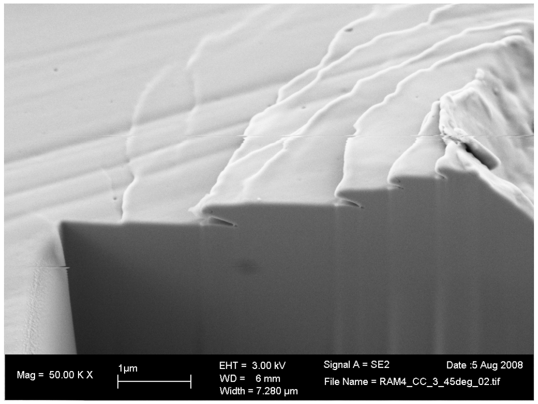


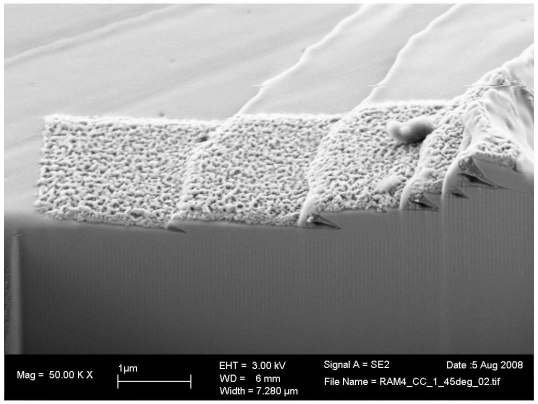
structurally-
relaxed

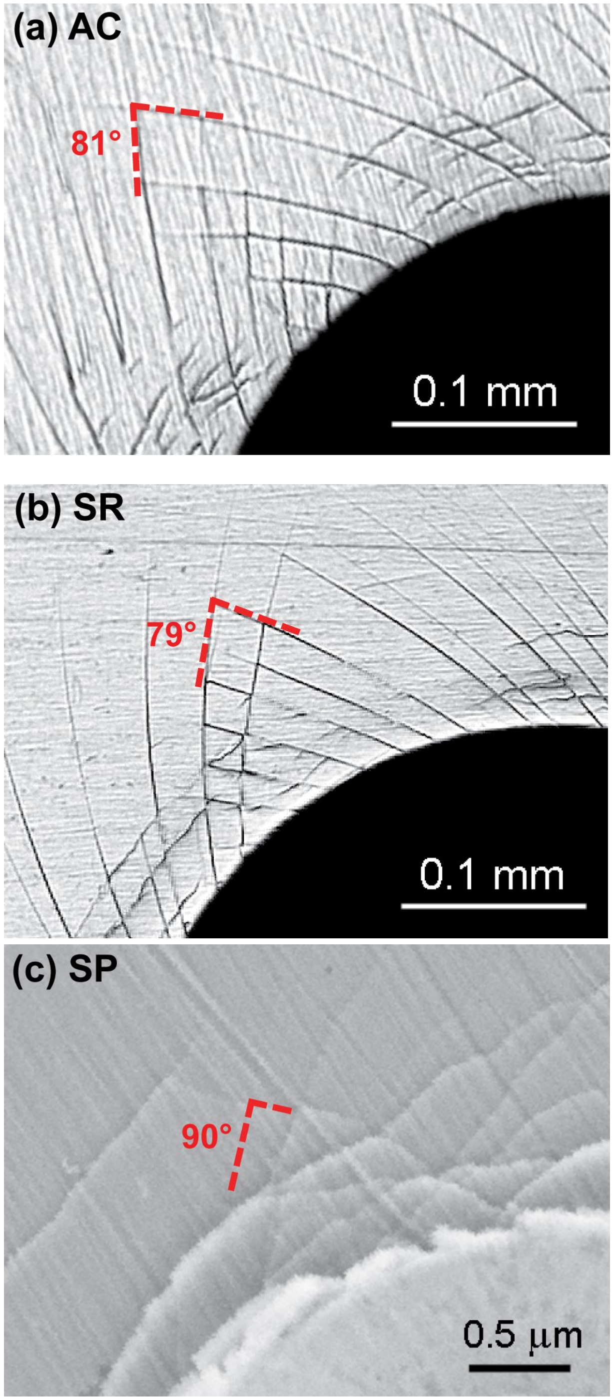




shot-
peened







Material condition	σ_y (MPa)	H (GPa)	C	Intersection angle, α (degrees)
as-cast	2079 ± *52*	6.07 ± *0.04*	2.92	80.9±*1.1*
structurally-relaxed	2137 ± *110* (+2.8%)	6.45 ± *0.05* (+6.3%)	3.02 (+3.4%)	79.8±*1.2*
shot-peened	2030 ± *49* (-2.4%)	5.22 ± *0.21* (-14%)	2.57 (-12%)	91.2±*3.2*