Fracture ~~and Fatigue~~ in Amorphous Alloys

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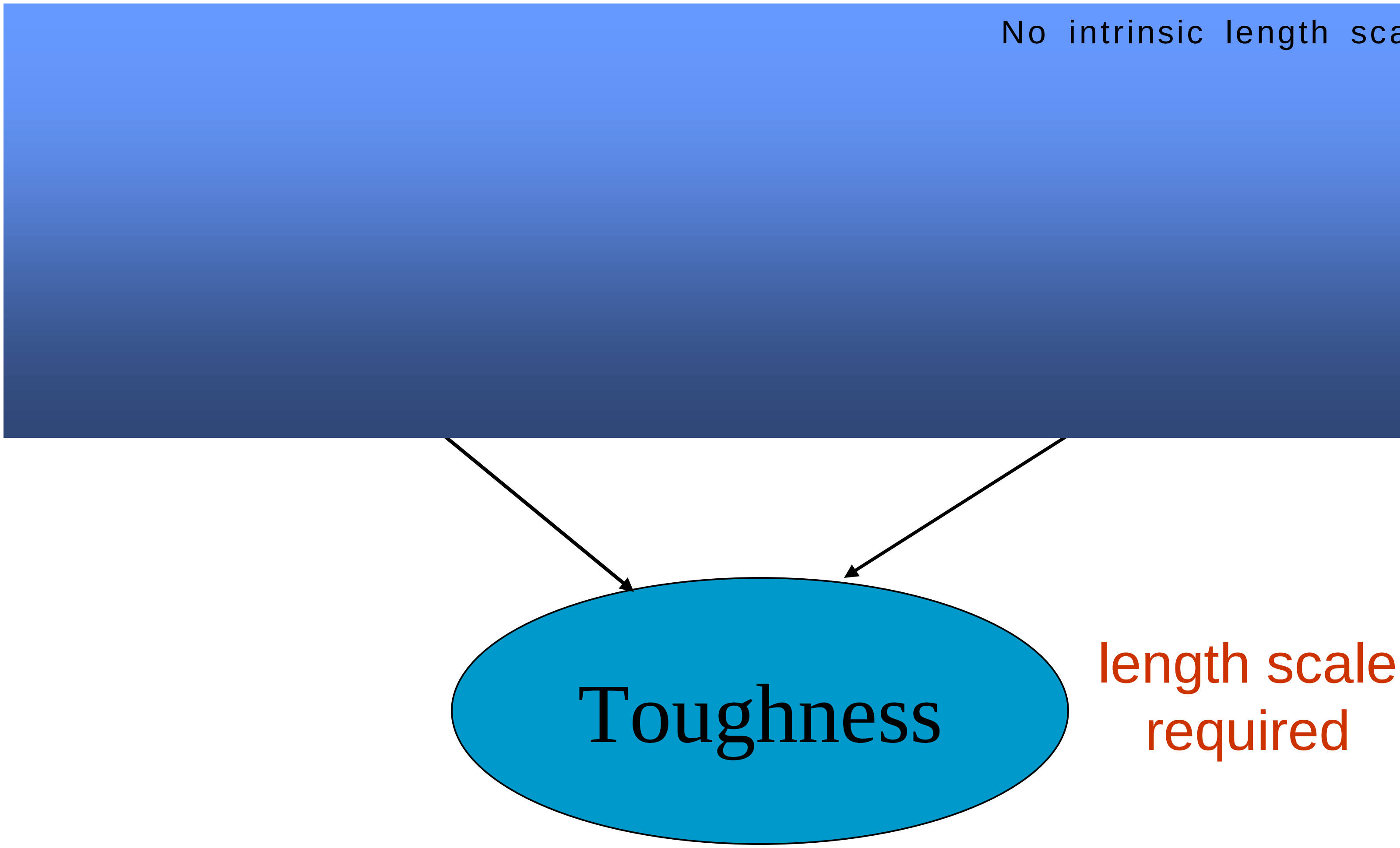
Fundamental Mechanical Properties*



*Quasi-static loading, room temperature

Basics of Fracture Mechanics

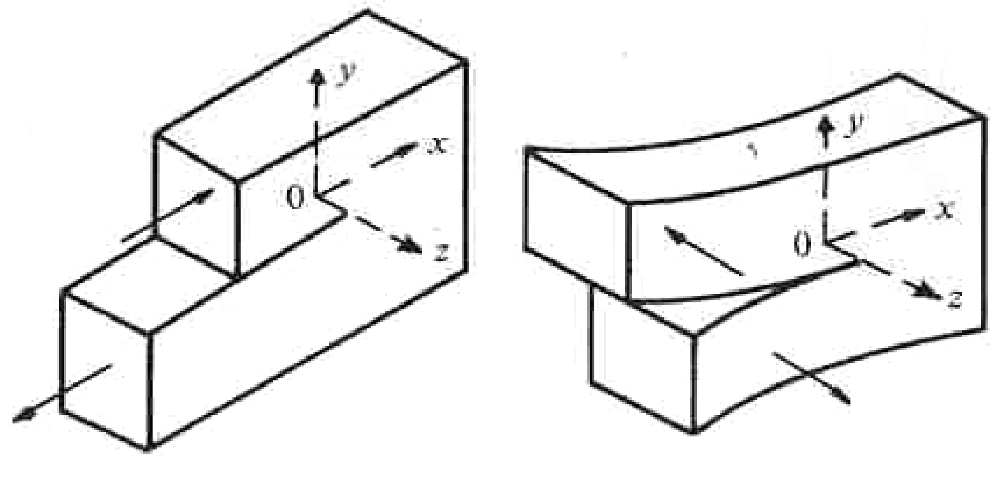
Importance of Fracture Mechanics :

All real materials contain defects: understand the influence of these defects on the strength of the material. Defect-tolerant design philosophy.

Relevance for Fatigue: understand the initiation and growth of fatigue cracks.

Modes of Fracture

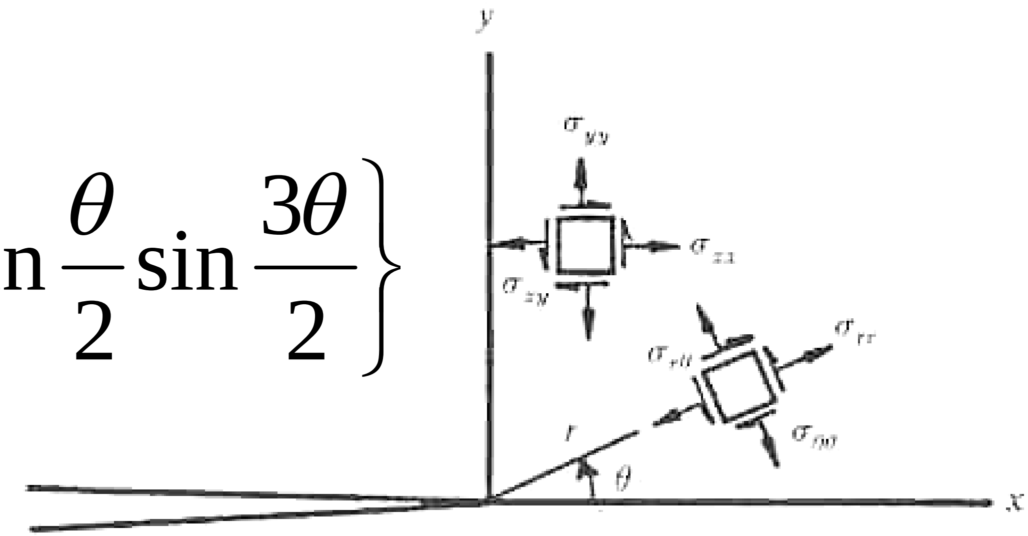
The three basic modes of separation of the crack surfaces (**modes of fracture)** are depicted below:



Combinations of modes (**mixed-mode loading**) are also possible.

Linear Elastic Fracture Mechanics (LEFM)

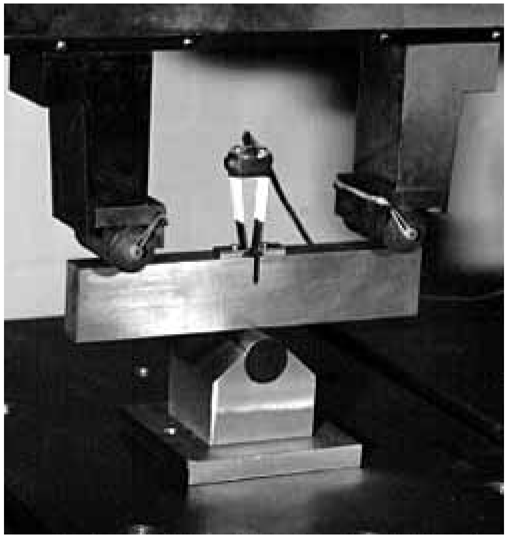
Stress analysis of a cracked body, within the framework of linear elasticity, with the goal to develop expressions for the stresses, strains and displacements around the crack tip .



$$\sigma_{yy} = \frac{K_I}{\sqrt{2\pi r}} \cos\frac{\theta}{2}\left\{1+\sin\frac{\theta}{2}\sin\frac{3\theta}{2}\right\}$$

$$u_y = \frac{K_I}{2E}\sqrt{\frac{r}{2\pi}}\left\{(1+\nu)\left[(2\kappa+1)\sin\frac{\theta}{2}-\sin\frac{3\theta}{2}\right]\right\}$$

Similitude

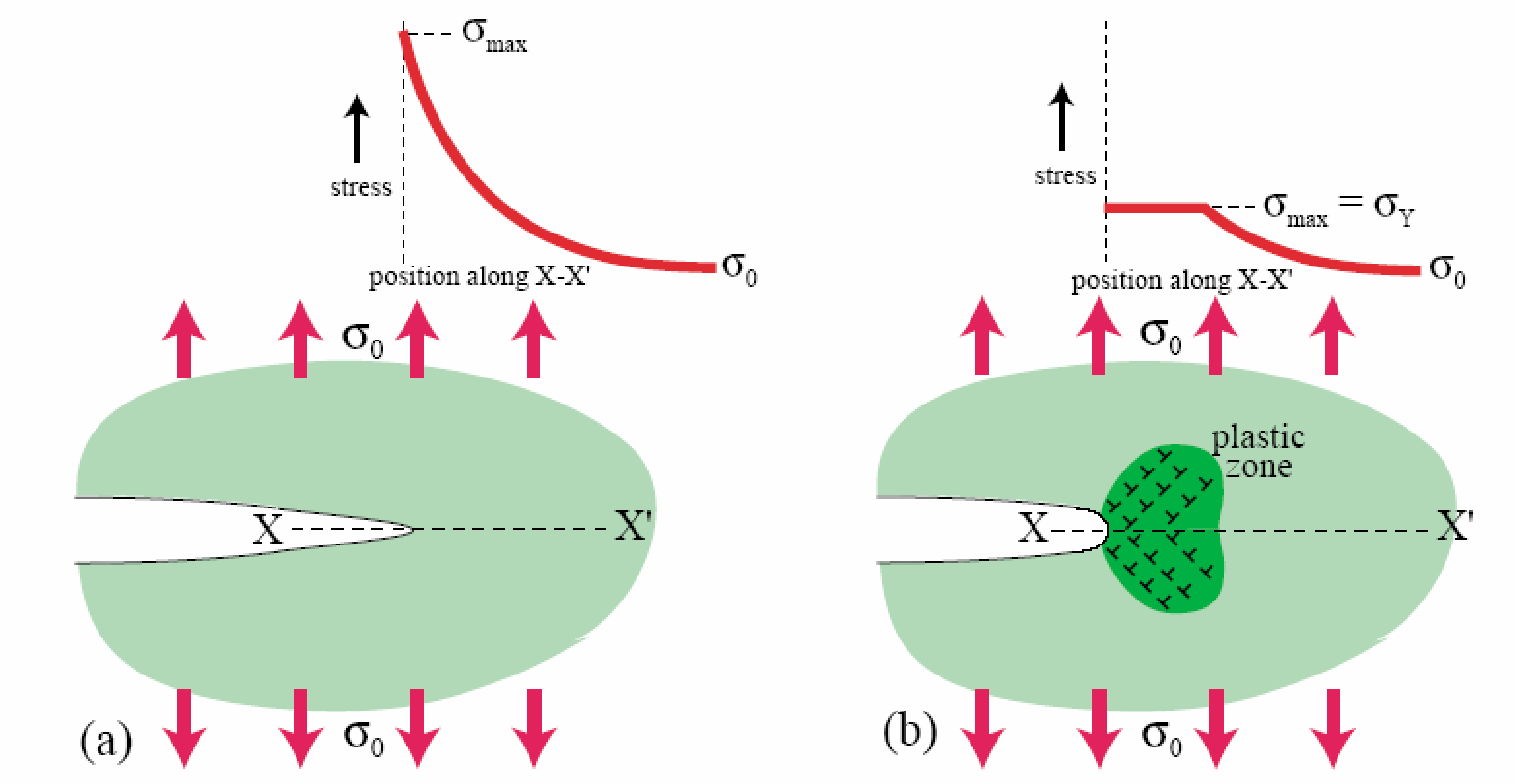
- 

$$K_I = \sigma_1 \sqrt{\pi a_1}$$

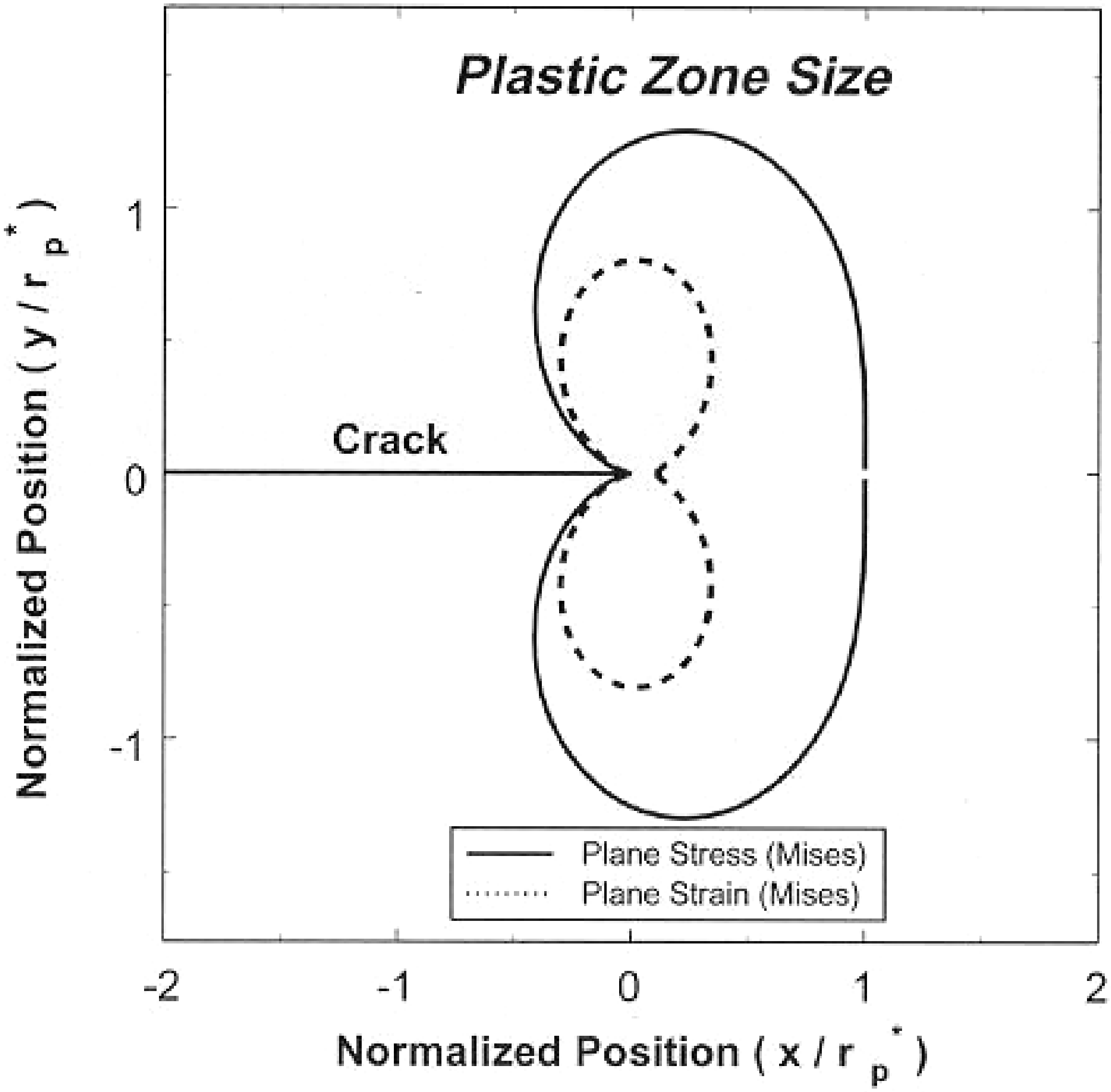
$$K_I^{(1)} = K_I^{(2)}$$

Material	K_c (MPa$\sqrt{m}$)
Glass	≈ 1
Al_2O_3	$\approx 3-4$
$Si_3\ N_4$	$\approx 4-8$
Polymers	$\approx 0.5-2$
Al alloys	$\approx 10-100$
Steels	$\approx 30-300$

Role of Crack Tip Plasticity



Plastic Zone Shape



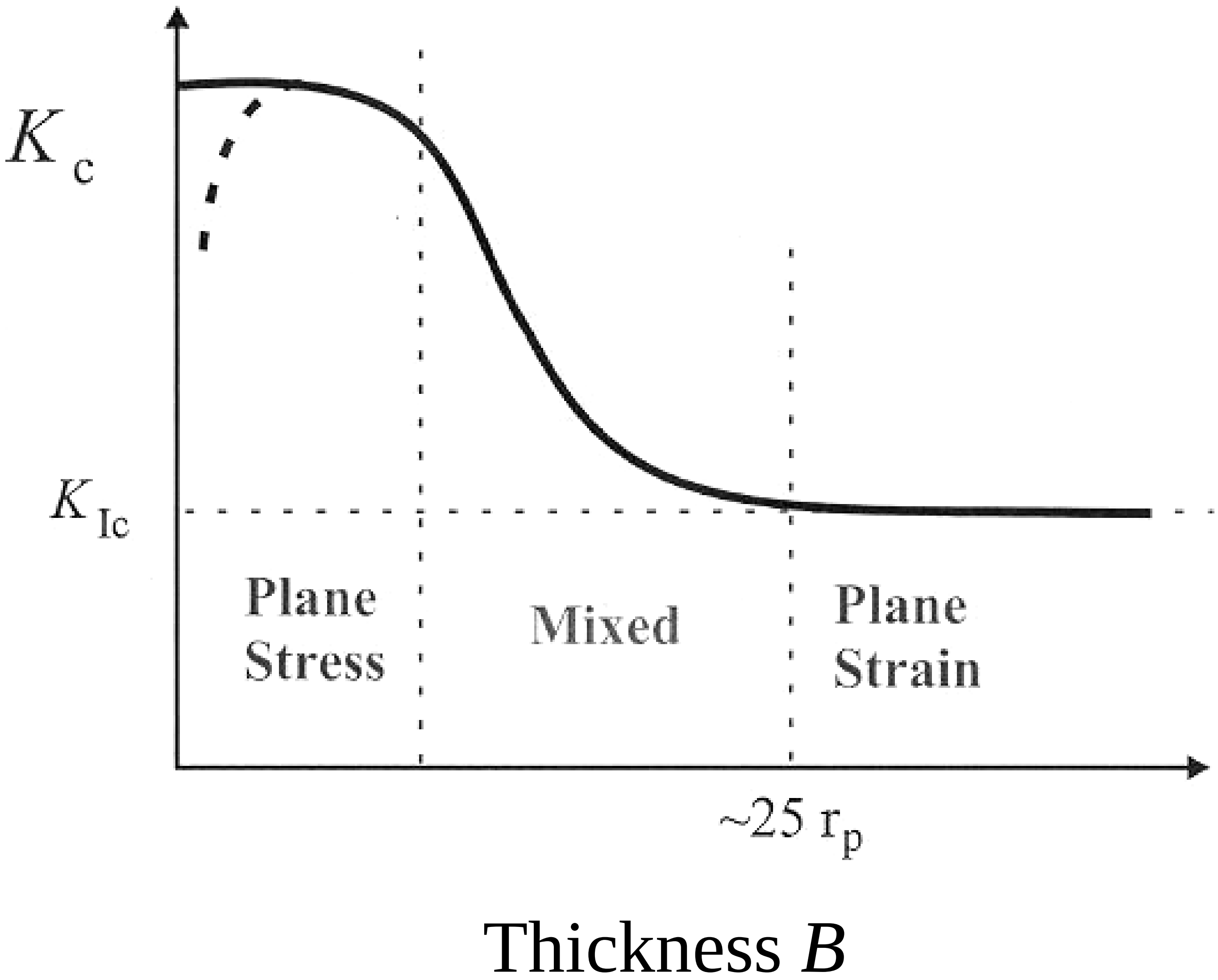
Plane Stress:

$$r_p = \frac{1}{\pi}\left(\frac{K_I}{\sigma_{ys}}\right)^2$$

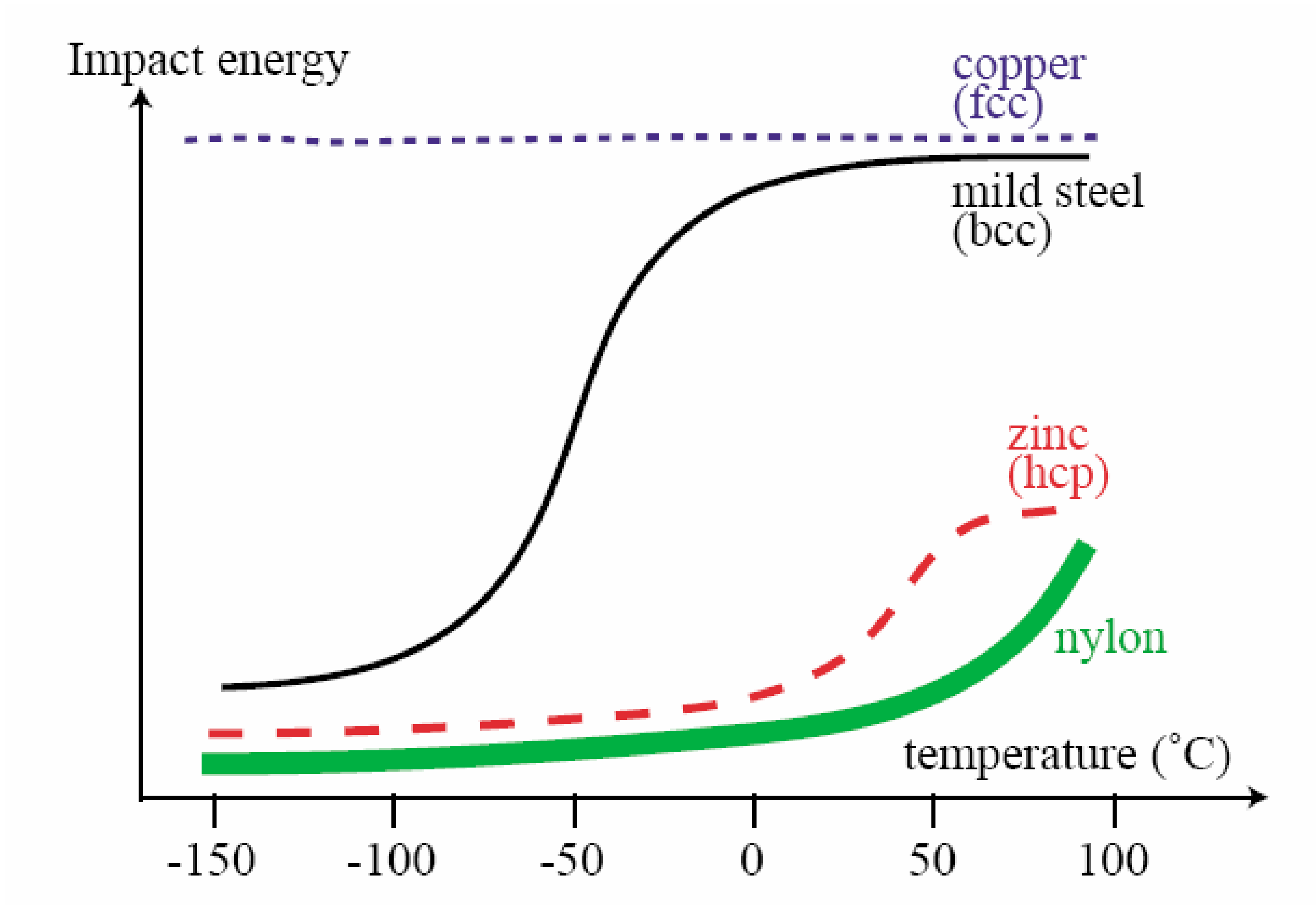
Plane Strain:

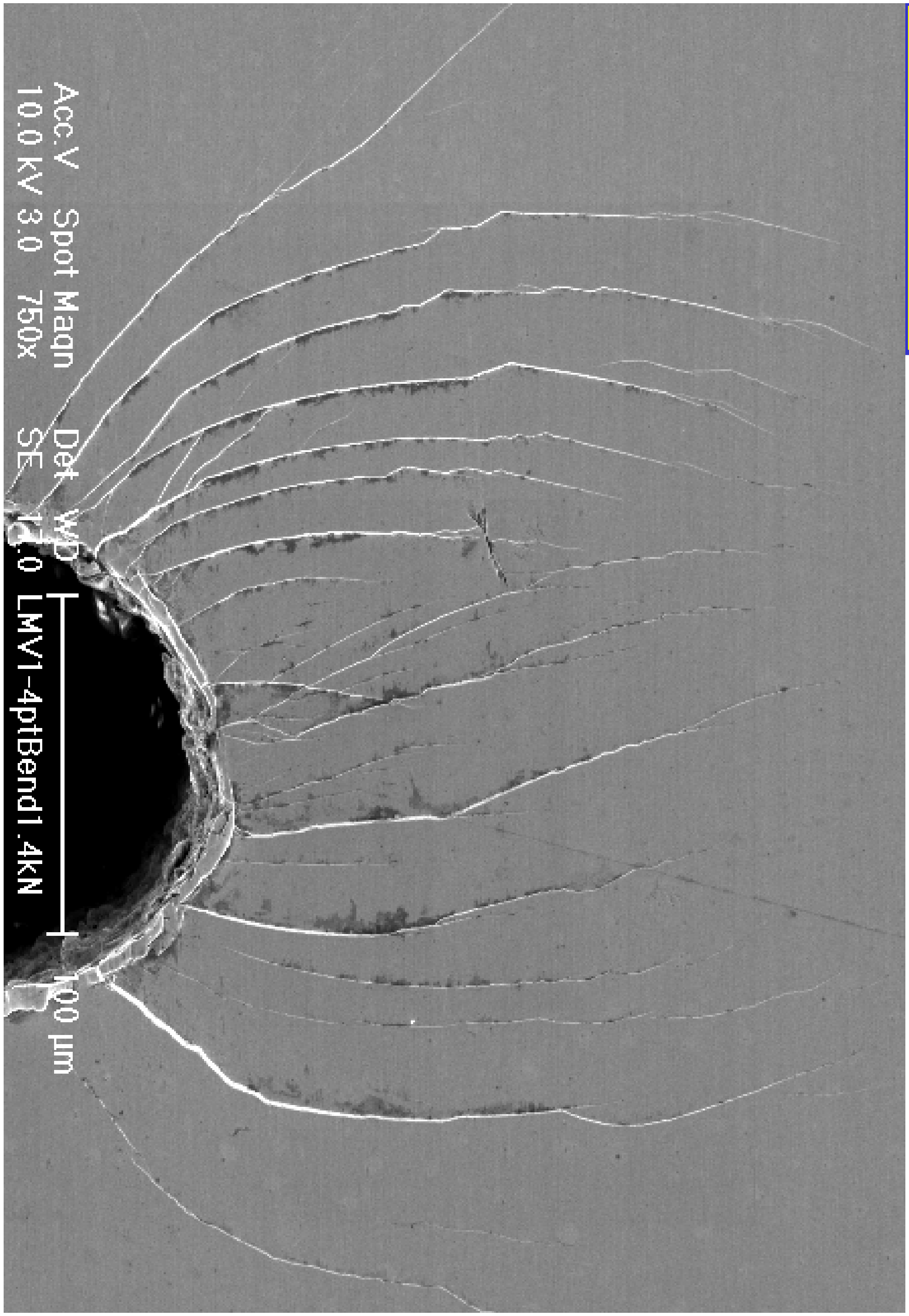
$$r_p = \frac{1}{3\pi}\left(\frac{K_I}{\sigma_{ys}}\right)^2$$

Specimen Thickness Effects



Ductile Brittle Transition





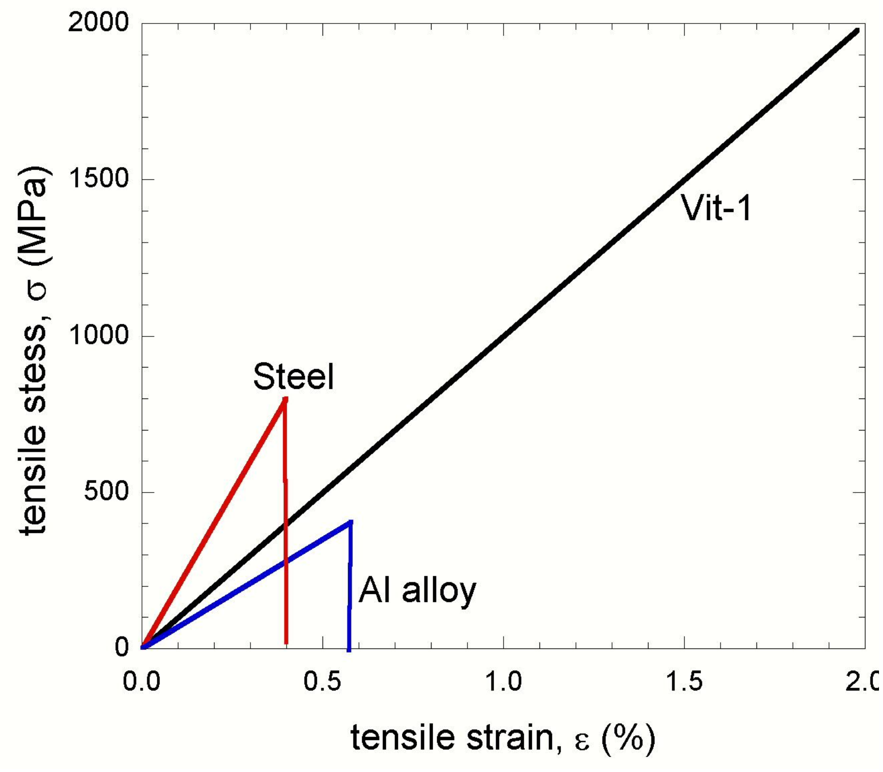
Fracture in amorphous alloys

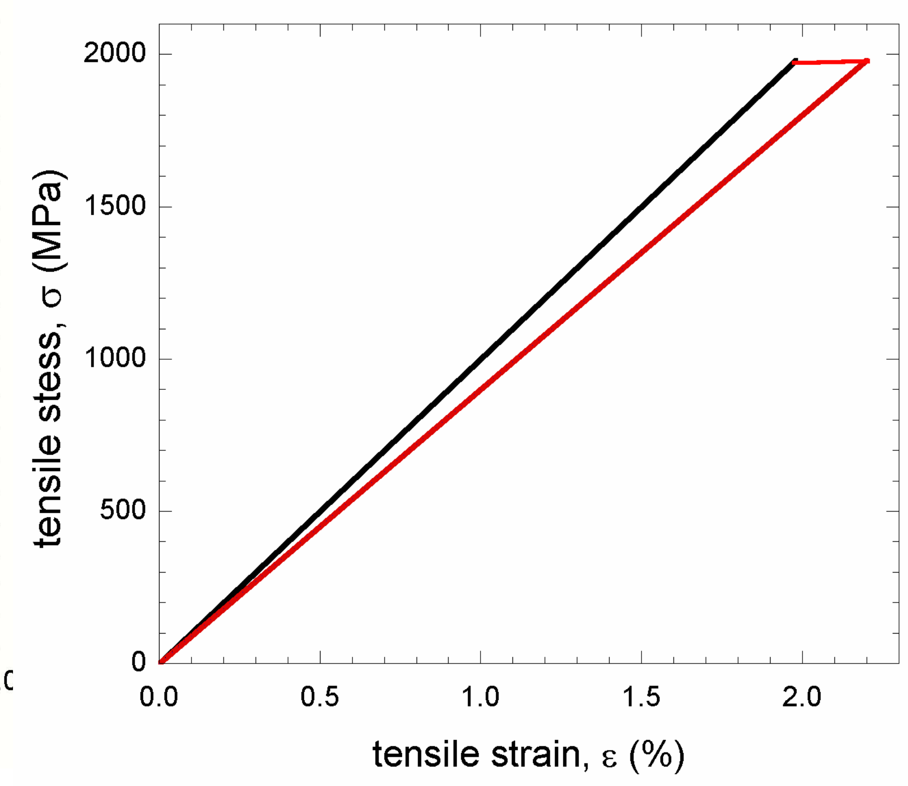
What are the connections between nano- and micro-mechanisms and toughness?

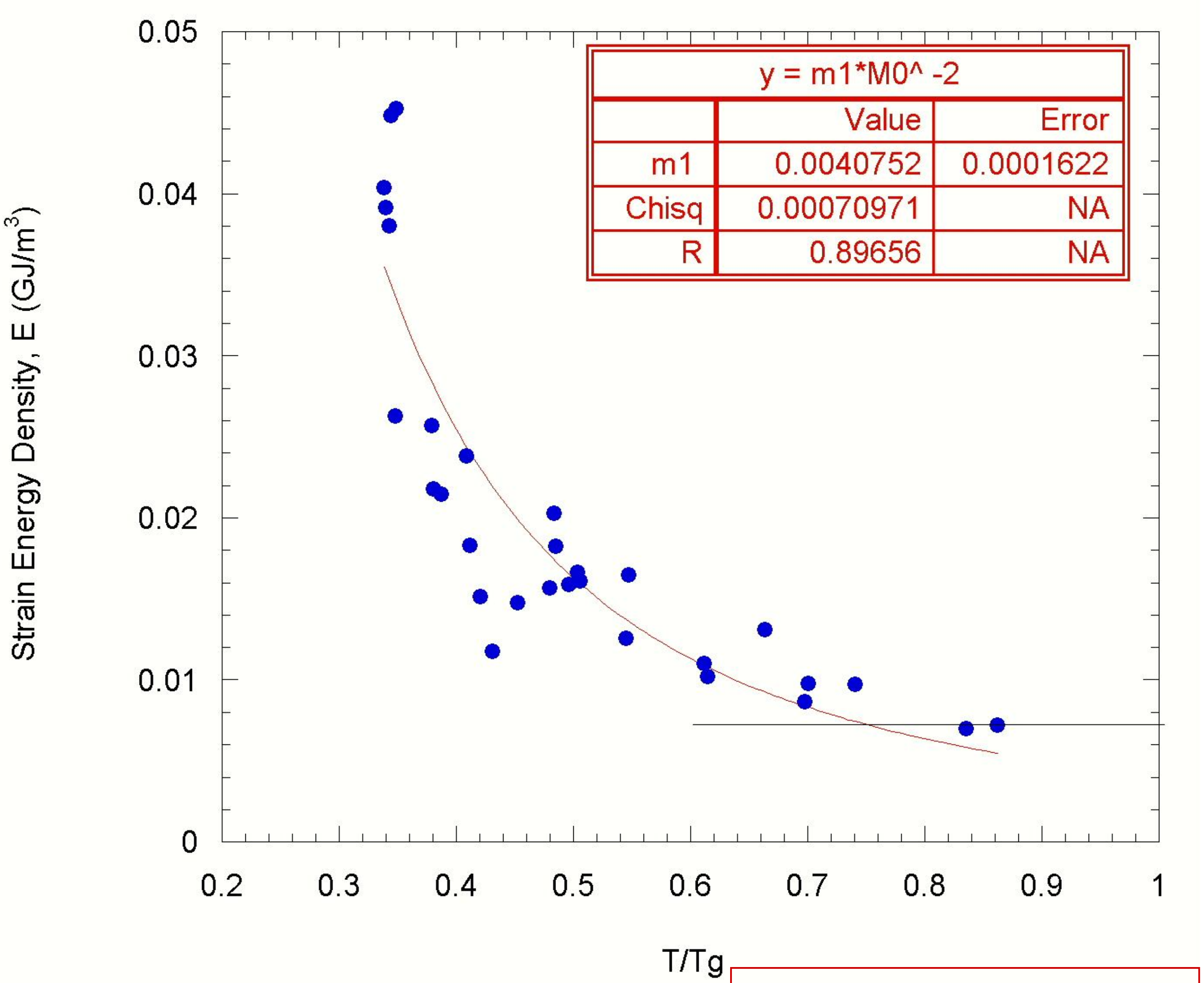
BMG	K_c (MPa√m)	Elastic Modulus (GPa)	Poisson's ratio	Hardness (GPa)
Vitreloy $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$	**30-68**	96	**0.36**	**5.9**
Amorphous steel $Fe_{48}Cr_{15}Mo_{14}Er_{2}C_{15}B_{6}$	**3.8 ± 0.3**	187	0.28-0.32	17.8±0.73

What controls the toughness of BMGs?

Elastic Strain Energies





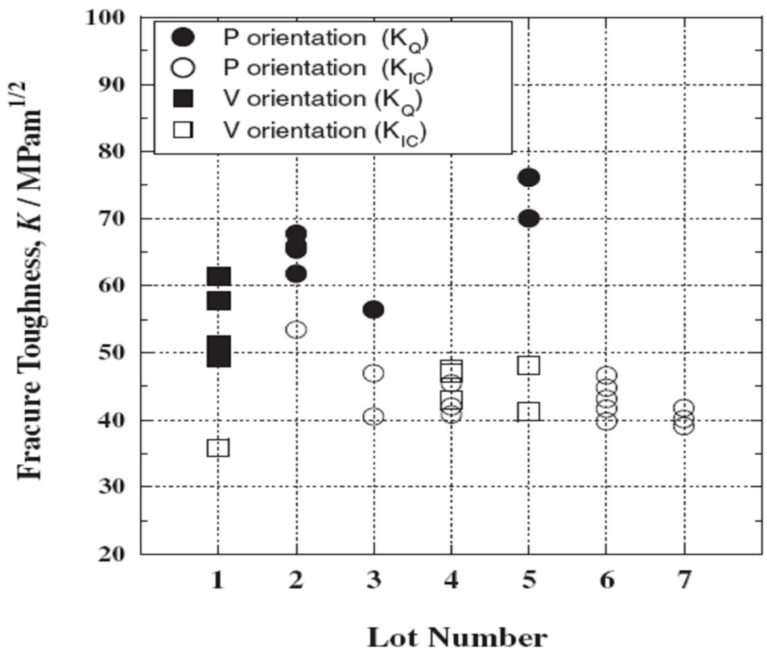


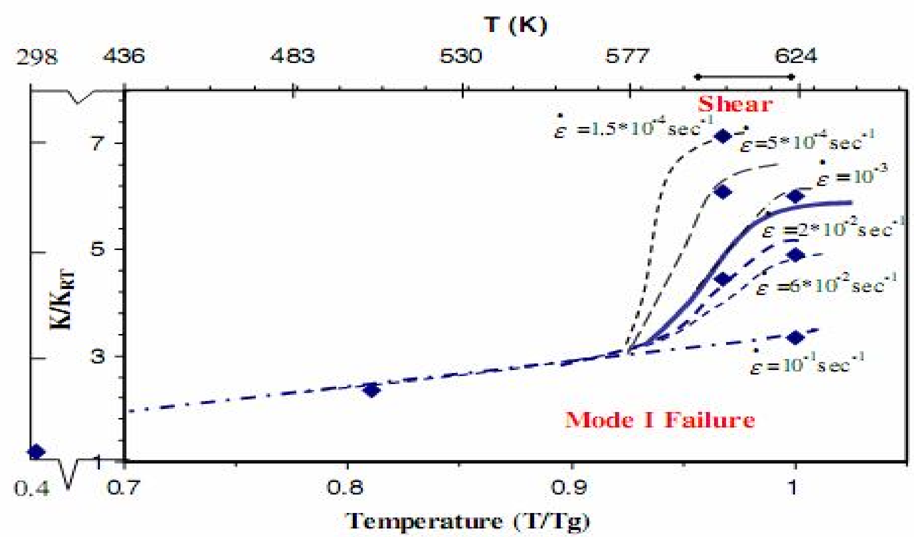
$$r_p = \frac{1}{3\pi}\left(\frac{K_I}{\sigma_{ys}}\right)^2$$ = 1/100 mm

Factors affecting Toughness

- ↑ Cooling Rates -> ↑ Free Volume
- Residual Stress on cooling -> Compressive stress on the surface. *M. E. Launey et al., Acta Mater. 2008*
- Compositional effect
- Oxygen Levels -> Nucleation of crystals, *Keryvin et al., J. Non-Cryst. Solids 2006*
- Sample Geometry
- Loading rates and Testing modes
- Temperature of Testing

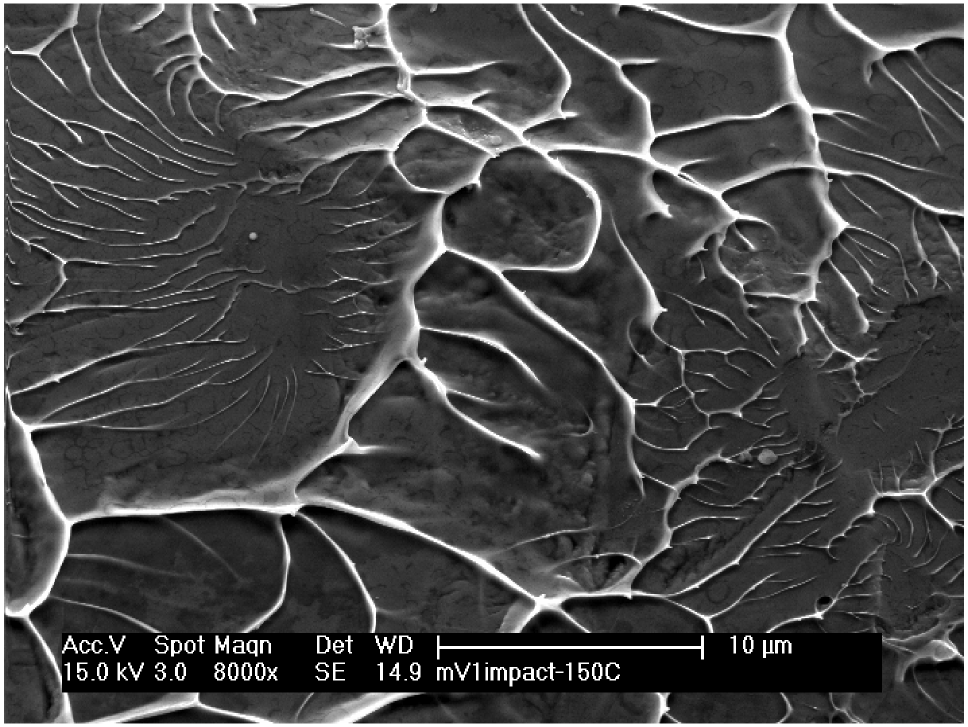
Kawashima *et al., Mater. Trans 2005*





H.A. Hassan *et al., Metall. Mater. Trans.* 2008

Ductile Fracture



•Material ahead of the crack-tip is fluid-like (aided by the free volume creation due to tension)

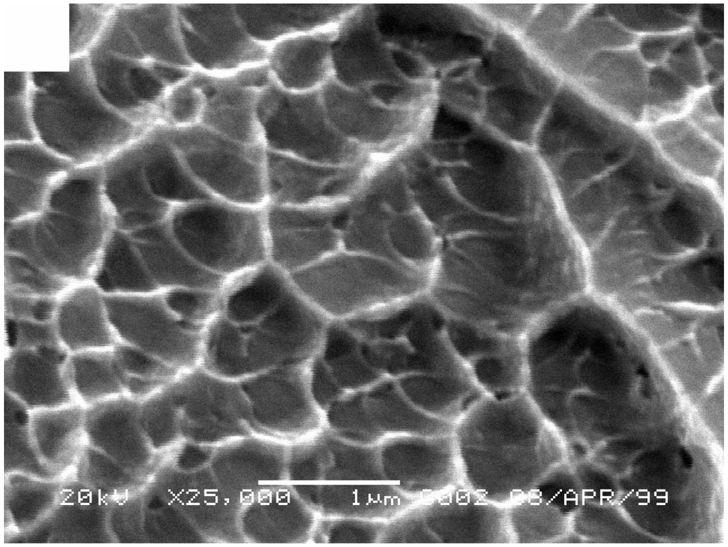
•Taylor's meniscus instability criterion applicable

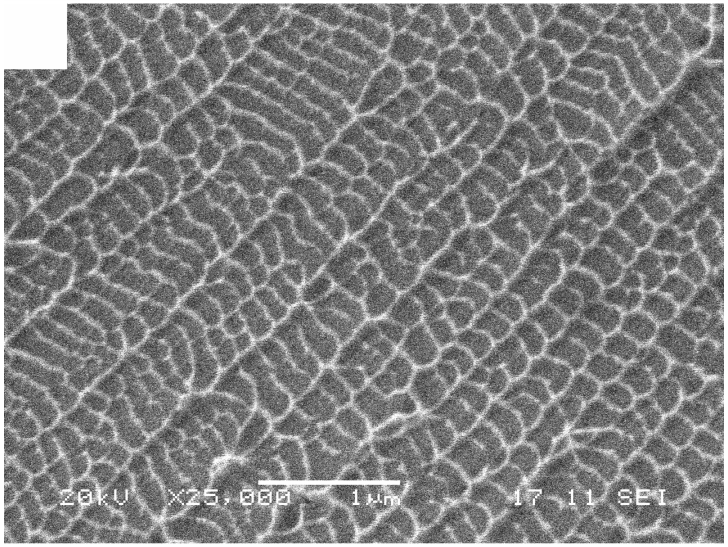
<u>Implications:</u>

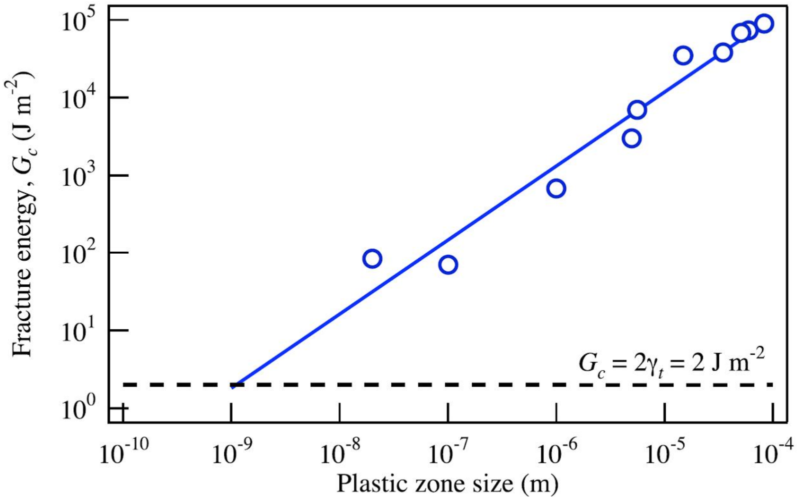
Whether a metallic glass will be ductile or brittle will depend on stress relaxation through homogeneous flow at the crack-tip.

→Fracture toughness should inversely scale with the characteristic relaxation time

Fracture Process Zone Size

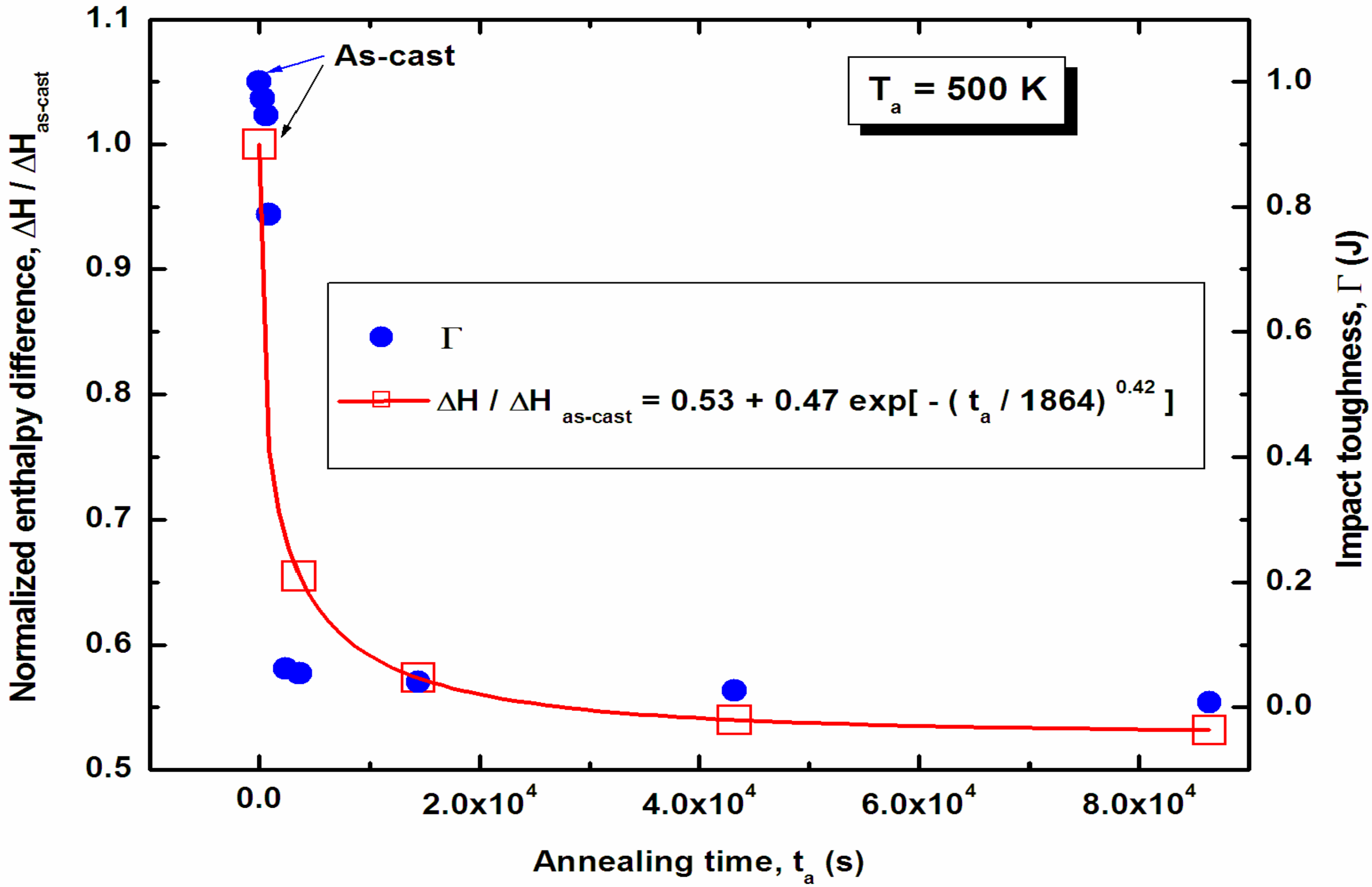






What controls the scale?

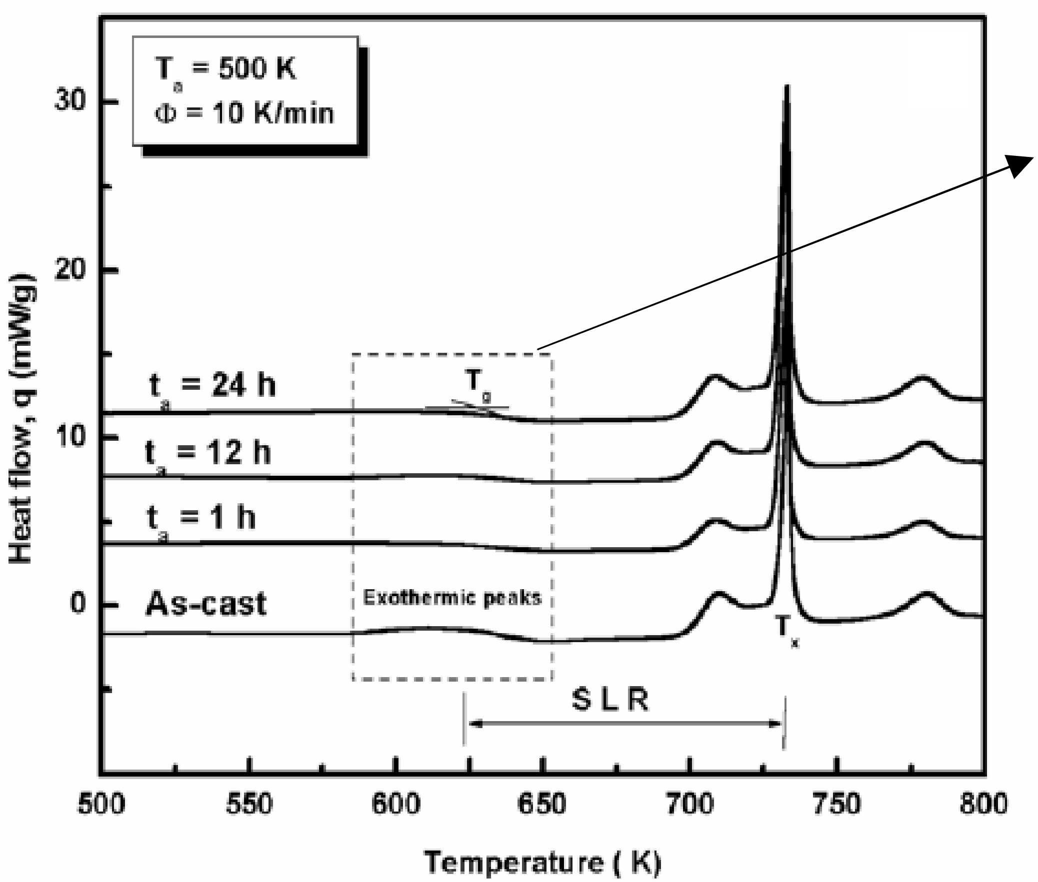
Free Volume and Embrittlement

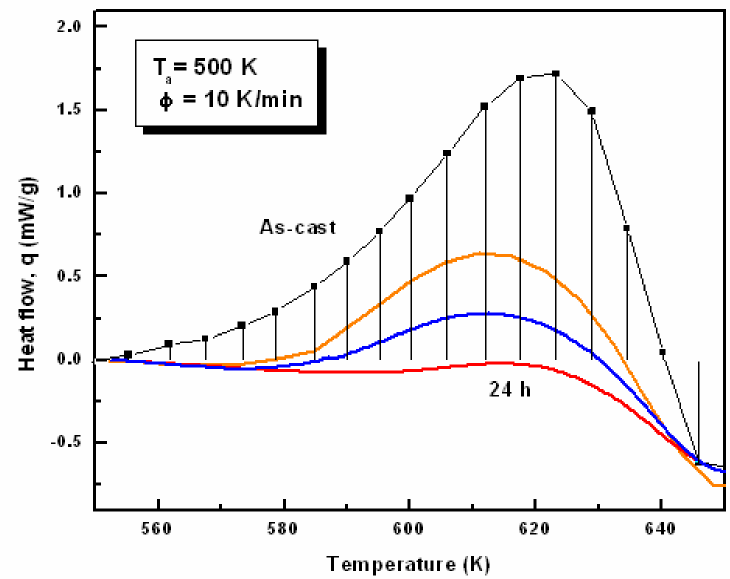


Murali & Ramamurty, Acta Mat. 2005

Calorimetric Observations

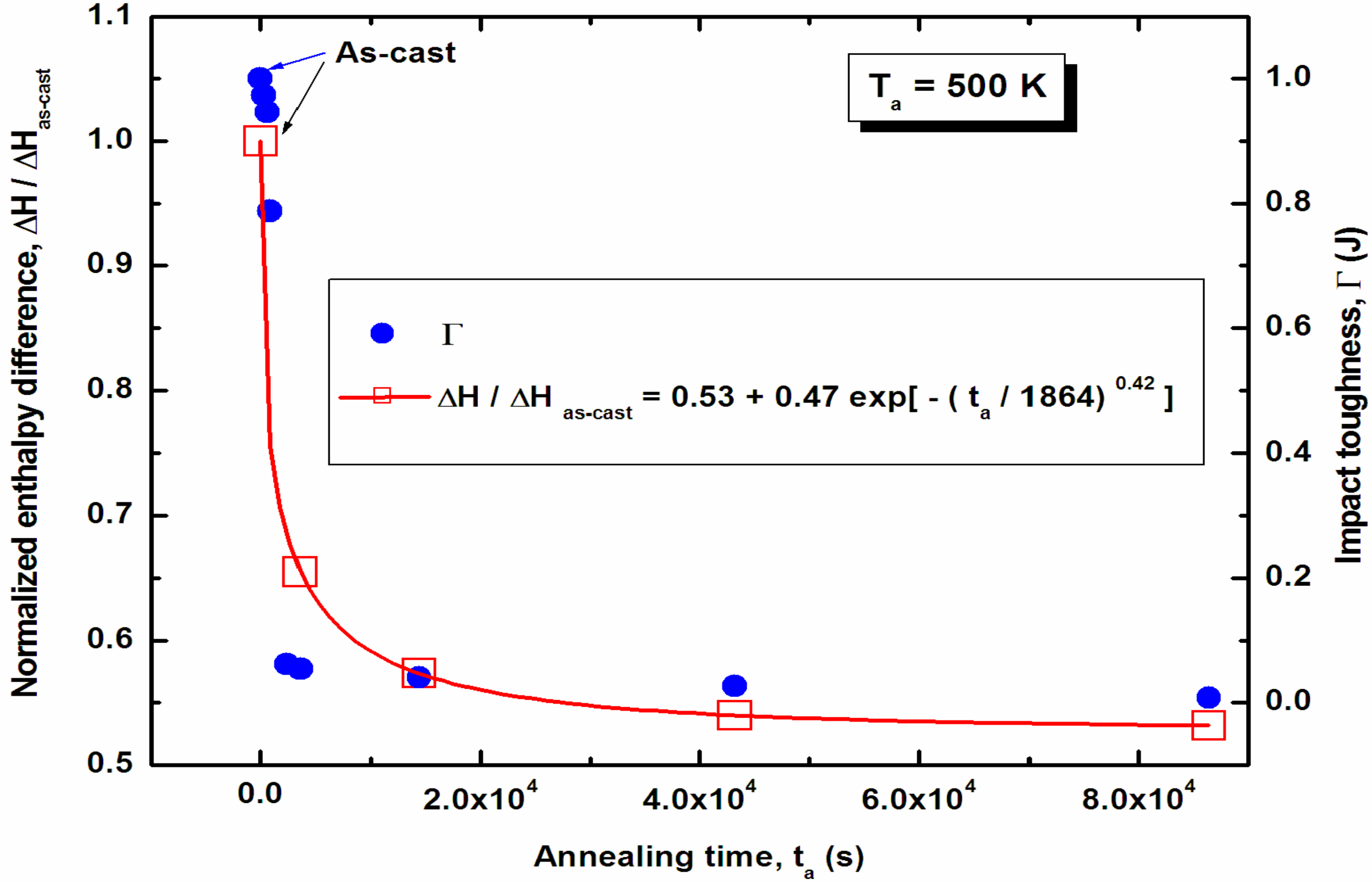
Isothermal Annealing



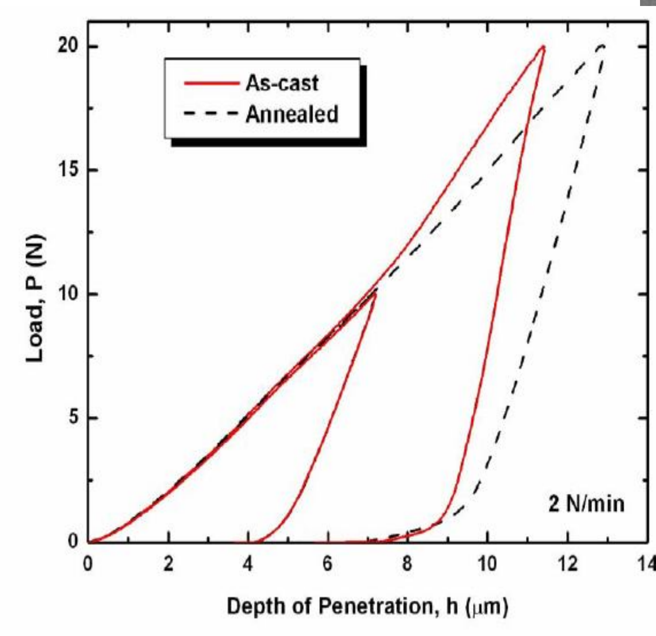


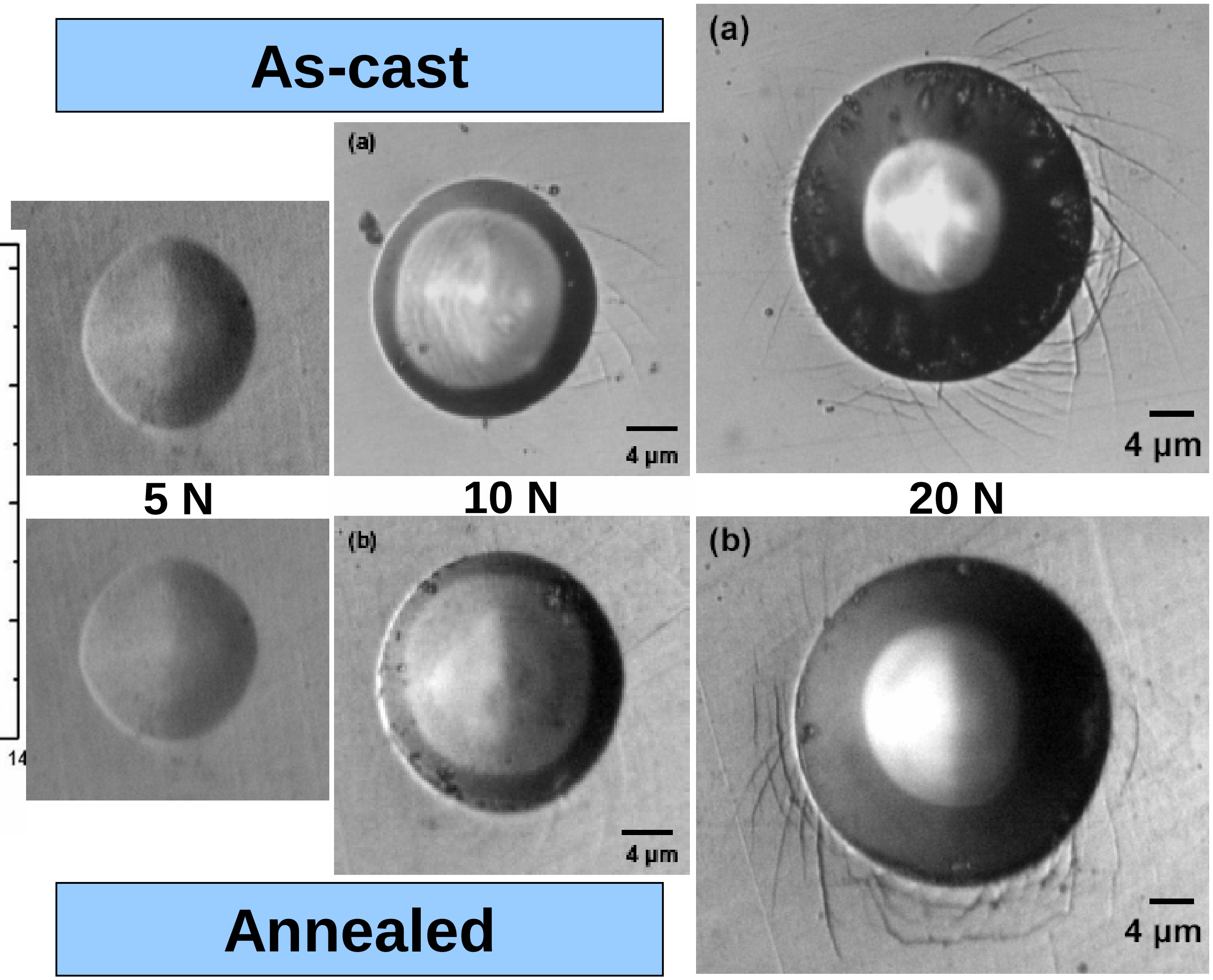
The decrease in the exothermic peak is used estimate free volume changes associated with structural relaxation

Free Volume and Embrittlement



Spherical Indentation





Free Volume and Shear Bands

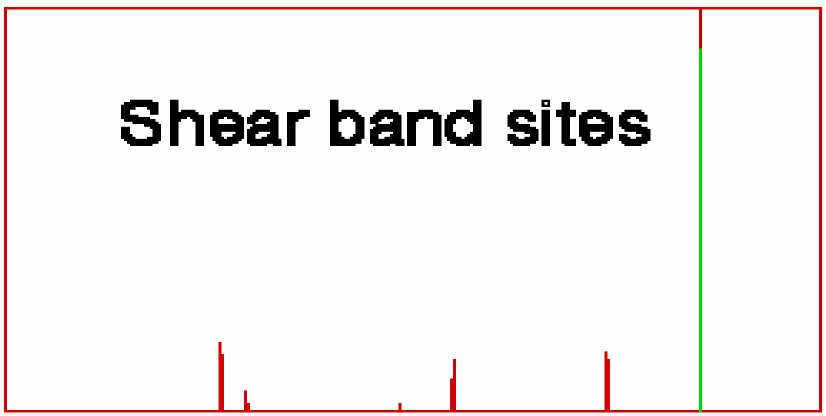
Decrease in Free Volume

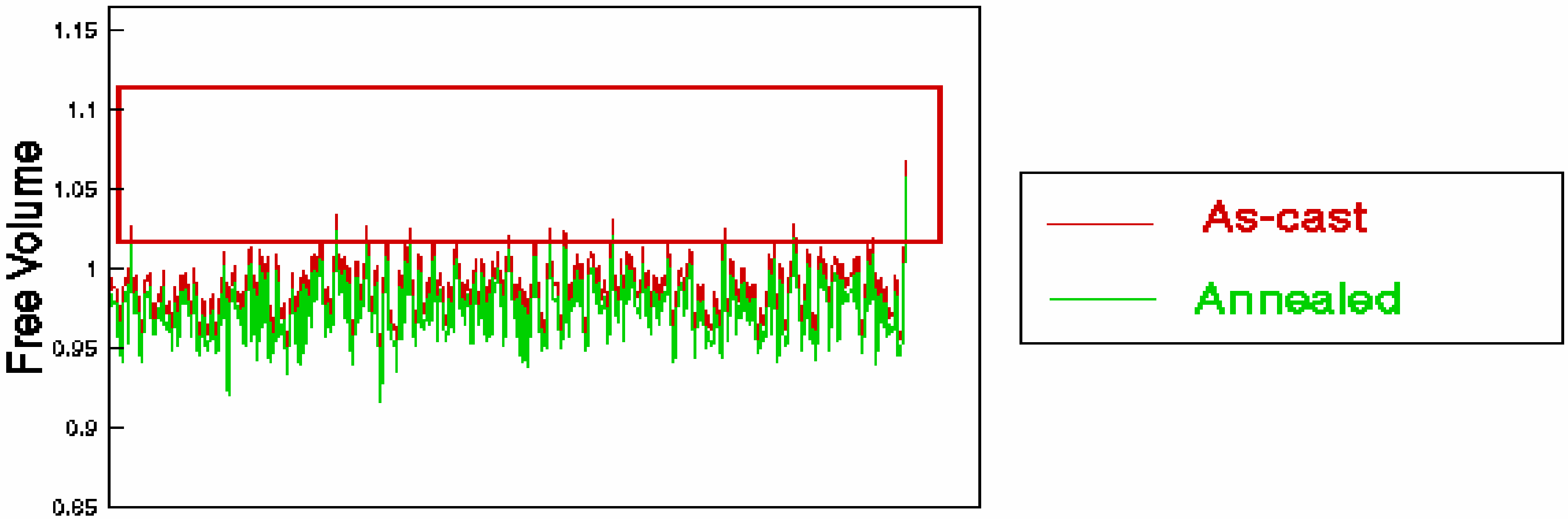
↓

Decrease in Shear Bands

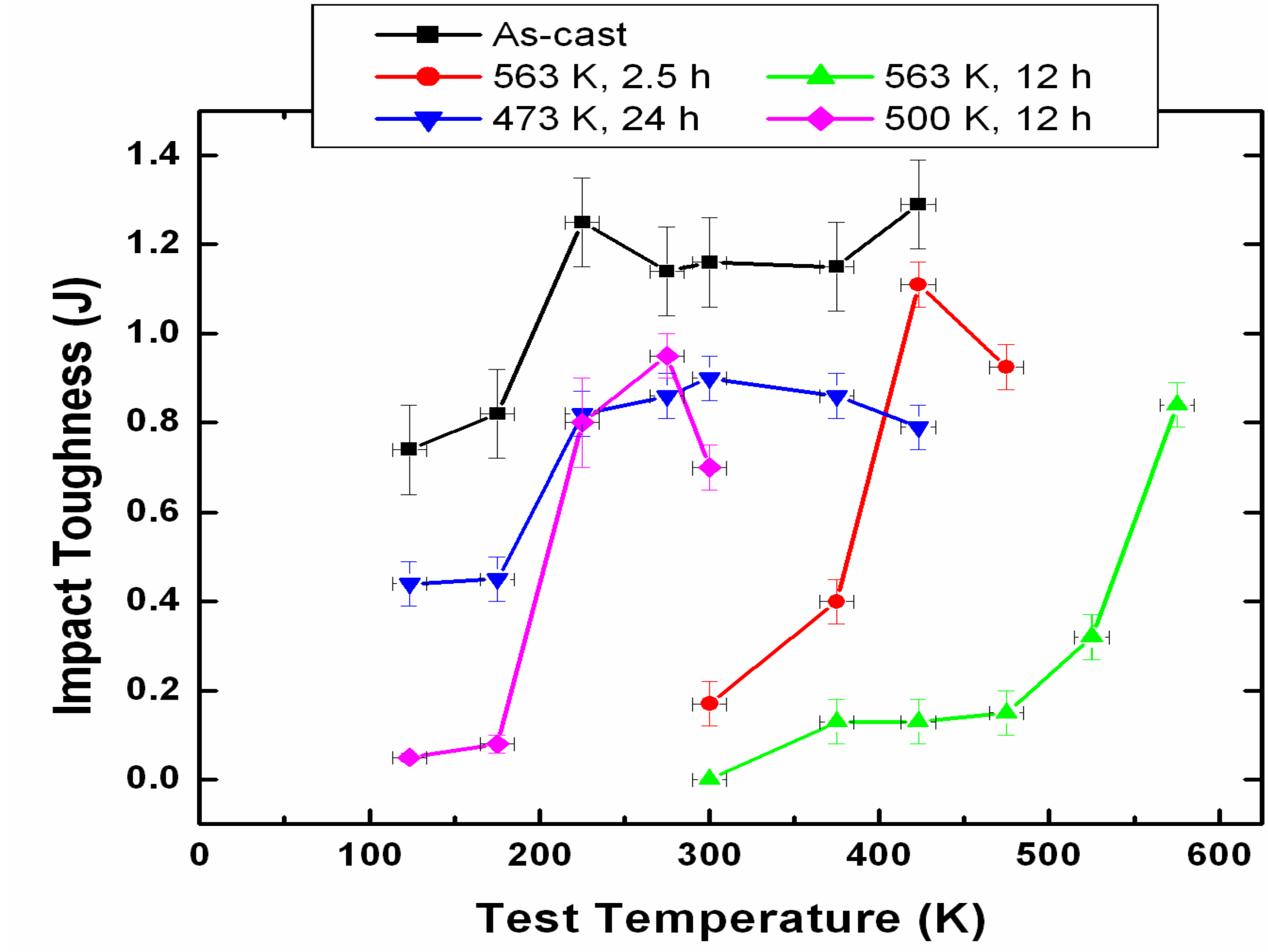
↓

Decrease in Toughness

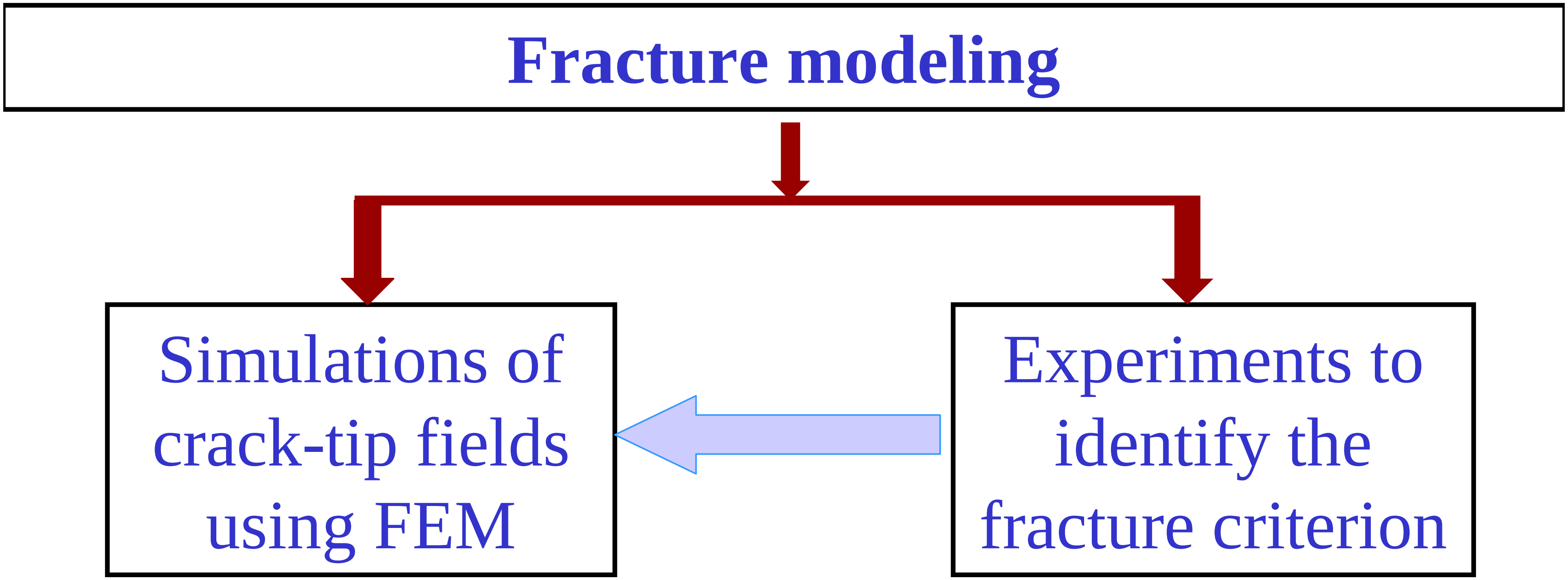




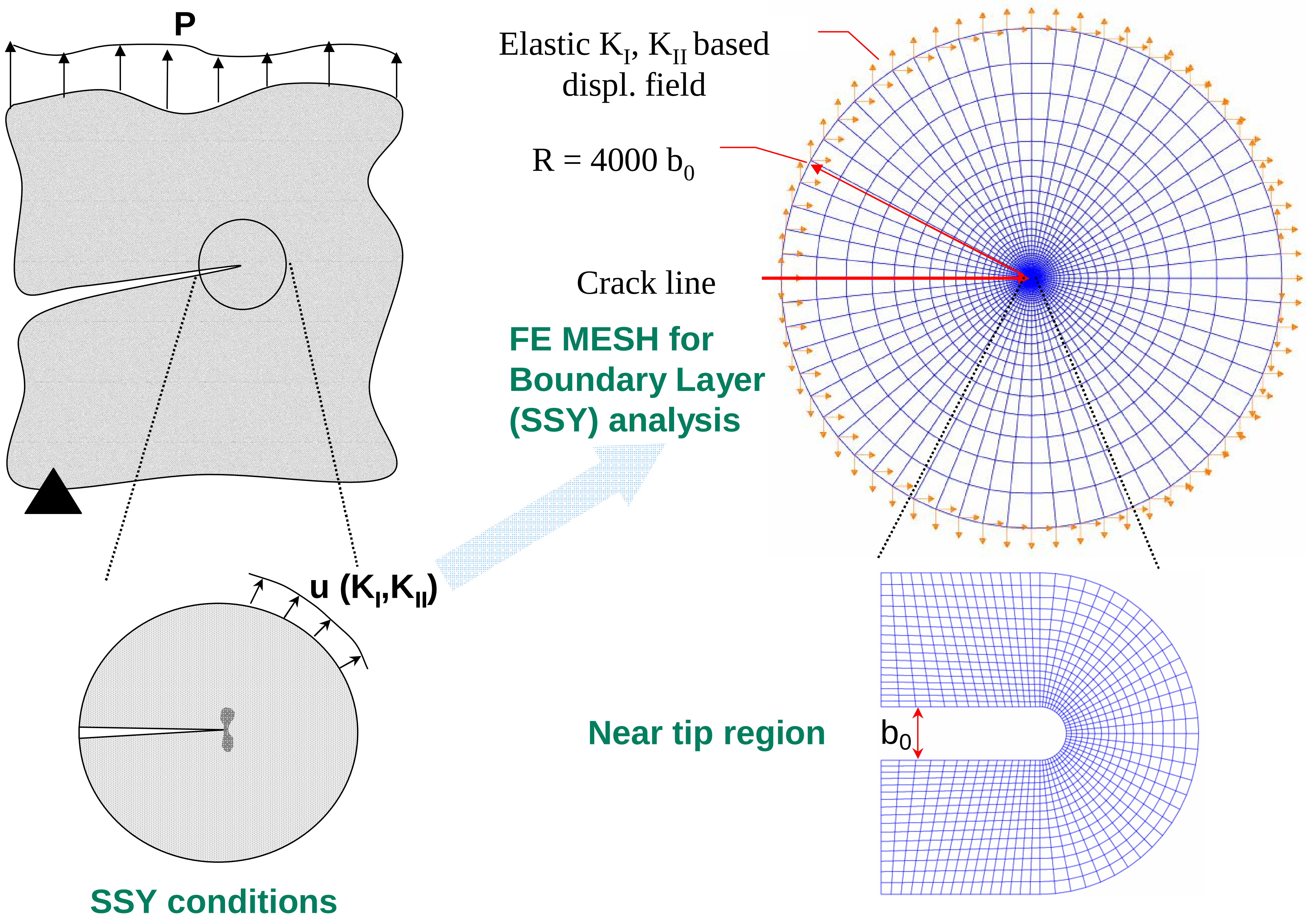
Ductile-to-Brittle Transition



Raghavan, Murali, Ramamurty. Acta mat. 2009


Fracture modeling
Simulations of crack-tip fields using FEM
Experiments to identify the fracture criterion

FE analysis of a stationary crack in BMGs



Material constitutive model

Anand-Su model for metallic glasses

- based on Mohr-Coulomb yield criterion
- involves discrete shearing accompanied by dilatation
- dilatation induced strain softening
- captures inhomogeneous deformation of BMGs well

$$\theta = \left\{ \frac{\pi}{4} + \frac{\phi}{2} \right\} \qquad \phi = \tan^{-1} \mu$$

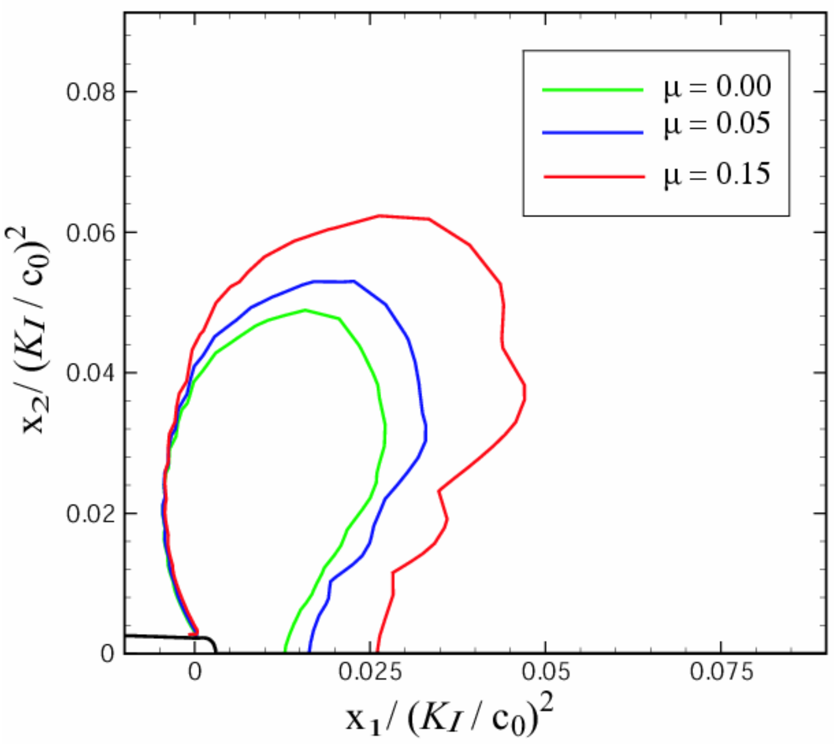
- **Plastic dilatancy function (*β*)**
- **Cohesion function**

Anand and Su (JMPS, 2005)

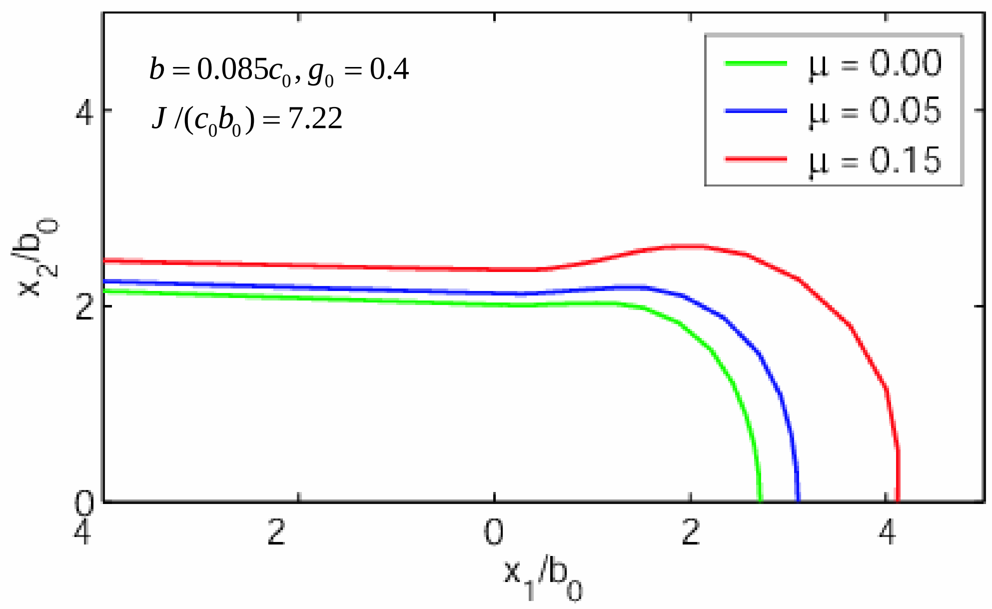
Effect of Mohr-Coulomb friction parameter

Tandaiya *et al.* Acta Mat (2007)

Plastic Zones

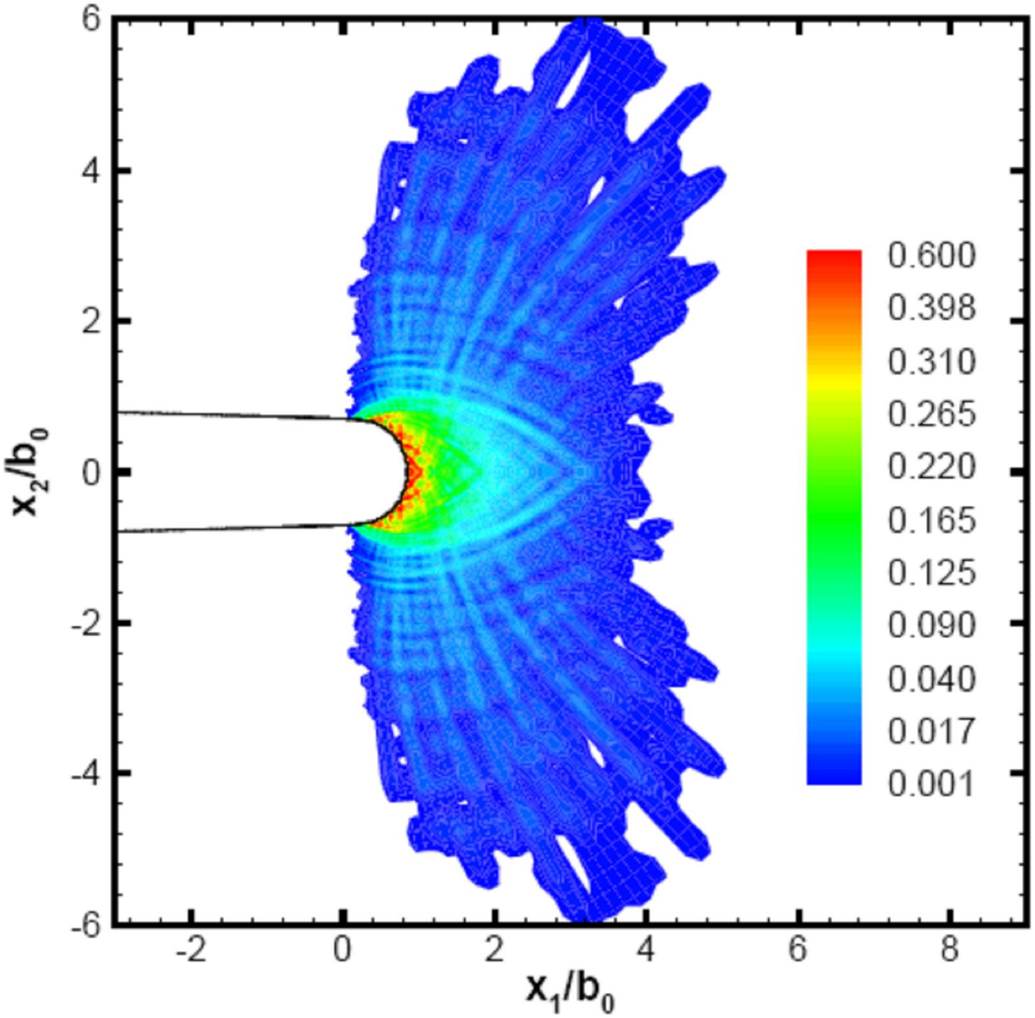


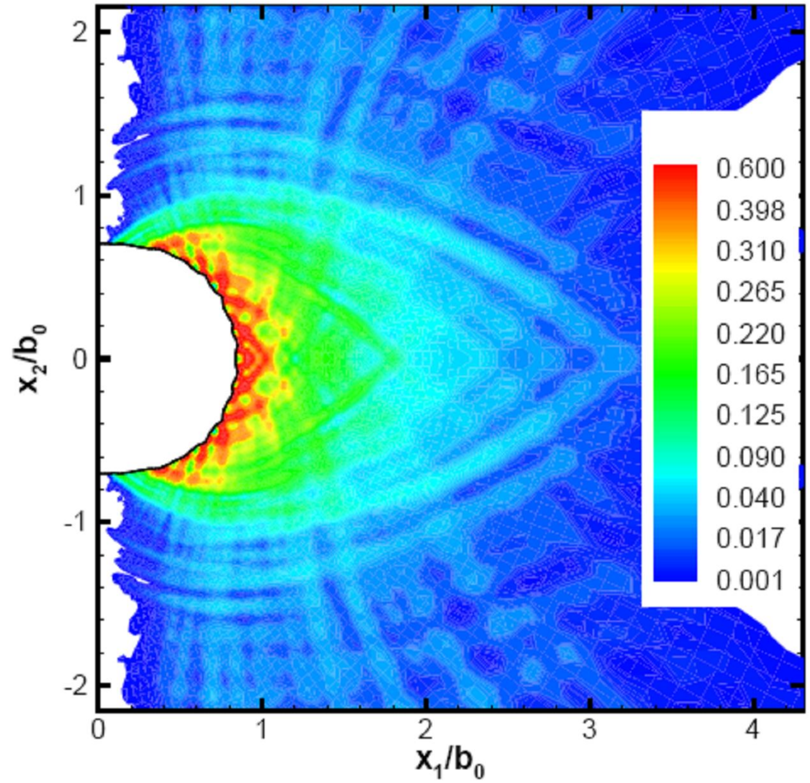
Notch profiles

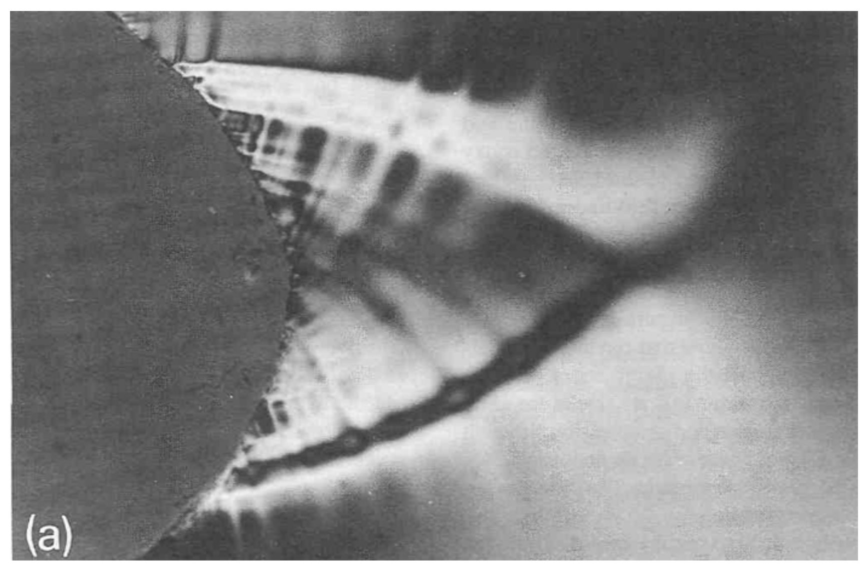


Higher μ → { Larger plastic zone; Enhanced notch opening profile }

Simulation of shear bands around the notch root

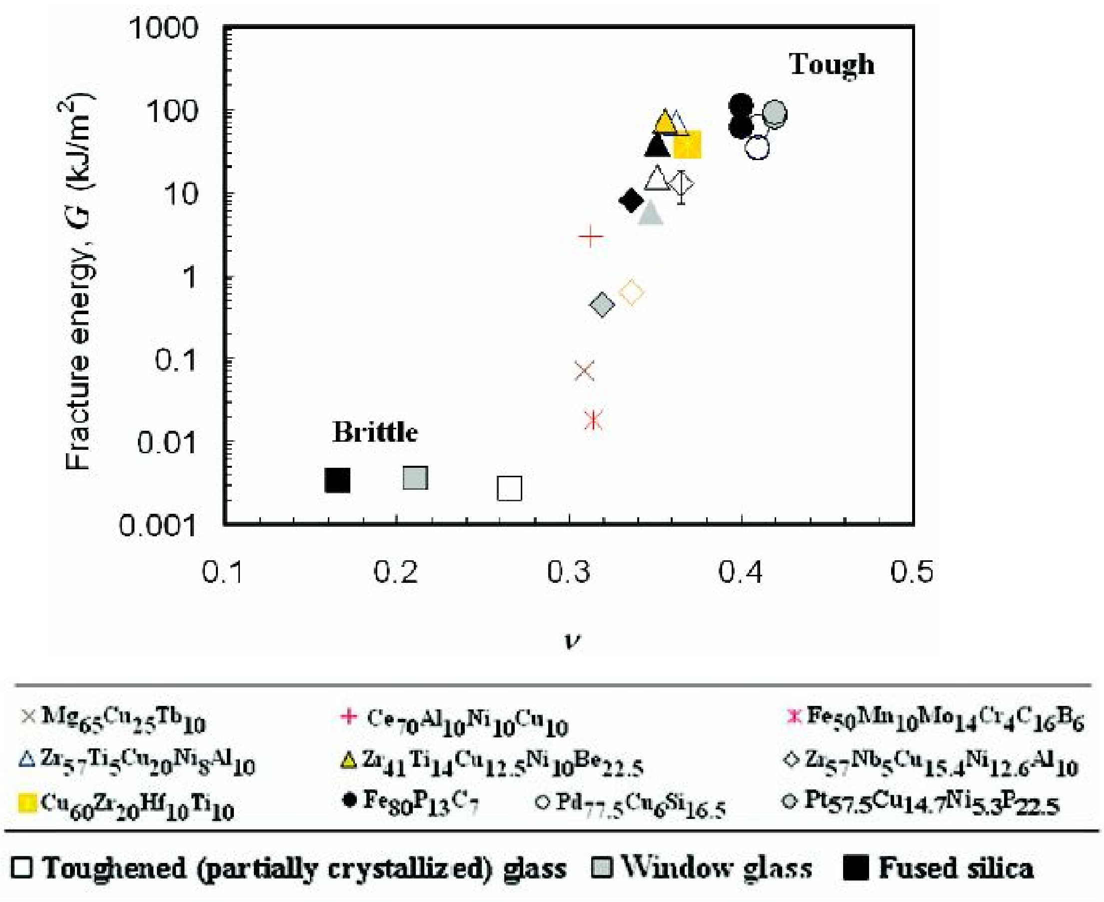


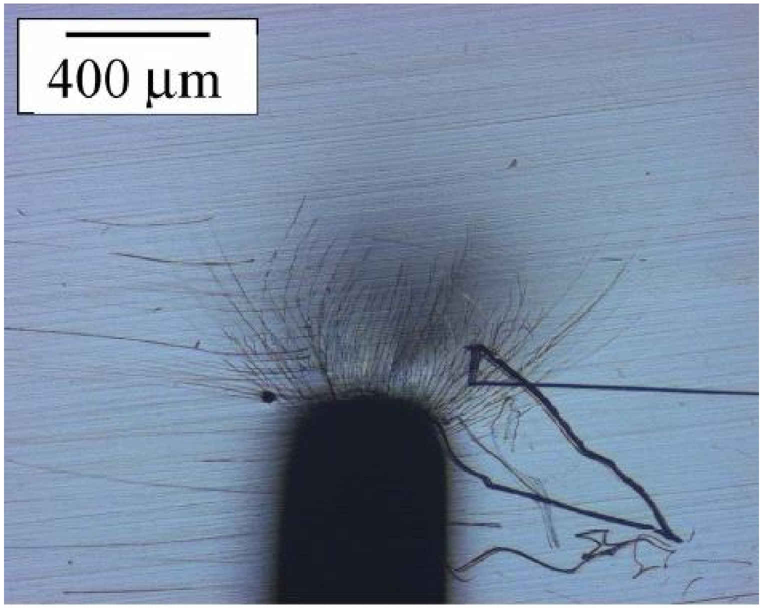




Simulation using statistical distribution of initial cohesion in the finite elements

Effect of Poisson's ratio





K_{Ic} = 80 MPa.m$^{0.5}$

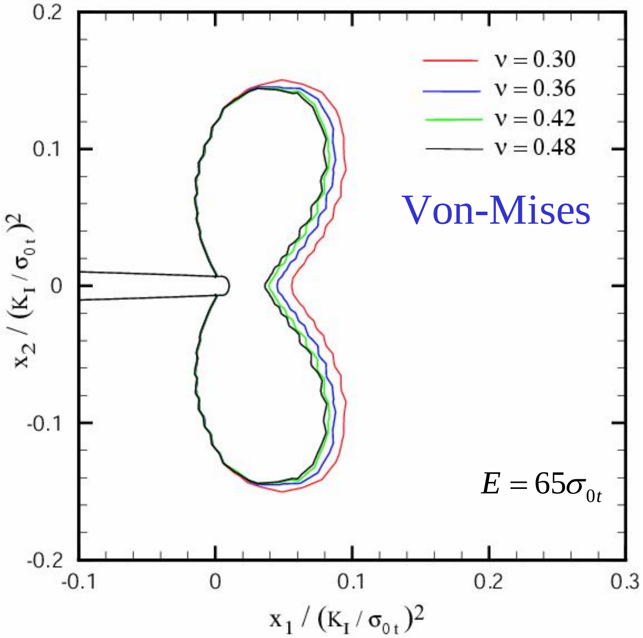
$Pt_{57.5}Cu_{14.7}Ni_{5.3}P_{22.5}$

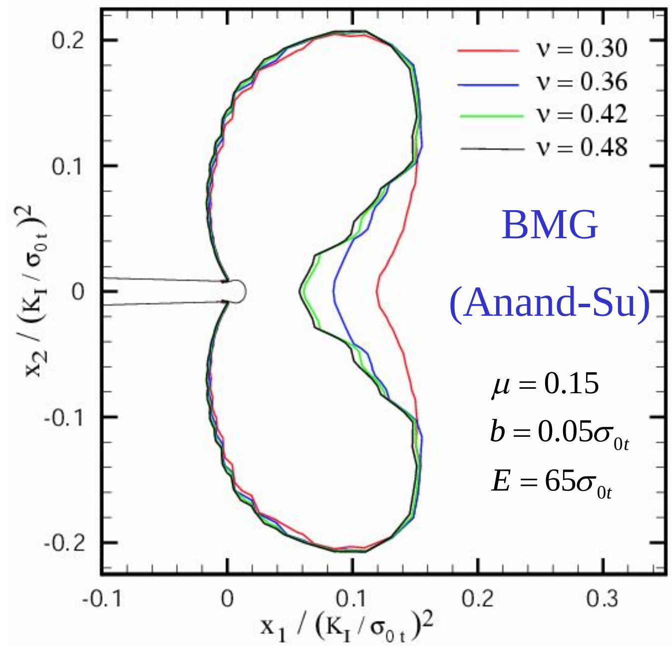
Poisson's ratio =0.42

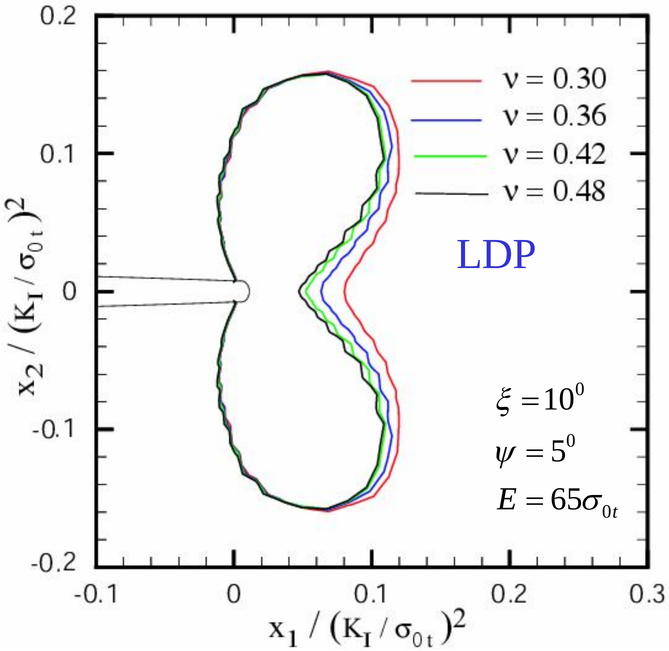
Lewandowski et al., Phil. Mag 2005

Schroers and Johnson, PRL 2004

Mode I plastic zones







Tandaiya *et. al.* Acta Mat (2008)

Stress based (RKR) fracture criterion

Models failure by brittle micro-cracking

(Ritchie et. al, 1973 and MTS theory of mixed mode fracture)

Failure occurs when $\sigma_{\theta\theta}$ exceeds a critical value σ_c over a critical distance r_c from the notch tip

Suitable for brittle materials

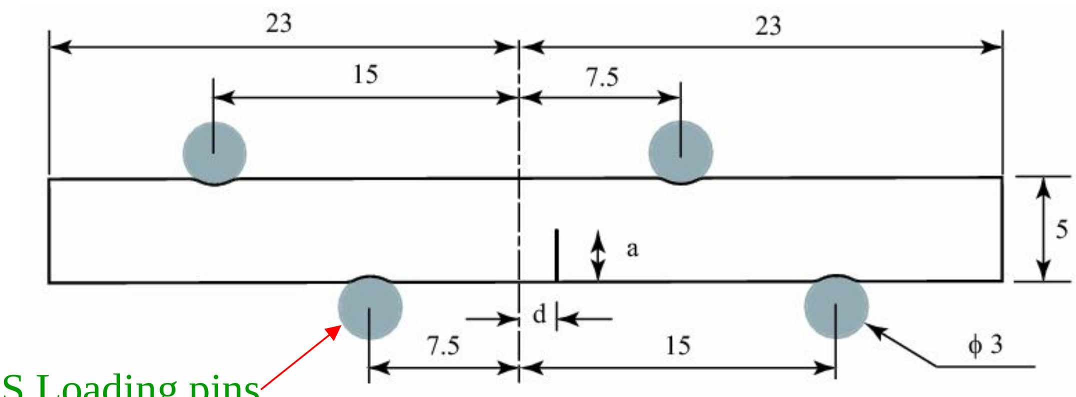
Strain based fracture criterion

Models failure by brittle micro-cracking

Failure occurs when $\ln e_p^1$ exceeds critical value ε_c over a critical distance r_c from the notch tip

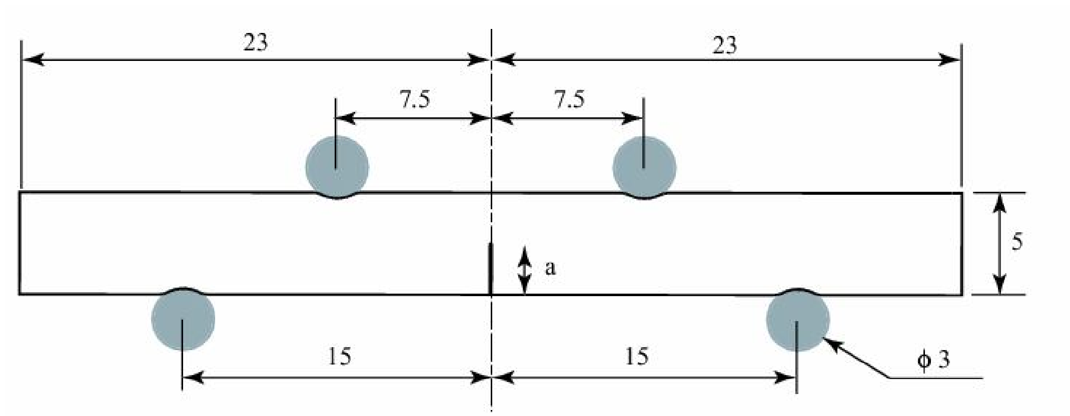
Suitable for ductile materials

Mixed-mode (I and II) Fracture
Asymmetric four-point bend specimen



- Material: Vitreloy 1 ($Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$)
- Wire-cut EDM machined
  46 mm x 5 mm x 3 mm (thickness)
- Notch diameter : 60 µm
- d controls mode mixity

● Pure mode I tests: Symmetric four-point bend specimen

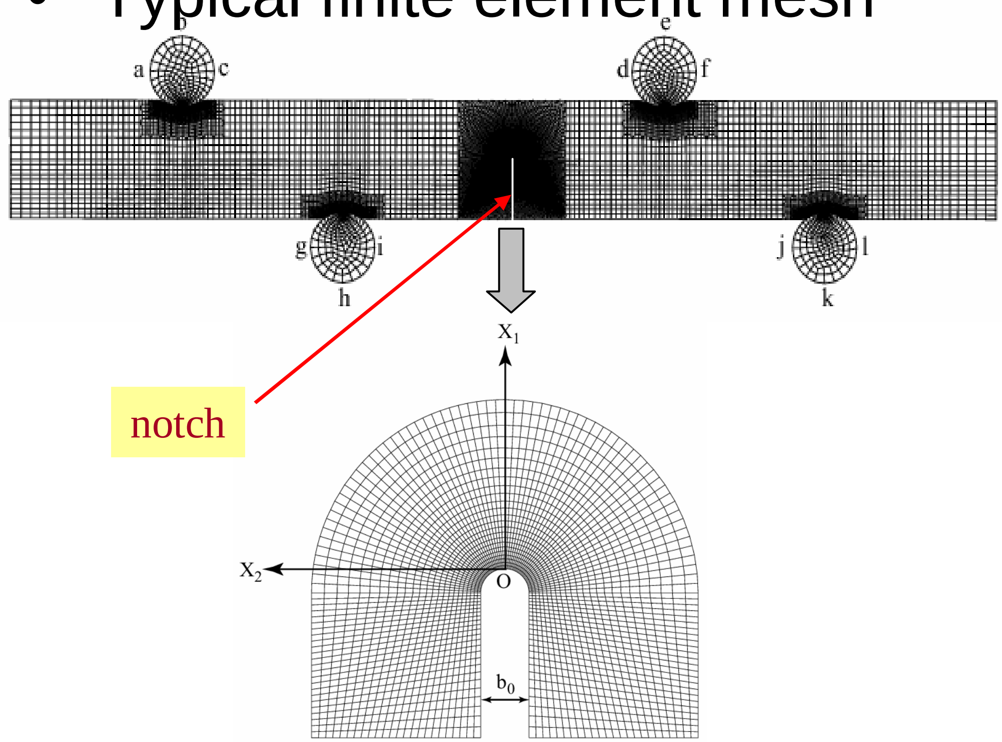


Specimen type	crack length, a (mm)	a/W	d (mm)
AS4PB-1	3.5	0.7	0
AS4PB-2	2.5	0.5	0.4
AS4PB-3	2.5	0.5	0.8
AS4PB-4	2.5	0.5	1.5
S4PB-1	2.5	0.5	-

(All dimensions are in mm)

Finite element analyses

- Typical finite element mesh



Near tip mesh

- No. of elements = 14394
- 64 elements around the notch root
- Frictionless contact
- Downward displacement prescribed for nodes on arcs abc and def
- Nodes on arc ghi and jkl are fixed

➢Two analyses:

a. Linear elastic

b. Elastic-plastic

➢Constitutive model:

Anand and Su model implemented through UMAT in ABAQUS/Standard

➢Material properties for Vitreloy 1:

E = 97 GPa; ν=0.36; c_0=890 MPa; μ=0.06; b=120 MPa

➢Determine:

a. Elastic mode mixity parameter M^e

b. Plastic mode mixity parameter M^p

$$M^p = \lim_{r\to 0}\left[\frac{2}{\pi}\tan^{-1}\left(\frac{\sigma_{\theta\theta}(r,\theta=0)}{\sigma_{r\theta}(r,\theta=0)}\right)\right]$$

c. Calibrate of J against P for each specimen using both the above analyses

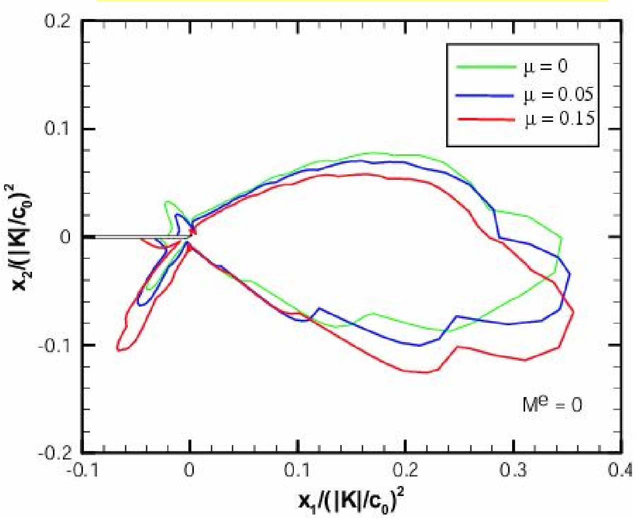
d. Find critical energy release rate J_c

e. Simulate near-tip shear band patterns

Effect of friction parameter on plastic zones

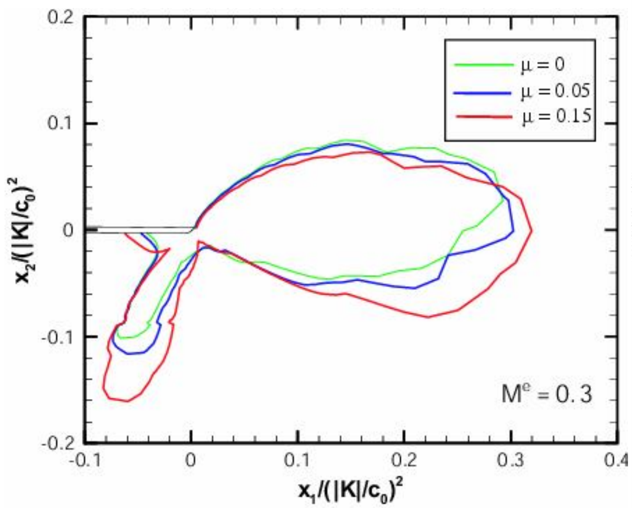
Pure Mode II loading

$M^e = 0$



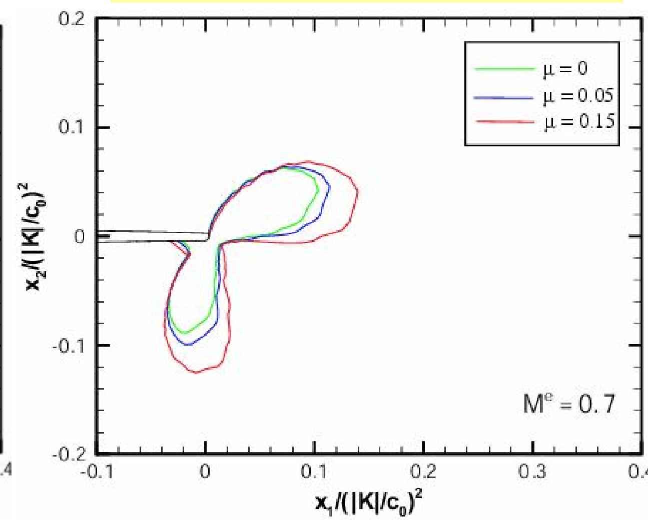
Mode II dominant loading

$M^e = 0.3$



Mode I dominant loading

$M^e = 0.7$

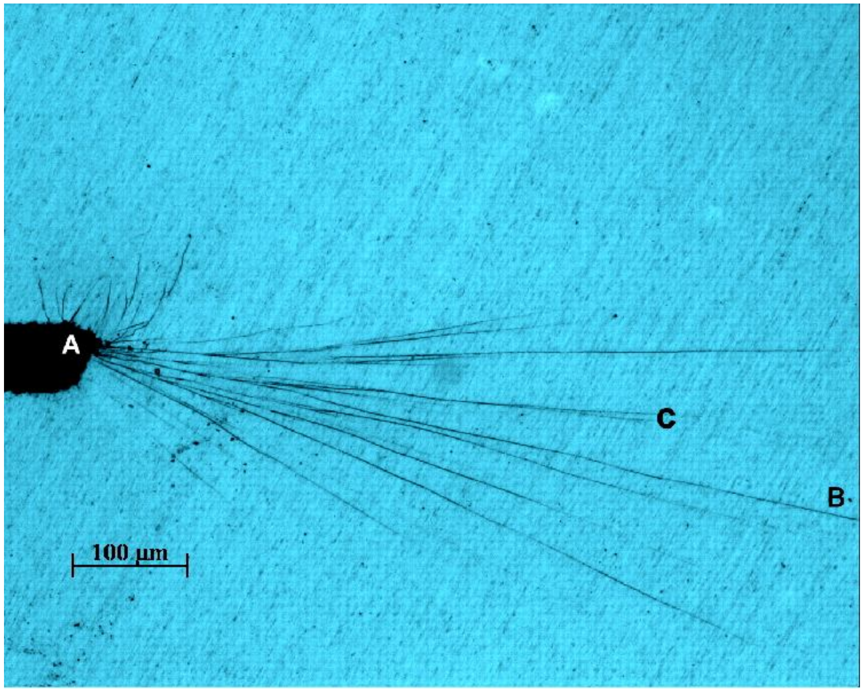


- Plastic zone size ↑ with ↑ in mode II component of loading
- $\mu > 0$ => For $M^e = 0$, plastic zone becomes unsymmetric and bends towards lower half-plane
  => For $M^e = 0.7$, both the lobes of plastic zone ↑ in size

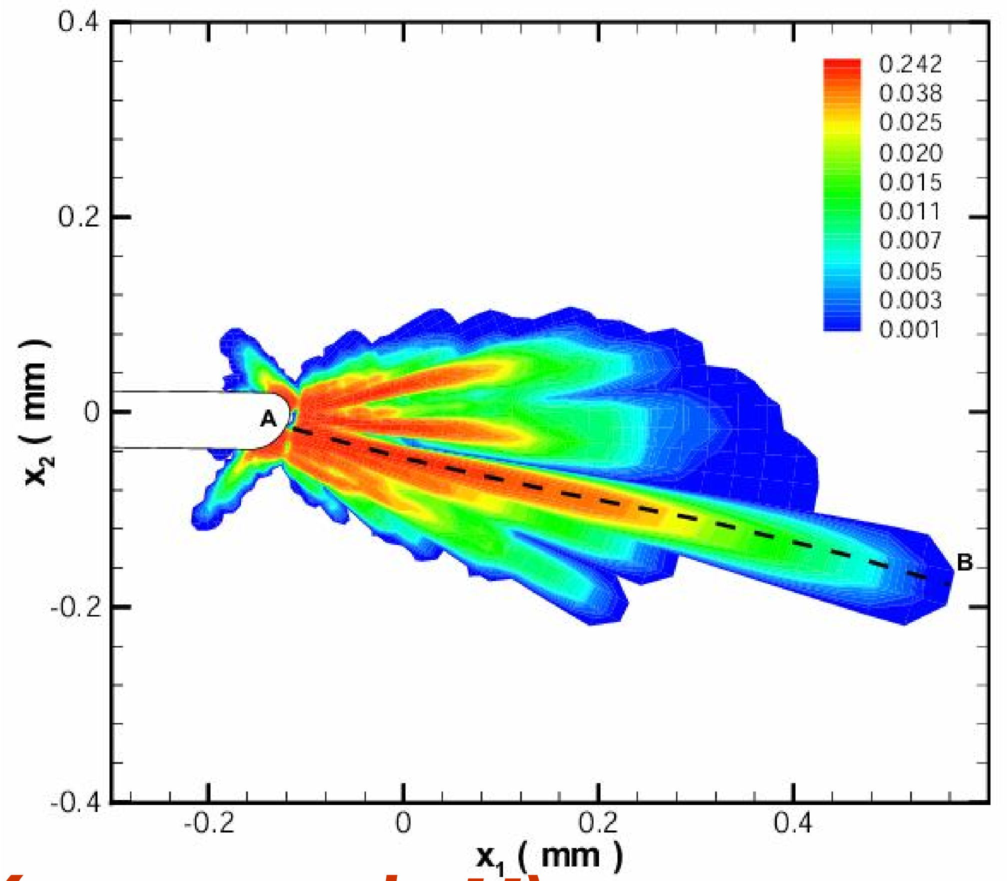
Lower mode mixity
Higher μ } ⟶ larger plastic zone

Mixed Mode Fracture

Experiment



Simulation

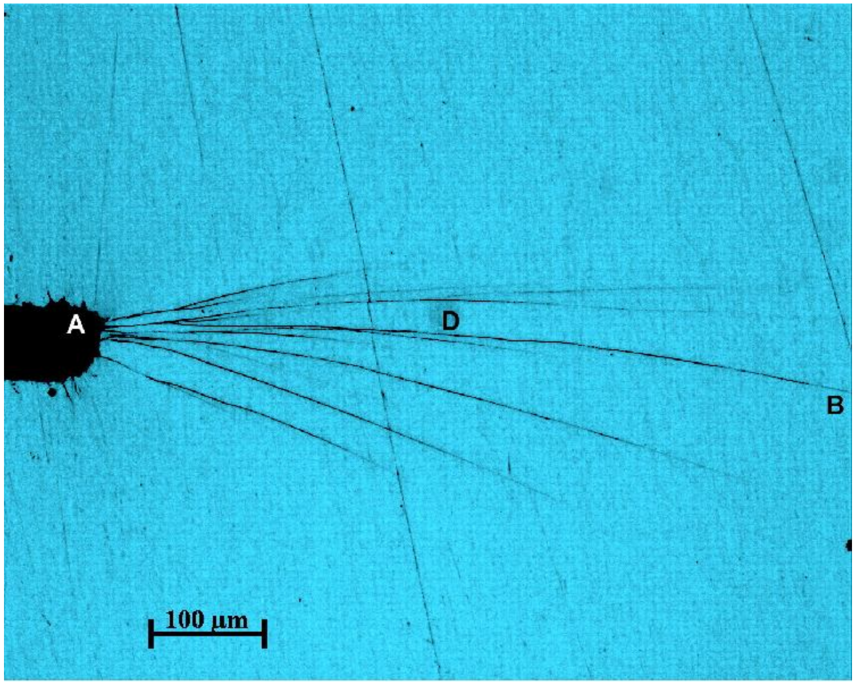


M^e = -0.089 (~ pure mode II)

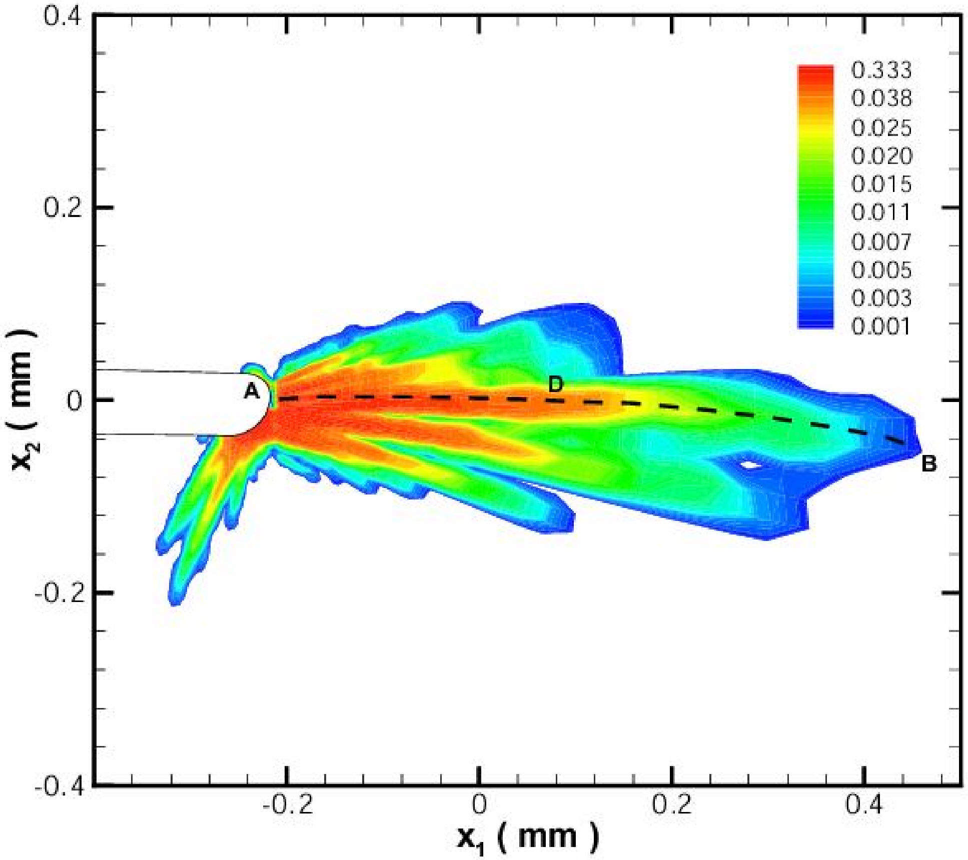
Tandaiya, Ramamurty, Narasimhan, JMPS 2009.

Mixed Mode Fracture

Experiment



Simulation

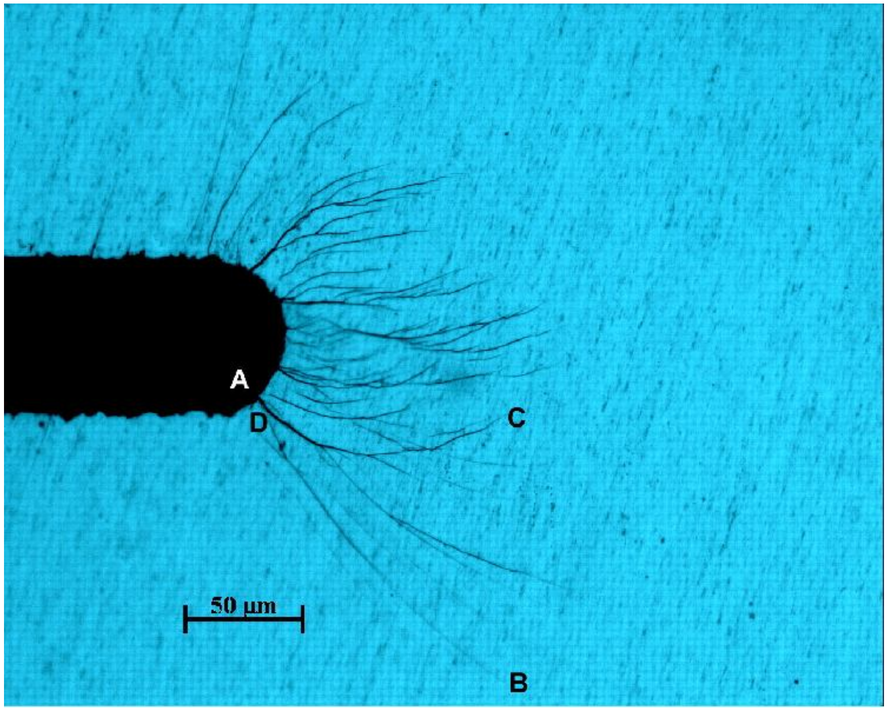


M^p= 0.484 (mixed mode)

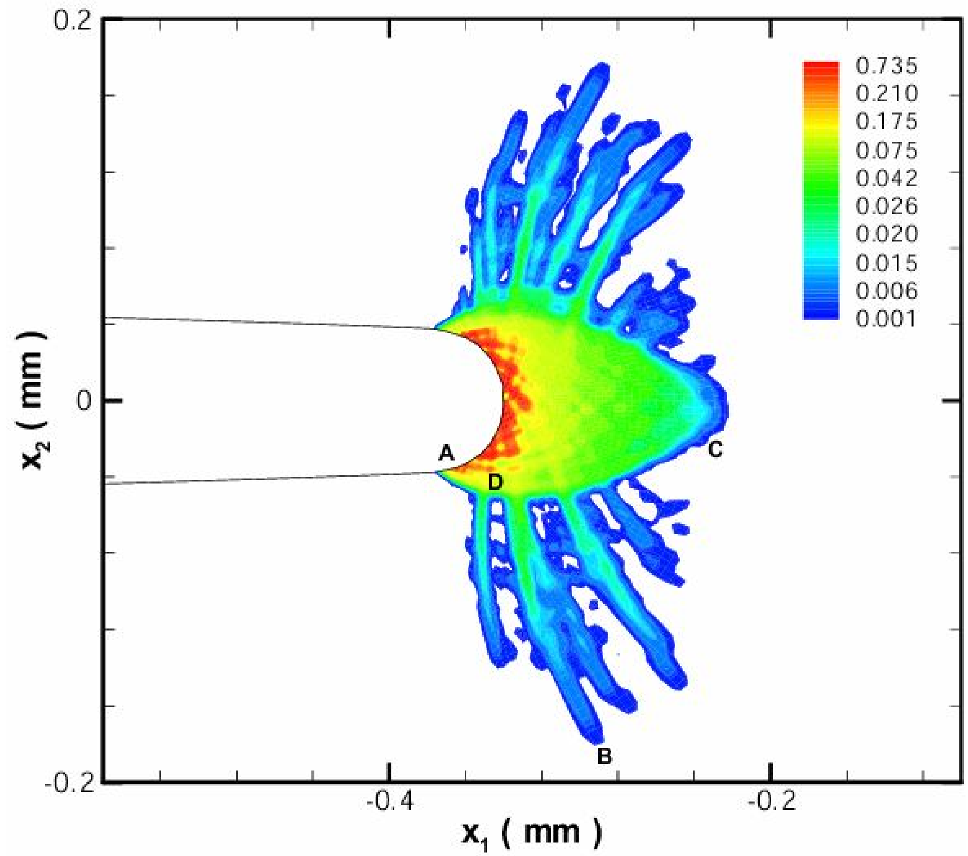
P = 14.1 kN

Shear band patterns near the notch root

Experiment



Simulation



P = 2.3 kN

M^e = 1 (pure mode I)

Approach

Understand the micromechanisms of fracture

Simulations of crack-tip fields using FEM

Experiments to identify the fracture criterion

Stress based (RKR) fracture criterion

Models failure by brittle micro-cracking

(Ritchie et. al, 1973 and MTS theory of mixed mode fracture)

Failure occurs when $\sigma_{\theta\theta}$ exceeds a critical value σ_c over a critical distance r_c from the notch tip

Suitable for brittle materials

Strain based fracture criterion

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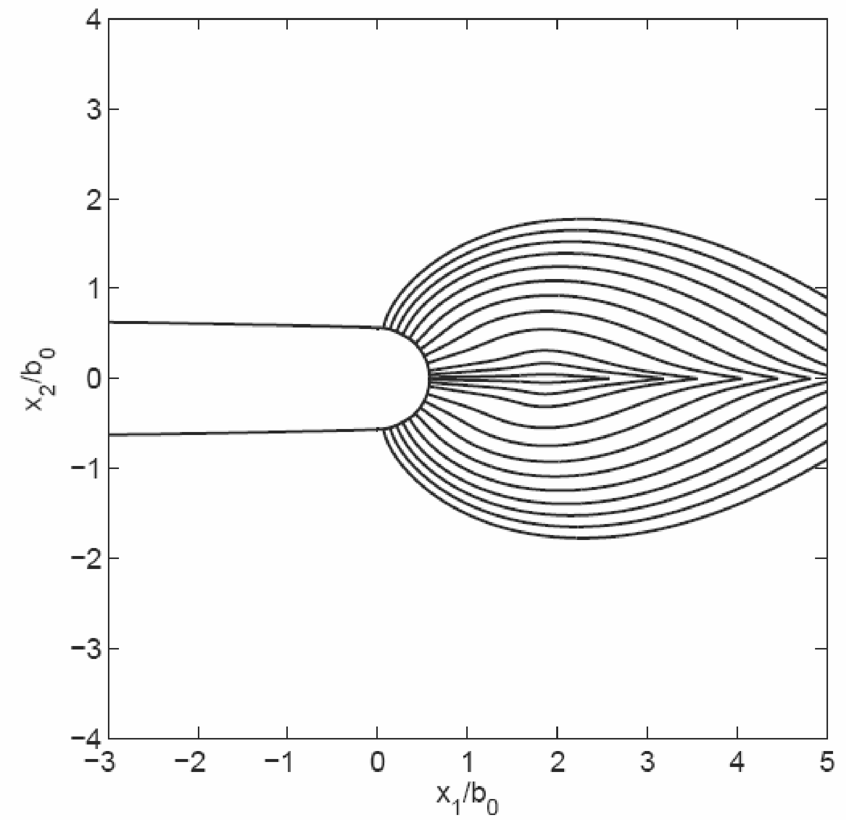
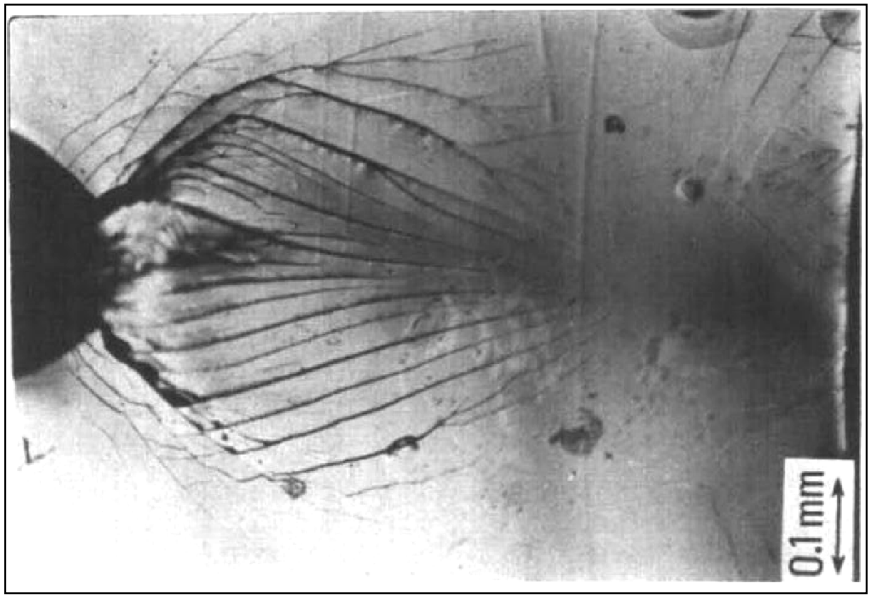
Suitable for ductile materials

Predictions of brittle crack trajectories



Loci of directions normal to the maximum principal stress direction



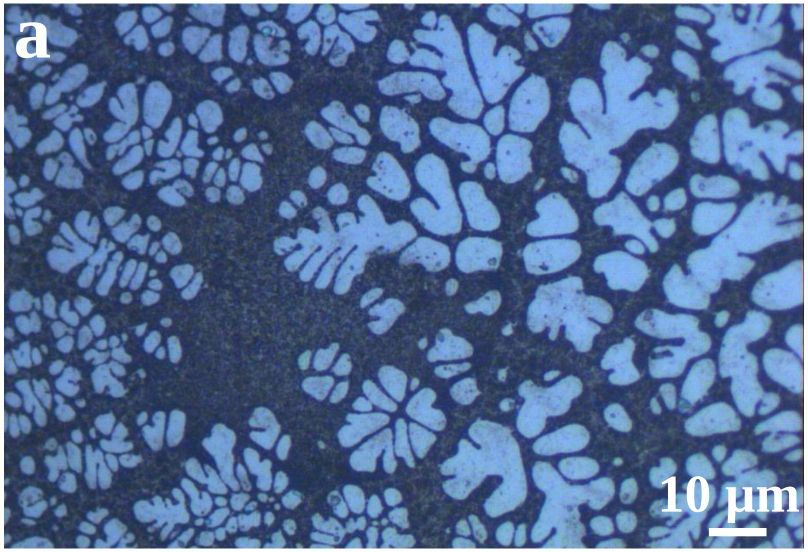
Kimura and Masumoto (1980)

-Pd-Cu-Si metallic glass

-Structurally relaxed

Other methods for toughening

Boopathy et al. JMR, 2009

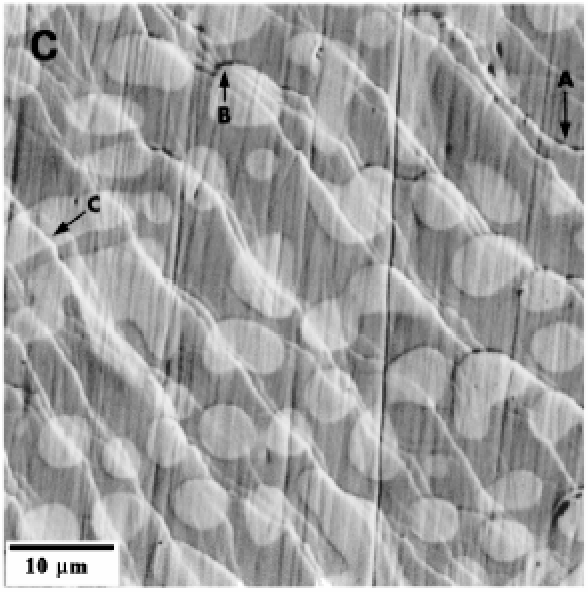


- Key problem: Absence of a microstructure to hinder shear bands
- Solution: BMG composite, *Johnson and Hofmann*

How they work?

- *Deflect or constrain Shear bands*
- *Initiation sites for shear bands(??)*
- *Dissipation by deformation of crystalline dentrites*

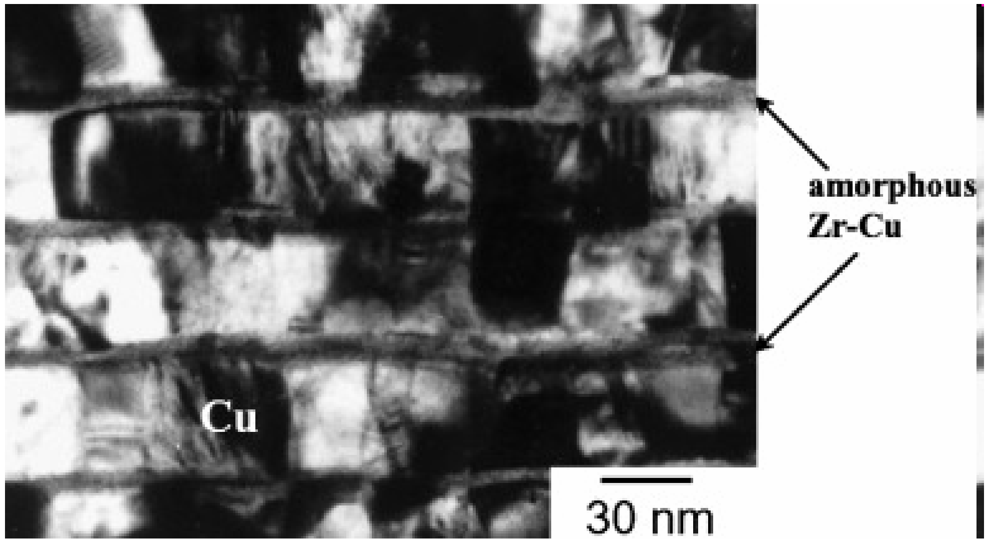
Cauiion: Inter'particle' spacing



Hays et al., PRL 2000

Other methods of Toughening

- Laminates
- Multiple shear banding
- Slip transmission effect



Note: Affects only crack growth, not nucleation

T.G. Nieh and J. Wadsworth, *Intermetallics* (2008)

Summary

- Still a long way to go before we understand plasticity and fracture in amorphous alloys

- Especially <u>fracture toughness</u> needs good understanding before we can find widespread applications for BMGs!

Thank you!!