Structural materials of the future
the case of bulk metallic glasses

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Metals are easy to work with…

can cast, forge, roll, extrude, bend, cut, stamp, and twist them….. **malleable**!

You can also drop them without worrying about breaking them… **tough**
The boon for metals is also their bane!

Several GPa

Alloy design for strengthening...... reaching the limit!
What are the alternatives?

Ceramics are difficult to shape and brittle

How about glasses?
Glasses......can also be shaped
...they are strong too

Strength of freshly drawn glass ~ 15 to 20 GPa

A 20 ton truck can be pulled by a 4-6 mm dia wire

Skywalk, Grand Canyon
but, glasses are brittle, hence extremely sensitive to defects.

“we never test the strength of glass: all we test is the weakness of its surface”  J. T. Littleton (1941)
what if we make glasses out of metals?

Metallic glasses or amorphous alloys

- Under normal conditions, metals crystallize upon cooling from liquid to solid state
- Crystallization can be prevented by applying high cooling rates (~ million K/s)
- Metastable amorphous phase known as metallic glass can be obtained
- Only thin ribbons or wires (10 – 100 µm) can be produced using rapid solidification techniques
In 1990, Inoue found new classes of metallic glasses that can be made in bulk.

- The bulk metallic glasses are composed of three or more metals in the alloy melt.
- Cooling rates of the new alloys are from 100 Ks⁻¹ to 1 Ks⁻¹.
- The possible thickness of the metallic glass increased from micrometers to centimeters.

Johnson & Peker (1992) discovered that Be-containing Zr-based alloys form BMGs.
Reduced glass transition temperature $T_{rg} = T_g/T_m \sim 0.71$

Supercooled liquid region $(\Delta T_X) = T_X - T_g \sim 75K$

Pd40Ni10Cu30P20

Scan Rate = 20°C/min
Structure Performance Relationships

“Seeing is Believing”

Performance
- Stiffness
- Inelastic deformation
- Ultimate failure
- Reliability

Microstructure

Allows for tailoring of the microstructure to obtain desired behavior

Processing
Scales in Crystalline Metals

Dislocation width

Dislocation substructure (0.1 μm)

Slip systems

Stacking fault width

Microstructure

Dislocation substructure

Fracture Process Zone

1 nm

0.1 μm

1 μm

1 μm

2 μm
Structure of a Glass
Fundamental Mechanical Properties

Toughness

No intrinsic length scale

Quasi-static loading, room temperature

length scale required
Fracture in metallic glasses

What are the connections between nano- and micromechanisms and toughness?

Metallic glasses are schizophrenic in the fracture sense
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 $\sigma_c$ over a critical distance $r_c$ from the notch tip.

Strain based fracture criterion
Models failure by brittle micro-cracking

Failure occurs when $\ln \varepsilon p1$ exceeds critical value $\varepsilon c$ over a critical distance $r_c$ from the notch tip.
<table>
<thead>
<tr>
<th>BMG</th>
<th>$K_c$ (MPa$\sqrt{m}$)</th>
<th>Elastic Modulus (GPa)</th>
<th>Poisson’s ratio</th>
<th>Hardness (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vitreloy Zr$<em>{41.2}$Ti$</em>{13.8}$Cu$<em>{12.5}$Ni$</em>{10}$Be$_{22.5}$</td>
<td>30-68</td>
<td>96</td>
<td>0.36</td>
<td>5.9</td>
</tr>
<tr>
<td>Amorphous steel Fe$<em>{48}$Cr$</em>{15}$Mo$<em>{14}$Er$</em>{2}$C$<em>{15}$B$</em>{6}$</td>
<td>$3.8 \pm 0.3$</td>
<td>187</td>
<td>0.28-0.32</td>
<td>17.8$\pm$0.73</td>
</tr>
</tbody>
</table>

What controls the toughness of BMGs?
FE analysis of a stationary crack in BMGs

Elastic KI, KII based displ. field

R = 4000 b0

Crack line

FE MESH for Boundary Layer (SSY) analysis

Near tip region

SSY conditions
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

\[
\tan \varphi \mu = \frac{\pi}{4} + \frac{\theta}{2} + \tan^{-1} \mu
\]

- Plastic dilatancy function \((\beta)\)
- Cohesion function

Anand and Su (JMPS, 2005)
Simulation of shear bands around the notch root

Simulation using statistical distribution of initial cohesion in the finite elements
Stress based (RKR) fracture criterion
Models failure by brittle micro-cracking
(Ritchie et. al, 1973 and MTS theory of mixed mode fracture)

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Strain based fracture criterion
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Failure occurs when $\ln \varepsilon_{p1}$ exceeds critical value $\varepsilon_c$ over a critical distance $r_c$ from the notch tip.
Mixed-mode fracture experiments

Pure mode I tests: Symmetric four-point bend specimen

- Material: Vitreloy 1
  \((\text{Zr}_{41.2}\text{Ti}_{13.8}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5})\)
- Wire-cut EDM machined
  \(46\ \text{mm} \times 5\ \text{mm} \times 3\ \text{mm}\) (thickness)
- Notch diameter: 60 \(\mu\text{m}\)
- \(d\) controls mode mixity

### Specimen Crack Length, \(a/W\), \(d\), \(M^p\), \(M^P\), Initiation \(J_c\) (Elastic), \(J_c\) (Elastic-Plastic)

<table>
<thead>
<tr>
<th>Specimen</th>
<th>(a) (mm)</th>
<th>(d) (mm)</th>
<th>(M^p) ((\text{N} \cdot \text{mm}))</th>
<th>(M^P) ((\text{N} \cdot \text{mm}))</th>
<th>Initiation (J_c) (Elastic) ((\text{N} \cdot \text{mm}))</th>
<th>(J_c) (Elastic-Plastic) ((\text{N} \cdot \text{mm}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>ASPB-1</td>
<td>3.5</td>
<td>0.7</td>
<td>-0.160</td>
<td>-0.089</td>
<td>9.22 ± 0.36</td>
<td>11.1 ± 0.57</td>
</tr>
<tr>
<td>ASPB-2</td>
<td>2.5</td>
<td>0.5</td>
<td>0.043</td>
<td>0.075</td>
<td>7.13 ± 0.39</td>
<td>8.38 ± 0.59</td>
</tr>
<tr>
<td>ASPB-3</td>
<td>2.5</td>
<td>0.5</td>
<td>0.215</td>
<td>0.444</td>
<td>14.31 ± 0.12</td>
<td>12.29 ± 0.32</td>
</tr>
<tr>
<td>ASPB-4</td>
<td>2.5</td>
<td>0.5</td>
<td>0.448</td>
<td>0.684</td>
<td>14.15 ± 0.12</td>
<td>20.50 ± 1.30</td>
</tr>
<tr>
<td>SLPB-1</td>
<td>2.5</td>
<td>0.5</td>
<td>1</td>
<td>1</td>
<td>26.6 ± 0.38</td>
<td>36.03 ± 7.73</td>
</tr>
</tbody>
</table>

(All dimensions are in mm)
Finite element analyses

- Typical finite element mesh

- 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:
  - $E = 97 \text{ GPa}$; $v=0.36$; $c_0=890 \text{ MPa}$; $\mu=0.06$; $b=120 \text{ MPa}$

- Determine:
  a. Elastic mode mixity parameter $M_e$
  b. Plastic mode mixity parameter $M_p$
  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

- 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
In-situ observations

- Notch deformation
- Shear banding
- Stable crack growth inside a dominant shear band
- Final failure

AS4PB-1 Specimen
P = 2.4 kN

Speed: 16x

100 μm
Mixed Mode Fracture

Experiment

Simulation

\[ M_e = -0.089 \text{ (~pure mode II)} \]

Tandaiya et al., JMPS 2009.
Mixed Mode Fracture

$M_p = 0.484 \ (mixed \ mode)$

$P = 14.1 \ kN$
Crack trajectories

Incipient crack growth occurs inside a dominant shear band for all the specimens.

AS4PB-1

AS4PB-2

AS4PB-4

S4PB-1
Variation of fracture toughness with mode mixity
Two types of morphologies

1. Smooth and shallow features involving highly smeared vein patterns within 45-60 µm from the notch front
2. Rough and deep features involving coarse dimple patterns superposed on ridges and valleys beyond 60 µm from the notch front

> Similar observations apply for other specimens also

Fracture mechanism is ductile involving growth of shear crack inside a dominant shear band

Process zone size ≈ 60 µm
in closing......

- Large scope for conducting exciting research on amorphous alloys, which are of interest from both technological as well as scientific stand points of view.
- Key is to identify relevant length scales that control deformation and fracture.
- Design alloys that have high strength and high toughness!!