RELATING NANOSCALE STRUCTURE AND PROPERTIES TO MACROSCALE FRACTURE TOUGHNESS FOR BULK METALLIC GLASSES

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Abstract
Bulk metallic glasses (BMGs) can range from exceptionally tough to brittle depending on their structural state; however, quantifying their structure-property relationships has been an unresolved challenge. Our findings revealed that local hardness variations within the BMG microstructure strongly affect the fracture behavior. Moreover, the hardness heterogeneities are controlled by the size and volume fraction of FCC-like medium-range order (MRO) clusters. We have proposed a model of ductile phase softening whereby relatively soft FCC-like MRO clusters sit in a matrix of harder icosahedral dominated ordering, while micropillar compression testing has revealed how the activation of these clusters into shear transformation zones can be negatively affected by oxygen impurities which in turn lower the fracture toughness.

1. Introduction
Bulk metallic glasses (BMGs) can demonstrate outstanding combinations of strength and fracture toughness; however, achieving high fracture toughness requires careful material processing to obtain desirable glassy microstructures and quantifying the glassy structure is an ongoing challenge. We overcame this challenge by utilizing nanobeam electron diffraction and fluctuation electron microscopy to understand how nanostructure variations create heterogeneous and high toughness microstructures in BMGs using three different Zr-based BMG compositions, two different manufacturing routes (casting and selective laser melting), and various thermo-mechanical histories (cryogenically-cycled, cold deformed, etc.).

2. Results
Our results show that depending on the microstructural arrangement of hard and soft regions (e.g., see example in Fig. 1f), the fracture toughness of a Zr–Cu–Ni–Al–Nb BMG can range from ~55 to 140 MPa√m and the fracture toughness of a Zr–Cu–Ni–Al–Ti BMG can range from ~40 – 100 MPa√m. Fig. 1 shows nanobeam electron diffraction results that reveal the nanostructural origins of the local hardness variations whereby the local hardness in the metallic glass microstructure decreases with increasing size and volume fraction of medium range order (MRO) clusters. Furthermore, the relationships between hardness and MRO for the various BMGs were maintained after different thermo-mechanical treatments (Fig. 1) where hardening and softening can be correlated with macroscopic embrittlement or toughening, respectively. Such results were explained using a model of ductile phase softening whereby relatively soft FCC-like MRO clusters sit in a matrix of harder icosahedral dominated ordering:

$$\frac{H_v}{3} = \sigma_y = \sigma_y^m - \sqrt{3}E^m(1-\beta)\gamma_{pl}^{MRO}\phi. \quad (1)$$

In Eq. (1), σ_y^m is the yield strength of the harder matrix, E^m is the elastic modulus of the harder matrix, γ_{pl}^{MRO} is the plastic strain of the MRO clusters at the point of overall composite yielding, and ϕ is the volume fraction of MRO clusters. β is the material constant of Eshelby's S-tensor for spherical inclusions, $\beta = 0.133(4-5\nu^m)/(1-\nu^m)$, where ν^m is the Poisson's ratio for the BMG matrix.

However, hardness alone is not a good predictor of fracture toughness and we have measured a Zr-Cu-Al-Nb BMG to have a toughness in the range of 24 – 29 MPa√m when produced by selective laser melting (SLM) and >160 MPa√m when produced by casting despite both materials having similar hardness. This difference can be explained by a suppression of the activation of the medium range order clusters into shear transformation zones due to much higher oxygen content in the SLM produced material (1271 vs. 168 ppm).

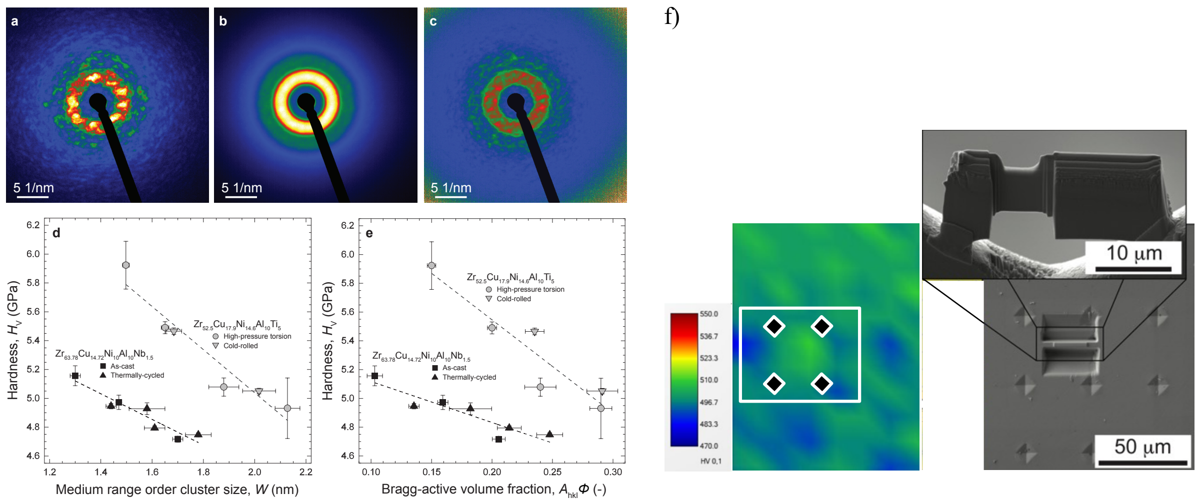

Fig. 1 – Nanobeam electron diffraction data showing a) a single pattern, b) the mean of 225 patterns, and c) the normalized variance used to deduce the relationships between local hardness and medium range order d) cluster size and e) volume fraction. f) shows how the sample was extracted from a region of known Vickers hardness HV0.1. Reprinted with permission from Elsevier.

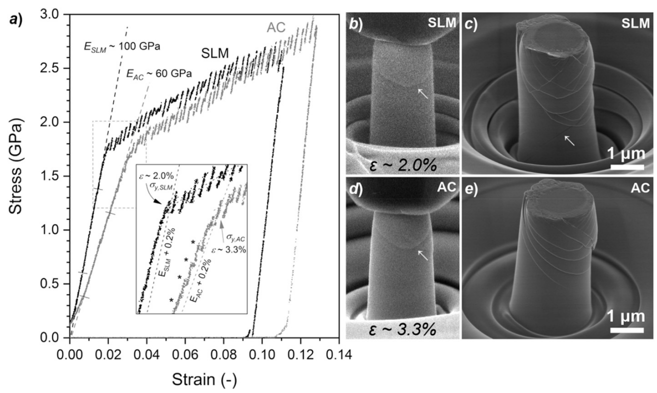

Fig.2 – a) Compression response of selective laser melted (SLM) and as-cast (AC) micropillars showing load-drops (*) for the AC material in the nominally elastic regime that indicate easier activation of MRO clusters into shear transformation zones. Also shown are micrographs at the first significant load-drop for each material in b), d) and post-compression in c), e). Reprinted with permission from Elsevier.

3. Conclusions

A hierarchy of nano- and microstructural features control the fracture toughness of bulk metallic glasses (BMGs). Excellent fracture toughness values >100 MPa√m can be achieved in BMGs by controlling the microstructural arrangement of hard and soft glassy regions, and the local hardness inside those regions is dictated by the size and volume fraction of nanoscale medium range order (MRO) clusters. A ductile phase softening model can explain the role of FCC-like MRO clusters in softening BMGs, while large amounts of oxygen impurities in additive manufactured BMGs can suppress the activation of those clusters into shear transformation zones, which in turn greatly decreases the BMG fracture toughness.

Acknowledgements

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