Atomistic Simulations of Metallic Glass and Nanoglass

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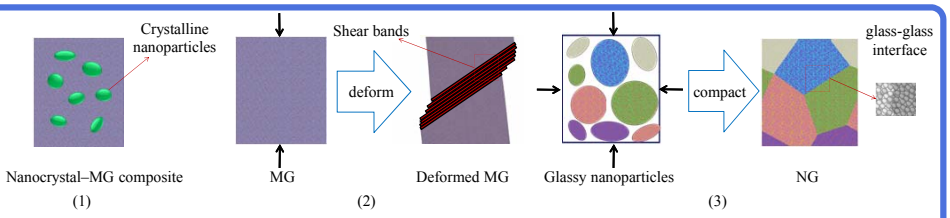
Background and Motivation

- Conventional Metallic glasses (MGs) exhibit high strength and high hardness, but severe lack of ductility.
- Some approaches to improve the ductility of MGs:
  1) Nanocrystalline inclusions [1]
  2) Preplastic deformation [2]
  3) Powder consolidation of glassy nanoparticles (Nanoglass (NG)) [3]



Objective: Investigate the mechanical properties and deformation mechanism, especially plasticity of NGs with different grain sizes and compare them with the case of MGs.

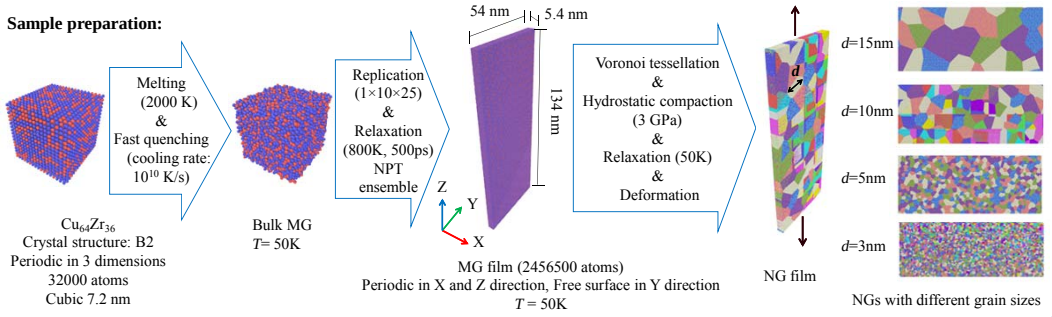
Material and Methodology

- NG nanostructure: MG grains separated by amorphous interface.

Molecular Dynamics (MD) simulation:

- Large scale MD simulations using LAMMPS [4].
- $Cu_{64}Zr_{36}$ MG and NG films over a range of grain sizes (d).
- Embedded atom model (EAM) potential [5].
- Uniaxial loading at strain rate of $\dot{\varepsilon} = 4\times10^{7}$ s^{-1}.

Sample preparation:



$Cu_{64}Zr_{36}$
Crystal structure: B2
Periodic in 3 dimensions
32000 atoms
Cubic 7.2 nm

Bulk MG
T= 50K

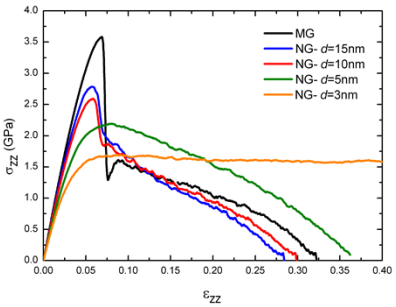
MG film (2456500 atoms)
Periodic in X and Z direction, Free surface in Y direction
T = 50K

NG film

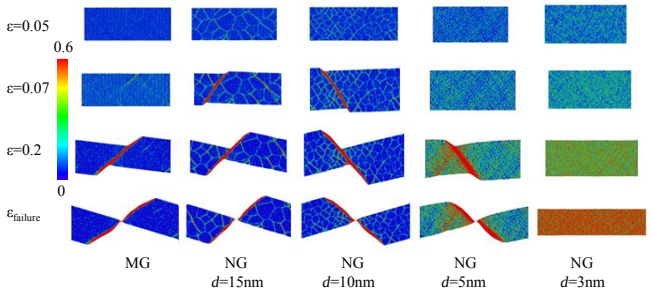
NGs with different grain sizes

Results and Discussion

- MG films fail catastrophically through localization due to formation of a single dominant shear band.
- NG films exhibit a transition from a localized deformation in the form of a single dominant shear band to a near homogeneous plastic deformation with decreasing grain size.
- NG films exhibit a consistent decrease in the yield stress with decreasing grain size.
- Multiple embryonic shear bands activate and propagate at the interfaces of NGs.
- Interfacial regions act as preferred channels for plasticity, causing the generation of an interconnected motif of shear bands that depends on the grain size.



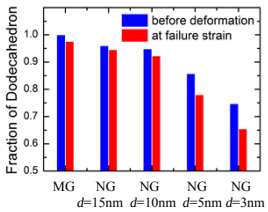
NG stress-strain curves as a function of grain size



Snapshots of atomic configurations of MG and NGs during tensile deformation at various strains (the color of the atoms is based on the local atomic shear strain)

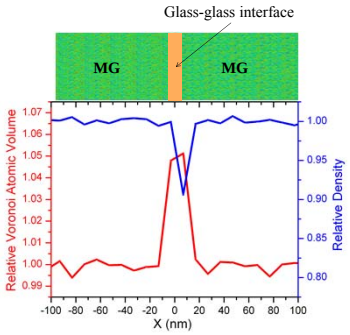
Shear band and NG interface compared to MG:

- Enhanced free volume.
- Softer region.
- Lower short range order.
- Lower fraction of Cu-centered Dodecahedron.



Population of Dodecahedron in NGs relative to undeformed MG

NG single interface analysis:



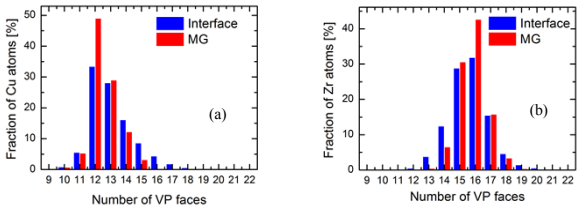
Relative Voronoi atomic volume and density along the specimen

Cu-centered Dodecahedron polyhedron:

- The most prominent Voronoi polyhedron (VP) for $Cu_{64}Zr_{36}$ MG.
- Defines activation barrier for shear transformation zones.
- Have high packing density.
- Have high shear resistance.

Dodecahedron VPs

Faces by sides: 12{5}
Voronoi Index: [0, 0, 12, 0]



Fraction of (a) Cu-centered and (b) Zr-centered VPs, in a MG and NG interface

Conclusion

- NGs are engineered nanostructures with soft interfaces separating MG grains.
- Glass-glass interfaces act as structural heterogeneities that promote shear band formation and prevent strain localization.
- Glass-glass interfaces in NGs are characterized by a lower fraction of Cu-centered dodecahedron and increased Voronoi atomic volume.
- Ductility of NGs can be tuned by varying powder particle size, and hence interface density.

Selected Literature

[1] Y. Shi, M. L. Falk, A Computational Analysis of the Deformation Mechanisms of A Nanocrystal–Metallic Glass Composite, Acta Materialia, 56, 995–1000 (2008).

[2] M. H. Lee, K. S. Lee, J. Das, J. Thomas, U. Kuhn, and J. Eckert, Improved Plasticity of Bulk Metallic Glasses Upon Cold Rolling, Scr. Mater, 62, 678 (2010).

[3] J. Jing, A. Kramer, R. Birringer, H. Gleiter, and U. Gonser, Modified Atomic Structure in a Pd-Fe-Si Nanoglass: A Mossbauer Study, J. Non-Cryst. Solids, 113, 167 (1989).

[4] Y.Q. Cheng, H.W. Sheng, E. Ma, Atomic Level Structure in Multicomponent Bulk Metallic Glass, Phys. Rev. Lett., 102, 245501 (2009).