Sandia Academic Alliance Spring UT Austin Research Poster Session | Sandia Day 2022

Spectroscopical Evaluation of Shear-induced Chemical Changes and Structural Transformations in Bulk Metallic Glass (BMG)

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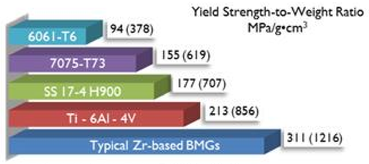
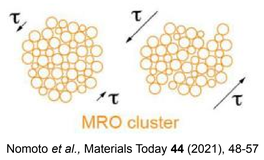
Introduction / Motivation

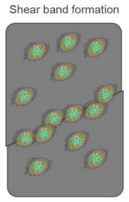
- Bulk Metallic Glasses (BMGs): a class of promising structural materials owing to its high elastic limit (~2%) and yield strength-to-weight ratio.
- Even though BMGs exhibit attractive tribological properties, the scientific basis for this behavior is not established due to the complex combination of plasticity, surface structural relaxation and transformation, material transfer, and atomic mixing.
- The determination of the structural properties of BMGs (local bonding configuration, local ordering) and their evolution during sliding is critical for correlating materials properties and tribological behavior



M. Telford, *Materials Today* **7** (2004), 36-43



Nomoto *et al.*, Materials Today **44** (2021), 48-57



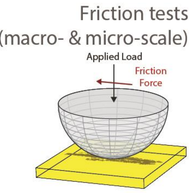
Aim: Understand the shear-induced surface chemical changes and structural transformations via advanced X-ray techniques

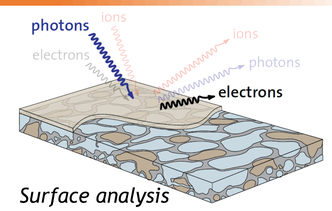
Approach

- **Evaluation of surface chemical changes upon sliding**

1) Tribological testing in glove box (UT-Austin)
2) X-ray photoelectron spectroscopy (XPS) (Texas Materials Institute, UT-Austin)

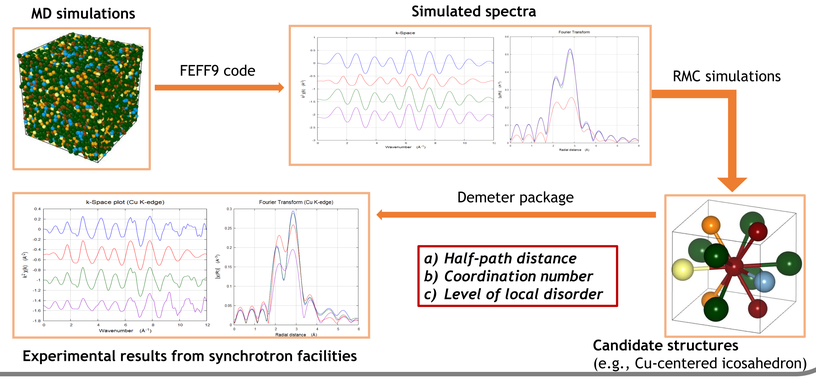
→ **Prevention of surface oxidation through the use of a dedicated interface developed at UT-Austin (Patent No. 9,945,761) to transfer air-sensitive specimens from glove boxes to ultra-high vacuum without any exposure to air**





- **Identification of changes in local atomic arrangements upon sliding**

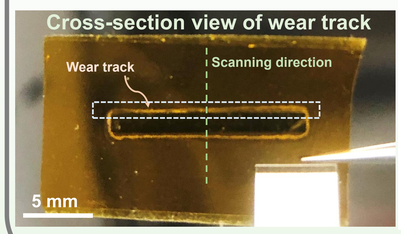
1) Synchrotron-based X-ray Absorption Fine Structure (XAFS) techniques (NSLS-II, APS, ALS, and SLAC)
2) Molecular Dynamic (MD) Simulations (Sandia and UT-Austin)
3) *Ab initio* simulation with FEFF9 code (UT-Austin)
4) Reverse Monte Carlo (RMC) Simulations (EvAX) (UT-Austin)
5) Demeter package for fitting experimental spectra

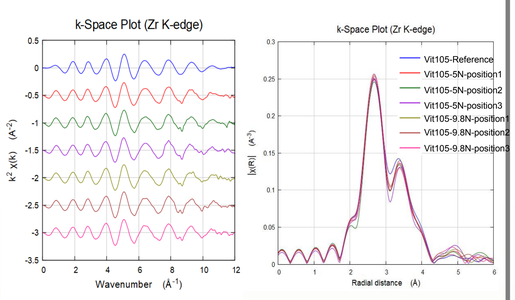


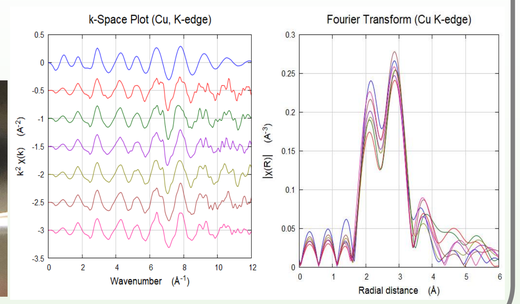
Brookhaven National Laboratory · ALS Advanced Light Source · Argonne National Laboratory · SLAC National Accelerator Laboratory

Current Status / XAFS Results

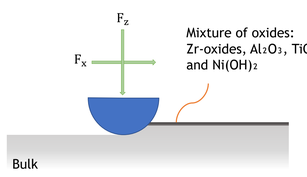
- Sample: $Zr_{52}Cu_{18}Ni_{15}Al_{10}Ti_5$ (Vit105)
- XAFS data acquired:
  - on cross-sections oriented along the sliding direction
  - as a function of depth from the sample surface
- Bond straining in Cu-centered polyhedra much more prominent than the one in Zr-centered polyhedra



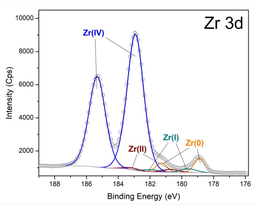


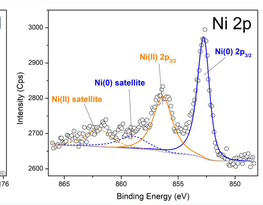


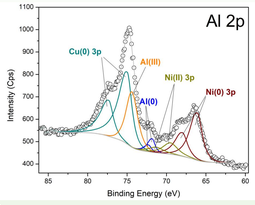
Current Status / XPS Results

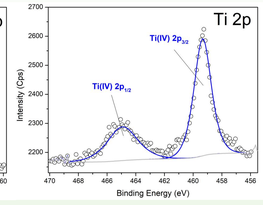


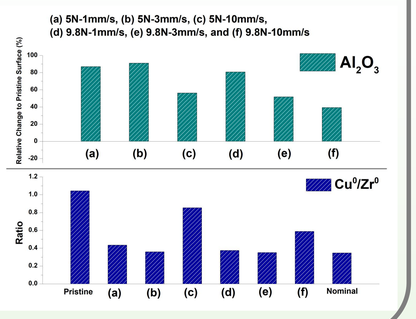
- Cu in metallic form (Cu^0), both in bulk and in the near-surface region
- Upon sliding in aerobic conditions, the composition of the oxide layer changes (much larger amount of aluminum oxide in the wear tracks)
  - Positive deviation of Cu^0 to Zr^0 ratio from the nominal value resulted from the preferential oxidation of newly exposed metallic Zr.











Next Steps / Future Work

Next Steps

- Evaluation of changes in surface chemistry upon sliding in inert environments
- Determination of temperature-dependent structural changes in BMG (XAFS analyses)
- RMC analysis of simulated XAFS data and use of the Demeter package to fit experimental XAFS spectra

Future Work

- Simulations of shear-induced changes in the MD-simulated BMG systems
- Spatially-resolved XPS measurements within the wear track with the incoming new XPS at Texas Materials Institute (NSF/MRI grant #2117623)
- Nano-scale friction force experiments on BMG with Atomic Force Microscopy (AFM)

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