Supporting Information for:

Mechanisms of Failure in Nanoscale Metallic Glass

X. Wendy Gu[†]*, Mehdi Jafary-Zadeh*[°]*, David Z. Chen*[‡]*, Zhaoxuan Wu*[°]*, Yong-Wei Zhang*[°]*, David J. Srolovitz*[+]*, Julia R. Greer*[‡]***

[†]Division of Chemistry and Chemical Engineering, and [‡]Division of Engineering and Applied Science, California Institute of Technology, 1200 E. California Blvd., Pasadena, CA 91125, United States

[°]Institute of High Performance Computing, 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632

[+]Departments of Materials Science and Engineering & Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, PA 19104, United States

CORRESPONDING AUTHOR:

Julia R. Greer

M/C 309-81, Division of Engineering and Applied Science, California Institute of Technology, 1200 E. California Blvd., Pasadena, CA 91125, United States

626-395-4127

jrgreer@caltech.edu

TEM sample preparation

TEM samples of notched and unnotched metallic glass nano-cylinders were prepared through a focus ion beam (FIB) free process that resulted in minimal damage to the nanostructures. Nano-cylinders with poor adhesion to the growth substrate were attached using

Van der Waals forces to a custom-fabricated tungsten needle attached to the indenter tip in the InSEM, an in-situ scanning electron microscope (SEM) nanomechanical testing instrument (Nanomechanics, Inc.). The W needle was used as a micromanipulator. Efforts were made to contact the W needle to the portion of the pillar between the lowest notch and the substrate, so that the notches would not be deformed during TEM preparation. The W needle carrying the pillar is then moved to the Cu TEM grid, and the pillar is glued to the TEM grid using carbon deposition using the SEM electron beam. The W needle is then removed from the pillar. A small amount of W is applied to the cap of the pillar, far from the notches in the gauge section, using deposition by electron beam (FEI Nova 200 Dual Beam) in order to secure the pillar to the TEM grid.

Molecular dynamics simulations

Simulations were conducted using the Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)[1]. The simulation samples were prepared from a melting-and-quenching simulation of a randomly substituted $Fe_{75}P_{25}$ solid solution whereby a $Fe_{75}P_{25}$ rectangular prism with periodic boundary conditions (PBC) in all directions was melted at 2000 K and equilibrated for 1 ns. Then, the sample was quenched to 1 K at a cooling rate of 0.5 Kps^{-1}. The time step for the melting-and-quenching was chosen to be 0.002 ps, and the isothermal-isobaric ensemble (NPT) was employed to maintain the pressure of the system at zero. The Verlet algorithm[2] and the Nose-Hoover thermostat/barostat[3,4] were used to integrate the equations of motion. After quenching, cylindrical nanocylinders were cut from the quenched bulk metallic glass. The samples were relaxed using the conjugate gradient (CG) minimization technique[5] as implemented in LAMMPS. The nanocylinders were then equilibrated at the temperature of the tensile test (1 K) and zero pressure for 0.5 ns using the NPT ensemble. Uniaxial tensile loading was applied to the nanocylinders by rescaling the simulation box and a time step of 0.001 ps.

During tensile loading, the PBC was applied just along the loading direction, and the temperature of the system was maintained at 1 K, which reduces the thermal fluctuation effects and facilitates the analyses of atomic quantities[6]. A strain rate of 5×10^7 s^{-1} was applied during tensile testing.

Supplementary movies

Movie S1. *In-situ* SEM video of an electroplated NiP metallic glass sample with diameter of ~75 nm tested in tension.

Movie S2. *In-situ* SEM video of a notched, electroplated NiP metallic glass sample with diameter of ~70 nm tested in tension.

Movie S3. Molecular dynamics movie of the tensile deformation of a FeP metallic glass with a diameter of 40 nm. The cross-section of the sample is shown, and the von Mises strain is plotted in the video.

Movie S4. Molecular dynamics movie of the tensile deformation of a notched FeP metallic glass with a diameter of 40 nm. The cross-section of the sample is shown, and the von Mises strain is plotted in the video.

References

(1) Plimpton, S. *J. Comput. Phys.* **1995**, *117*, 1-19.
(2) Verlet, L. *Phys. Rev.* **1967**, *159*, 98-103.
(3) Nosé, S. *The Journal of Chemical Physics* **1984**, *81*, 511-519.
(4) Hoover, W. G. *Phys. Rev. A* **1985**, *31*, 1695-1697.
(5) Štich, I.; Car, R.; Parrinello, M.; Baroni, S. *Phys. Rev. B* **1989**, *39*, 4997-5004.
(6) Murali, P.; Guo, T. F.; Zhang, Y. W.; Narasimhan, R.; Li, Y.; Gao, H. J. *Phys. Rev. Lett.* **2011**, *107*, 215501.