Determining the 3D Atomic Structure of Metallic Glass

Yao Yang[1], Jihan Zhou[1], Fan Zhu[1], Yakun Yuan[1], Dillan J. Chang[1], Dennis S. Kim[1], Minh Pham[2], Arjun Rana[1], Xuezeng Tian[1], Yonggang Yao[3], Stanley J. Osher[2], Andreas K. Schmid[4], Liangbing Hu[3], Peter Ercius[4] and Jianwei Miao[1*]

[1.] Department of Physics & Astronomy, STROBE NSF Science & Technology Center and California NanoSystems Institute, University of California, Los Angeles, CA, USA.
[2.] Department of Mathematics, University of California, Los Angeles, CA, USA.
[3.] Department of Materials Science and Engineering, University of Maryland, College Park, MD, USA
[4.] National Center for Electron Microscopy, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California, USA.
* Corresponding author: miao@physics.ucla.edu

Since the first discovery in 1960 [1], metallic glasses have been actively studied for both fundamental interest and practical application [2-9]. However, due to the lack of long-range order, the three-dimensional (3D) atomic structure of metallic glasses has eluded direct experimental determination. To understand the structure property relationships, it is essential to characterize the 3D structure of metallic glasses at the atomic resolution. A powerful method that can in principle solve this long-standing problem is atomic electron tomography (AET) [10]. AET determines the 3D atomic structure of materials without assuming crystallinity and has been used to image grain boundaries, anti-phase boundaries, stacking faults, dislocations, point defects, chemical order/disorder, atomic-scale ripples, bond distortion and strain tensors with unprecedented 3D detail [10-14]. More recently, 4D AET (3D space and 1D time) has been developed to observe crystal nucleation, showing that a theory beyond classical nucleation theory is needed to describe early-stage nucleation at the atomic scale [15].

In combination of newly developed REal Space Iterative REconstruction (RESIRE) algorithm and the TEAM microscope at the National Center for Electron Microscopy, we have advanced AET to determine the 3D atomic structure of a multi-component metallic glass and amorphous materials with a precision of ~20 picometers [16,17]. Figure 1 shows the 3D atomic model of the metallic glass sample, in which 8 different atomic species were grouped into three types: Co, Ni (type 1), Ru, Rh, Pa, Ag (type 2), Ir and Pt (type 3). We quantitatively characterized the short- and medium-range order (SRO and MRO) of the 3D atomic arrangement. We found that, the 3D atomic packing of the SRO is geometrically disordered, which was quantified by the Voronoi tessellation [16]. We observed that some SRO structures connect with each other to form crystal-like superclusters and give rise to MRO. We identified four types of crystal-like MRO —face-centered cubic, hexagonal close-packed, body-centered cubic and simple cubic — coexisting in the metallic glass, which exhibit translational but not orientational order. Figure 2 show two representative structures of fcc- and sc-like MRO in the metallic glass sample. But we did not observe icosahedral-like MRO in the metallic glass sample. These experimental results provide direct experimental evidence to support the general framework of the efficient cluster packing model for metallic glasses [3,5-7]. We expect that this work will pave the way for the determination of the 3D atomic structure of a wide range of amorphous solids, which could transform our fundamental understanding of non-crystalline materials and related phenomena [18].

CrossMark
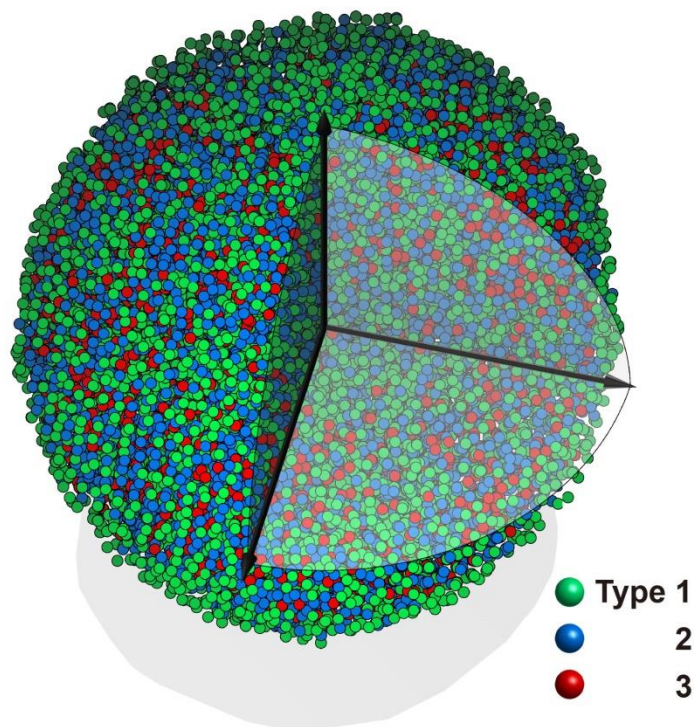
Figure 1. Experimental 3D atomic model of the metallic glass nanoparticle.
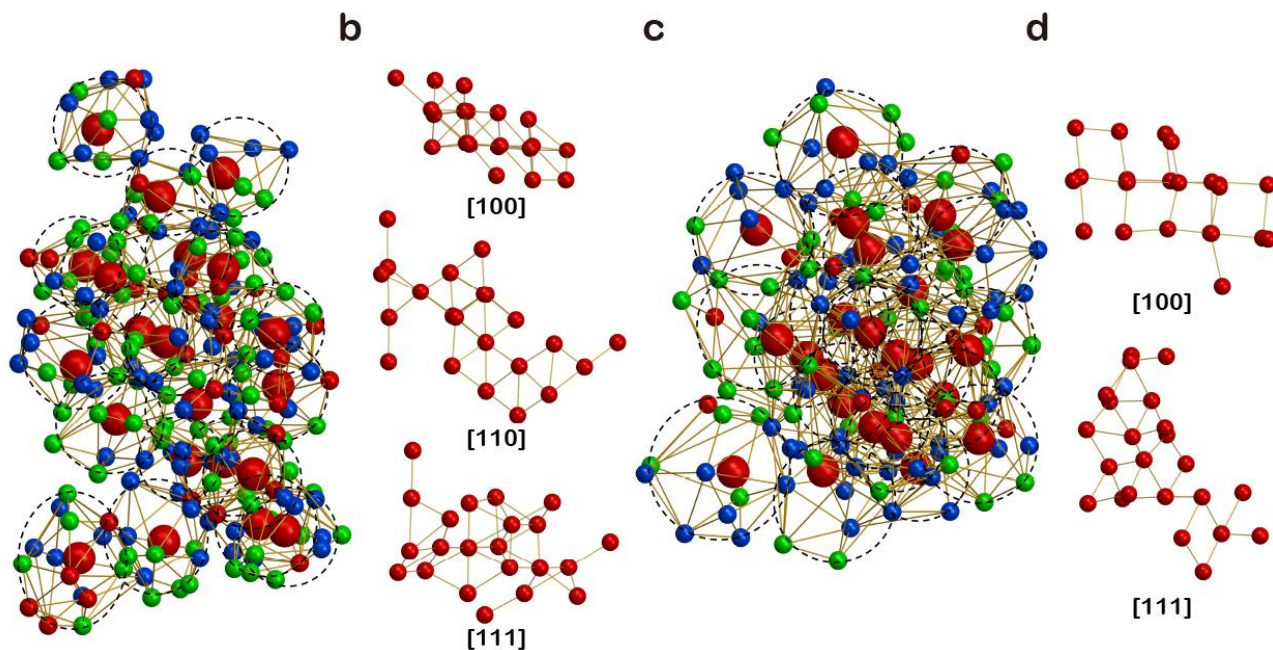
Figure 2. Representative fcc- (a) and sc-like (c) MROs, consisting of 22 and 23 solute centers (large red spheres), respectively, where the individual solute-center clusters (dashed circles) are randomly oriented. To better visualize the crystal-like MROs, the solvent atoms have been removed and the solute centers are orientated along the fcc (b) and sc (d) zone axes, showing that the MROs have anisotropic 3D shapes and strongly deviate from the crystal lattices.

References:

[1] Klement, Jun et al., Nature **187** (1960), p. 869.
[2] Nelson, D. R. and Spaepen, F. Solid State Phys. **42** (1989), p. 1.
[3] Miracle, D. B., Nat. Mater. **3** (2004), p. 697.
[4] Sheng, H. W. et al., Nature **439** (2006), p. 419.
[5] Miracle, D. B. et al., MRS Bull. **32** (2007), p. 629.
[6] Cheng, Y. Q. and Ma, E., Prog. Mater. Sci. **56** (2011), p. 379.
[7] Miracle, D. B., JOM **64** (2012), p. 846.
[8] Greer, A. L., Science **267** (1995), p. 1947.
[9] Chen, M.W., NPG Asia Mater. **3** (2011), p. 82.
[10] J. Miao et al., Science **353** (2016), p. aaf2157.
[11] M. C. Scott et al., Nature **483** (2012), p. 444.
[12] C. C. Chen et al., Nature **496** (2013), p. 74.
[13] R. Xu et al., Nature Mater. **14** (2015), p. 1099.
[14] Y. Yang et al., Nature **542** (2017), p. 75.
[15] J. Zhou et al., Nature **570** (2019), p. 500.
[16] Y. Yang et al., Nature **592** (2021), p. 60.
[17] Y. Yuan et al., Nature Materials **21** (2022), p. 95.