ADVANCED MATERIALS

Supporting Information

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# Unveiling the Local Atomic Arrangements in the Shear Band Regions of Metallic Glass

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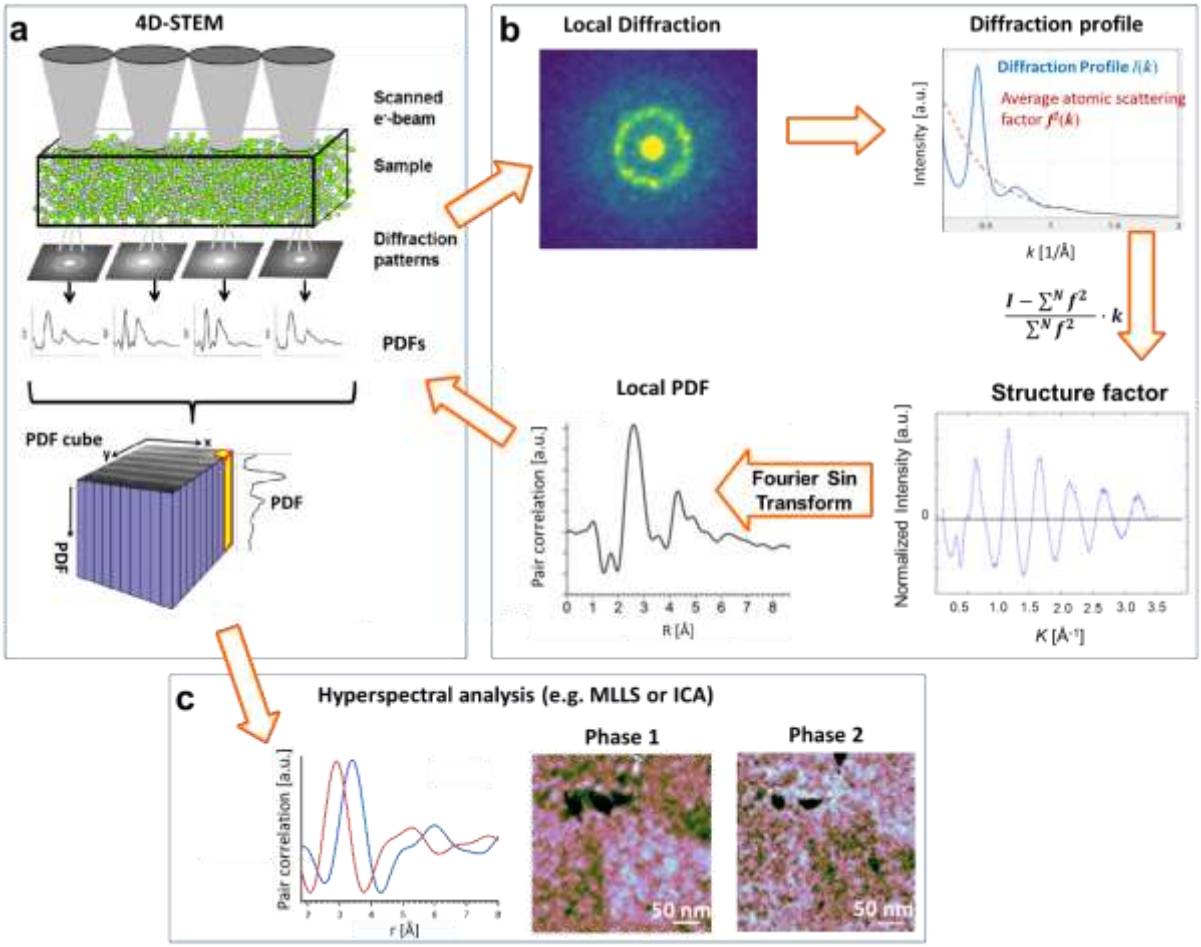


**Figure S1.** Work flow for the STEM pair distribution function (STEM-PDF). **a**, 4D-STEM acquisition and PDF cube creation. **b**, details of PDF calculation from individual local nanobeam electron diffraction. **c**, Hyperspectral analysis of the PDF data cube to obtain the structural map and PDFs for individual structural phases.

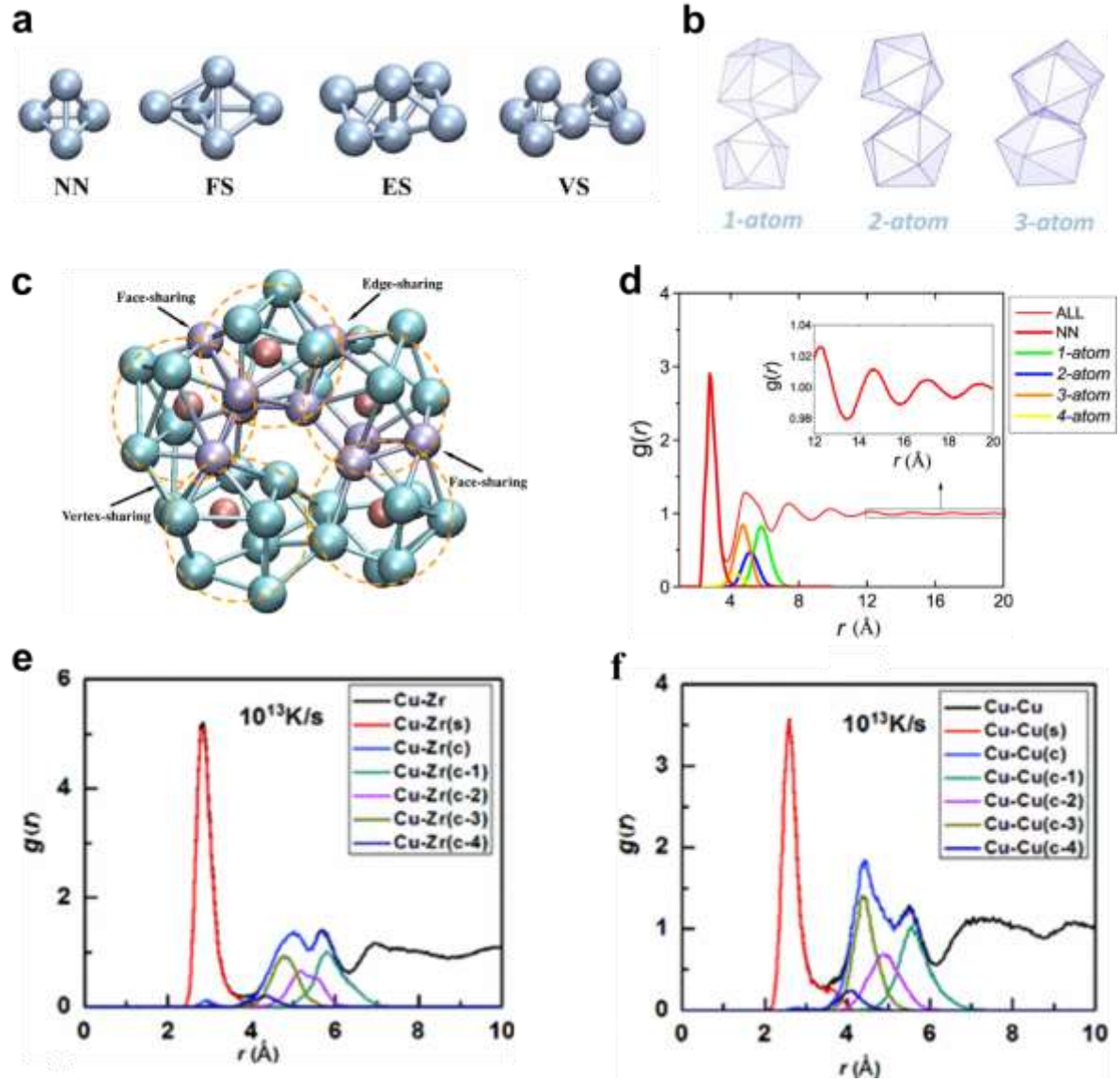


**Figure S2.** Connection Schemes for the tetrahedral and their influence on the PDFs in metallic glasses. Taken from literature for the convenience of readers. **a,** sharing schemes of tetrahedra in MGs[1], NN denotes nearest neighbor, FS is face share, ES is edge share and VS is vertex share. **b**, Connection schemes of polyhedral motifs[2]. **c,** interconnected polyhedra through the connection of tetrahedra illustrated in **a**[1]. **d**, PDF for $Zr_{46}Cu_{46}Al_8$ MGs obtained by MD simulation[2]. **e** and **f,** partial Cu–Zr and Cu–Cu PDFs for $Cu_{50}Z_{50}$ MG obtained by MD simulation[3] showing that the second peak of PDFs strongly reflects the polyhedra connection. Figure S2a and S2c Reprinted from [W. K. Luo, H. W. Sheng, E. Ma, *Appl. Phys. Lett.* **2006**, *89*, 131927], with the permission of AIP Publishing. Figure S2b and S2d Reprinted from [J. Ding, E. Ma, M. Asta, R. O. Ritchie, *Sci. Rep.* **2015**, *5*, 1.], (CC BY 4.0). Figure S2e and S2f reprinted from [S. P. Pan, J. Y. Qin, W. M. Wang, T. K. Gu, *Phys. Rev. B - Condens. Matter Mater. Phys.* **2011**, *84*, 092201], with permission of APS.

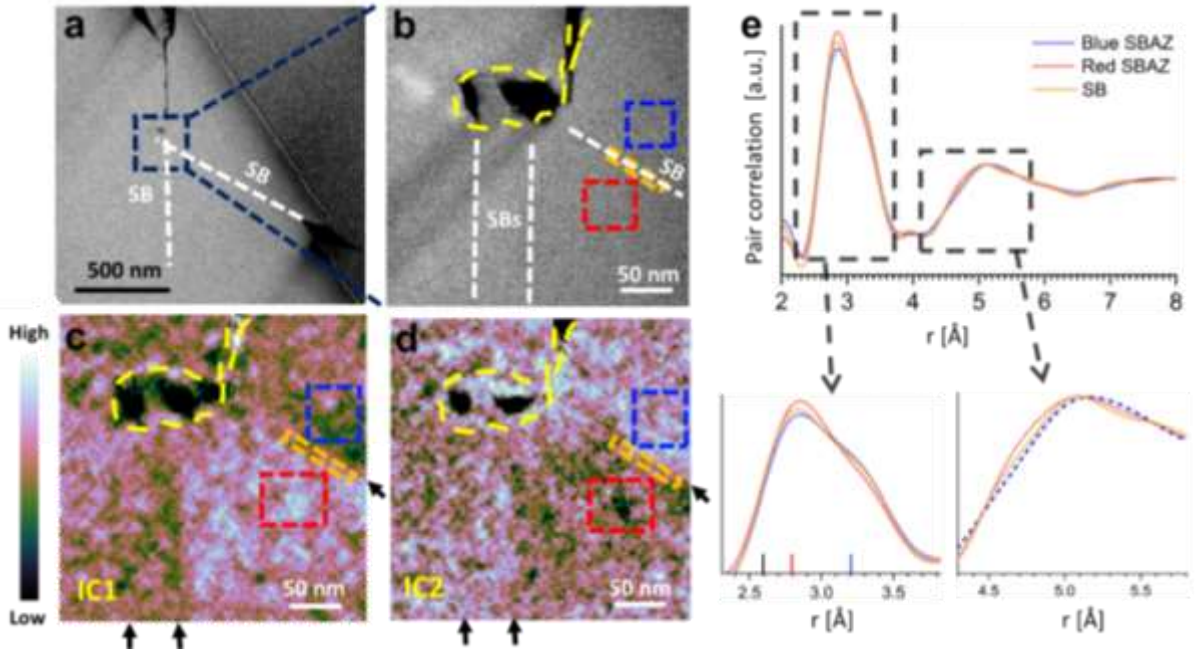


**Figure S3.** STEM-PDF analysis conducted in the intersection of two SBs. **a** and **b**, STEM-HAADF images of intersected SBs. The crack is circled by the yellow dashed curve. **c** and **d**, Distribution map of the IC1 and IC2, SB (black arrows) and two type of SBAZs can be observed. **e**, PDFs taken from the SB and SBAZs highlighted by the orange, red and blue dashed boxes in **b-d**. Reference marks at 2.6, 2.8 and 3.2 Å correspond to the Cu–Cu, Cu–Zr and Zr–Zr NN distance in $Zr_{50}Cu_{50}$ glass[3,4].

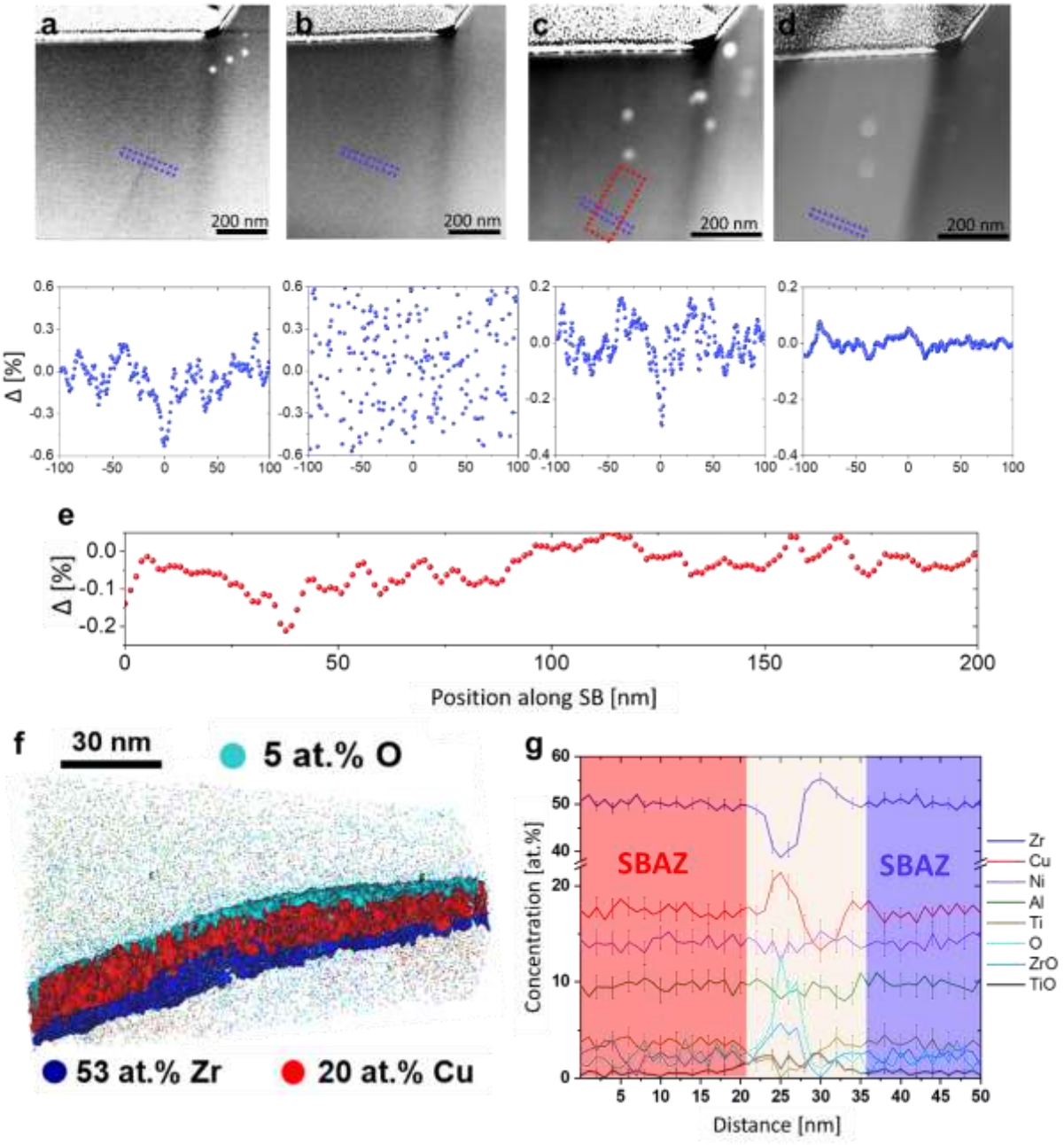


**Figure S4.** Shear band oxidation observation with STEM-HAADF and APT. **a-d**, STEM HAADF image of a SB in the same sample. **a**, after 20 days sample storing. **b**, after FIB thinning of **a**. **c**, 10 days after **b**, the SB alternating contrast is visible. **d**, FIB re-thinning of **c**. The relative intensity change profile standard deviations (error bar of intensity) are 0.14%, 0.55%, 0.08%, 0.02% for a-d, respectively. **e**, contrast profile extracted from the SB inside the red rectangle in **c. f**, 3D atom probe reconstruction of oxidized deformed sample including Oxygen, Cu and Zr depicted as aqua, red and blue isoconcentration surfaces, respectively. **g,** one-dimensional concentration profile perpendicular to the SB. Refer to Figure 4e for the schematic representation of extracted chemical concentration profiles in APT analysis

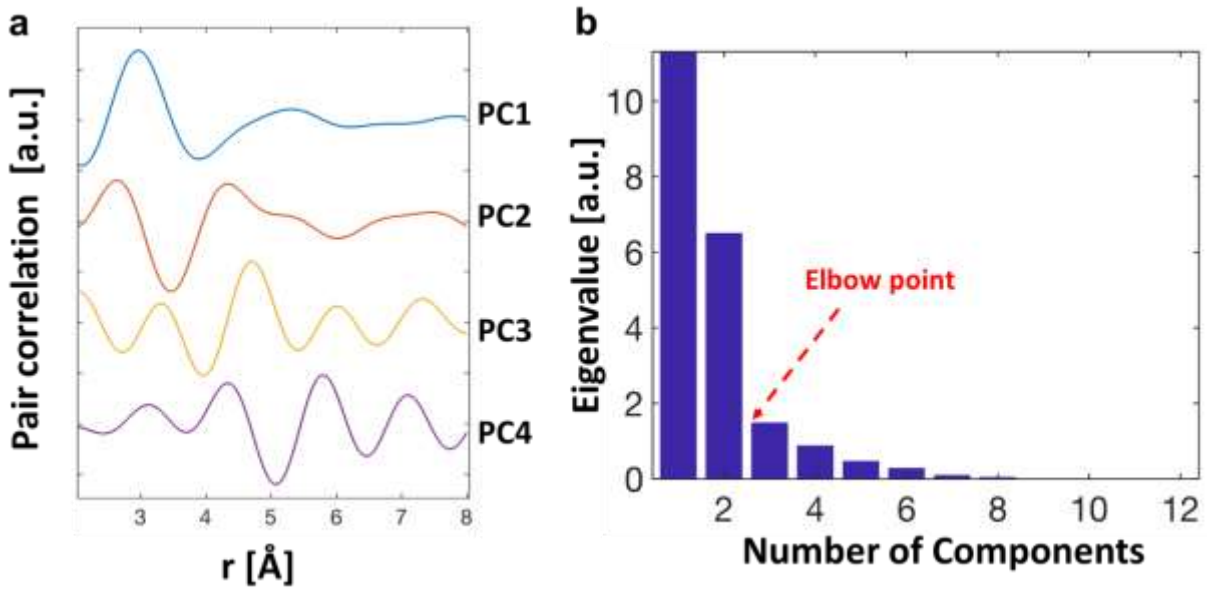


**Figure S5**. PCA analysis of the STEM-PDF data. **a**, the first four component PDFs in the order from top to bottom (PC is principal component). **b**, Eigenvalue scree plot for each component. The abrupt truncation (elbow point) after the 2$^{nd}$ component suggests the first two components should be considered as principal components.

## References

[1] W. K. Luo, H. W. Sheng, E. Ma, *Appl. Phys. Lett.* **2006**, *89*, 131927.

[2] J. Ding, E. Ma, M. Asta, R. O. Ritchie, *Sci. Rep.* **2015**, *5*, 17429.

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