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

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The prospective application of metallic glasses (MGs) are limited by the lack of toughness under plastic deformation [1-2], attributed to shear banding inducing catastrophic failure. A concise depiction of the local atomic arrangement (local atomic packing and chemical short-range order), induced by shear banding, is quintessential to understand the deformation mechanism, however still not clear. An explicit view of the complex interplay of local atomic structure and chemical environment is presented by mapping the atomic arrangements in shear bands (SBs) and in their vicinity in a deformed Vitreloy 105 metallic glass, using the 4-dimensional scanning transmission electron microscopy (4D-STEM) (Figure a) based pair distribution function (PDF) mapping (Figure b) [3-4]. The results [5] experimentally prove that plastic deformation causes a reduction of geometrically favored polyhedral motifs (GFMs). As shown in Figure c and d, localized motifs variations and antisymmetric (bond and chemical) segregation extend for several hundred nanometers from the SB, forming the shear band affected zones. Moreover, the variations within the SB are found both perpendicular and parallel to the SB plane, also observable in the oxidation activity. The knowledge of the structural–chemical changes provides a deeper understanding of the plastic deformation of metallic glasses especially for their functional applications and future improvements.

Keywords: Shear band, Metallic glass, Atomic structure, Pair distribution function (PDF), 4-dimensional scanning transmission electron microscope (4D-STEM)

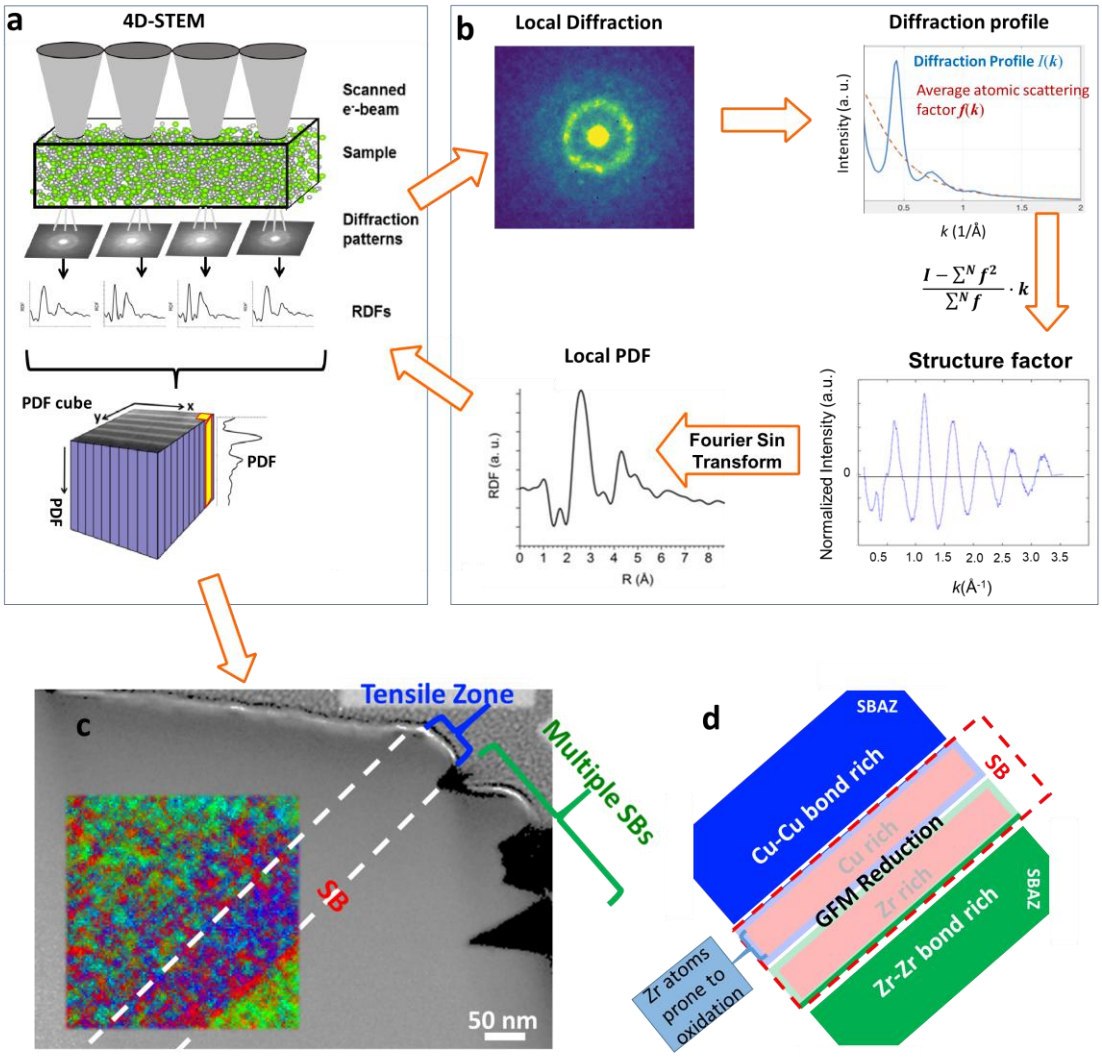

Figure: **a**, Schematic illustration of STEM-PDF used for this study. **b**, PDF process. **c**, superposition of the PDF maps with the HAADF image of the deformed area in a SB, where green corresponds to rich of Zr-Zr bonds, blue to rich of Cu-Cu bonds and red to GFMs reduction. **d**, representation of the different structures found in this study.

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