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In-situ synchrotron X-ray diffraction study of dual-step strain variation in laser shock peened metallic glasses

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ABSTRACT

Atomic-structure evolution is significant in understanding the deformation mechanism of metallic glasses. Here, we firstly find a dual-step atomic strain variation in laser-shock-peened (LSPed) metallic glasses during compression tests by using in-situ synchrotron X-ray diffraction. Under low compressive load, LSP-deformed zone's atomic-structure shows low Young's Modulus (*E*); with load increase, atomic-structure are re-hardened, showing high *E*. An atomic deformation mechanism is proposed by using flow unit model, that LSP could induce interconnected flow units and homogenize the atomic-structure. These interconnected flow units are metastable and start to annihilate during compressive loading, causing the dual-step atomic strain variation.

Due to the absence of long-range order, bulk metallic glasses (BMGs) exhibit excellent mechanical properties, such as high strength, large elastic strain limit, and high hardness [1,2]. Different from crystalline solids, BMGs do not possess a microstructure with dislocations, twins, or stacking faults. The structural origin of BMG deformation has been investigated for decades but still not fully understood, mainly due to the absence of direct experimental characterization of atomic-structure evolution. High energy synchrotron X-ray diffraction (HESXRD) is an effective tool to explore the details of BMG deformation mechanism in atomic level [3–8]. Poulsen et al. [3] demonstrated that the atomic strain tensor of BMGs could be quantitatively estimated by considering the shift of peak positions of the pair-distribution-function (PDF) curves. Based on this approach, it was found that during elastic deformation in BMGs, the atomic strain in atomic shells varied linearly with the applied stress [4,6–8]; and the bonds in 1st atomic shell are much stiffer against external loading compared to high order shells, showing the structure heterogeneity. However, the atomic-structural evolution in plastic deformed BMG is still unclear. The main reason is that in BMG, the plastic flow usually localizes in nano-scaled shear bands and brittle fracture happens quickly, the plastic deformation zone is narrow and difficult to be researched experimentally.

Laser shock peening (LSP), which can induce high impact stress (>10GPa) with high strain rate (>10^6 s^{-1}) on materials, is an effective method to induce large plastic deformation zone with high energy in BMGs. Free volume and multiple shear bands can be generated by LSP [9–11]. The deformed zone is obviously softened and the depth is >500 μm [12,13]. This large plastic deformed zone provides an opportunity to research the structure evolution in plastic deformed MGs directly.

Here, we used LSP to induce intense plastic deformation in Ti-based BMGs. In-situ HESXRD process and PDF analysis were employed to investigate the atomic-structure evolution in LSPed BMGs during compression. We found that not only high-order shells, but also 1st atomic shell were greatly softened. A dual-step atomic strain variation with different Young's Modulus (*E*s) in LSPed BMGs was observed during compression tests. By using a flow unit model, an atomic deformation mechanism is proposed, that metastable interconnected flow units were induced by LSP and the structure heterogeneity were weakened. The increase of *E* in high load region reveals the structure relaxation.

$Ti_{32.8}Zr_{30.2}Ni_{5.3}Cu_9Be_{22.7}$ (at.%) BMG plates with dimensions of 50 × 50 × 3 mm^3 were prepared by flip casting into a copper mold. BMG plates were shocked by laser pulse with wavelength of 1064 nm, the power density of a single laser pulse with 3 mm diameter is

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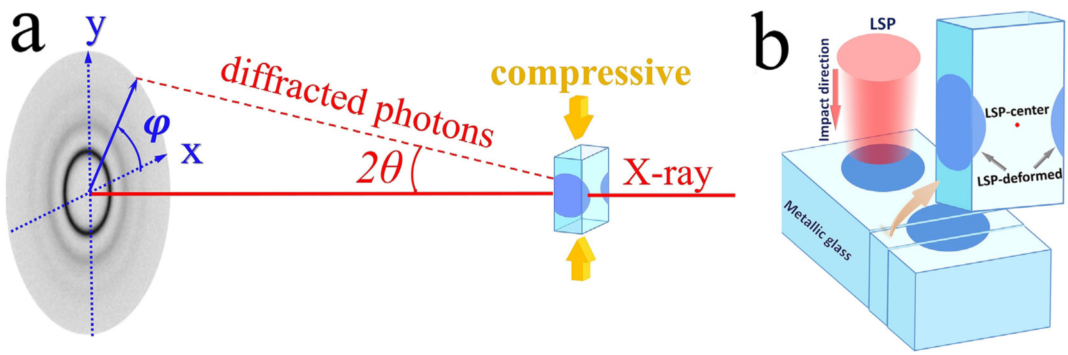

Fig. 1. The schematic diagram of the HESXRD measurement (a) and sample preparation (b).

25 GW/cm^2 and the pulse duration is 30 ns (see details in supplementary material). In-situ HESXRD technique was used to study the atomic-structural evolution of LSPed BMG at the 11-ID-C beamline of Advanced Photon Source, Argonne National Laboratory, USA. The process of the measurement is schematically shown in Fig. 1a. For the LSPed sample, plastic deformed zone and center zone (referred as LSP-deformed and LSP-center, respectively, as illustrated in Fig. 1b) were select to be measured by HESXRD. Based on the XRD patterns, the reduced pair distribution function (PDF), $G(r)$, were calculated using the software package of Fit2D [14] and PDF getX2 [15] (see HESXRD measurement and PDF analysis details in supplementary material).

Fig. 2a presents the reduced PDFs, $G(r)$, of the as-cast BMG, LSPed BMG samples before loading ($\sigma=0$ MPa). The inset of Fig. 2a shows that the first peak of $G(r)$ shifts to lower r after LSP, indicating that the 1st atomic shell in BMGs was obviously compressed.

The isotropic atomic packing structure of BMGs can become anisotropic under loading [5], and the atomic strain ε_i of the ith atomic shell caused by the applied stress σ can be calculated according to the following eq. [4]:

$$\varepsilon_i(\varphi)=\frac{r_i(0,\varphi)-r_i(\sigma,\varphi)}{r_i(\sigma,\varphi)} \tag{1}$$

The angular variation of strain can be fitted to the following expression [4]:

$$\varepsilon_i(\varphi)=\varepsilon_{i\,x}\,sin^2\varphi+\gamma_{i\,xz}sin\varphi cos\varphi+\varepsilon_{i\,z}\,cos^2\varphi \tag{2}$$

Fig. 2b shows the atomic strain distribution in different directions (φs, as shown in Fig. 1a) of LSP-deformed before loading. The strain distribution of the 1st atomic shell has a good consistency with that of the 3rd atomic shell, indicating a similar mechanical response to LSP process shared by the 1st and the 3rd atomic shells. The inhomogeneous strain distribution reveals that LSP induced anisotropic residual stress in the BMG sample [12], leading to the anisotropic atomic packing [8].

To analyze the LSPed atomic-structure evolution in compression tests, atomic strain variation along the compressive loading direction ($\varphi=90°$) in the as-cast BMG, LSP-center, and LSP-deformed zone are extracted and compared, the 1st shell strain results are shown in Fig. 2c. For the as-cast BMG and LSP-center, the atomic strain varies linearly with the stress, which agrees well with previous studies [4,6–8]. However, the strain variation in LSP-deformed zone is quite complicated. Firstly, the initial strain of LSP-deformed is not 0, showing the residual strain in 1st shell. Secondly, dual-step variation with inflection point at $\sigma_i=$ ~400 MPa was observed during compressive loading (hereafter $\sigma<400$ MPa is called step A and 400 MPa $<\sigma<1200$ MPa is called step B), indicating that an atomic-structure transformation appears around 400 MPa. When the applied stress $\sigma>1200$ MPa, the atomic strain became constant, and the BMG structure yielded [8]. Young's modulus E can be estimated from the slope of the stress-strain curves in Fig. 2c, and the results are presented in the inset of Fig. 2c. Compared with as-cast sample, E values of the LSP-center and the step A of LSP-deformed zone are much lower, indicating that the LSP process clearly decreases the atomic bond strength [16] and softens the atomic-structure. Such softening in LSP-center shows that LSP could change BMG structure as deep as 1500 μm. In step B, the E recovered, suggesting the re-hardening of the structure.

Moreover, in as-cast BMG and LSP-center, the higher stress-strain curve slope of 1st shell than that of 3rd shell (shown in Fig. S2a and S1b) indicates that 1st shell is stiffer than 3rd shell. This phenomenon demonstrates the structure heterogeneity. However, in LSP-deformed zone, there is some overlap of the stress-strain curves between 1st shell and 3rd shell (shown in Fig. S2c), showing the similar Es in 1st and 3rd shell. Combined with the similar residual strain distribution between 1st shell and 3rd shell in LSP-deformed zone (Fig. 2b). We found that LSP process clearly weakened the structural heterogeneity between the 1st shell and high order shells, indicating an atomic-structural homogenization in BMG. To further understand the atomic-structural homogenization and the mechanism of the dual-step atomic strain variation in LSP-deformed zone, the flow units, which could be regarded as the basic deformation units in MGs [17–19], is necessary to be

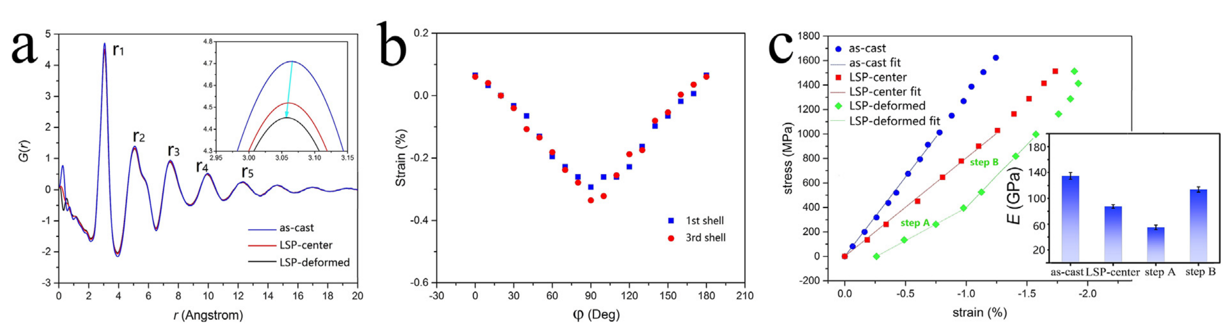

Fig. 2. (a) $G(r)$ of as-cast BMG, LSP-center and LSP-deformed. (b) Strain distribution of the 1st shell and 3rd shell of LSP-deformed. (c) Experiment and three-parameter viscoelastic model fit stress-strain results in the 1st shell of as-cast sample, LSP-center, and LSP-deformed zone respectively, the inset is the Young's modulus variation of 1st shell.