Free Volume in a cold-worked Zr$_{55}$Cu$_{30}$Ni$_{5}$Al$_{10}$ Bulk Metallic Glass

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1 Introduction

It was reported that the volume fluctuation called the free volume is introduced into a plastically deformed amorphous alloy and metallic glass [1, 2]. However, the change in the glass structure of a deformed metallic glass has been insufficiently studied for recent years. The discovery of bulk metallic glasses (BMGs) gives us much opportunity to elucidate the structural properties in a deformed metallic glass. The high intensity x-ray of PF enables us to obtain new information of the details of plastically deformed BMGs.

2 Experiment

The Zr$_{55}$Cu$_{30}$Ni$_{5}$Al$_{10}$ BMG was prepared by the tilted copper mold-casting technique [3] with a size of 14 mm in diameter and 30 mm in length. Two disks with a thickness of about 2 mm were cut from the rod shape BMG. One piece was thinned down into a fraction of about 90% by cold working at room temperature and another was regarded as the standard sample. The change in the glass structure of a deformed metallic glass was obtained. The result was interpreted as the decrease of free volume.

3 Results and Discussion

The reduced radial distribution function, $G(r)$, was calculated by Fourier transformation of $S(Q)$. Figure 1 exhibits, $Ql(Q)=Q(S(Q)-1)$, of standard as-cast and 10% cold-worked BMGs and the difference of $S(Q)$, $\Delta S(Q)=S_{cw}(Q)-S_{as}(Q)$. The change in $S(Q)$ representatively appears around its first peak, i.e. a peak shift to lower side and a small broadening of peak. The corresponding $G(r)$’s are shown in Fig. 2 together with the difference, $\Delta G(r)$. $G_{as}(r)$ and $G_{cw}(r)$, meaning that the amplitude of $G_{as}(r)$ became smaller than the $G_{cw}(r)$. The result suggests that the topological disorder of the as-cast BMG increased by cold working. The change in the glass structure by the structural relaxation was quantitatively investigated by the atomic level stress model [4]. Following this model, the $\Delta G(r)$ for structural relaxation was expressed as,

$$\Delta G(r) = -\gamma r^2 \partial^2 G_{as} / \partial r^2 \left( \langle p^2 \rangle_\text{as} - \langle p^2 \rangle_\text{relax} \right),$$

where $\langle p^2 \rangle$ is the fluctuation of the atomic level hydrostatic pressure, and $\gamma$ is the $r$-dependent parameter approximately equivalent to a constant over first peak of $G(r)$. The $G_{as}(r)$ is the reduced radial distribution function from the region with almost 0 pressure, and it is actually approximated by the $G(r)$ in as-cast state. In case of structural relaxation, the $\Delta G(r)$ changed in phase to a minus second derivative of $G_{as}(r)$, $-\partial^2 G_{as} / \partial r^2$, and consequently a positive change in $\langle p^2 \rangle_\text{as} - \langle p^2 \rangle_\text{relax}$ was obtained. The result was interpreted as the decrease of topological disorder, i.e. the fluctuation of atomic level stress. Figure 3 plots $-\partial^2 G_{as} / \partial r^2$ against the distance, $r$. 

Fig. 1: $Ql(Q)$’s of as-cast, deformed BMGs and the difference of $S(Q)$.

Fig. 2: $G(r)$’s of as-cast, deformed BMGs and the difference of $G(r)$.

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where the curve was smoothed by cubic spline functions after the subtractive calculation. We can easily see an anti-phase behavior of $-\partial^2 G_0/\partial r^2$ against $\Delta G(r)$, meaning that $<p_\text{as}^2>-<p_{\text{cw}}^2>$ becomes a negative value, and it is an opposite sign to the structural relaxation. Thus we conclude that the volume fluctuation, which is characterized by the atomic-level stress, increases after plastically deforming BMG. The result consists with the volume and enthalpy change of cold-worked Zr$_{55}$Cu$_{30}$Ni$_{5}$Al$_{10}$ BMG [5].

References

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