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Effect of hydrostatic pressure on reinforcing bulk metallic glasses investigated by synchrotron radiation and molecular dynamics simulations

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ABSTRACT

Volume change of bulk metallic glasses (BMGs) during the repeated loading and unloading was investigated using in situ high-pressure synchrotron diffraction. Molecular dynamics simulations, which were used for further research of the microstructure change, were presented on an approximately 5.0×10^5 atom sample of an amorphous $Fe_{80}P_{20}$ model. The results show that the first compression process includes irreversible annihilation of free volume and elastic volume change. The main form of annihilation of free volume is that smaller atoms are extruded into the larger atomic clearance. Hydrostatic pressure can make the microstructure of BMGs more stable and dense. As a result of the decrease in free volume, hardness and bulk modulus of BMGs treated with hydrostatic pressure are obviously improved.

1. Introduction

Bulk metallic glasses (BMGs), with unique advantages of possessing isotropic properties, high strength, low coefficient of friction, high wear resistance and high corrosion resistance, are expected to extend their applications to several specific fields [1–3]. Thus, studies on reinforcing amorphous materials are particularly important. As such, we propose an effective reinforcement method for amorphous materials. Hydrostatic pressure acts comprehensively and evenly on the surface of all components. An increase in this type of stress can make the volume of objects smaller but will not affect their shapes, which is beneficial for the annihilation of free volume in amorphous materials. Hardness and bulk modulus of amorphous materials increase with the reduction of free volume [4–6]. Therefore, the purpose of reinforcing amorphous materials can be achieved. In this paper, the effect of hydrostatic pressure on reinforcing amorphous materials was investigated through synchronous radiation experiments, molecular dynamics (MD) simulations and nanoindentation.

2. Experiment

Powder was carefully scraped using a 4Cr13 stainless-steel scalpel from an amorphous rod of $Fe_{80}P_{11}C_9$ BMG in at%, which was prepared by copper mold casting for pressure experiments [7]. The amorphous nature of the scraped powder was confirmed by X-ray diffraction (XRD). Pressure was generated by using a diamond anvil cell. The culet of the diamond anvil was 400 μm in diameter. Amorphous powder sample, together with the pressure-calibrator ruby, was loaded into a 120 μm-diameter hole of a T301 stainless steel gasket, which was preindented to a thickness of approximately 40 μm. Silicone oil was used as pressure-transmitting media. In situ angle-dispersive XRD (ADXRD) measurements were carried out in the Beijing Synchrotron Radiation Laboratory. Debye rings were recorded by using an image plate in transmission mode, and XRD patterns were integrated from the images using FIT2D software [8]. The size of the X-ray spot was $45\ \mu m^2 \times 26\ \mu m^2$. A Li detector was used to collect diffraction signals under various pressure values. Experimental pressure was determined from the position of the diffraction peak of ruby.

In addition, we performed classical MD simulations for amorphous $Fe_{80}P_{20}$, which further studied the microstructure change. Glass sample was prepared by melt quenching. A large-scale atomic/molecular massively parallel simulator with an embedded-atom method potential [9] was used to carry out MD simulations. After relaxation at 2000 K for 2 ns which ensures the chemical

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homogeneity, the melt was quenched to 300 K, with a cooling rate of 0.01 K/ps. Hydrostatic pressure was applied to the $Fe_{80}P_{20}$ sample, with dimensions of 16.3 $nm^3 \times 18.2$ $nm^3 \times 19.6$ nm^3 and $\sim 5.0 \times 10^5$ atoms. Volume change of block sample was recorded under different pressure values.

3. Results and discussion

Stability of $Fe_{80}P_{11}C_9$ BMGs under high pressure at room temperature was investigated using ADXRD. Fig. 1(a) shows the synchrotron radiation XRD spectrum under different pressure values during the loading and unloading processes. In this figure, the broad diffusive amorphous halo obviously shifts to a higher angle with the increase in pressure, which shows the compression behavior of bulk amorphous alloys. Then, the amorphous halo shifted to a lower angle during the unloading process. No new diffraction peak was detected from curves up to approximately 32 GPa. The structure of BMGs was stable at room temperature, and compression behavior did not affect the amorphous structure. However, the broad diffusive amorphous halo cannot return to its original position when pressure decreases to 0 GPa after the loading process. The original broad diffusive amorphous halo appeared at $2\theta = \sim 17.34$ and $2\theta = \sim 17.67$ after the loading and unloading processes, respectively. This finding indicates that the microscopic structure has changed, and that the structure became denser. The same results were obtained in the pressure experiments for $Co_{56}Ta_9B_{35}$ and $Yb_{60}Ca_{2.5}Zn_{20}Mg_{17.5}$ BMGs, as shown in Fig. 1(b).

The peak position θ_{max} of the broad halo reflected change in interatomic spacing d_{max} ($d_{max} = \lambda/(2 \sin \theta_{max})$), where λ is equal to 0.61993 Å. Volume change was determined by the reduced volume ratio of the sample V_P/V_0, which could be calculated by the parameter of $(d_{max,P}/d_{max,0})^3$, where the subscript P and 0 denote a given high-pressure and zero-pressure conditions, respectively [10,11]. Therefore, relative volume change $\Delta V/V_0 = V_P/V_0 - 1$ could be plotted as a function of pressure at ambient temperature. The loading and unloading processes were repeated twice on the amorphous $Fe_{80}P_{11}C_9$. Fig. 2(a) shows the $\Delta V/V_0 - P$ relationship of the two loading and unloading processes from 0 GPa to approximately 32 GPa. Reference V_0 was the initial volume in all courses. The volume after the first loading and unloading processes was

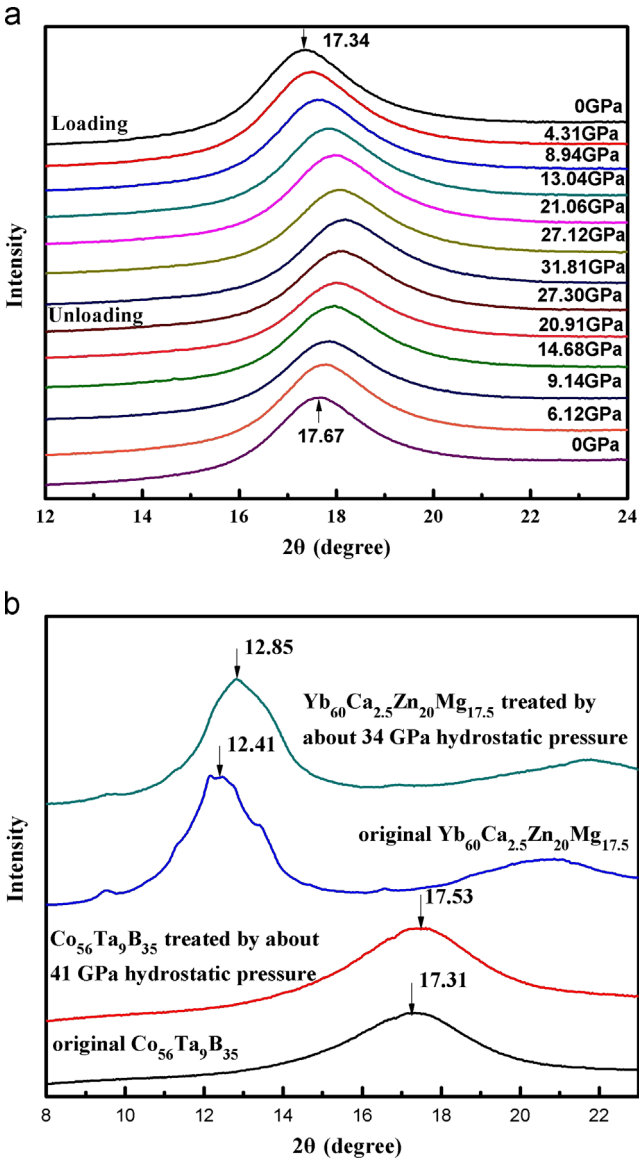

Fig. 1. (a) In situ ADXRD patterns of $Fe_{80}P_{11}C_9$ BMG at different pressure values in the loading and unloading processes. (b) In situ ADXRD patterns of $Yb_{60}Ca_{2.5}Zn_{20}Mg_{17.5}$ and $Co_{56}Ta_9B_{35}$ BMGs before and after hydrostatic processing.

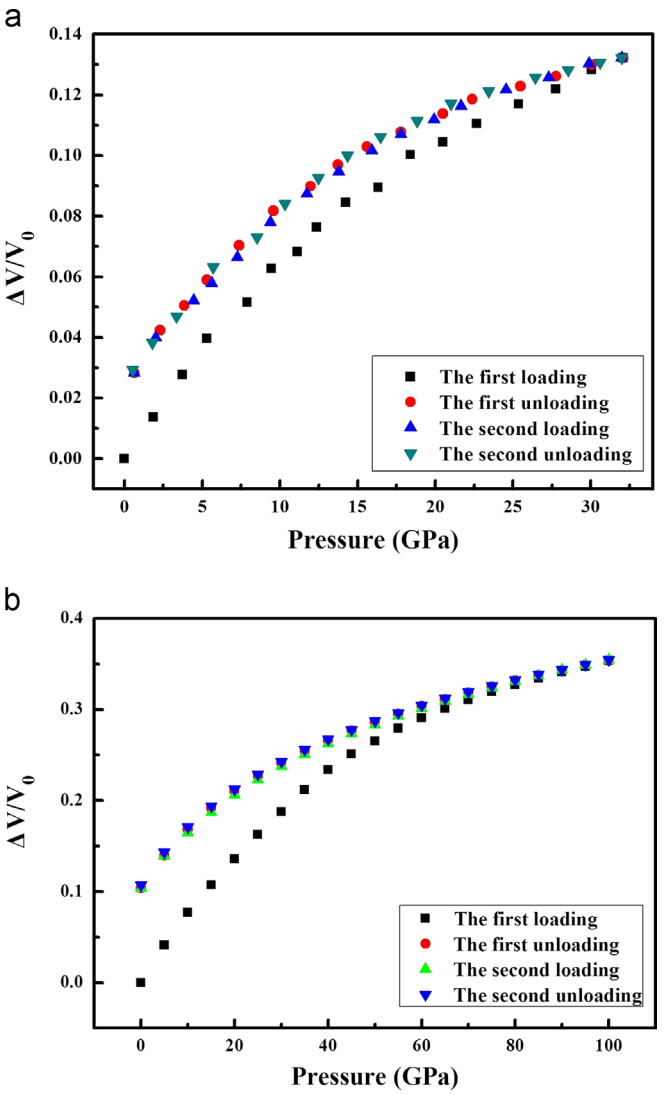

Fig. 2. (a) The experimental pressure dependence of relative volume change $\Delta V/V_0$ of $Fe_{80}P_{11}C_9$ BMG at ambient temperature. (b) The simulative pressure dependence of relative volume change $\Delta V/V_0$ of $Fe_{80}P_{20}$ BMG at ambient temperature.