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# Short-range structure of $\text{Zr}_{41}\text{Ti}_{14}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5}$ glass prepared by shock wave

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Short-range structure of a  $\text{Zr}_{41}\text{Ti}_{14}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5}$  bulk metallic glass prepared by shock-wave treatment was investigated by x-ray diffraction using synchrotron radiation with a wavelength of  $0.11271 \text{ \AA}$ . The radial distribution function was obtained from  $S(Q)$  with a large  $Q$  value up to  $20 \text{ \AA}^{-1}$ . The oscillation in  $S(Q)$  of the glass definitely persists up to  $Q \sim 14 \text{ \AA}^{-1}$ . The shoulder on the high  $Q$  side of the second peak is observed in the bulk glass. It is found that the glass has higher coordination numbers in the range of  $r \sim 2.4\text{--}5.6 \text{ \AA}$  and lower numbers in the range of  $r \sim 5.6\text{--}9.5 \text{ \AA}$  than those for a water-quenched glass while the shell distances are similar in both glasses prepared by shock-wave and water-quenching methods. In the shock-waved glass, atomic configurations in the first, fourth, or fifth coordination shells are modified, i.e., atoms are packed denser in the first two coordination shells and less (or more free volume) in the third and fourth coordination shells as compared to those for the water-quenched glass. This atomic configuration for shock-waved glass might have different physical properties. © 2004 American Institute of Physics. [DOI: 10.1063/1.1763214]

Microstructure of metallic glasses is a long-standing issue for disordered materials.<sup>1,2</sup> The defect density contained in metallic glasses strongly depends on the sample preparation. According to the free volume theory in metallic glasses, the slower the cooling rate, the lower the free volume during the solidification process.<sup>3</sup> Most bulk metallic glasses (BMG), thickness larger than 1 mm, are prepared by copper mold casting or water-quenching, in which a cooling rate is about 100 K/s.<sup>4</sup> During shock-wave treatment, the alloy solidifies from high temperature in extreme short duration under extremely large pressure.<sup>5</sup> Consequently, different atomic configurations of BMG as compared to conventional preparation methods might be expected. It should be stressed that such shock-wave experiments are very difficult. In this letter, we report high resolution radial distribution function of a  $\text{Zr}_{41}\text{Ti}_{14}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5}$  bulk metallic glass, one of the most widely studied bulk metallic glasses,<sup>6</sup> prepared by shock-wave treatment in comparison with that of a water-quenching sample.

Bulk  $\text{Zr}_{41}\text{Ti}_{14}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5}$  amorphous alloys were prepared by water-quenching and shock-wave treatment as shown in the following. The ingots of water-quenched alloy

with nominal composition of  $\text{Zr}_{41}\text{Ti}_{14}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5}$  were prepared from a mixture of pure elements in an arc-melting furnace under a Ti-gettered Ar atmosphere. The ingots were remelted in quartz tube, and then were water quenched with a cooling rate of about 100 K/s to form a BMG of 10 mm in diameter. The structure of BMG was identified by x-ray diffraction (XRD) and no crystalline phase was detected. The preparation method of the BMG by shock wave was relatively complicated. First, we prepared a bulk amorphous alloy of 18 mm in diameter by water-quenching. Small cylinders with a length of 10 mm were cut out from the alloy rod. The full amorphous structure of the cylinders was verified by XRD. These small cylinders were then utilized to carry out impact experiments of hypervelocity by a two-stage light gas gun. The amorphous cylinder was embedded in the cylindrical concave of copper cylinder with diameter of 40 mm. Their axes were superposition to each other. A steel cylinder was mounted tightly beneath the copper cylinder and an aluminum cylinder was mounted tightly beneath the steel cylinder. The polyethylene cylinder was mounted tightly beneath the aluminum cylinder. Finally, the assembly of these cylinders was inserted into a steel cylinder with 40 mm inside diameter and 120 mm outer diameter. The end against impact direction of the cylinder assembly was ringed. The other end was fixed by bolts. The above content described the recovery

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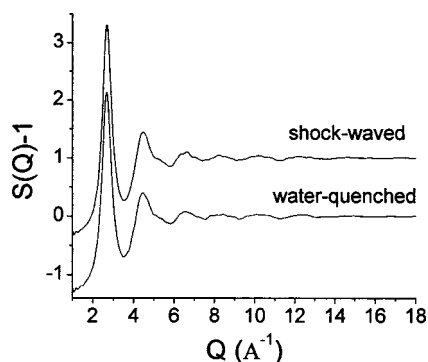


FIG. 1. Structure factor,  $S(Q)-1$ , of  $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$  bulk glass prepared by shock-wave and water-quenching methods.

erable device in detail. The amorphous cylinder samples were impacted by the hypervelocity copper and aluminum cylinder projectiles of 22 mm diameter and 2 mm thickness at a speed about 3 km/s. The axis of the cylinder projectile is coincident with the steel cylinder assembly. The impact pressure reached up to about 100 GPa. At the same time, the impact temperature can exceed about 3000 K. The duration of the shock wave was about  $10^{-6}$  s. The surface of the recovered amorphous cylinder was slightly polished and the composition of the recovered amorphous sample was examined to be the same as the water-quenched sample within the experimental uncertainty.

To obtain high resolution radial distribution function information, XRD data with a large  $Q$  value are necessary.<sup>7</sup> Thus, x-ray diffraction measurements were performed at experimental station BW5 at HASYLAB at DESY using a short wavelength of 0.11271 Å. Samples were measured at room temperature and illumination time was 90 s. XRD patterns were recorded by a two-dimensional detector MAR image plate in asymmetric mode (to get high  $Q$  range). The XRD data were integrated by using the FIT2D program.<sup>8</sup> The background was properly subtracted and the image was integrated into  $Q$  space. The data were corrected for inelastic scattering and the total structural factor was obtained by using the Faber-Ziman formula.<sup>9</sup> The pair correlation functions,  $g(r)$ , from corresponding  $S(Q)$  were obtained by using the MCGR program based on Monte Carlo algorithms.<sup>10</sup>

Figures 1 and 2 show structure factor,  $S(Q)-1$ , of  $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$  bulk glass prepared by shock-wave and water-quenching methods and their difference curve, respectively.  $S(Q)$  curves look very similar for both glasses in

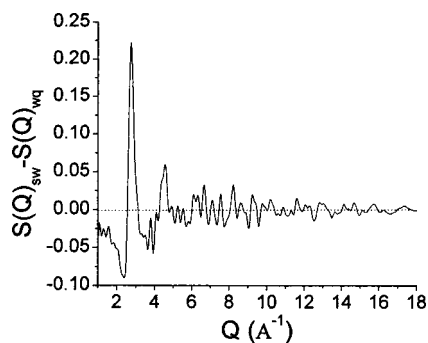


FIG. 2. The difference of structure factor of  $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$  bulk glass prepared by shock-wave,  $S(Q)_{sw}$ , and water-quenching,  $S(Q)_{swq}$ , methods.

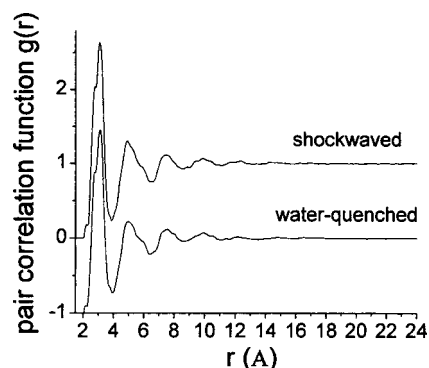


FIG. 3. Atomic pair correlation function,  $g(r)$ , of  $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$  bulk glass prepared by shock-wave and water-quenching methods in a large range of atomic distance.

term of peak intensity, position, and width. The oscillation in  $S(Q)$  of both glasses definitely persists up to  $Q \sim 14 \text{ Å}^{-1}$ . The shoulder on the high  $Q$  side of the second peak, which is the common feature in  $S(Q)$  of conventional metallic glasses, is still observed in both bulk glasses. The fine difference in  $S(Q)$  can be detected in Fig. 2, where the two clear peaks are revealed at  $Q \sim 2.8$  and  $4.5 \text{ Å}^{-1}$ . At large  $Q$  values, no obvious difference in  $S(Q)$  was observed between both samples. Figures 3 and 4 show the atomic pair correlation function,  $g(r)$ , of  $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$  bulk glass prepared by shock-wave and water-quenching methods in a large range of atomic distance and their difference curve, respectively. Figure 5 shows the atomic pair correlation function,  $g(r)$ , of  $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$  bulk glass prepared by shock-wave and water-quenching methods in a range of atomic distance 2–4 Å together with interatomic bond lengths and corresponding weight factors.  $g(r)$  curves of both glasses display similar features, i.e., the first peak split into two peaks and the second peak having a few small humps. The fine difference is illustrated in Fig. 4. The glass after shock-wave treatment clearly shows a higher  $g(r)$  in the first two coordination shells  $r \sim 2.4\text{--}5.6 \text{ Å}$  as compared to the water-quenched glass. The relative change in the first peak height is about 10%, but the change in the second peak is of the order of 20%. In higher coordination shells,  $r \sim 5.6\text{--}9.5 \text{ Å}$ ,  $g(r)$  in water-quenched glass becomes higher. For  $r > 10 \text{ Å}$ , no obvious difference was detected. For a pure structural relaxation effect by annealing treatment at a temperature far below crystallization temperature, the difference in  $g(r)$  could remain up to  $r \sim 20 \text{ Å}$ .<sup>11</sup> This indicates that

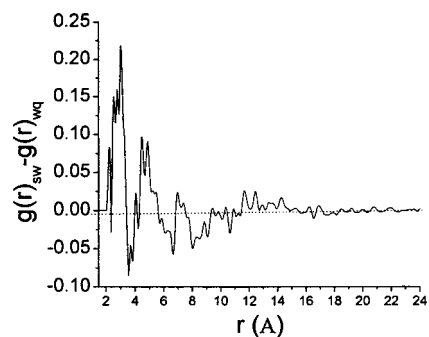


FIG. 4. The difference of atomic pair correlation function of  $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$  bulk glass prepared by shock-wave,  $g(r)_{sw}$ , and water-quenching,  $g(r)_{swq}$ , methods in a large range of atomic distance.

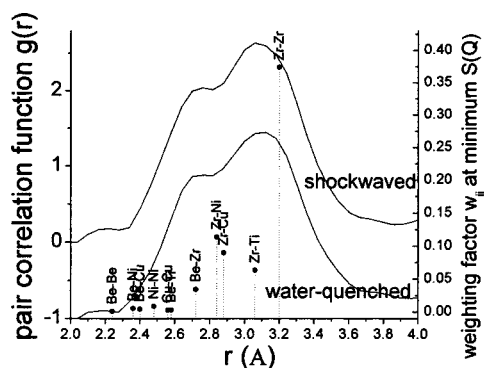


FIG. 5. Atomic pair correlation function,  $g(r)$ , of  $\text{Zr}_{41}\text{Ti}_{14}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5}$  bulk glass prepared by shock-wave and water-quenching methods in a range of atomic distance 2–4 Å together with interatomic bond lengths and corresponding weight factors.

shock-wave treatment mainly modifies the atomic configuration in the first, fourth, or fifth coordination shells. In the five-component  $\text{Zr}_{41}\text{Ti}_{14}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5}$  alloy the measured structure factor  $S(q)$  and the estimated  $g(r)$  curves represent the weighted sum of the 15 partial functions  $S_{ij}(q)$  and  $g_{ij}(r)$ :<sup>7</sup>

$$S(q) = \sum_i \sum_j w_{ij} S_{ij},$$

$$g(r) = \sum_i \sum_j w_{ij} g_{ij} \quad \text{with} \quad w_{ij} = c_i c_j f_i f_j / \left( \sum_i c_i f_i \right)^2, \quad (1)$$

where  $w_{ij}$ ,  $c_i$ , and  $f_i$  are the weight factor for the  $i$ – $j$  correlation, the concentration fraction, and atomic scattering length of the  $i$ th atom in the alloy, respectively. An interpretation of the data for the multicomponent alloy is therefore difficult and ambiguous. However, the subpeak on the low  $r$  side ( $r \sim 2.7$  Å) of the first peak in Fig. 5 mainly corresponds to the Zr–Be correlation together with Zr–Ni and Zr–Cu correlations. The peak at  $r \sim 3.1$  Å is mainly contributed by the Zr–Zr together with Zr–M ( $M = \text{Ti}, \text{Cu}, \text{and Ni}$ ) correlations. The first coordination number,  $N = 14.4$  and 14.0, was estimated from a distance of 2.1–3.7 Å for  $\text{Zr}_{41}\text{Ti}_{14}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5}$  bulk glasses prepared by shock-wave and water-quenching methods, respectively. Such higher first coordination numbers strongly indicate a dense packing atomic structure in the BMG. For the higher shells determination of  $N$  becomes ambiguous because it is difficult

to set the onset and end of shells in  $g(r)$  curves. However, it is clear that after shock-wave treatment, the glass has higher coordination numbers in the range of  $r \sim 2.4$ –5.6 Å and lower ones in the range of  $r \sim 5.6$ –9.5 Å than those in the water-quenched glass in Fig. 4.

In summary, the short-range structure of the  $\text{Zr}_{41}\text{Ti}_{14}\text{Cu}_{12.5}\text{Ni}_{10}\text{Be}_{22.5}$  bulk metallic glass prepared by shock-wave treatment was investigated by x-ray diffraction using synchrotron radiation. The radial distribution function was obtained from  $S(Q)$  with a large  $Q$  value up to  $20 \text{ Å}^{-1}$ . The oscillation in  $S(Q)$  of the glass definitely persists up to  $Q \sim 14 \text{ Å}^{-1}$ . The shoulder on the high  $Q$  side of the second peak is observed in the bulk glass. It is found that the glass has higher coordination numbers in the range of  $r \sim 2.4$ –5.6 Å and lower numbers in the range of  $r \sim 5.6$ –9.5 Å than those for the water-quenched glass while the shell distances are similar in both glasses. Under shock-wave treatment, i.e., rapid solidification under high pressure, atomic configurations in the first, fourth, or fifth coordination shells are modified, i.e., the atoms in glass are packed even denser in the first two coordination shells and less (or more free volume) in the third and fourth coordination shells as compared to those for conventional water-quenched glass. This atomic configuration for shock-waved glass might have different physical properties, which are in progress.

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