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Direct observation of the changes in atomic arrangement of $Cu_{50}Zr_{50}$ metallic glass during tensile deformation by EXAFS

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Abstract

The purpose of this research is to investigate the micro-mechanism of anelastic behavior of metallic glass. The changes of atomic arrangement in $Cu_{50}Zr_{50}$ metallic glass were observed directly by EXAFS method during tensile deformation. The transmission-mode EXAFS measurements around Zr K-edge and Cu K-edge of the sample in various amounts of tensile deformation conditions were done. The interatomic distance between Cu–Zr increased, and that between Zr–Zr decreased simultaneously, with the amount of tensile deformation increase of the sample at first stage of deformation. When the atomic distances reached certain values, respectively, they recovered to the initial values of no tensile deformation condition at first stage, and then the atomic distances changed in same manner as the first stage of deformation, respectively.

Keywords: Metallic glass; Anelasticity; $Cu_{50}Zr_{50}$ alloy; Tensile deformation; EXAFS; Radial structure function; Short range structure change

1. Introduction

The anelastic behaviors of amorphous alloys had been well known from the early 1970s [1]. The researches on micro-mechanism of anelasticity of amorphous alloy were done by computer simulation [2] and EXAFS method [3]. The changes of atomic arrangement around Pd atom in $Pd_{83}Si_{17}$ amorphous alloy during tensile deformation were done [3]. Recently, Inoue et al. have succeeded in synthesizing bulk glassy alloys (BGAs) [4]. In those BGAs, Zr-based alloys exhibit good glass forming ability, high strength and ductility [5]. Deformation behavior of bulk metallic glass both in elastic region and plastic region are different from those of crystalline alloys. Computational investigations of deformation of bulk metallic glass were described successfully for showing the insight during deformation [6–8]. The purpose of this research is to investigate the micro-mechanism of anelastic deformation behavior of metallic glass. The changes of atomic arrangement in $Cu_{50}Zr_{50}$ metallic glass were observed directly by EXAFS method during tensile deformation.

2. Methods

A master alloy of $Cu_{50}Zr_{50}$ was made by arc melt in high purity argon atmosphere. A metallic glass sample in the shape of ribbon (1.5 mm width and 25 μm thickness) was made by rapid quenching method using single roller in argon atmosphere. The size of copper roller was 200 mm in diameter. Rotation speed of roller was 4000 rpm. Tensile deformation of the sample was made by using special equipment (Imoto: IMC-0087) adopted for EXAFS measurements. The length between two chucks for sample holding was 20 mm. The cross-head speed was 1 mm/min. The amount of strain of the sample was checked semi-quantitatively by using strain gauge (Kyowa: SKF-22111) and its amplifier (Kyowa: UCAM-5BT). The amount of strain increases with grade number, i.e. grades 1–7, here grade 1 indicates that the strain of the sample equals 0.0%, and grade 7 indicates that the strain of the sample almost equals 1.2%. The transmission-mode EXAFS measurements of the sample in various amounts of tensile deformation conditions around Zr K-edge and Cu K-edge were done at Beam-Line 10B of Photon Factory, KEK in Tsukuba and Beam-Line 7C of National Synchrotron Radiation Laboratory, University of Science and Technology of China in Hefei. By Fourier transform of the measured EXAFS signals, the radial structure functions (RSF) around the Zr atom and Cu atom were obtained.

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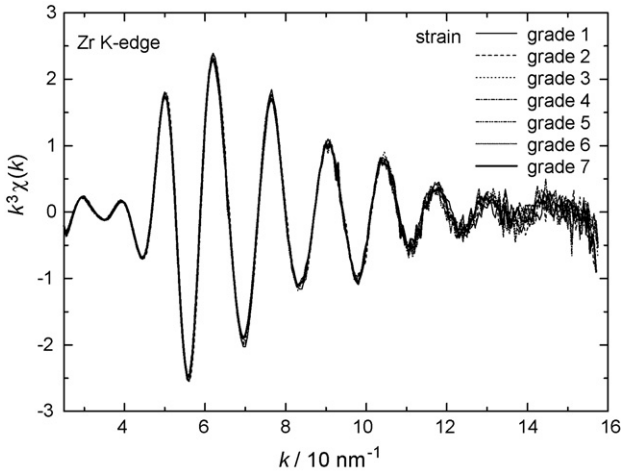

Fig. 1. k^3-weighted Zr K-edge EXAFS, $k^3\chi(k)$, of $Cu_{50}Zr_{50}$ metallic glass ribbon in the various amount of strain conditions during tensile deformation. The amount of strain increases with grade number: grade 1 (strain is equal to 0.0%) to grade 7 (strain is equal to almost 1.2%).

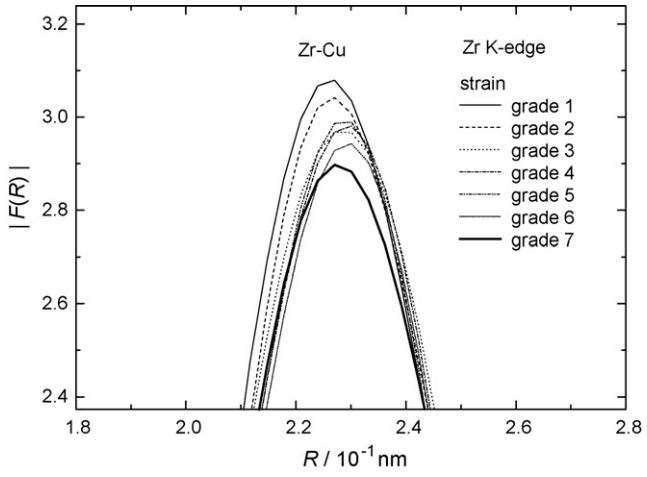

Fig. 3. Radial structure function (Fourier transform of EXAFS $k^3\chi(k)$), $F(r)$, magnified near main peak (Zr–Cu correlation) around the Zr atom of $Cu_{50}Zr_{50}$ metallic glass ribbon in the various amount of strain conditions during tensile deformation. The amount of strain increases with grade number: grade 1 (strain is equal to 0.0%) to grade 7 (strain is equal to almost 1.2%).

3. Results

The backgrounds-subtracted Zr K-edge EXAFS spectra, $k^3\chi(k)$ versus k (nm^{-1}), of $Cu_{50}Zr_{50}$ metallic glass ribbon in the various amounts of strain conditions are shown in Fig. 1. The amount of strain increases with grade number, i.e. grades 1–7, here grade 1 indicates that the strain of the sample equals 0.0%, and grade 7 indicates that the strain of the sample almost equals 1.2%. The radial structure functions (RSF), $F(r)$, around the Zr atom provided by the Fourier transform of Zr K-edge EXAFS spectra are shown in Fig. 2. RSF has a main peak at 0.22 nm together with a small peak of a second coordination shell at 0.29 nm. The first peak is considered to be Zr–Cu correlation and the second peak is considered to be Zr–Zr correlation. These peak positions are shifted a few hundreds of a nanometer from actual interatomic distances because of the phase shift, respectively. The interatomic distance between Cu–Zr increased gradually with the amount of tensile deformation increase in $Cu_{50}Zr_{50}$ metallic glass at first stage of deformation as shown in Fig. 3, and that between Zr–Zr had an inclination to decrease gradually with the amount of tensile deformation increase as shown in Fig. 4. When these interatomic distances reached to certain values, respectively, at strain condition of 1.2%, they recovered close to the initial values of no tensile deformation condition at first stage, respectively. This means that the interatomic distance between Cu–Zr increased, and that between

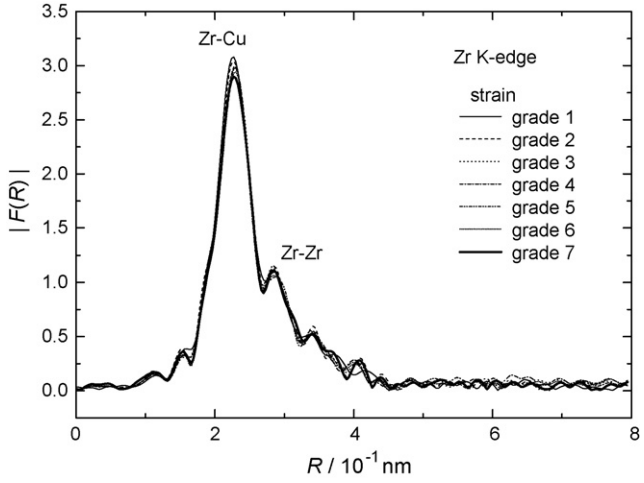

Fig. 2. Radial structure function (Fourier transform of EXAFS $k^3\chi(k)$), $F(r)$, around the Zr atom of $Cu_{50}Zr_{50}$ metallic glass ribbon in the various amount of strain conditions during tensile deformation. The amount of strain increases with grade number: grade 1 (strain is equal to 0.0%) to grade 7 (strain is equal to almost 1.2%).

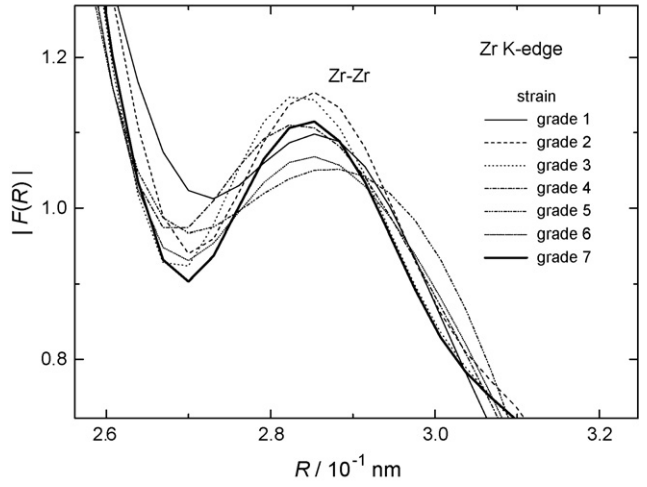

Fig. 4. Radial structure function (Fourier transform of EXAFS $k^3\chi(k)$), $F(r)$, magnified near second peak (Zr–Zr correlation) around the Zr atom of $Cu_{50}Zr_{50}$ metallic glass ribbon in the various amount of strain conditions during tensile deformation. The amount of strain increases with grade number: grade 1 (strain is equal to 0.0%) to grade 7 (strain is equal to almost 1.2%)

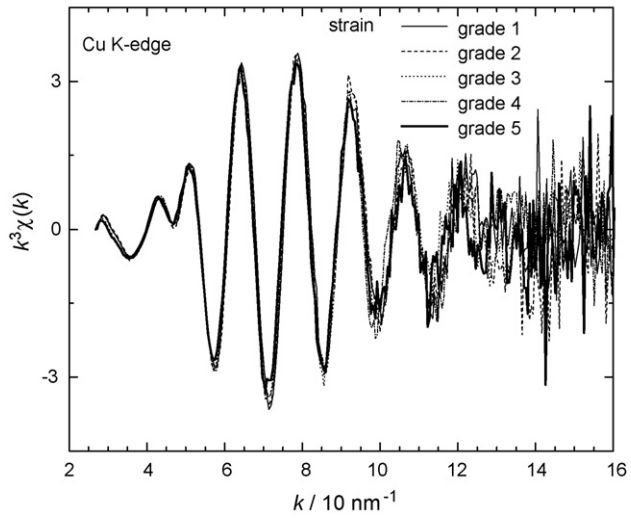

Fig. 5. k^3-weighted Cu K-edge EXAFS, $k^3\chi(k)$, of $Cu_{50}Zr_{50}$ metallic glass ribbon in the various amount of strain conditions during tensile deformation. The amount of strain increases with grade number: grade 1 (strain is equal to 0.0%) to grade 5 (strain is equal to almost 1.2%).

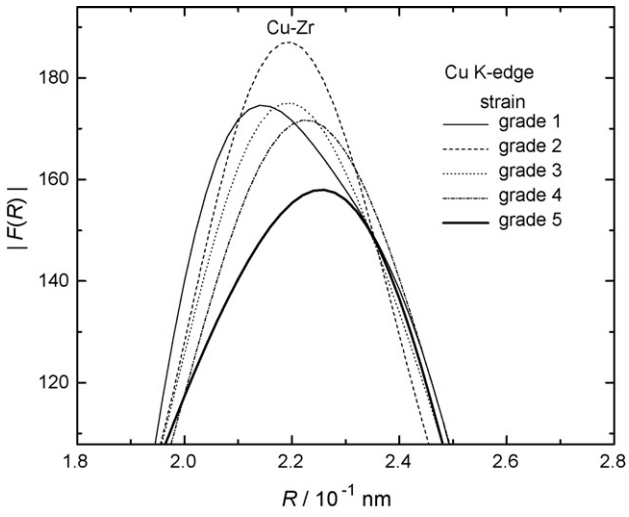

Fig. 7. Radial structure function (Fourier transform of EXAFS $k^3\chi(k)$), $F(r)$, magnified near main peak (Cu–Zr correlation) around the Cu atom of $Cu_{50}Zr_{50}$ metallic glass ribbon in the various amount of strain conditions during tensile deformation. The amount of strain increases with grade number: grade 1 (strain is equal to 0.0%) to grade 5 (strain is equal to almost 1.2%).

Zr–Zr decreased, with the amount of tensile deformation increase in $Cu_{50}Zr_{50}$ metallic glass again. The backgrounds-subtracted Cu K-edge EXAFS spectra, $k^3\chi(k)$ versus k (nm^{-1}), of $Cu_{50}Zr_{50}$ metallic glass ribbon in the various amounts of strain during tensile deformation are shown in Fig. 5. The RSFs, $F(r)$, around the Cu atom provided by the Fourier transform of Cu K-edge EXAFS spectra are shown in Fig. 6. The main peak position, Cu–Zr interatomic distance, increased gradually with the amount of tensile deformation increase of $Cu_{50}Zr_{50}$ metallic glass as shown in Fig. 7. In this case, recovery of Cu–Zr interatomic distance was not observed during the tensile deformation increase.

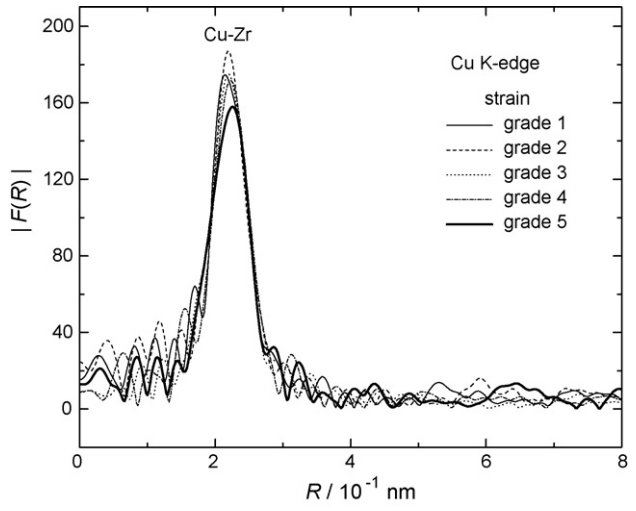

Fig. 6. Radial structure function (Fourier transform of EXAFS $k^3\chi(k)$), $F(r)$, around the Cu atom of $Cu_{50}Zr_{50}$ metallic glass ribbon in the various amount of strain conditions during tensile deformation. The amount of strain increases with grade number: grade 1 (strain is equal to 0.0%) to grade 5 (strain is equal to almost 1.2%).

4. Discussions

The result of EXAFS measurements suggests that the Zr–Cu interatomic distance increase and the Zr–Zr interatomic distance decrease with the amount of tensile deformation increase, and then stress relaxation occurred in atomic level during tensile deformation as shown in Figs. 3 and 4. When the interatomic distances reached certain values, respectively, they recovered close to the initial values of no tensile deformation condition at the first stage, respectively. The same kind of behavior as this EXAFS result in Cu–Zr metallic glass was found by Ogata et al. [6] by using computer simulation. Atomic simulation of shear deformation in Cu–Zr bulk metallic glass revealed that the stress–strain curve has small discontinuous points, where the relaxation occurs at the stress accumulated part by shear deformation [6]. From the computer simulation and the results of our EXAFS measurements the following hypothesis seems to be available, i.e. the interatomic distance between Cu–Zr increase, and that between Zr–Zr decreases, with the amount of tensile deformation increase of the $Cu_{50}Zr_{50}$ metallic glass sample at first stage of deformation. When the atomic distances reach certain values, respectively, they recover to the initial values of no tensile deformation condition at first stage and then the atomic distances may change in the same manner as the first stage of deformation, respectively. These relaxation behaviors of atomic arrangement during the deformation process may correlate with “anelasticity” of metallic glass. In the crystalline metals, when the stress increases over the elastic limit, a dislocation will appear and move, and then the elastic deformation changes to plastic deformation. The relaxation behavior of atomic arrangement during deformation process in metallic glass may be analogous to the appearance of dislocation under the stress over the elastic limit in crystalline metal. More EXAFS data over the relaxation behavior

during tensile deformation of metallic glass should be collected to make clear the mechanism of deformation in metallic glass.

Structure parameter fittings of the coordination number (N) and interatomic distance (r) for the first and second nearest coordination peaks in $F(r)$ around the Zr and Cu atoms are now in progress.

5. Conclusions

The interatomic distance between Cu–Zr increased, and that between Zr–Zr decreased, with the amount of tensile deformation increase of the $Cu_{50}Zr_{50}$ metallic glass sample at first stage of deformation. When the atomic distances reached certain values, respectively, they recovered to the initial values of no tensile deformation condition at first stage. These relaxation behaviors of atomic arrangement during tensile deformation process may correlate with "anelasticity" of metallic glass.

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