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Glass forming ability and bending plasticity evolutions in Zr-Co-Al bulk metallic glasses and their structural origin

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ABSTRACT

The effect of composition tuning on glass forming ability (GFA), mechanical properties and atomic structure in $Zr_xCo_{84-x}Al_{16}$ bulk metallic glasses (BMGs) with x = 51–58 has been investigated by using copper-mold suction casting, nanoindentation, high-energy X-ray diffraction, extended X-ray absorption fine structure experiments and ab initio molecular dynamics simulations, respectively. It is found that GFA firstly increases then decreases with increasing Zr content, exhibiting a maximum diameter of 7 mm with the Zr content of 55 and 56, while an abrupt reduction of bending plasticity occurs as the Zr content drops below 55. Both experimental and theoretical results find that GFA is remarkably enhanced, due to the abnormal reduction in the fractions of the Co-centered ⟨0, 2, 8, 1⟩, ⟨0, 3, 6, 2⟩ and ⟨0, 3, 6, 3⟩ polyhedra, and the denser atomic packing of Zr atoms around center Co atom, as the Zr content increases from 51 to 56. Meanwhile, the simultaneously improved plasticity is associated with the increased Co-centered ⟨0, 3, 6, 0⟩, and Al-centered ⟨0, 2, 8, 1⟩ and ⟨0, 3, 6, 2⟩ polyhedra, which provide more fertile sites for the nucleation of shear transformations. Further Zr addition to 58 increases remarkably the fractions of Zr- and Al-centered ⟨0, 1, 10, 2⟩ and ⟨0, 3, 6, 4⟩ polyhedra, and causes looser atomic packing of Co atoms around center Zr atom, leading to the reduction in GFA. However, the plasticity is not enhanced further but remains nearly constant, which may be related to the deteriorated effect on plasticity of the decreased fractions of Zr-centered ⟨0, 1, 10, 5⟩ and Co-centered ⟨0, 3, 6, 0⟩ polyhedra, and the increased fractions of Zr-centered ⟨0, 1, 10, 3⟩ and ⟨0, 2, 8, 4⟩ and Co-centered ⟨0, 2, 8, 0⟩ polyhedra. Compositional tuning, with internal structure tuned to favor both GFA and plastic flow, offers new possibilities in developing ductile BMG materials.

1. Introduction

Due to the lack of periodic atomic arrangement, bulk metallic glasses (BMGs) with high strength, excellent corrosion-resistance and good soft-magnetic property, are promising for future structural, chemical and magnetic applications as compared with their crystalline counterparts [1–3]. However, strain softening often causes catastrophic failure through unhindered shear localization, significantly limiting the actual application in structural materials [4–6]. Therefore, how to overcome the brittleness and enhance plasticity has become one of the most key issues in the community, and heterogeneous microstructures have been designed in virtue of the interaction between amorphous matrix and second phases to restrict the propagation of shear bands [7,8]. The second phases in the composites include in situ formation of crystalline dendrites during solidification, and ex situ addition of toughening particles [9]. However, the realization of ductilization/toughening of the composites still relies on a reasonable ductility of the amorphous matrix, which has recently been revealed to be related to the structural in-homogeneities in monolithic BMGs [10]. In order to improve ductility, the microstructure of BMGs should be tailored to suppress severe strain location and encourage spread-out distribution of the plastic flow. The increased structural in-homogeneity, as reflected by more “geometrically unfavored motifs” (GUMs) and higher vibrational degree of freedom, leads to improved deformability and restrained shear banding instability.

Tuning alloy composition has been confirmed to be an effective way to enhance the plasticity of monolithic BMGs through adjusting Poisson's ratio ν and the free-volume content. Larger ν, allowing shear bands to occur readily before the structure collapse caused by normal stresses, results in better plasticity [11]. The plasticity is also correlated

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with the free-volume content, and minor Ti adding induce higher free volume and improve the compressive plasticity of Cu-Zr-Al BMG without obvious change in ν [12]. However, detailed structural origin for the enhancement of plasticity via compositional tuning still remains unclear. Recently, the composition of $Zr_{56}Co_{28}Al_{16}$ (at.%), which can be cast into glassy rod with 18 mm in diameter by conventional copper-mold casting, was successfully developed [13]. The excellent GFA of $Zr_{56}Co_{28}Al_{16}$ provides a wide window for the compositional optimization with good plasticity and high GFA simultaneously. Tan et al. [14] reported that with increasing Al/Co concentration ratio, Zr-Co-Al BMGs present an obvious improvement of plasticity. In this work, Zr/Co composition tuning in the Zr-Co-Al alloy system around $Zr_{56}Co_{28}Al_{16}$ was performed, and thermal, mechanical properties and atomic structure of these newly developed Zr-Co-Al BMGs were studied.

2. Experimental procedures and simulation method

Alloy ingots with nominal compositions of $Zr_xCo_{84-x}Al_{16}$ (at.%) with x ranging from 51 to 58 were prepared by arc melting pure elements of Zr, Co and Al with purity higher than 99.9 at.% under a Ti-gettered high purity argon atmosphere. All the ingots were remelted at least five times to improve the chemical homogeneity. Cylindrical rods with different diameters and flat plates with thickness of 1 mm and width of 10 mm were produced by using water-cooled copper mold suction casting technique. The amorphous nature of all samples was verified by X-ray diffraction (XRD, Thermo ARL X'TRA) with Cu Kα radiation and differential scanning calorimetry (DSC, NETZCH DSC 404C) at a heating rate of 20 K/min. Structural analyses of Zr-Co-Al BMGs were also conducted by using synchrotron radiation X-ray diffraction (SRXRD) at P07 station Petra III/DESY, Hamburg, Germany. The beam size was 0.4 × 0.4 mm^2 and the wavelength (λ) used was 0.1783 Å. High-resolution XRD patterns were recorded by a MAR345 image plate, and then scattering intensity $I(q)$ was extracted after subtracting the background by program FIT2D [15]. Then, the output data were normalized to get the structure factor $S(q)$ after standard corrections by removing the effects of self-absorption, polarization, fluorescence absorption and Compton scattering by PDFgetX2 [16]. The corresponding pair distribution function $G(r)$ was obtained by Fourier transformation of $S(q)$, and the pair correlation function $g(r) = 1 + \frac{G(r)}{4\pi r\rho_0}$ where ρ_0 is average atomic number density. Zr and Co K-edge extended X-ray absorption fine structure (EXAFS) spectra were collected in transmission mode at the beamline 1W1B-XAFS of BSRF, Beijing, China. Each spectrum was repeated three times to minimize the noise disturbance, and the standard data analysis was conducted by using the software of Ifeffit package [17].

Based on the Archimedean principle, the densities ρ for all studied BMGs, were measured using a microbalance (Mettler Toledo XS105) having a sensitivity of 0.01 mg. The acoustic longitudinal velocity (V_l) and shear velocity (V_s) of the cylindrical specimens (2 mm in diameter and 4 mm in height) were measured by an Olympus 5072PR model ultrasonic system with a measuring sensitivity of 0.5 ns. The carrying frequency of longitudinal wave and shear wave was 15 MHz and 10 MHz, respectively. The shear modulus G, Poisson's ratio ν, Young's modulus E and bulk modulus K of the specimen were derived from the acoustic velocities and the density [18].

Three-point bending (3 PB) specimen with dimensions of 20 × 4 × 0.8 mm^3 were cut from the as-cast plates, and polished by 1000-grit SiC paper and diamond polishing solution. Bending tests with the span of 10 mm were conducted on a computer-controlled universal testing machine (SANS CMT5205) at a displacement rate of 0.02 mm/min. For each composition, eight 3 PB tests were performed using the specimen cut from similar positions of as-cast plates to evaluate the plastic deformability. The specimens after failure were ultrasonically cleaned in ethanol, and both the tensile surface near the fracture edge and the fracture surface were observed by scanning electron microscopy (SEM, Zeiss Supra 55). Microhardness was measured under 200 g load by a Vickers diamond pyramidal microhardness tester (HVS-1000, China) at room temperature. All the data obtained from multiple measurements were analyzed to get the standard deviation. Nanoindentation tests were carried out at room temperature on the plate specimen by Agilent Nano Indenter G200 equipped with a spherical indenter with the tip radius (R) of 3.8 μm, which was calibrated by measuring the elastic modulus of fused silica. Tests were conducted in load-control mode with the loading and unloading rates of 1 mN/s, and maximum load of 100 mN was adopted. The holding time at maximum load was set to be 60 s. For each composition, > 100 indentations spaced 25 μm apart on the surface were conducted. In nanoindentation experiments, thermal drift rate was set to be 0.05 nm/s to keep the reliability of the results, and the thermal drift correction was performed at about 10% of maximum load during unloading.

The ab initio molecular dynamics (AIMD) simulations for $Zr_xCo_{84-x}Al_{16}$ (x = 51, 53, 56, 58) were performed on the basis of density functional theory by using the Vienna Ab initio Simulation package (VASP) [19], along with canonical NVT ensemble and Nosé-Hoover thermostat [20,21]. The Vanderbilt-type ultrasoft pseudopotentials based on generalized gradient approximation were used to describe the exchange-correlation function. A typical time step of 3 fs was adopted with the Verlet algorithm to integrate Newton's equations of motion. Only Γ point was used to sample the Brillouin zone of the supercell, containing 200 atoms with periodic boundary conditions. The systems were melted and equilibrated at 2000 K for 6000 AIMD steps in order to remove the configuration thermal history, then quenched to 1500 K, 1200 K, 900 K, 600 K and 300 K with a cooling rate of 0.1 K/step. At each temperature, the equilibrium volume was established by keeping the internal pressure to zero within about ± 1.0 kBar. At 300 K, the optimized densities of $Zr_xCo_{84-x}Al_{16}$ (x = 51, 53, 56, 58) were found to be 6.599 g/cm^3, 6.545 g/cm^3, 6.472 g/cm^3 and 6.439 g/cm^3, respectively, which is quite in accord with the experimental values 6.622 g/cm^3, 6.567 g/cm^3, 6.496 g/cm^3 and 6.450 g/cm^3. Here, the experimental densities were measured using the Archimedean method for bulk specimens.

Voronoi tessellation [22] is a commonly used approach to describe local atomic structure of liquid and glassy solids. In this approach, the perpendicular bisectors unweighted by the atomic size between the central atom and the neighboring atoms will form a Voronoi cell, also called Voronoi polyhedron (VP). In this work, the neighboring atoms were identified within a cut-off distance 4.0 Å. The VP can be indexed as $\langle n_3, n_4, n_5, n_6, \ldots, n_i\rangle$ in order to describe the arrangements of the nearest-neighbor atoms around the center atom, where n_i is the number of i-edge faces on the VP. The total face number of a VP is equivalent to the coordination number ($\Sigma n_i = CN$) for a given center atom. In our case, the vertex is ignored if the cross section area is < 1% of the total.

3. Results and discussion

3.1. Glass forming ability and thermal stability

To explore how GFA changes in $Zr_xCo_{84-x}Al_{16}$ alloy series, dozens of compositions with x varying from 48 to 72 were chosen to prepare the plate specimens with thickness 1 mm and width 10 mm using copper-mold suction casting technique, and only $Zr_xCo_{84-x}Al_{16}$ with x = 51–58 are entirely in the glassy state. Therefore, we focus on this compositional range, and typical XRD patterns of $Zr_xCo_{84-x}Al_{16}$ (x = 51–58) rods with various diameters from 2 to 8 mm were shown in Fig. 1a and b, respectively. The critical diameter (D_c) for glass formation was clearly seen and plotted in Fig. 1c. It is obvious that GFA firstly increases then decreases with increasing Zr content, and displays a maximum of D_c = 7 mm at x = 55 and 56. Furthermore, glass transition and crystallization events can be clearly seen from the DSC curves, as shown in Fig. 1d. Characteristic temperatures, such as T_g (glass transition temperature), T_x (onset crystallization temperature), T_m (melting

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