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Poisson's ratio and plasticity in CuZrAl bulk metallic glasses

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Abstract

The study of compositional dependence of Poisson's ratio and compressive plasticity in a CuZr-based bulk metallic glass (BMG) forming system demonstrates that the plasticity of the BMGs is very sensitive to the change of composition. The sensitivity can be well characterized by the Poisson's ratio. The Poisson's ratio and plasticity have a homologous evolution with regard to the adjustment of composition in the alloys. The work has implication that the correlation between the Poisson's ratio and plasticity might provide useful guideline for the development of plastic BMGs in known or unknown BMG-forming alloys.

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Bulk metallic glasses (BMGs) have received much attention due to their excellent mechanical properties, which offer potential applications as structural materials [1–3]. However, most BMGs have a shortcoming of low plasticity at ambient conditions that limits the practical utilization. Efforts had focused on conquering the demerit by searching for experimental approaches to improve the plasticity [4–6] and the fundamentally understanding the deformation mechanism of BMGs. It is generally known that the unique properties of BMGs are straightly determined by the lack of long-range atomic order in the materials. The elastic moduli are apparently important parameters as a chain to understand the correlation between the structural characteristics and relevant mechanical properties. Lewandowsiki et al. found, by summarizing a large number of data, that the intrinsic plasticity or brittleness of BMGs correlates with their Poisson's ratio, υ [7]. The larger the υ is, the more ductile the BMGs become. Metallic glasses with a higher Poisson's ratio $\upsilon > 0.31 - 0.32$ or, equivalently, a ratio of shear modulus G to bulk modulus K less than 0.41–0.43, are ductile. This correlation was verified in annealing-induced embitterment in a given BMG system [7], in ductile Pt-based BMG [8], and in brittle Fe-based BMGs which display crossover from brittle to ductile via controlling υ [9]. Furthermore, it is also found that elastic constants of metallic glasses scale with the weighted average of those of their components [10]. Therefore, the correlation provides useful guidelines for the development of plastic BMGs by appropriate choice of components with the υ control strategy.

In this letter, we report the investigation of the evolution of the elastic moduli and ductility in an individual BMG-forming alloy by tuning the composition. We find minor content deviation can drastically change the plasticity of the BMGs, and the composition sensitivity of plasticity can be well characterized by the Poisson's ratio. The results indicate that the correlation between the Poisson's ratio and plasticity with regard to the adjustment of composition might helpful for the accurate determination of plastic BMG in a known or unknown BMG-forming system.

The $(Cu_{50}Zr_{50})_{100-x}Al_x$ ($x = 0$–10) alloys were prepared by melting pure Cu, Zr and Al in an arc-melting furnace under a Ti-gettered argon atmosphere. These alloys were remelted for several times and cast by suction of the melt into a copper mold to obtain a 50-mm-long cylindrical rod. The diameter of the $(Cu_{50}Zr_{50})_{100-x}Al_x$ rods was in the range of 2–5 mm. The structure of the cylindrical alloys (cross-sectional surface) was characterized by X-ray diffraction (XRD) using a MAC M03 XHF diffractometer (Cu Kα radiation), and a differential scanning calorimeter (DSC). Cylindrical specimens with a 2:1 aspect ratio were prepared and tested in an Instron 5500R1186 under quasi-static loading at an initial strain rate of $8 \times 10^{-4}\ s^{-1}$ at room temperature. The fracture surfaces after failure were

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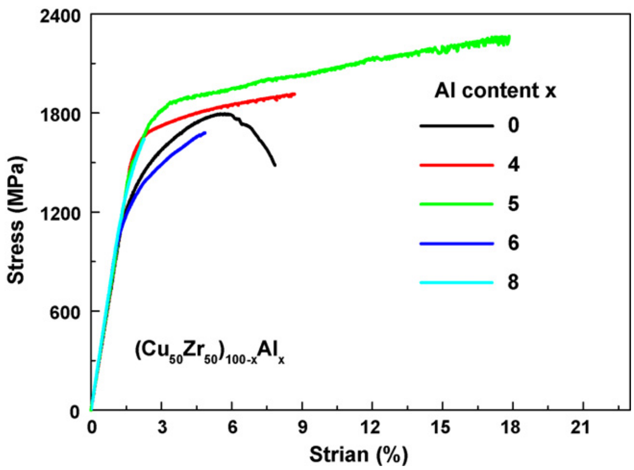

Fig. 1. (Color online) Stress–strain curves of $(Cu_{50}Zr_{50})_{100-x}Al_x$ (x = 0, 4, 5, 6, 8) under compression at a strain rate of $8 \times 10^{-4}\,s^{-1}$, showing the different plastic flowability of the BMGs.

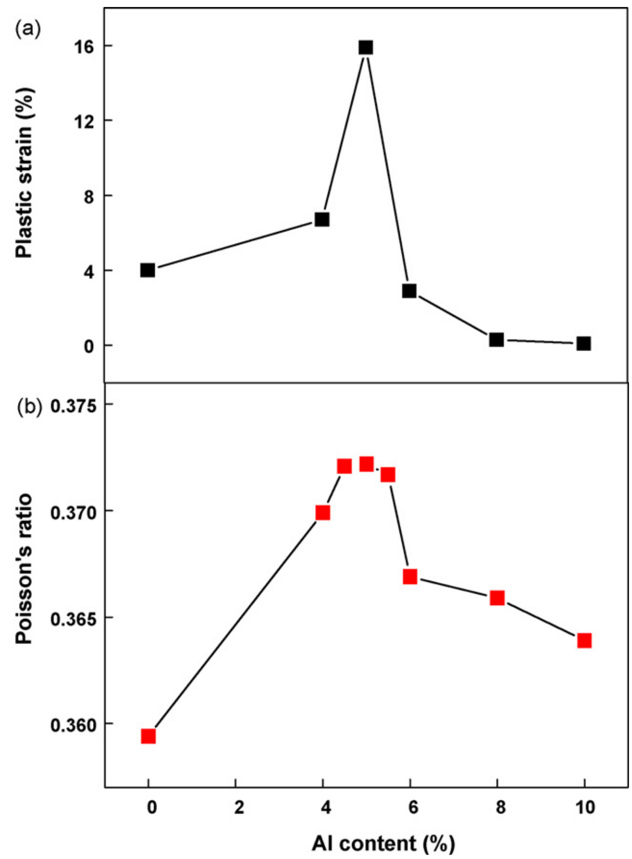

Fig. 2. (Color online) The dependence of plastic strain and Poisson's ratio on Al content for the $(Cu_{50}Zr_{50})_{100-x}Al_x$ BMGs. The homologous relation between plastic strain and Poisson's ratio can be seen.

investigated by scanning electron microscopy (SEM) using a Philips XL 30 SEM. The BMG rods were cut into a length of 7 mm and its ends were polished flat and parallel for the ultrasonic measurement. The acoustic velocities of the BMG were measured at ambient conditions by using a pulse echo overlap method. The travel time of ultrasonic waves propagating through the rod with a 10 MHz carry frequency was measured by using a MATEC 6600 ultrasonic system with x- and y-cut quartz transducers. The measuring sensitivity was of the order of 0.5 ns. The density was measured by the Archimedean technique and the accuracy lies within 0.1%. Elastic constants (e.g., Young's modulus E, shear modulus G, bulk modulus K, and Poisson's ratio v) were derived from the acoustic velocities and the densities [11].

The fully amorphous structure of the samples is confirmed by XRD as well as thermal analysis of DSC [12]. Fig. 1 shows the compressive stress-strain curves of the as-cast glassy $(Cu_{50}Zr_{50})_{100-x}Al_x$($x$ = 0, 4, 5, 6, 8) rods. It is seen that all the samples exhibit similar elastic elongation about 1.7% at the early stage of the deformation. However, these samples behave much different plastic deformations with regard to Al percentage composition as shown in Fig. 2(a). The $(Cu_{50}Zr_{50})_{95}Al_5$ exhibits the maximum plastic deformation of 16% [13], but $(Cu_{50}Zr_{50})_{92}Al_8$ only has a plasticity of less than 0.5%. The distinct contrast implies the ductility of the BMGs is sensitive to the change of composition, and the ductile BMGs could be obtained by appropriately adjustment of the compositions in the BMG-forming alloys.

Table 1 summarized the longitudinal, transverse ultrasonic velocities, density and the calculated elastic moduli of the CuZr-based BMGs with the Al content variation from 0 to 10%. The corresponding data of Cu, Zr, and Al elements are also listed [14]. Because Al has relative high acoustic velocities and low density, the increase of Al content leads to the higher acoustic

Table 1
The density ρ, longitudinal, transverse ultrasonic velocities (V_l and V_s), elastic moduli (e.g. $E, G, K,$ and v) for the $(Cu_{50}Zr_{50})_{100-x}Al_x$ BMGs, and the corresponding data of Cu, Zr, and Al elements

Samples	ρ (g/cm^3)	V_l (km/s)	V_s (km/s)	E (GPa)	G (GPa)	K (GPa)	v
Cu	8.960	4.711	2.320	130	48	140	0.34
Zr	6.511	4.572	2.251	88	33	92	0.34
Al	2.702	6.460	3.103	70	26	76	0.35
$Cu_{50}Zr_{50}$	7.404	4.436	2.079	87	32	103	0.36
$(Cu_{50}Zr_{50})_{96}Al_4$	7.221	4.661	2.118	88.7	32.4	113.7	0.3699
$(Cu_{50}Zr_{50})_{95.5}Al_{4.5}$	7.212	4.695	2.119	88.9	32.4	115.8	0.3721
$(Cu_{50}Zr_{50})_{95}Al_5$	7.195	4.699	2.120	88.7	32.3	115.8	0.3722
$(Cu_{50}Zr_{50})_{94.5}Al_{5.5}$	7.174	4.706	2.126	89.0	32.4	115.6	0.3717
$(Cu_{50}Zr_{50})_{94}Al_6$	7.129	4.722	2.179	92.4	33.8	113.8	0.3669
$(Cu_{50}Zr_{50})_{92}Al_8$	7.076	4.787	2.202	93.7	34.3	116.4	0.3659
$(Cu_{50}Zr_{50})_{90}Al_{10}$	7.204	4.855	2.246	99.1	36.3	121.4	0.3639

velocities and the decrease of density for these BMGs. Previous studies show that the elastic constants (M) of various BMGs can be calculated in the form of $M^{-1} = \sum f_i M_i^{-1}$, where M_i and f_i denote any elastic constant and the atomic percentage of the constituent element [10]. However, the Al composition dependence of Poisson's ratio or G/K shows anomalous considering the elastic moduli of the alloying elements. Fig. 2(b) shows the Al composition dependence of the Poisson's ratio in the $(Cu_{50}Zr_{50})_{100-x}Al_x$ BMGs. All the BMGs have high Poisson's ratios (>0.36) larger than the plastic transition value of 0.31–0.32 Ref. [7]. It can be clearly seen that the Poisson's ratios have a maximum around the composition of $(Cu_{50}Zr_{50})_{95}Al_5$. Elastic moduli give a global and often macroscopic view of a material stiffness. They reflect both the interatomic bonding energies and the connectivity. The result indicates that the change of the Al content leads to dramatically microstructural change in certain composition of the CuZr-based BMGs, and furthermore, adjusts the elastic properties of the BMGs. The phenomenon may be due to the intrinsic structural characteristics of BMGs consisting of packed atomic clusters [15]. This kind of microstructure allows efficient packing of atom clusters in fixed compositions that show markedly different properties [15].

Both Poisson's ratio and plastic strain have a similar change tendency upon the variation of Al content, and show the maximum peak around the same composition of $(Cu_{50}Zr_{50})_{95}Al_5$ as shown in Fig. 2. The sample with the largest plastic strain of 16% has the largest Poisson's ratio value of 0.372 among the BMGs. The similar variation tendency of plastic strain and Poisson's ratio upon the change of the Al content reveals that they are well correlated.

Fig. 3 shows the relationship between the glass transition temperature T_g and the Al percentage composition. The T_g of these BMGs changes with the increasing of Al content. A sharper increase of T_g happens in 5% Al content of the BMG (Fig. 3). It is known that the T_g is dominated by the bonding force among the constituents and reflects the structural characteristics of an alloy [16]. This result confirms the sharper alteration of structure happens in the composition of $(Cu_{50}Zr_{50})_{95}Al_5$. Recent work also confirms that 5% Al addition can lead to a dense liquid structure and higher value of viscosity compared to that of the CuZr glass [17].

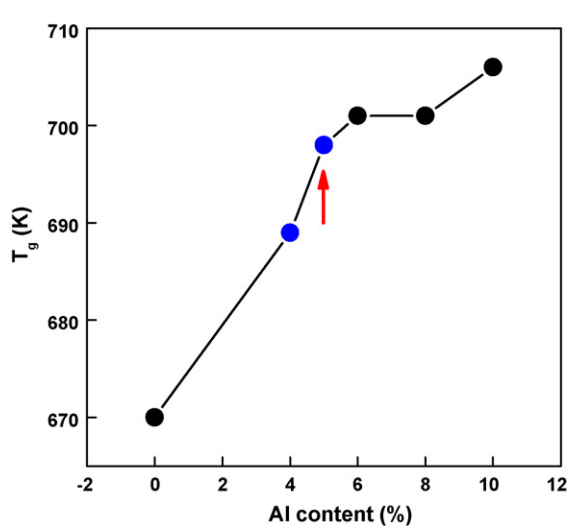

Fig. 3. (Color online) The relationship of T_g and Al content for the $(Cu_{50}Zr_{50})_{100-x}Al_x$ BMGs. The arrow points the sharp increase of T_g in 5% Al content.

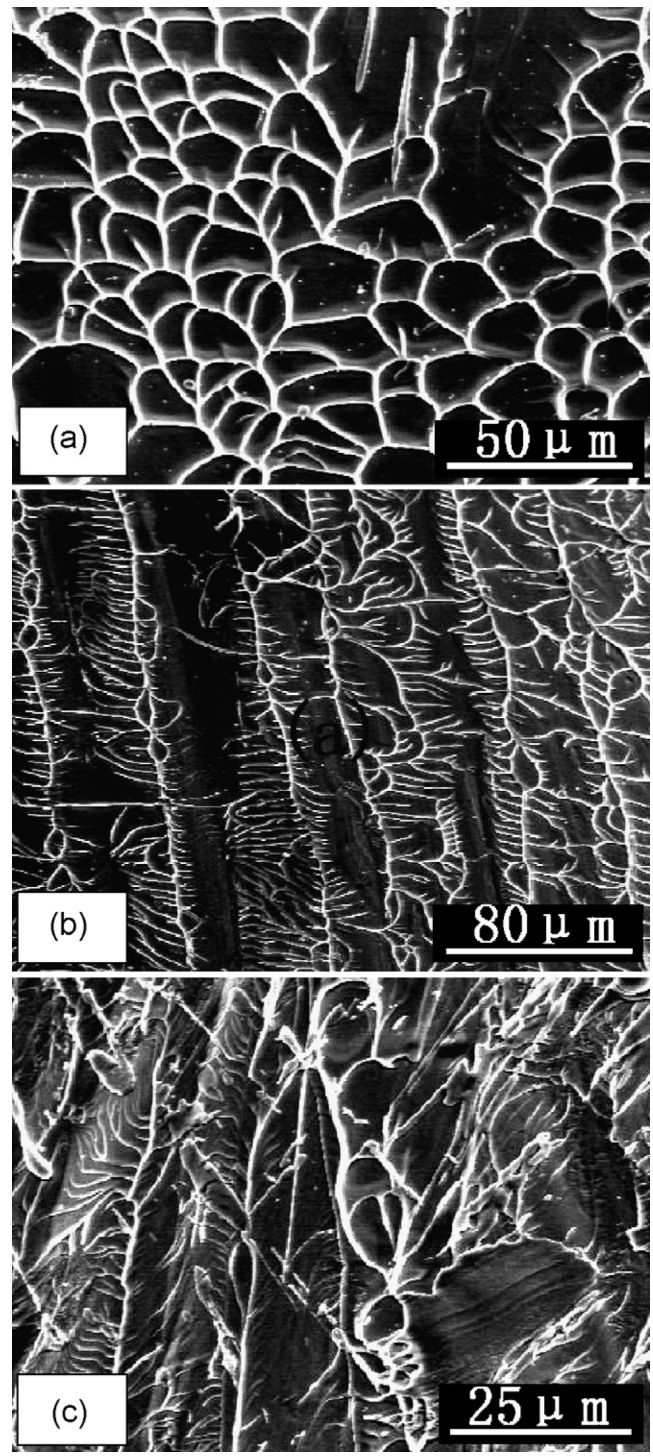

Fig. 4. SEM micrographs of fracture surfaces of (a) $(Cu_{50}Zr_{50})_{95}Al_5$, (b) $(Cu_{50}Zr_{50})_{94}Al_6$, and (c) $(Cu_{50}Zr_{50})_{92}Al_8$ samples. The evolution of fracture patterns indicates the different plastic flow ability for the BMGs with different Al contents.

The resultant phenomenon of ultimate fracture often gives information for uncovering the mechanism of deformation [18]. Fig. 4 shows SEM micrographs of fracture surfaces of (a) $(Cu_{50}Zr_{50})_{95}Al_5$, (b) $(Cu_{50}Zr_{50})_{94}Al_6$, and (c) $(Cu_{50}Zr_{50})_{92}Al_8$ sample. Even though the three BMGs have very close compositions, they show markedly different micrographs of fracture surfaces. The image of fracture surface of $(Cu_{50}Zr_{50})_{95}Al_5$ shows a typical dimple-like structure of a characteristic scale of 20 μm, which indicates the ductile fracture mechanism. For the $(Cu_{50}Zr_{50})_{94}Al_6$, the main feature is a vein-like structure in the fracture surface. However, for the $(Cu_{50}Zr_{50})_{92}Al_8$ sample, an obvious melting residual pattern displays over all the fracture surface without any obvious dimple-like or vein-like structure. The dramatic contrast for the three fracture patterns confirms the different fracture behaviors, the atomic bonding features, and the structural difference for the BMGs [18]. The 5% Al addition to CuZr alloy may make the structure and atomic bonding reach an appropriate state and yield the excellent plastic flowability in the alloy.

The Poisson's ratio υ is directly related to the ratio of bulk and shear moduli and can be calculated as: $\upsilon = (1/2) - (3/6\,K/G + 2)$, it characterizes the relative value of the compressive and shear deformation and correlates with the atomic configuration in glassy materials [11,19,20]. So the subtle changes of the compositional dependent structure and plasticity of the alloy can be clearly reflected by the Poisson's ratio. Our results indicate that, similar to glass forming ability of BMG-forming alloys, which is very sensitive to their composition [2], the plasticity of BMGs is also susceptive to the composition. Minor content deviation can drastically change the plasticity of the BMGs through alteration of the microstructure. The composition sensitivity of the plasticity can be characterized by the Poisson's ratio, which further supports the previous reported universal correlation between the Poisson's ratio and the plasticity [7]. Similar results have also been reported in ZrCuNiAl BMG-forming system, the extraordinarily plastic ZrCuNiAl BMGs are obtained by appropriate choice of the composition utilizing the Poisson's ratio and plasticity correlation [21].

In summary, the study of the compositional dependence of the elastic properties and the plasticity in CuZr-based BMGs shows that the Poisson's ratio and plasticity have a homologous evolution with the adjustment of composition. The plasticity of the CuZr-based BMGs is very sensitive to the change of composition characterized by anomalous Poisson's ratio change considering the elements alloying. The results imply that even in the reported BMG systems, plastic BMGs are possible to be obtained by appropriate choice of the composition utilizing the Poisson's ratio and plasticity correlation. It is expected that the Poisson's ratio and plasticity correlation would provide useful guidelines for the development of plastic BMGs in other known or unknown BMG-forming alloys.

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References

[1] A.L. Greer, Science 267 (1995) 1947.
[2] W.H. Wang, Prog. Mater. Sci. 52 (2007) 540.
[3] W.H. Wang, C. Dong, C.H. Shek, Mater. Sci. Eng. R 44 (2004) 45.
[4] H. Bei, S. Xie, E.P. George, Phys. Rev. Lett. 96 (2004) 105503.
[5] M.W. Chen, A. Inoue, W. Zhang, T. Sakurai, Phys. Rev. Lett. 96 (2006) 245502.
[6] Y. Zhang, W.H. Wang, A.L. Greer, Nat. Mater. 5 (2006) 857.
[7] J.J. Lewandowski, W.H. Wang, A.L. Greer, Philos. Mag. Lett. 85 (2005) 77.
[8] J. Schroers, W.L. Johnson, Phys. Rev. Lett. 93 (2004) 255506.
[9] X.J. Gu, S.J. Poon, G.J. Shiflet, Appl. Phys. Lett. 88 (2006) 211905.
[10] W.H. Wang, J. Appl. Phys. 99 (2006) 093506.
[11] D. Schreiber, Elastic Constants and Their Measurement, McGraw-Hill, New York, 1973.
[12] P. Yu, H.Y. Bai, M.B. Tang, J. Non-Cryst. Solids 351 (2005) 1328.
[13] M.B. Tang, D.Q. Zhao, M.X. Pan, W.H. Wang, Chin. Phys. Lett. 21 (2004) 901;
J. Das, M.B. Tang, K.B. Kim, R. Theissmann, F. Baier, W.H. Wang, J. Eckert, Phys. Rev. Lett. 94 (2005) 205501.
[14] A.M. James, M.P. Lord, Macmillan's Chemical and Physical Data, Macmillan, London, 1992.
[15] D. Miracle, Nat. Mater. 3 (2004) 697.
[16] P. Wen, R.J. Wang, W.H. Wang, J. Mater. Res. 17 (2002) 1785;
W.H. Wang, R.J. Wang, F.Y. Li, D.Q. Zhao, M.X. Pan, Appl. Phys. Lett. 74 (1999) 1803.
[17] G.J. Fan, M. Freels, H. Choo, P.K. Liaw, J.J.Z. Li, W.K. Rhim, W.L. Johnson, P. Yu, W.H. Wang, Appl. Phys. Lett. 89 (2006) 241917.
[18] X.K. Xi, D.Q. Zhao, M.X. Pan, W.H. Wang, Y. Wu, J.J. Lewandowski, Phys. Rev. Lett. 94 (2005) 125510.
[19] S. Bossuyt, S. Giménez, Y. Schroers, J. Mater. Res. 22 (2007) 533.
[20] E. Pineda, Phys. Rev. B 73 (2006) 104109.
[21] Y.H. Liu, G. Wang, D.Q. Zhao, M.X. Pan, W.H. Wang, Science 315 (2007) 1385.