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Understanding the correlations between Poisson's ratio and plasticity based on microscopic flow units in metallic glasses

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In metallic glasses (MGs), a clear correlation has been established between plasticity and the Poisson's ratio. Such a correlation between the two distinctive macroscopic mechanical properties is challenging to explain from a microstructure perspective. We studied the microstructural origin of the Poisson's ratio and plasticity criterion in various MGs and find a correlation between the relative concentration of flow units and Poisson's ratio: the MGs with higher concentration of flow units show a larger Poisson's ratio and better plasticity. We have explained the empirical correlation between ductility and the Poisson's ratio based on microscopic flow units in MGs.
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I. INTRODUCTION

In crystalline metals and alloys, the knowledge of deformation and fracture is gained by systematic experimental and simulation studies, which correlate microstructure and mechanical properties.[1,2] However, the lack of a periodic structure and the inability to conduct systematic parametric studies are the main impediments for gaining such knowledge in metallic glasses (MGs). Recently, a clear correlation between Poisson's ratio ν and plastic deformation in MGs with diverse systems, compositions, and significant disparity in toughness and plasticity has been established.[3–7] From this criterion, the intrinsic plasticity or brittleness of MGs is related with the value of Poisson's ratio, which is equivalent to the ratio of the bulk modulus K to the shear modulus G. The higher Poisson's ratio or lower G/K ratio is predicted to result in higher toughness or plasticity in MGs,[4,5] because the small ratio of G/K causes the extension of the tip of a shear band rather the initiation of a crack, and this results in the formation of multiple shear bands and high global ductility.[3–7] This correlation has benefits including better understanding of the plastic and elastic deformations and fracture mechanisms, as well as providing a strategy in the design of a glass with improved performance in applications.[8–13] However, the structural origin and the fundamental mechanism for the Poisson's ratio and plasticity criterion are not fully understood yet even though the Poisson's ratio has been widely used to search the tough MGs. The Poisson's ratio and plasticity criterion does not capture the essential features of the structural mechanism of plasticity in MGs, and a comprehensive description for the plastic flow behaviors of MGs requires the understanding of the interplay between their structure and properties.

In parallel with the development of the Poisson's ratio and plasticity correlation, a revelation from various experimental studies shows that the microstructural heterogeneity plays nontrivial roles in the observed mechanical properties of MGs.[14–20] The MG can be regarded as a composite with solid like regions, which are the source of elasticity, and another liquid like regions with less stress resistance.[19–31] The liquid like regions can be activated to form the flow units which are embodied in the elastic matrix and accommodate the plastic deformation in MGs.[20–30] The flow units are a group of atoms exhibiting a lower packing density, a higher energy dissipation rate, and lower modulus, and at high energy states in the energy landscape.[20–30] The flow units are found to play nontrivial roles in determining and controlling the properties and the performance of MGs, such as elastic properties, density, glass transition, relaxations, and mechanical properties.[19–30] Therefore, the implication can be drawn that the flow units might have possible relation to the empirical Poisson's ratio and plasticity correlation, and provide insight into microstructural understanding on the correlation.

Along this idea, in this work, we studied the density of the flow units of a series of MGs with various plasticity and Poisson's ratio by annealing the MGs at the same normalized glass transition temperature T_g because the isothermal annealing can tune the density of flow units.[21–23] The variations of elastic moduli including K, G, ν, and the relative concentration of flow units of these MGs are monitored during the structural relaxation. We show these two apparently universal phenomena in MGs: plasticity with Poisson's ratio and concentration of flow units are related.

II. EXPERIMENTAL

The various MGs we studied were prepared by arc-melting the mixture of the elements under a Ti-gettered argon atmosphere and then sucked in a water cooled copper mold to get the $2 \times 10 \times 100$ mm glassy plates. The fully glassy structures of the as-cast and annealed samples were verified by the differential scanning calorimetry and X-ray diffraction. The annealed samples were obtained by annealing the as-cast samples encapsulated in a quartz crucible with vacuum of 10^{-4} Pa, at a normalized 0.8 T_g for each MG for 48 h. Elastic constants of the MGs, including Yong's modulus E, G, and ν, were measured using resonant ultrasound spectroscopy (RUS). Rectangle samples about $2 \times 2.5 \times 4$ mm with known volume and mass were placed

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TABLE I. Summary of elastic properties for various MGs. G_0 and ν are the shear modulus and Poisson's ratio of MGs in as-cast state. The G_a is the shear modulus of the MGs annealed for 48 h at 0.8 T_g.

Composition	G_0 (GPa)	G_a (GPa)	$(G_a - G_0)/G_0$ (%)	Poisson's ratio ν
$Mg_{65}Cu_{25}Tb_{10}$	20.41 ± 0.23	20.57 ± 0.04	0.81 ± 0.39	0.307 ± 0.003
$Mg_{65}Cu_{25}Gd_{10}$	19.82 ± 0.10	19.97 ± 0.03	0.72 ± 0.41	0.308 ± 0.008
$Ce_{68}Al_{10}Cu_{20}Co_2$	11.18 ± 0.09	11.41 ± 0.03	2.26 ± 0.40	0.336 ± 0.006
$La_{55}Al_{25}Co_{20}$	15.46 ± 0.05	15.90 ± 0.03	2.82 ± 0.10	0.353 ± 0.003
$Cu_{46}Zr_{46}Al_8$	34.52 ± 0.05	35.61 ± 0.03	3.16 ± 0.16	0.370 ± 0.002
$Cu_{48}Zr_{48}Al_4$	32.00 ± 0.09	33.06 ± 0.09	3.34 ± 0.10	0.381 ± 0.002
$Cu_{45}Zr_{47}Al_7Fe_1$	33.75 ± 0.13	34.86 ± 0.21	3.30 ± 0.41	0.360 ± 0.002
$Zr_{56}Co_{28}Al_{16}$	33.89 ± 0.05	35.19 ± 0.08	3.84 ± 0.25	0.369 ± 0.002
$Cu_{47.5}Zr_{47.5}Al_5$	32.41 ± 0.22	33.76 ± 0.13	4.22 ± 0.34	0.377 ± 0.003
Zr_{46} $Cu_{45}Al_7Ti_2$	33.61 ± 0.09	35.33 ± 0.06	5.04 ± 0.20	0.383 ± 0.003

between the piezoelectric transducers, and the two independent elastic constants C_{11} and C_{44} for each alloy were obtained and used to calculate the elastic moduli. The elastic moduli of the various MGs are listed in Table I. Specimens about 4 mm long and 2 mm in diameter were cut from MG rods and then carefully ground into compression specimens with an aspect ratio of 2:1. Uniaxial compression tests were performed with an Instron 3384 electromechanical test system at a constant strain rate of 1×10^{-4} s^{-1} at room temperature.

III. RESULTS AND DISCUSSIONS

Figure 1 presents the plasticity against Poisson's ratio for ten various MGs with diverse compositions and mechanical properties. It can be seen that the plasticity is clearly correlated with the Poisson's ratio in these typical MGs. The MGs with larger value of Poisson's ratio have better plasticity. For example, a Mg-based MG with a low Poisson's ratio of 0.307 shows very brittle fracture, while for a Zr-based MG with a high Poisson's ratio of 0.382, its plastic strain can reach as high as 32%.[32] There does exist a critical Poisson's ratio value, and above the value, the fracture mechanism changes from brittle to ductile.

Metallic glasses undercooled from the liquid are in a metastable state and tend to undergo structural rearrangement alternatively the activation of the flow units when excited by external agitations either in the form of stress or temperature.[19–30] During the process of annealing much below T_g, the properties such as elastic moduli, hardness, and density will be changed arising from the annihilation of the "defect" or the flow units in MGs.[21–30] According to the flow unit model, the flow unit in MGs is generally perceived to be a local rearrangement of atoms that are microstructural origin for plastic deformation and relaxations in MGs, and a relationship of the effective concentration of flow units c and the properties such as shear modulus G of MGs can be expressed as[21–24]

$$G = G_\infty/(1 + c), \quad (1)$$

where the G_∞ is the shear modulus of the MG when annealing time approaches unlimited, which is roughly equal to the shear modulus of the corresponding perfect crystal of a crystallized MG.[33,34] Based on Eq. (1), the relative concentration change of effective flow units Δc in a MG can be reflected by the change of the shear modulus after isothermal annealing as

$$\Delta c \propto (G_a - G_0)/G_0, \quad (2)$$

where the G_0 is the shear modulus of the as-cast MG, and the G_a in our case is the shear modulus of the MG annealed for 48 h. The value of Δc reflects the relative density of the effective flow units of a MG in the as-cast state.[23,24,33,34]

We then compare the relationship among the plasticity, Poisson's ratio, and the relative concentration of flow units of the MGs in as-cast state. Figure 2 is the plot of relative concentration of flow units and plasticity of various MGs in as-cast state. We can see that the plasticity and Δc follow the same change trend in these MGs, and the MG with high concentration of flow units has better plasticity. Figure 3 is the plot of the Poisson's ratio vs. the change of the shear modulus, or the change of the relative concentration of flow unit Δc for various MGs in as-cast state. There is also a roughly linear correlation between these two parameters. That is the MG with higher Poisson's ratio has higher concentration of the flow units because the same isothermal annealing condition can annihilate more flow units in a MG with higher Poisson's ratio. This indicates that the value of Poisson's ratio in a MG is partly dependent on the relative concentration

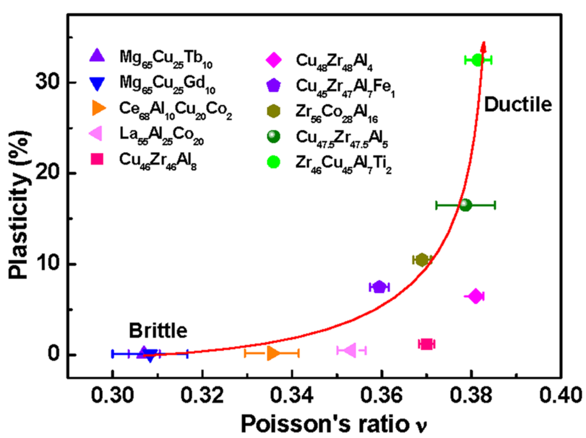

FIG. 1. The correlation of room-temperature comprehensive plasticity and Poisson's ratio for ten as-cast MGs with diverse compositions and properties.

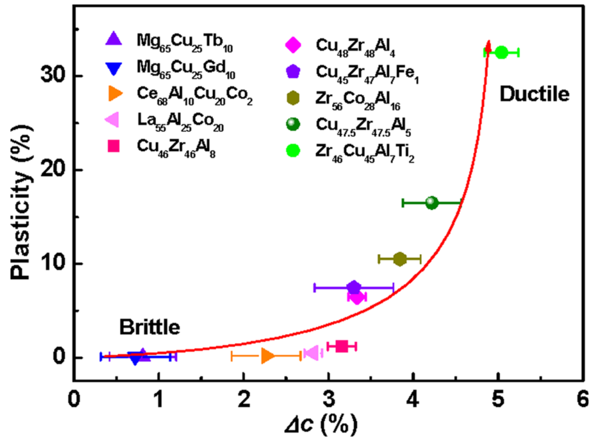

FIG. 2. The correlation of room-temperature comprehensive plasticity and the relative change of the concentration of the flow units Δc for ten as-cast MGs.

of effective flow units. Ichitsubo *et al.*[35] estimated the macroscopic elastic constants using the effective-mean-field theory for the model MG composed of strongly bonded regions and weakly bonded regions, and found that a very small amount increase of weakly bonded regions exist in the strongly bonded regions can arouse markedly decrease in Poisson's ratio. This result also demonstrates the weakly bonded regions or flow units can significantly affect the value of Poisson's ratio in a MG, which is consistent with our observations. Therefore, based on our above results, the Poisson's ratio criterion for the plasticity intrinsically actually reflects the effect of the concentration of flow units on the plastic deformation of a MG. In other words, the plasticity of a MG is determined by its density of flow units, and the MG with high density of flow units will have higher value of Poisson's ratio and larger plasticity. The results also suggest that any MG can be ductile or brittle if it has enough high or low concentration of flow units.[36] Therefore, the results indicate that the flow unit is a key structural parameter for understanding and controlling the plasticity of MGs. For a MG with larger Poisson's ratio, it has more flow units and will show better plasticity; for a MG with lower Poisson's ratio, it has less density of flow units and shows poor plasticity.

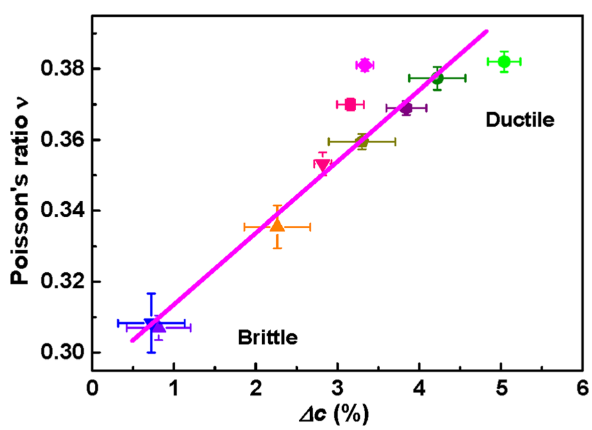

FIG. 3. Poisson's ratio vs. the relative change of the concentration of the flow unit Δc for various MGs in as-cast state. The MGs with larger density change of flow units show larger Poisson's ratio and better plasticity.

The correlation between Poisson's ratio and Δc is helpful for plastic MG designing through increase the concentration of flow units or liquid like regions in a MG. For example, a $La_{68.5}Ni_{16}Al_{14}Co_{1.5}$ MG with remarkable high concentration of flow units had been developed, and it indeed exhibits a large global plasticity, even the pronounced macroscopic tensile plasticity near room temperature, because high density of flow units activated in the MG can alleviate the strain localization and more homogenously accommodate the plastic deformation.[37] The correlation between Poisson's ratio and Δc can also explain the widely observed embrittlement by annealing in MGs. Annealing of MGs is known to induce embrittlement as demonstrated by the correlation of fracture energy G_c, plasticity with the ratio K/G or ν as the MGs isothermal annealed much below T_g.[4,23,38] The transition from ductility/plasticity to brittleness on annealing occurs at the same critical value of Poisson's ratio as found in the as-cast MGs of different compositions.[4] By monitoring the change of the compression plasticity, Poisson's ratio, and the relative change of concentration of flow units Δc of the MGs upon the isothermal annealing, both the plasticity and Poisson's ratio show the similar change tendency with the change of Δc, and the Poisson's ratio decreases and the MG becomes brittle with more flow units annihilated by the isothermal annealing.[23]

Previous studies have shown that the cooling rate and previous deformation have great influence on the properties especially for the plasticity of MGs.[14,33,39–42] It is also found that there exist a critical fictive temperature for plasticity in MGs, which can explain the sensitivity of mechanical properties of MGs to cooling rate and annealing-induced embrittlement.[33] These phenomena can also be understood from the correlation between the density of flow units and plasticity: when a MG sample is made in a high cooling rate or a MG is previous deformed, more flow units will be frozen in or induced into the MG, when the concentration of flow units reaches a critical value (corresponding to the critical fictive temperature[22]), the MG will have a large Poisson's ratio and better plasticity.

IV. CONCLUSIONS

We interpret the correlation between plasticity and Poisson's ratio in microstructural point of view. We show that both plasticity and ν are linked with the density of flow units in various MGs in as-cast state, and the found correlation indicates that the Poisson's ratio criterion for the plasticity intrinsically reflects the effect of the concentration of flow units on the plastic deformation of a MG in as-cast state. The result is helpful for MG designing and for understanding of deformation mechanisms and some phenomena such as annealing induced embrittlement, cooling rate, and creep effects on the plasticity, and the existence of critical fictive temperature for mechanical properties in MGs.

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[1]G. I. Taylor, Proc. R. Soc. A **145**, 362 (1934).
[2]S. S. Brenner, J. Appl. Phys. **27**, 1484 (1956).
[3]H. S. Chen, J. T. Krause, and E. Coleman, J. Non-Cryst. Solids **18**, 157 (1975).
[4]J. J. Lewandowski, W. H. Wang, and A. L. Greer, Philos. Mag. Lett. **85**, 77 (2005).
[5]W. H. Wang, J. Appl. Phys. **99**, 093506 (2006).
[6]J. Schroers and W. Johnson, Phys. Rev. Lett. **93**, 255506 (2004).
[7]Y. H. Liu, G. Wang, R. J. Wang, M. X. Pan, and W. H. Wang, Science **315**, 1385 (2007).
[8]X. J. Gu, A. G. McDermott, S. J. Poon, and G. J. Shiflet, Appl. Phys. Lett. **88**, 211905 (2006).
[9]P. Yu and H. Y. Bai, Mater. Sci. Eng. A **485**, 1 (2008).
[10]A. Castellero, D. I. Uhlenhaut, B. Moser, and J. F. Löffler, Philos. Mag. Lett. **87**, 383 (2007).
[11]W. H. Wang, J. Appl. Phys. **110**, 053521 (2011).
[12]Q. He, J. K. Shang, E. Ma, and J. Xu, Acta Mater. **60**, 4940 (2012).
[13]A. Caron, R. Wunderlich, D. V. Louzguine-Luzgin, G. Q. Xie, A. Inoue, and H.-J. Fecht, Acta Mater. **58**, 2004 (2010).
[14]H. B. Yu, J. Hu, X. X. Xia, B. A. Sun, X. X. Li, W. H. Wang, and H. Y. Bai, Scr. Mater. **61**, 640 (2009).
[15]T. Fujita, Z. Wang, Y. H. Liu, H. Sheng, W. H. Wang, and M. W. Chen, Acta Mater. **60**, 3741 (2012).
[16]T. Ichitsubo and E. Matsubara, Mater. Sci. Eng. A **521**, 236 (2009).
[17]W. Dmowski, T. Iwashita, C. P. Chuang, J. Almer, and T. Egami, Phys. Rev. Lett. **105**, 205502 (2010).
[18]H. Wagner, D. Bedorf, S. Küchemann, M. Schwabe, B. Zhang, W. Arnold, and K. Samwer, Nature Mater. **10**, 439 (2011).
[19]J. C. Ye, J. Lu, C. T. Liu, Q. Wang, and Y. Yang, Nature Mater. **9**, 619 (2010).
[20]Z. Wang, P. Wen, L. S. Huo, H. Y. Bai, and W. H. Wang, Appl. Phys. Lett. **101**, 121906 (2012).
[21]R. J. Xue, D. P. Wang, Z. G. Zhu, D. W. Ding, B. Zhang, and W. H. Wang, J. Appl. Phys. **114**, 123514 (2013).
[22]Z. G. Zhu, P. Wen, D. P. Wang, R. J. Xue, D. Q. Zhao, and W. H. Wang, J. Appl. Phys. **114**, 083512 (2013).
[23]D. P. Wang, Z. G. Zhu, R. J. Xue, D. W. Ding, H. Y. Bai, and W. H. Wang, J. Appl. Phys. **114**, 173505 (2013).
[24]L. S. Huo, J. F. Zeng, W. H. Wang, C. T. Liu, and Y. Yang, Acta Mater. **61**, 4329 (2013).
[25]S. T. Liu, W. Jiao, B. A. Sun, and W. H. Wang, J. Non-Cryst. Solids **376**, 76 (2013).
[26]W. Jiao, P. Wen, H. L. Peng, H. Y. Bai, B. A. Sun, and W. H. Wang, Appl. Phys. Lett. **102**, 101903 (2013).
[27]W. Jiao, B. A. Sun, P. Wen, H. Y. Bai, Q. P. Kong, and W. H. Wang, Appl. Phys. Lett. **103**, 081904 (2013).
[28]S. T. Liu, Z. Wang, H. L. Peng, H. B. Yu, and W. H. Wang, Scr. Mater. **67**, 9 (2012).
[29]H. L. Peng, M. Z. Li, and W. H. Wang, Phys. Rev. Lett. **106**, 135503 (2011).
[30]H. B. Yu, W. H. Wang, H. Y. Bai, Y. Wu, and M. W. Chen, Phys. Rev. B **81**, 220201(R) (2010).
[31]W. H. Wang, Prog. Mater. Sci. **57**, 487 (2012).
[32]L. Y. Chen, Z. D. Fu, G. Q. Zhang, X. P. Hao, and Q. K. Jiang, Phys. Rev. Lett. **100**, 075501 (2008).
[33]S. V. Khonik, A. V. Granato, D. M. Joncich, A. Pompe, and V. A. Khonik, Phys. Rev. Lett. **100**, 065501 (2008).
[34]A. V. Granato, Phys. Rev. Lett. **68**, 974 (1992).
[35]T. Ichitsubo, E. Matsubara, T. Yamamoto, H. S. Chen, N. Nishiyama, J. Saida, and K. Anazawa, Phys. Rev. Lett. **95**, 245501 (2005).
[36]G. Kumar, P. Neibecker, Y. H. Liu, and J. Schroers, Nat. Commun. **4**, 1536 (2013).
[37]H. B. Yu, X. Shen, Z. Wang, L. Gu, W. H. Wang, and H. Y. Bai, Phys. Rev. Lett. **108**, 015504 (2012).
[38]W. H. Wang, R. J. Wang, W. T. Yang, and B. C. Wei, J. Mater. Res. **17**, 1385 (2002).
[39]Y. Q. Cheng, A. J. Cao, and E. Ma, Acta Mater. **57**, 3253 (2009).
[40]H. B. Ke, P. Wen, W. H. Wang, and A. L. Greer, Scr. Mater. **64**, 966 (2011).
[41]K. Zhao, X. X. Xia, H. Y. Bai, D. Q. Zhao, and W. H. Wang, Appl. Phys. Lett. **98**, 141913 (2011).
[42]B. Huang, H. Y. Bai, P. Wen, D. W. Ding, D. Q. Zhao, M. X. Pan, and W. H. Wang, J. Appl. Phys. **114**, 113508 (2013).