Journal of Alloys and Compounds 637 (2015) 44–54

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: www.elsevier.com/locate/jalcom

Yield strength and yield strain of metallic glasses and their correlations with glass transition temperature

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ARTICLE INFO

Article history:
Received 12 January 2015
Received in revised form 11 February 2015
Accepted 1 March 2015
Available online 5 March 2015

Keywords:
Metallic glass
Yield strength
Yield strain
Glass transition temperature
Shear transformation zone

ABSTRACT

Strength should be the most outstanding mechanical property for metallic glasses (MGs). Here we analyze the strengths of MGs with more than 300 compositions in ~30 alloy systems covering nearly all strength levels, ranging from 0.3 GPa to 6 GPa. With these abundant experimental data available, we find that the yield strain is not always constant but depends on glass transition temperature, T_g, ranging from 1% to 2.5% for normal strain and from 1.2% to 3.4% for shear strain. This can be well explained by assuming an equivalent energy barrier for yielding and glass transition. Relations derived based on this assumption show that MGs with high T_g may yield with larger critical strain and higher strength, implying that high elasticity, high strength and high thermostability can be synchronously achieved for MGs.

1. Introduction

Strength, which determines the resistance to mechanical failure (e.g., plastic deformation or brittle fracture), is one of the most important mechanical properties for structural materials [1,2]. Seeking for high strength is always one important direction of efforts for materials scientists. In conventional metallic crystalline materials, their strengths are often limited by crystal defects such as dislocations or interfaces [2,3]. Due to the dislocation-free structures, metallic glasses (MGs) usually exhibit very high strengths approaching to the theoretical values [4]. A recent report indicated that the Co–Ta–B MG can achieve strength as high as ~6 GPa [5], which is the highest value for bulk metallic materials in the world. The ultra-high strength endows MGs with promising structural materials, and activates lots of research interests [4,6]. Thus one may wonder that what factors intrinsically determine the strength of various MGs.

Recently, it is suggested by several research groups that the yielding of MGs may intrinsically correlate to the glass transition [7–11]. Based on the physical analogy between the mechanical yielding and glass transition, Yang et al. [7] found that the strength at the ambient temperature can be determined by the glass transition temperature and molar volume with a simple linear equation. Later Liu et al. [8] derived a similar universal law based on the fundamental thermodynamics without the employment of any microscopic model, which demonstrates the intrinsic correlation between yielding and glass-supercooled liquid transition. With molecular dynamics (MD) simulation, Guan et al. [9], on the other hand, considered the effect of temperature on the steady-state flow stress and found a parabola equation which predicted equivalent results for stress and temperature on reducing the viscosity of MGs. Very recently, Wang [10] suggested that yielding and glass transition might have identical physical origin, i.e., a relaxation process called α-relaxation. Although some experimental data have been found to verify above models, owing to the variety of MGs and the very wide range of strength, it is far from enough to confirm the generality of the equivalent relation between mechanical yielding and glass transition for any MGs by using only limited experimental evidences by the previous authors.

In this work, we systematically studied the experimental data of MGs with ~300 different compositions in ~30 systems collected from ~100 research papers. From the strongest MGs such as Co-based MGs and refractory metal-based MGs to the softest MGs such as Ca-based, Sr-based and some rare-earth (RE) based MGs, the data we collected here nearly cover all strength levels of MGs developed to date, which guarantees the rationality to find general equations for any MGs. With these data in hand, we shall firstly depict the limits of strength and elastic strain, and then some theoretical models on yielding and strength will be examined. Finally assuming an identical energy barrier for mechanical yielding and glass transition, the expressions for yield strain as well as strength will be derived.

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http://dx.doi.org/10.1016/j.jallcom.2015.03.005
0925-8388/

2. Method and data

Physical data including glass transition temperature (T_g), Young's modulus (E), shear modulus (G), molar volume (V_m) and yield strength (σ_y) of 301 MGs were directly collected from literature [5,6,8,12–108]. The yield strengths were measured at room temperature (T_{RT}) and quasistatic strain rates, i.e., ranging from 10^{-5} to 10^{-3} s^{-1}, via uniaxial compression or tension with large (mm-scale) samples. Most of strength data were measured by uniaxial compression, and only strengths of 4 MGs were obtained by uniaxial tension. For MGs fabricated with refractory metals (9 MGs in total) such as W-based, Re-based MGs, due to the limited sample thickness [76,86–88], the yield strengths were derived according to $\sigma_y = H_V/3$ [109], where H_V is Vickers hardness. The elastic constants E and G were determined either by quasistatic compression or tension at T_{RT} or via ultrasonic method. The collected T_g data were usually examined with differential scanning calorimeter at a heating rate in the range of 20–40 K/min. The similar conditions for measurement ensure the validity of examining the intrinsic relations between these properties. MG alloy systems include Al-based, Au-based, Ca-based, Co-based, Cu-based, Fe-based, RE-based (Ce-, Dy-, Er-, Gd-, Ho-, La-, Lu-, Nd-, Pr-, Tb-, Tm-, Y-, Yb-), Hf-based, Mg-based, Ni-based, Pd-based, Pt-based, Re-based, Sr-based, Ti-based, W-based and Zr-based MGs. All the data used in this work are summarized in Table 1.

3. Results

3.1. Strength levels of 301 MGs

In order to present the range and overall trend for strengths of MGs in various glass families, we plotted directly σ_y vs T_g for 301 different MGs in 29 alloy systems, as shown in Fig. 1. Apparently, the data show that the strength is mostly determined by the base element of the alloy. For Co-based MGs and MGs fabricated with refractory metals such as W-based, Re-based MGs, the strength level is the highest among all MGs, i.e., 4–6 GPa. However, for Ca-, Ce- and Sr-based MGs, the strength level is the lowest, i.e., 0.3–0.5 GPa. MGs with other base elements exhibit relatively moderate strength levels among all MGs, but still very strong comparing with their crystalline counterparties. For example, the strength range for Fe-based MGs is from ~2 GPa to ~4.5 GPa, higher than high-strength steels [110]; and the strength range is ~2 GPa to ~4 GPa for Ni-based MGs, ~1 GPa to ~2.5 GPa for Cu-based MGs and ~1 GPa to ~2 GPa for Zr-based MGs. For Al-based MGs, the strengths can achieve as high as ~1.5 GPa, which makes them be the metallic alloys with almost the highest specific strength [13].

The data trend also reveals a clear positive correlation between strength and T_g. For Co-based MGs and MGs fabricated with refractory, besides the highest strength they also have nearly the highest T_g (~1000 K), while Ca- and Sr-based MGs with the lowest strength level have almost the lowest T_g (~320 K) near T_{RT}. Based on the data in Fig. 1, we can fit the empirical relation between σ_y vs T_g as,

$$\sigma_y \propto T_g^2, \tag{1}$$

The fitted curve of Eq. (1) was plotted in Fig. 1 as dashed line. Although the data are still much dispersed, Eq. (1) grossly captures the positive trend of the relation between yield strength and glass transition temperature. This means tuning composition to achieve enhanced T_g may be an effective way to design MGs with high strength. Eq. (1) also demonstrates that high thermostability and high strength can be synchronously achieved in MGs. This advantage is rather unique as compared to materials with another nonequilibrium structure, i.e., nanocrystals, in which the thermostability and yield strength are often mutually exclusive [111]. This is because as refining grains into nano-scale to enhance strength, the driven force for grain growth dramatically increases due to the increased free energy of grain boundary. However, the positive relation between σ_y and T_g suggests that the stability of the structure in MGs seems to be energetically determined by stress and temperature in equivalent ways. This should be of significance for designing MGs for high temperature applications.

3.2. Yield strains of 175 MGs

Many researchers found that MGs yield at almost constant elastic strain of ~2%, or constant shear elastic strain of ~2.67%, although their compositions may be different [6,18]. In Fig. 2(a), σ_y vs the Young's modulus, E, of 175 MGs was plotted. Good linear relation can be obviously seen, further illustrating the generality of yielding conditions for MGs. The slope of the fitting line gives the average yield strain of 2.01%, well consistent with the previous report. However, the rule of 2% yield strain seems to be not very good for the high strength Co-based MGs and for the low strength Mg-based, Au-based and some RE-based MGs; some Co-based MGs exhibit elastic strain as high as ~2.5%, while some RE-based MGs show low elastic strain of ~1%.

Fig. 2(b) shows the shear strength, τ_y (here for simplicity neglecting the normal stress effect and assuming $\tau_y = \sigma_y/2$ [18]) vs the shear modulus, G, of 116 MGs. Similar to Fig. 2(a), the data give good linear relation, which indicates a "*general*" yield strain among various MGs in many alloy systems. Linear fitting gives the value of the average critical shear strain of 2.74%, similar to the value of 2.67% by fitting data of 30 MGs by Johnson and Samwer [18]. Also, if observing Fig. 2(b) carefully, one can see that some Co-based MGs have elastic shear strain limit of higher than 3%, while some RE-based MGs exhibit critical shear strain as small as 1.2%.

The good linear relation between strength and elastic modulus for various different MGs demonstrates that the strength should be primarily dependent on the type of atomic bonds represented by elastic modulus. However, the deviation from the constant elastic strain for some MGs should imply that the physical mechanism of yielding should be also associated with the specific structural arrangement.

3.3. Validation of previous models on yield strength and yield strain

As mentioned above, a unified equation on strength of MGs has been found by Yang et al. [7] and later derived by Liu et al. [8] from fundamental thermodynamics. This equation can be written as,

$$\sigma_y = 6R(T_g - T_{RT})/V_m, \tag{2}$$

where R is the gas constant, T_{RT} is the room temperature and V_m is the molar volume. In Fig. 3, we plotted σ_y vs $(T_g - T_{RT})/V_m$ for 132 different MGs. We can see that there is a good linear relation, demonstrating that Eq. (2) well captures the general variation of strengths for various MGs with a much wide strength range from 0.3 GPa to ~6 GPa. Considering the physical connotation behind Eq. (2), the observed good accordance with experimental data suggests the inherent correlation between mechanical yielding and glass transition. On the other hand, large scatters still exist if one only considers experimental data with strength lower than 2.5 GPa, under which there are strength levels of the most Zr-based, Cu-based, Ti-based, Pd-based, Pt-based, Mg-based, Al-based and RE-based MGs, as shown in Fig. 3(b). This discrepancy may imply that the intrinsic relation between yield strength and glass transition temperature may be more complicated than only simply considering thermodynamics.

Johnson and Samwer [18] considered the plastic yielding as activations of shear transformation zones (STZs), which were considered as basic plastic units of amorphous materials. Following Frenkel they developed a cooperative shear model (CSM), according to which the shear yield strain γ_C at T_{RT} can be written as,

$$\gamma_C = \gamma_{C0} - \gamma_{C1}(T_{RT}/T_g)^{2/3}. \tag{3}$$

Alternatively, the normal yield strain ε_C can be written as,

$$\varepsilon_C = \varepsilon_{C0} - \varepsilon_{C1}(T_{RT}/T_g)^{2/3}. \tag{4}$$