

On Mechanical Properties of Metallic Glass and its Liquid Vitrification Characteristics

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Abstract. A systematic survey of the available data such as elastic constants, density, molar mass, and glass transition temperature of 45 metallic glasses is conducted. It is found that a critical strain controlling the onset of plastic deformation is material-independent. However, the correlation between elastic constants of solid glass and vitrification characteristics of its liquid does not follow a simple linear relation, and a characteristic volume, viz. molar volume, maybe relating to the characteristic size of a shear transformation zone (STZ), should be involved.

Introduction

Metallic glasses, especially bulk metallic glasses (BMGs), are a relatively recent addition to the large family of glass systems [1,2], providing perfect model materials to investigate the relationship among their physical properties. The availability of various BMGs has permitted better characterization of their mechanical and elastic properties, and significant data have been collected on the mechanical properties, glass transition and elastic constants for various metallic glasses. Besides, the bonding in metallic glasses is essentially a central force isotropic character; thus the interactions between atoms are sufficiently simple to allow widely applicable common descriptions of the phenomena. In a manner, searching for intrinsic correlation in this simple glassy system could assist in understanding the relation between microstructure and macroscopic properties [3,4], and even fundamental physical questions relating to glass formation [5,6]. In this paper, we endeavor to collect massive new data available for metallic glasses to present that there are striking linear correlation among mechanical properties and liquid vitrification characteristics. Further, underlying physics of these correlations observed are explored.

Physical Properties

Based on Table I in Ref. 7 and further using the relevant data in the latest literature such as Refs. 4, and 8-12, the measured physical properties, including density ρ , molar mass M , yield strength σ_y , bulk modulus K , shear modulus G , glass transition temperature T_g , and fragility m , of 45 metallic glasses were obtained. The elastic constants of a glass are apparently important parameters for determining many of its mechanical quantities. Besides, their change under pressure or temperature

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treatments gives information of the changes in the atomic structure of the glass. The values of the elastic constants can be obtained experimentally by many methods in solids, such as mechanical deformation or ultrasonic propagation. The glass transition temperature T_g always occurs as an adjustable parameter, but is also dominated by the bonding force among the constituent atoms. Its value can be determined by differential scanning calorimetry (DSC) or differential thermal analysis (DTA). Besides, the molar volume V_m , as a “characteristic” volume of atomic structure, is given by

$V_m = M / \rho$. Because of the limit plasticity in BMGs before fracture, we identify fracture strength

with yield strength σ_y in compression or tension, ignoring the small normal stress dependence of yield [10]. Therefore, it would be intriguing to see if there exist some relations among the physical properties mentioned above.

Results and Discussion

We find that although G exhibits a very good linear correlation with E , there seems no clear linear relation between G and K , as shown in Fig. 1. Using a model developed by Knuyt et al. based on a Gaussian distribution for the nearest-neighbor distance in an ideal unicomponent metallic glass [13], the K/G can be expressed by [14]

$$\frac{K}{G} = \frac{5}{3} \left[1 + \frac{3}{2} \frac{\langle \sum r_k U'(r_k) \rangle}{\langle \sum r_k^2 U''(r_k) \rangle} \right]^{-1} \quad (1)$$

where r_k is the positions of any atom k , $U(r)$ is the interatomic potential, and

$\langle \sum r_k^n U'(r_k) \rangle = \int_{r=0}^{\infty} r^n U'(r) \text{RDF}(r) dr$, ($n=1,2$), here the RDF is defined by a mean position

r_1 and a width σ_1 for the atoms in the first shell around a central atom. Thus, K/G is determined

by the atomic structure and highly material dependent. But, the Young's-shear modulus ratio is given by $E/G = 3/(1 + G/3K)$. Note that the dependence of G/K on E/G is very slight, although

G/K is material dependent. For BMGs, G/K mostly ranges from 1/6 to 1/2; thus, the range of E/G is about 2.57 ~ 2.84. This value is consistent with the fitting parameter of 2.678 in Fig. 1(b).

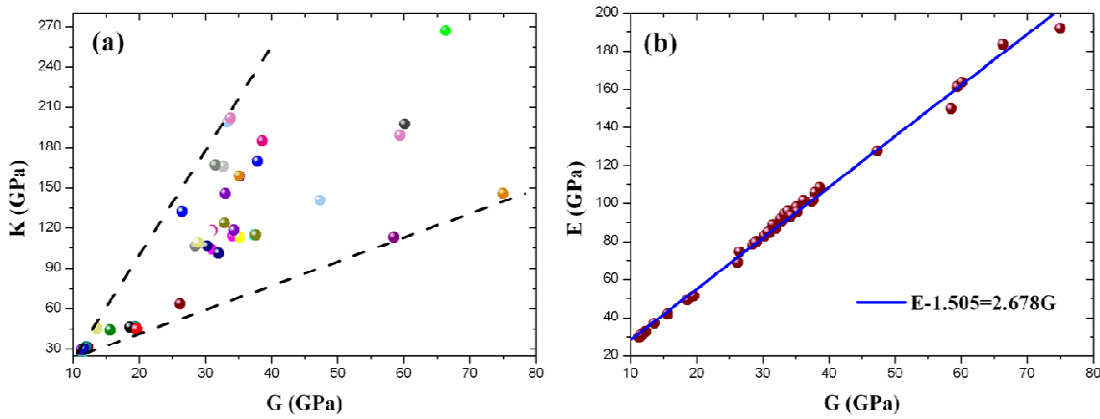


Fig. 1 Correlation of (a) K and (b) E with G .

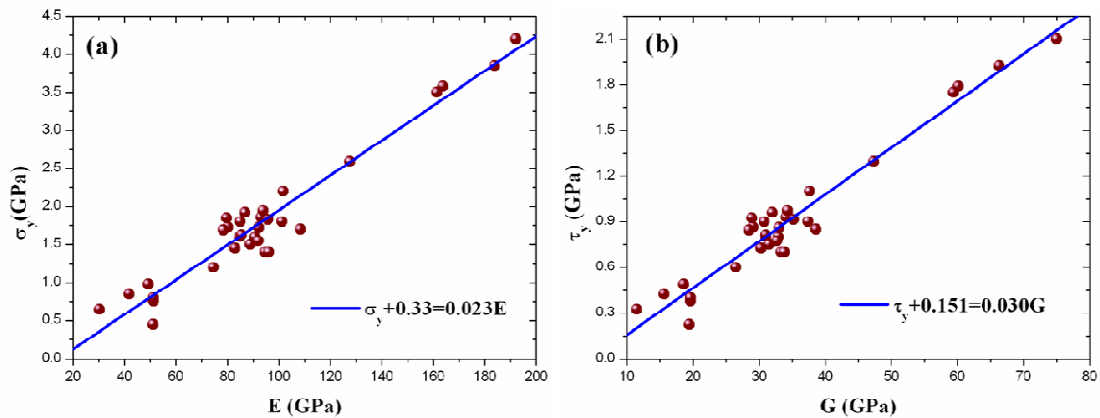


Fig. 2 (a) σ_y vs. E , (b) τ_y vs. G .

Based on relevant data from metallic glasses, Wang shows a clear linear relationship between σ_y and E ($E \approx 50\sigma_y$) [4]. A similar relationship between shear yield stress $\tau_y \approx 0.5\sigma_y$ and G ($\tau_y = 0.0267 \pm 0.0020G$) is revealed by Johnson *et al.* [9]. Using the collected data, a striking linear correlation between σ_y and E is also observed, as shown in Fig. 2(a). This linear correlation can be best fit by $\sigma_y \approx 0.023E$. Following Johnson *et al.* [9], the other linear relation $\tau_y \propto 0.03G$ is also obtained, as shown in Fig. 2(b). Such relationships clearly demonstrate that the elastic and plastic properties are mutually related to each other in all the classes of BMGs, unlike the crystalline alloys. Further, there is a constant critical strain of about 2%, controlling the onset of plastic deformation for BMGs. This means that the atomistic structure and bonding strength, i.e., the density and Young's modulus, produce no influence on the critical strain in BMGs. As with most materials, the mechanism of plastic deformation of BMGs is closely linked to their structure. There is general consensus that the fundamental unit process underlying plastic softening must be a local rearrangement of atoms, referred to as "shear transformation zone" (STZ) that can accommodate local shear strain [15,16]. The material-independence of macroscopic critical flow strain provides powerful evidence for the universally valid STZ in BMGs.

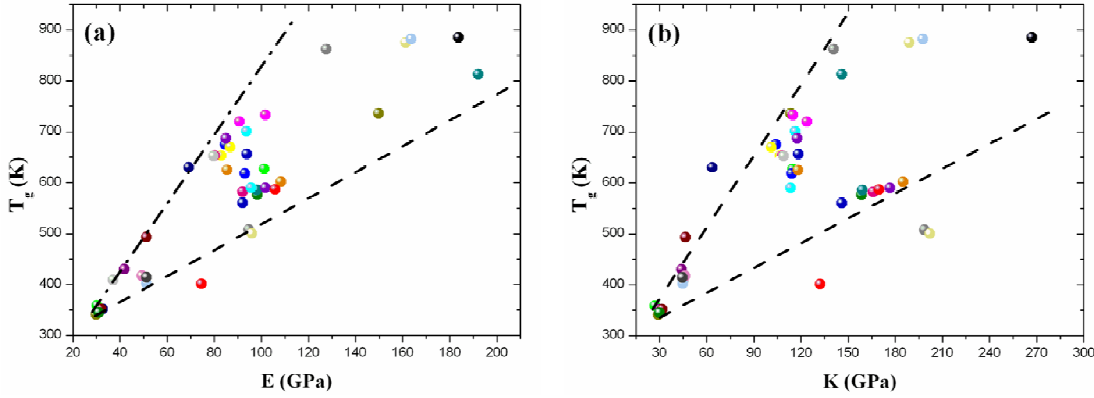


Fig. 3 Correlation of T_g with (a) E and (b) K .

Primary analysis based on limited data show that the glass transition temperature T_g is in scale with E [4]. The free volume model for the glass transition predicts that $T_g \propto K_\infty$ [17], here K_∞ is the instantaneous bulk modulus of liquid. Our results show that there seems no clear linear relation between T_g and E (or K), as shown in Fig. 3. Since $E \propto G$, the relation between T_g and G must be also nonlinear. In the elastic models (in particular, the shoving model), a “characteristic” volume is suggested by Dyre to enter the correlation between T_g and G [18]. The most obvious thing would be to take the characteristic volume to be proportional to the molecular volume V_m defined above. In fact, Heuer *et al.* [19] proposed that T_g has to scale with a energy scale which can be chosen as $B = Mv^2$, here v is the velocity of sound. Remember $G \propto \rho v^2$; hence $T_g \propto V_m G$. To examine the validity of this equation, we plot the ratio $RT_g/(M/\rho)$ against G in Fig. 4(a). Surprisingly, a striking linear correlation is observed, which can be best fitted by

$$RT_g/(M/\rho) - 0.056 = 0.014G \quad (2)$$

where the value of “-0.056” reflects the temperature softening effect on modulus [7]. Based on the physical analogy between the STZ deformation and glass transition, Yang *et al.* found that the shear yield strength of BMGs at ambient temperature T_0 can be predicted well by a unified parameter, $R(T_g - T_0)/V_m$ [3]. Compared to Eq. (2), we find that a compound parameter, RT_g/V_m , can be regarded as a scale on shear yield strength at zero temperature. The constant of 0.014 corresponds to the average shear yield strain γ_c observed by Johnson *et al.* [9] and can be considered as an apparent shear yield strain $\hat{\gamma}_c$. The linear correlation between RT_g/V_m and G implies that G

is a controlling quantity in real flow events [18]. Fig. 4(b) exhibits that σ_y does be proportional to $RT_g/(M/\rho)$, which confirms the validity of our analysis.

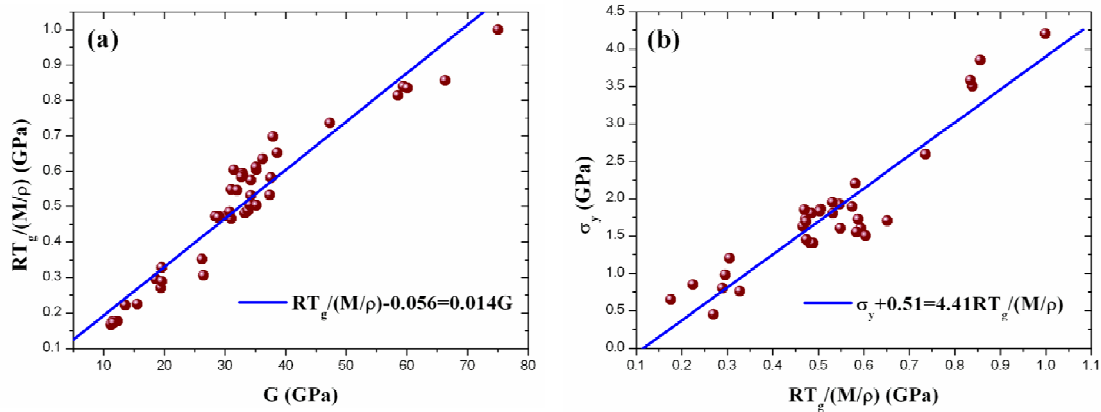


Fig. 4 (Color online) Correlation of $RT_g/(M/\rho)$ with (a) G and (b) σ_y .

Summary

The survey of large scale experimental data available on 45 BMGs reveals striking systematic correlations among elastic constants, mechanical properties, molar volume, and the glass transition temperature of the glass-forming liquid. Their underlying physics are rationalized based on the atomic structure information. The correlations imply that the BMGs may exhibit universal behavior due to their similar structure. A common element process such as STZ with a characteristic volume, relating to molar volume, may underpin the deformation and fracture behavior of BMGs. Our results could assist in understanding the relation between microstructure and macroscopic properties, and even fundamental physical questions relating to glass formation and the nature of glass.

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