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Universal percolation threshold for ductile-brittle transition of amorphous alloys

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ABSTRACT

Based on the free volume, shear transformation zone and percolation theory, a new percolation model has been established to investigate the ductile-brittle transition in amorphous alloys. Taking the binary $Cu_{25}Zr_{75}$ amorphous alloy for example, the influence of the free volume concentration and flow unit dispersity on its percolation threshold value was analyzed. The results show that the concentration of flow units reach a critical value when the ductile-brittle transition occurs in the $Cu_{25}Zr_{75}$ amorphous alloy, and this critical value is independent of the concentration of the free volume but dependent on the dispersity of flow units. Furthermore, the percolation threshold values of La-, Zr-, Cu-, Pd-, Fe-, Sr- and Tm-based amorphous alloys were also calculated, a percolation threshold value of ~0.516 for ductile-brittle transition in these amorphous alloys was obtained. Therefore, our analysis results suggest that ~0.516 appears to be a universal percolation threshold value for ductile-brittle transition in amorphous alloys.

1. Introduction

Since a glassy state is usually obtained by rapidly freezing the liquid to avoid crystallization, the structure and many properties of amorphous alloys (or metallic glasses, MGs) are inherited from supercooled liquid [1,2]. Many exotic mechanical properties of MGs have attracted a lot of interest, such as ultrahigh strength, superior elasticity, and excellent thermo-plasticity [3–6], originating from the disordered atomic structures [7,8]. However, due to some common structural defects (for instance, dislocations and slips) do not exist in amorphous alloys, most MGs exhibit poor ductility at room temperature because their plastic deformation is highly localized into shear bands [9–11]. Therefore, the solution to the key problem of plastic deformation will be very beneficial for the extensive application of MGs.

It seems to be well-known that an amorphous solid that exhibits a glass transition is called a glass, and the glass transition can take place upon applying stress or heating, cause they have the same evolutionary process of microscopic structure, i.e., “strain-temperature equivalence” [12–14]. Thus, several significant theoretical models in describing this flow and evolution of structure have been made in the past years. A free volume model based on the single atom transition was proposed by Spaepen [15], a shear transformation zone (SZT) model based on the cooperative shear motion of atomic clusters (ACs) was proposed by Argon [16], in addition, the flow unit model was introduced by Wang [17] and the tension transformation zone (TTZ) model was introduced by Jiang [18]. Anyhow, although these theoretical models have their own scope of application, they do have considerable implications for understanding “flow events” and plastic deformation of amorphous alloy.

According to the free volume model, a critical reduced free volume (RFV) value of $x_C \sim 2.4\%$ for the onset of yielding in most MGs has been found by Wang [19]. So another interesting question about what is the critical value of STZ for the onset of yielding attracted us, whereas this question is not so easy to be solved because STZ is a dynamic defect, which cannot be determined beforehand from an amorphous solid atom image at a certain time. Therefore, in this paper, a percolation model for the critical volume fraction of atomic clusters (ACs) in STZ as shear bands initiate is established, we here regard ACs as the flow units. When the density of ACs reaches a critical value, the percolation of flow units occurs and the entire STZ can unjam from a frozen state into a supercooled liquid state, so the different sizes of the shear bands will be formed through the interconnectedness of some STZs, but only single main shear band will expand rapidly through the self-organized behavior of STZs and eventually lead to failure of MGs. The present work may supplement a new result on studying the ductile-brittle transition of MGs.

2. Methods

As shown in Fig. 1(a), there are some local sites in the MGs because

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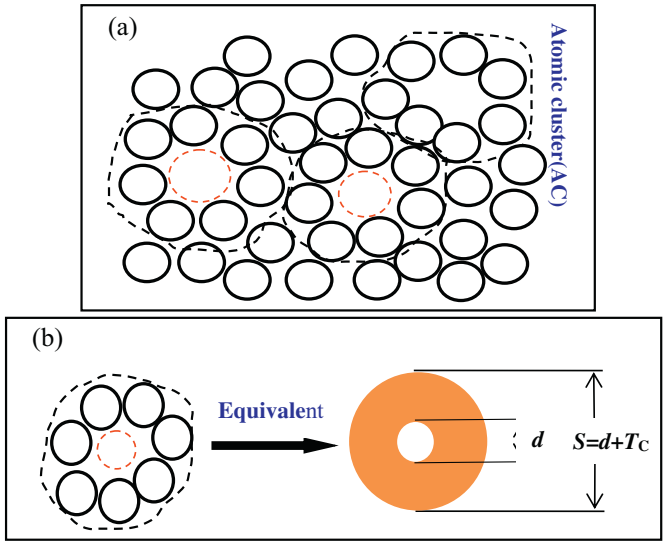

Fig. 1. (a) The schematic of atomic structure of MGs in a 2-D system, the black dotted line areas are ACs, the red dotted line areas are free volume; (b) The schematic of equivalent SSV, and d is diameter of SFV, S is diameter of SSV, T_C is the critical thickness between SSVs. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

of the statistical distribution of free volume [15], these liquid-like regions where are rich in free volume, like black dotted line areas, have a smaller viscosity, on the contrary, the viscosity of another solid-like regions where are short of free volume is larger. In Fig. 1(b), all atoms and free volume within black dotted line areas are called an Atomic Cluster (AC), which is equivalent to the sphere stress volume (SSV) according to the concept of BDT theory proposed by Wu [20], and the free volume within AC can regard as the sphere free volume (SFV). When shearing stress τ exceeds critical value τ_C, multiple SSVs will yield and form a percolating network in STZ. Actually, the purpose of our hypothesis is to take SSV as a "toughening particle", the plastic deformability of MGs can attribute to the effect of the concentration of "toughening particles" on the toughening of sample, such as amorphous alloy foam material [21]. So what is the optimum concentration of these "toughening particles" or the percolation threshold for ductile-brittle transition of amorphous alloys?

2.1. The diameter d and volume fraction θ_f of SFV

In the free volume model, Spaepen thinks the strain rate of amorphous alloys is closely related to the free volume:

$$\dot{\gamma} = 2f\Delta f \exp\left(-\frac{\alpha v^*}{v_f}\right) \times \sinh\left(\frac{\tau v_a}{2kt}\right) \times \exp\left(-\frac{\Delta G^m}{kt}\right) \tag{1}$$

where f is the frequency of atomic vibration, Δf is volume ratio fraction, α is a geometric factor between 0.5 and 1(our article is 0.75), $v^*(v_a = 1.25v^*$, v_a is atomic volume) is the hard-sphere volume of an atom, v_f is the average free volume per atom, $\tau$is shearing stress, k is the Boltzmann constant, t is the temperature, ΔG^m is the activation energy of atomic motion. RFV x is thus introduced by Wang [19]:

$$x = v_f/(\alpha v^*) \tag{2}$$

They found a critical RFV value of $x_C \sim 2.4\%$ for the onset of yielding is universal for MGs. Furthermore, as shown in the Fig. 1(b), the RFV x can also be written as:

$$x = \frac{v_f}{\alpha v^*} = \frac{1.25v_f}{\alpha v_a} = \frac{1.25 \times (4\pi/3)(d/2)^3}{(4\pi/3)(\overline{D}/2)^3 n\alpha} = \frac{1.25}{n\alpha}\left(\frac{d}{\overline{D}}\right)^3 \tag{3}$$

where n is the number of atoms within AC, and $\overline{D}$ is atomic average diameter, but the atomic average radius [22] is $\bar{R} = \left(\sum_i^n A_i r_i^3\right)^{1/3}$, A_i is the volume fraction of atom which radius is r_i in the amorphous alloy. According to Eq. (3), the diameter d of SFV is determined from x and n because $\overline{D}$ is a constant for a given MG. In addition, the volume fraction of SFVs is:

$$\theta_f = v_f/(v_f + v^*) \tag{4}$$

By Eqs. (2), (3) and (4), the relationship between diameter d and volume fraction θ_f of SFVs can be obtained:

$$d = \left[\frac{n\theta_f}{(1-\theta_f)1.25}\right]^{1/3} \overline{D} \tag{5}$$

So the relationship between θ_f and d will be affected by the number of atoms n, in fact, different n reflects the different size of flow units in MGs. Therefore, we take the binary $Cu_{25}Zr_{75}$ amorphous alloy as an example to investigate the relationship between θ_f and d under different size of flow units.

Initially, $D_1 = 0.256$ nm and $D_2 = 0.32$ nm are from Ref [23], where D_1 and D_2 are respectively the minimum and maximum atomic diameter of $Cu_{25}Zr_{75}$ amorphous alloy system. Atomic average diameter $\overline{D}$ is 0.306 nm, moreover, the critical diameter d_C is between $d_{min} = D_1/(1.25)^{1/3}$ and $d_{max} = D_2/(1.25)^{1/3}$ for the onset of yielding in MGs based on free volume model, so the size of flow units in $Cu_{25}Zr_{75}$ amorphous alloy system, namely, the n will vary from 33 to 64 calculated by Eq. (3). Then, considering that the RFV x varies from the initial value 0.008 [24] to critical value 0.024 [21], the volume fraction $\theta_f$of SFVs is thus from 0.006 to 0.018, correspondingly. Last, scatter points in Fig. 2 show the nonlinear relation between θ_f and d when n is 35, 45, 55 and 65, respectively.

We noticed that the critical values d_C are in the range of 0.2–0.3 nm, it is generally understood that voids of this size are not stable in MGs, but it does not mean that our model is wrong, SFV does not really exist and is just a hypothesis. Furthermore, According to Wu's research on polymers, the relationship between d and θ_f can also be approximately expressed as following:

$$\theta_f = (\pi/6)*(d/S)^3 = (\pi/6)*[d/(d + T_C)]^3 \tag{6}$$

or:

$$d = T_C\{[\pi/(6\theta_f)]^{1/3} - 1\}^{-1} \tag{7}$$

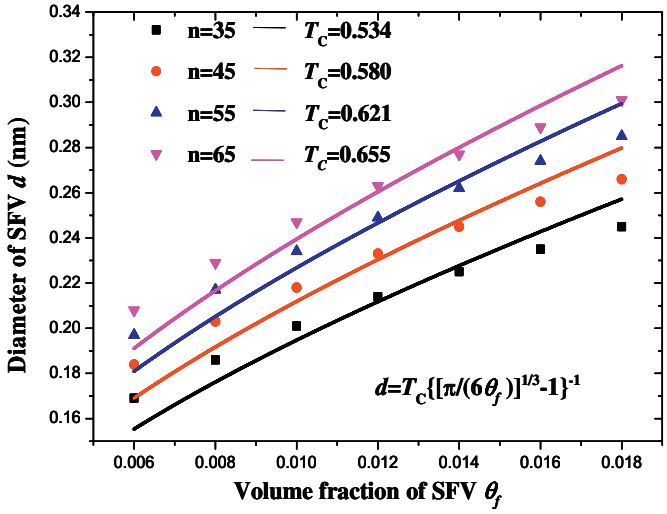

Fig. 2. The evolution of diameter d of SFV under different volume fraction θ_f of SFV when n is 35, 45, 55 and 65, respectively. The scattered points are theoretical results, the solid curves are correspondingly fitted results. The parameter T_C is obtained by fitted function $d = T_C\{[\pi/(6\theta_f)]^{1/3} - 1\} - ^1$, the correlation coefficient R^2 of the fit for four curves is all about 0.88.