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Letter to the editor

Relation between ideal and real strengths of metallic glasses

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ABSTRACT

Available experimental data of about 110 metallic glasses show that the ratios of room-temperature strengths to low-temperature ideal strengths have universal upper and lower bounds. The two bounds are rationalized by taking cooperative shearing of shear transformation zone (STZ) operations into consideration in the potential energy landscape thermodynamics. It is striking to find that the real-to-ideal strength gap results from both configurational and thermo-vibrational contributions to STZs. The former determines the upper bound, while the latter further decreases strengths to the lower bound. The results may shed new insight into metallic glass strength and flow.

1. Introduction

The scientific interest in strength of materials could be traced back to the famous notebooks of Leonardo da Vinci [1]. However, not until the early years of the twentieth century did people relate strength of materials with their atomic structure. In 1926, Jacov Frenkel [2] calculated the ideal shear strength of a perfect fcc metal to be about a tenth of its shear modulus *G*. However, real crystalline materials yield strengths two to three orders of magnitude lower. This discrepancy was attributed to dislocations. The real strengths for crystalline materials have been widely estimated according to the resistance of dislocation motion such as Peierls–Nabarro force, grain size, dislocation junction, etc. [3–6]. In contrast, metallic glasses or glassy alloys, representing a young class of advanced materials, are free of dislocations [7–10]. It is highly expected that strengths of such amorphous materials could approach the theoretical limit. These materials receive therefore much attention from both scientific and engineering points of view [11–20].

In this aspect, a key finding is the intrinsic correlation of strength for inhomogeneous deformation with glass transition temperature [14,16,17], which indicates the similarity between stress-driven yielding and temperature-caused glass transition in metallic glasses [16,21,22]. Actually, both physical processes are underpinned by collective motions of atomic clusters, termed shear transformation zones (STZs) [23–25]. By developing the cooperative shearing model (CSM) of STZs, Johnson and Samwer [13] proposed a universal power-law of 2/3 of temperature dependent yield strength. In particular, Cheng and Ma [18] applied this power law to homogeneous deformation by atomistic calculations, and successfully predicted the ideal strengths for metallic glasses. Their prediction has recently been confirmed by employing an in situ TEM tension technique [20]. These intriguing progresses greatly motivate us to understand metallic glass strengths from real value to ideal/theoretical limit. In fact, their relationship has not been established theoretically up to now, which is a major scientific challenge. In this letter, we analyze the experimental data of both real and ideal strengths for more than 100 metallic glasses from 24 different alloy systems. The relationship between room-temperature (RT) and low-temperature ideal strengths is quantitatively bridged combining the potential energy landscape (PEL) theory, the CSM of STZs with fracture mechanics.

2. Experimental observations

Fig. 1 presents the macroscopic shear strength τ_{yT} at RT versus the athermal theoretical shear strength τ_0 for ~110 metallic glasses. Here, we roughly adopt τ_{yT} as half of the yield strength σ_{yT} in monotonic loading (Tresca's yield criterion), ignoring the small normal stress dependence [13,17,26]. It must be pointed out that the "thermal" actually means a temperature as low as possible rather than the absolute zero temperature. Following the previous works [16,18,27], τ_0 maybe recall the origin of $G/10$, skirting its very small temperature dependence [13,28,29]. It is believed that these approximations cannot significantly change the essential physics. The experimental data for σ_{yT} and G at RT can be found in the literature [13,21,30–33]. It can be observed from Fig. 1 that the real strengths are indeed quite close to their theoretical strengths, being of the same order of magnitude. The former is only a fraction smaller than the latter. Very interestingly however, all experimental data can be bounded by two straight lines. More specifically,

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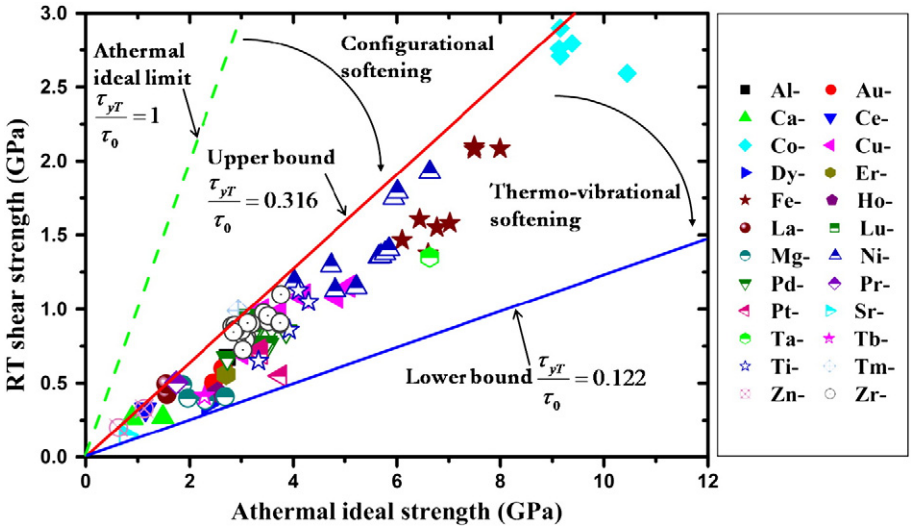

Fig. 1. Real shear strength τ_{yT} at RT versus "athermal" ideal shear strength τ^0 for about 110 metallic glasses from 24 different alloy systems, showing the upper and lower bounds. The upper bound, i.e., the red solid line is best fitted by Eq. (5). The lower bound, i.e., the blue solid line is best fitted by Eq. (7). The green dashed line is the athermal ideal strength limit.

the ratio of the RT strength to the athermal theoretical strength obeys the following universal relationship:

$$\Gamma_{\text{upper}} \geq \frac{\tau_{yT}}{\tau_0} \geq \Gamma_{\text{lower}}. \tag{1}$$

The fitting to the experimental data in Fig. 1 shows that the two bounds, Γ_{upper} and Γ_{lower}, are very close to values of 0.316 and 0.122, respectively. It is clear that there exists a gap between the real strengths and their ideal limit, i.e. $\tau_{yT}/\tau_0 = 1$, marked by the green dashed line in Fig. 1. Some questions should arise from our observations. What is the physical meaning of the upper and lower bounds of the real strengths? Due to absence of dislocations in metallic glasses, what should be responsible for the gap of the real-ideal strengths? Undoubtedly, definitive answers originate from the unique response of atomic structures of metallic glasses to applied stress. Considering the complexity of disordered structures, we resort to the PEL theory [34–37] to reveal the underlying physics of our observed phenomena.

3. Theory and discussion

PEL is a multidimensional surface describing the potential energy function of a glassy system that depends on the spatial location for its constituent particles. Intuitively, the state of such a system can be well represented by a point on or above the hypersurface. By analogy to Earth's topographic maps, Stillinger and Weber [34,35] provided a formally exact portioning of the configurational space as a sum of distinct basins, associating with each local minimum of the potential energy surface, namely, an inherent structures (IS). The PEL picture provides a natural separation of the system's state into sampling distinct ISs and vibration within an IS. The PEL approach thus permits identification of the IS in an ideal metallic glass at very low temperature and a real sample at RT. As illustrated on the left in Fig. 2, the ideal sample should correspond to the IS with the lowest potential energy (deepest "megabasin") that is devoid of substantial regions with local crystalline order [38]. At a low enough temperature the ideal system becomes stuck in the single IS with almost frozen vibration, unable to surmount the highest energy barrier. As temperature increases to RT, the depth of ISs in the real sample decreases and the vibration intensifies, as shown on the right in Fig. 2. Meanwhile, the real system displays a proliferation of well-separated megabasins, corresponding to the increase of the configurational entropy. Consequently, the difference of the IS between the ideal system and the real one has the configurational and vibrational aspects. It is such difference that results in the gap of their strengths, because the strength of systems *per se* reflects the mechanical instability of their ISs that is normally obscured by the thermal vibration [13,39–41]. Hence, the ratio of the real-ideal strengths can be expressed as a sum of the configurational contribution r_{conf} and the thermo-vibrational one r_{ther}, that is

$$\frac{\tau_{yT}}{\tau_0} = r_{\text{conf}} + r_{\text{ther}}, \tag{2}$$

where $r_{\text{conf}} = \left[\tau_{y0}/\tau_0\right]_{\text{conf}}$ measures the ratio between the ideal strengths and the real strengths at the athermal limit, and $r_{\text{ther}} = \left[\tau_{yT}/\tau_{y0}\right]_{\text{ther}}$ denotes the thermal softening effect on the real strengths due to temperature increase from very low temperature to RT. Next, the main task is to quantitatively determine the configuration and vibration terms in Eq. (2).

Recent studies have identified solute-centered polyhedra as the fundamental building blocks of metallic glasses, constituting short-range-order; these polyhedra subsequently pack together to fill three-dimensional space obeying a certain rule, giving rise to medium-range-order [42–45]. Driven by external stress, the short-to-medium-range order could be lost via STZ operations. Therefore, it is reasonable to treat the virgin metallic glass as a composite consisting of potential STZ sites within the elastic confinement of a surrounding matrix [23,46]. Here we consider a semi-infinite metallic glass plate containing an edge-crack subject to a remote shear stress. The edge-crack has finite size that is so small

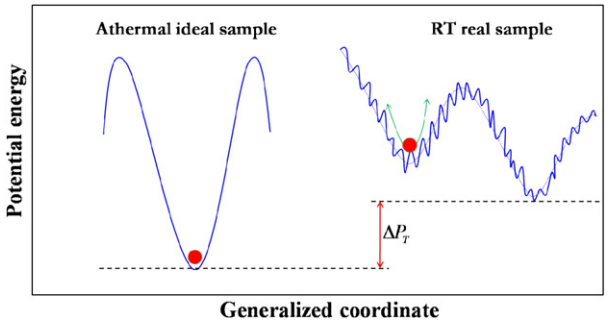

Fig. 2. Schematic illustration of archetypal potential energy landscapes of athermal ideal and RT real metallic glass.