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Review

On the source of plastic flow in metallic glasses: Concepts and models

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ABSTRACT

We briefly review the state-of-the-art study on plastic flow in metallic glasses. Especially, we survey the features and behaviors, percolation, and response of the basic deformation units to the activation of stress and temperature, and various models and notions on microscopic flow in metallic glasses. The discussion, comments and perspective on possible unified notation, terminologies and models on plastic flow in metallic glasses are presented. The purpose is to reach a consensus within the community with a hope to eventually unify the notations and models on the deformations in metallic glasses.

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1. Introduction

Glassy state is a universal property of liquids if they are cooled rapidly enough, and is regarded as the fourth state of matter [1–5]. As a liquid is cooled, its atomic motions or dynamics slow down, resulting in a material just as solid as any crystal but without obvious long-range structural order of a crystal. Metallic glasses (MGs, also often referred to as amorphous alloys) are the simplest atomic glasses, which have spherical or nearly spherical constituents. Metallic glasses do not possess a microstructure in the traditional sense, where structural defects, such as dislocations, twins, stacking faults in a crystalline solid, are well defined and largely determine the mechanical and other properties of the solid. The atomistic mechanism of mechanical deformations, the atomic flow responded to stress or temperature, and failure in metallic glasses are very different from those in crystalline solids, and also different from the conventional picture [6]. In glasses, the medium-range topological heterogeneity in the order of only a few nanometers [7–9], is regarded as a result of density and/or compositional fluctuations, becomes an important parameter [7,8]. However, exact correlation between structural heterogeneity and resulting mechanical behavior remains mostly unresolved [7–9].

Studies have clearly demonstrated that in MGs, atomic processes in plastic flow is not so simply perceived [10]. Scientists both in material science and physics fields have made intensive efforts to elucidate the flow mechanism in MGs. Because plastic deformation

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of crystalline materials occurs due to motion of dislocations, search for similar "defects" in MGs has been attempted for long time. The current majority view on the phenomenon of flow, including mechanical failure and relaxations, and glass transition in MGs, appears to be that it is triggered by the activity of some structural "defects", such as free-volumes [11–13], shear transformation zones (STZs) [14–16], or soft liquid-like regions [17–20]. The concentrations of such defects are assumed to be low, for instance, the free volume in a MG is only in the order of a percent in volume fraction [15,17,21–23]. Despite a small fraction, mechanical properties of the MGs depend sensitively on their "defects" [11,15,17,21–34]. In crystalline solids, defects such as dislocations can be directly imaged using transmission electron microscopy, but such characterization techniques are considerably more difficult to apply to MGs in the absence of a long-range lattice. To find a direct evidence to correlate microscopic "defects" with plastic flow has proven to be extremely challenging. Macroscopically, MGs fail by forming well-defined shear bands. Many efforts were, therefore, made to study shear band formation. However, the shear banding process itself is very complicated and involves the interplay among temperature, local structural heterogeneity, free volume, and stresses. As a shear band propagates, it becomes intensively heated and, sometimes, melted by the dissipated energy of mechanical work [35], and this local melting essentially wipes out any structural change made by mechanical deformation. Consequently, it is almost impossible to relate the plastic deformation to the microstructure through shear bands.

There is yet another great challenge in discussing the flow behavior of metallic glasses in the community. Specifically, various terminologies/notations have been used to describe the onset of plasticity, plastic flow and fracture in metallic glasses. It often causes confusion and, sometimes, unnecessary dispute. Therefore, it might be useful to discuss the different terminologies and models at this stage. The purpose of the paper is, therefore, to summarize various notations/terminologies and models on plastic flow in MGs with an attempt to compare and comment the physical assumptions behind these terminologies used in the description of different models. It may never be impossible to get a universal consensus within the community. However, a comparison of various models and notations/terminologies used in each model, the similarity and dissimilarity among them, and their mutual connections can certainly benefit the advance of the field.

2. The notation, terminologies and models on plastic flow in MGs

2.1. Shear-transformation-zone modeling

Classical theories that posit flow defects in MGs commonly refer to these as free volumes. As illustrated in Fig. 1(a), free-volume is defined as excess space among atoms which is necessary for atomic rearrangements in glassy solids [11–13]. The free-volume is probably the most widely used phenomenological concept in explaining flow, diffusion, structural relaxation, glass transition and mechanical properties. Free volumes facilitate atomic motion, including interatomic slips which would result in plastic deformation. However, the free-volume model was created for hard-sphere systems. In metallic materials, because of the harmonic nature of the interatomic potential, atoms can squeeze through tight space without free-volume when sufficient shear stress is applied. It was demonstrated that diffusivity in metallic liquids is surprisingly insensitive to pressure, whereas in the free-volume theory diffusivity is expected to be suppressed by pressure [36,37]. Lewandowski have shown that the mechanical strength of metallic glasses is almost the same in tension and compression, and thus nearly independent of pressure [38], indicating that pressure has only minor effects. This result is consistent with the absence of the pressure effect on diffusion, and casts doubt on the free-volume mechanism for deformation. The free volume model has also been decisively challenged by diffusion studies, which demonstrated that atomic diffusion occurs in a collective manner rather than individual atom jumps as assumed by the free-volume theory [39,40].

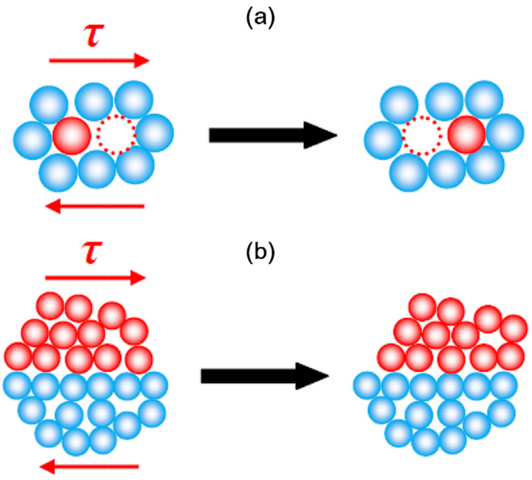

Fig. 1. The schematic illustration of (a) the free-volume model and (b) the shear-transformation-zone model.

Alternatively, Argon [14] proposed the seminal concept of 'shear transformation zone' (STZ) in the late 1970s to explain plastic flow in metallic glass. Since then, extensive research interest has been stimulated in the field of metallic glasses, with an attempt to understand the nature and characteristics of STZs. Today, STZ may have become the most popular term used by us for explaining our experimental data; however, little attention has been paid to the fact that, indeed, there is more than one type of STZ models. In general, existing STZ models could be categorized into two types, with one picturing STZ as a "defect" and the source of plastic flow, and the other picturing STZ as an "event" and the consequence of plastic flow. The STZ model of Argon belongs to the latter type, according to which STZ is an event involving small collective atomic movements across tens of atoms [14,16], as illustrated in Fig. 1(b). In the early development of the STZ model, it was assumed that these STZ events tend to occur in the regions of low atomic density [11,12,14]; however, through tracking the local intensive shear events in atomistic simulations, it was found that there is no deterministic correlation between local density and STZ event [41]. By comparison, STZs were ascribed to bond switching events in the atomic stress theory, which result from local topologic instability and can be triggered in both high and low density regions where unstable atomic configurations reside [42]. Here, it is worth mentioning that Johnson and Samwer [43] extended Argon's concept of STZ and merged it into the potential energy landscape perspective, and proposed a cooperative shear model to understand the deformation mechanisms and rheological properties of MGs. According to the cooperative shear model, activation of isolated STZs locally confined within an elastic matrix could be associated with the reversible fast β relaxations, while percolation of these β events leads to an irreversible collapse of the confining matrix and breakdown of elasticity that is associated with the slow α process. In such a sense, the mechanical response of MGs should be correlated with their relaxation behavior and the attributes of the underlying potential energy landscape. Namely, local hopping