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Origin of stress overshoot in amorphous solids

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ABSTRACT

Based on the shear-transformation-zone (STZ) theory, we propose a constitutive model for describing homogeneous elastoplastic deformation of amorphous solids where the interaction of shear transformations and free volume dynamics is incorporated. This theoretical model can reproduce the stress overshoot behavior that shows the dependence of strain rate, temperature, STZ population and dilatancy of systems. It reveals that the stress overshoots its steady state value due to the delayed activation of shear transformations that results from the insufficient free volume in the system. However, the subsequent strain softening (stress drop) is attributed to the shear-induced dilatation that is a result of the positive interplay between shear transformations and free volume creation, the latter playing the dominant role. Our analysis also demonstrates that the STZs, as basic carriers of amorphous plasticity, govern the yielding of the system, whereas the free volume dynamics significantly affects the post-yielding behaviors.

1. Introduction

Understanding of plasticity, i.e., how solids flow, is a classical problem (Hill, 1998), however it remains a challenge, particularly in the absence of a crystal lattice. Dislocation-mediated plasticity of crystals breaks down in the face of amorphous solids without long-range order (Falk, 2007; Chen, 2011). Regarding plastic flow of amorphous solids, ranging from glassy polymers to metallic glasses, a common feature is the stress overshoot (Hasan and Boyce, 1995; Kawamura et al., 1997; de Hey et al., 1998; Koumakis et al., 2012): the stress versus the applied strain first increases to a maximum and then decreases towards its steady-state value. The universality of this behavior implies that certain fundamental processes should underlie amorphous plasticity, albeit the diversity of microscopic constituents.

In the past few decades, theories concerning the plasticity of amorphous solids have developed along two main avenues. (i) The free-volume theory (Spaepen, 1977) argues that the plastic flow results from a series of stress-driven creation events of free volume via individual atomic jumps. (ii) The “shear transformation (ST)” theory (Argon, 1979) proposes that the basic carries of amorphous plasticity are irreversible rearrangements of small clusters of particles (i.e., atoms and molecules). However, an integrated picture for amorphous plasticity is emerging that (Falk and Langer, 1998; Langer, 2001; Lemaître, 2002; Argon and Demkowicz, 2008; Henits et al., 2012): free volume has a “catalytic” capability to trigger STs and meanwhile is enriched by the latter; free volume can be depleted by relaxation, which may cause potential STs to extinguish. Recently, Langer and co-workers (Langer, 2004; Bouchbinder et al., 2007a,b; Langer, 2008; Bouchbinder and Langer, 2009) have developed an athermal version of the shear-transformation-zone (STZ) theory where an

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effective disorder temperature (analogous to the free volume in some sense) is introduced to directly relate with the STZ density. They revealed that the stress overshoot occurs due to a lack of the initial STZ density or effective disorder temperature in systems; new STZs must be generated by a stress higher than the steady state flow stress. This basic picture motivates us to further ask: what roles do the STs and free volume play, respectively, during the overshoot process? The present work attempts to answer this question. For this purpose, we propose a constitutive model for amorphous solids, within the framework of the classical STZ theory developed by Falk and Langer (1998).

2. Theoretical model

Consider an amorphous solid at temperatures T near the glass transition temperature T_g. The deformation is expected to be spatially homogeneous, modeled for a simple-shear case. The overall shear-strain rate $\dot{\varepsilon}$ can be decomposed into elastic and plastic parts, $\dot{\varepsilon} = \dot{\varepsilon}^{el} + \dot{\varepsilon}^{pl}$. The elastic deformation obeys Hooke's law $\sigma = \mu\varepsilon^{el}$, where σ is the shear stress and μ is the shear modulus. The plastic deformation results from the accumulation of unit STs occurring within local clusters (Argon, 1979; Falk and Langer, 1998; Johnson and Samwer, 2005; Jiang et al., 2009; Lemaître and Caroli, 2009). Here we adopt the mean-field approximation of STs, i.e., the STZ theory that ignores the spatial correlations between STs (Falk and Langer, 1998; Langer, 2001; Argon and Demkowicz, 2008; Lemaître and Caroli, 2009). Nevertheless, this assumption of spatial homogeneity is sufficient to capture the homogeneous flow of amorphous solids.

The core of the STZ theory (Falk and Langer, 1998; Langer, 2001) is that STZs, localized regions where potential STs take place, are two-state systems; they can switch forth and back between only two orientations. In the present simple-shear case, the two orientations correspond to the shear "positive" and "negative" directions, respectively. We denote the original state of a STZ as the "+" state, and its post-transformation state as the "−" state. Populations (number density) $n_\pm$ of two STZ states are natural order parameters to construct the constitution. Following Falk and Langer (1998) and Langer (2001), the plastic strain rate can be obtained by considering the dynamic balance of STs between "+" and "−" states:

$$\dot{\varepsilon}^{pl} = V_a(R_+ n_+ - R_- n_-), \tag{1}$$

where V_a is the STZ activation volume that is the product of characteristic STZ volume and shear strain, $R_\pm$ are the ST rates from a $\pm$ to a $\mp$ state. Equations of motion for the populations are (Falk and Langer, 1998; Langer, 2001):

$$\dot{n}_\pm = n_\mp R_\mp - n_\pm R_\pm + \bar{\varphi}\left|\sigma\dot{\varepsilon}^{pl}\right|(n_\infty/2 - n_\pm). \tag{2}$$

The first two terms on the right-hand side describe internal reconstructions between two STZ states. The last two terms in parentheses account for the rates of creation and annihilation of STZs, proportional to the plastic work rate $\left|\sigma\dot{\varepsilon}^{pl}\right|$ with a coefficient $\bar{\varphi}$. Physically, the plastic flow constantly agitates the particles, thus creating and destroying local configurations (Lemaître, 2002). Note that n_∞ is the total populations of STZs generated in the system that is in a steady flow state.

For a low-temperature system, STs are free-volume or entropy activated, in which the applied stress is the driving force and the thermal activation is negligible (Falk and Langer, 1998; Bouchbinder et al., 2007a,b). However, as originally proposed by Argon that STs are stress-driven thermally activated events initiated around free volume regions (Argon, 1979), which is more applicable to our present thermal system. Actually, our recent work (Jiang et al., 2014) substantiates the idea that stress-driven STZs need thermal assistance, and further predicts that athermal or very-low-temperature STZs are prone to suffer a dilatation mode (we call it tension transformation zone, TTZ (Jiang et al., 2008)) due to their relatively low critical stress. Therefore we modify the ST rates to involve the internal dependence of free volume, thermal and stress fluctuations. First, only a particle group that resides in a "fertile" site with a typical free volume v^* has the possibility to transform. According to the free-volume theory (Cohen and Turnbull, 1959; Spaepen, 1977), the probability that a particle group is in this "fertile" site can be calculated as $\exp(-xv^*/v_f)$ where x is a geometrical factor, v_f is the free volume that the group surrounds. If no external stress is applied, subsequent STs are triggered by thermal activation across an energy barrier ΔG (Fig. 1). However the applied stress can tilt the activation energy barrier. Along the shear "positive" direction, the activation barrier from "+" to "−" becomes $\Delta G - \sigma V_a/2$; a backward activation should surmount the barrier $\Delta G + \sigma V_a/2$. Thus, the ST rates become:

$$R_\pm = \exp\left(-\frac{xv^*}{v_f}\right) f \exp\left(-\frac{\Delta G \mp \sigma V_a/2}{k_B T}\right), \tag{3}$$

where f is an attempt frequency, k_B is the Boltzmann constant. It must be pointed out that, in the present model, the free volume is not directly correlated to the STZ density, but definitely facilitates the STZ operations. In other words, the free volume (together with temperature and stress) directly influences the STs rates, instead of the absolute value of the STZ density. We believe that such a treatment

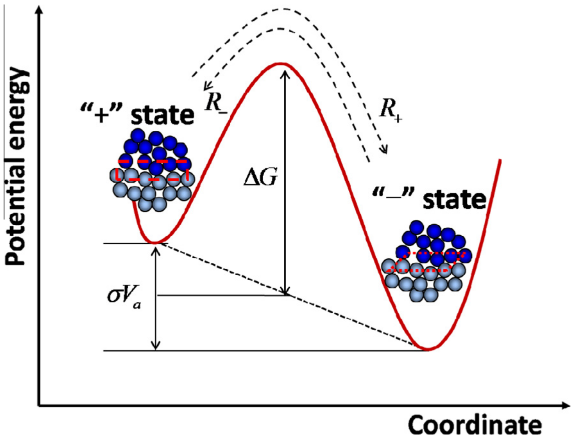

Fig. 1. Illustration of a shear transformation, the basic step for macroscopic plastic flow in amorphous solids.