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Atomistic mechanism of elastic softening in metallic glass under cyclic loading revealed by molecular dynamics simulations

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ABSTRACT

Metallic glasses (MGs) have a great potential for structural applications due to their high strength; however, they soften under cyclic loadings and exhibit low fatigue endurance limits. To understand the softening mechanism, molecular dynamics simulations were carried out to study the $Cu_{50}Zr_{50}$ MG within the nominal elastic regime, which clearly show that the quasi-static elastic modulus of the MG softens with either the decreasing cyclic frequency or increasing stress amplitude. Through the extensive analysis of the atomic trajectories, we found the complex elastic softening behavior is related to the activation of string-like liquid-like sites and atomic bond breaking in the cyclically deformed amorphous structure. Our current finding provides a quantitative insight into the atomistic mechanism of damage in MGs under cyclic loadings, also shedding light on the important mechanisms for fatigue damage initiation in amorphous solids.

1. Introduction

Metallic glasses (MGs) are well known for their great potential as a structural material; however, the lack of room-temperature plasticity has hindered their use in various structural applications [1–5]. Unlike crystalline alloys, MGs possess an amorphous structure without any dislocation-like crystalline defects [6] and, therefore, yielding and plasticity in them are commonly due to shear banding, which arises due to stress-induced softening in an amorphous structure [7–12]. Under monotonic loadings, the MG's yield strength which corresponds to the shear band formation is quite high, about ~2% of the corresponding quasi-static elastic modulus or even higher [13]. This is in sharp contrast to the cases of cyclic loading, in which relatively low fatigue endurance limits, being 10–50% of the corresponding yield strength, could be found for shear band initiation [14–16]. Extensive studies have been carried out exploring the mechanism for shear banding in MGs under monotonic loadings [9,13,17,18]; however, only few works were carried out for the study of the mechanisms of mechanical softening and shear banding under cyclic loadings [19–24]. Here it is worth mentioning that, using the cyclic spherical indentation method, Packard et al. [20] reported that MGs could be cyclically hardened rather than softened. The hardening mechanism was then attributed to confined microplasticity and the presence of a hydrostatic pressure beneath an indenter [19,20]. This mechanism was later found to be consistent with the molecular dynamics (MD) simulation of Delogu et al. [23], which shows that cyclic hydrostatic compression could slow down the dynamics of shear transformation zones (STZs). Different from the above works, our current focus of research is on the effect of cyclic loading on the mechanical properties of MGs without a hydrostatic pressure.

In general, there are two types of views to understand yielding and shear band initiation in MGs. The first one simply treats MGs as an elastic solid and, therefore, their yielding point is essentially an elasto–plastic transition triggered by the nucleation and growth of some local defects [8,10]; by comparison, the second one treats MGs as a viscoelastic solid and follows a rheological approach [2,4,25–27]. As such, yielding of MGs can be related to atomic-scale relaxation processes [2,4,24–27] and to different rheological properties, such as the glass transition temperature T_g and viscosities [28–31]. In this work, our goal is to first testify which view is more applicable to the cyclic deformation in MGs and, after that, to elucidate the underlying atomistic mechanisms through molecular dynamics simulations.

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2. Simulation details

The binary $Cu_{50}Zr_{50}$ (in atomic %) alloy is chosen as the simulation system with the dimensions of ~10 nm × 10 nm × 10 nm and 50,000 atoms, as shown in Fig. 1(a). The embedded atom method (EAM) potential [32] of Cu and Zr is applied in the MD simulation. To obtain the glassy state, the binary metallic liquid was first equilibrated at the temperature $T = 2000$ K for 100 ps and subsequently quenched to 100 K at the rate of 10^{11} K s^{-1}. After that, a series of uniaxial stress cycles, with the peak stress and frequency listed in Table 1, were applied along the Z axis using the Nose-Hoover chain method [33,34] with a periodic boundary condition and at the temperature of 100 K. Note that the maximum peak stress was set to be much lower than the corresponding quasi-static yielding strength (>2 GPa) obtained at the similar stress rate [Fig. 1(b)].

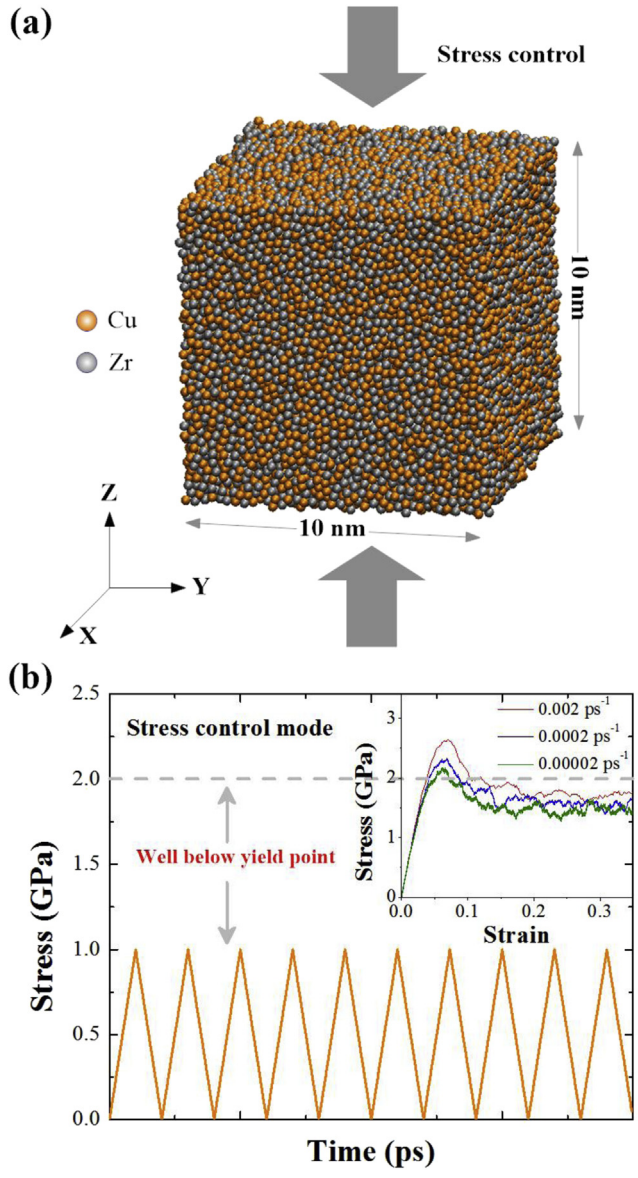

Fig. 1. (a) Illustration of the computer generated $Cu_{50}Zr_{50}$ MG under cyclic compression (the arrows indicate the stress direction). Note that the orange and gray ball represent the Cu and Zr atom respectively. and (b) the applied cyclic stress with the peak value well below the corresponding quasi-static yield point (the inset shows the monotonic stress–strain curves obtained at the strain rates of 0.002 ps^{-1}, 0.0002 ps^{-1} and 0.00002 ps^{-1} respectively). Note that 10 load cycles were applied for each run of the MD simulation. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

For the sake of completeness, listed below are the equations of motion that are adopted by the Nose-Hoover chain method [33,34]:

$$\dot{\vec{r}}_i = \frac{\vec{P}_i}{m_i} + \frac{p_\varepsilon}{W}\vec{r}_i \tag{1}$$

$$\dot{\vec{P}}_i = \vec{F}_i - \left(1 + \frac{1}{N}\right)\frac{p_\varepsilon}{W}\vec{P}_i - \frac{p_\eta}{Q}\vec{P}_i \tag{2}$$

$$\dot{V} = \frac{dVp_\varepsilon}{W} \tag{3}$$

$$\dot{p}_\varepsilon = dV(p_{\text{int}} - p_{ext}) + \frac{1}{N}\sum_{i=1}^{N}\frac{\vec{p}_i^{\,2}}{m_i} - \frac{p_\eta}{Q}p_\varepsilon \tag{4}$$

$$\dot{\eta} = \frac{p_\eta}{Q} \tag{5}$$

$$\dot{p}_\eta = \sum_{i=1}^{N}\frac{\vec{P}_i^{\,2}}{m_i} + \frac{p_\varepsilon^2}{W} - (dN+1)kT \tag{6}$$

where ε, p_ε and W denote the logarithm of the volume, the associated momentum and the mass parameter related to the barostat, respectively; while η, p_η and Q denote, respectively, the coordinate, the associated momentum and mass parameter related to the thermostat. Finally, P_{ext} is the external applied pressure and P_{int} the instantaneous internal pressure given by

$$P_{\text{int}} = \frac{1}{dV}\left[\sum_{i=1}^{N}\frac{\vec{P}_i^{\,2}}{m_i} + \sum_{i=1}^{N}\vec{r}_i\vec{F}_i - (dV)\frac{\partial U}{\partial V}\right] \tag{7}$$

3. Results and discussions

Fig. 2(a) displays a typical cyclic stress–strain curve obtained at the peak stress of 1 GPa, from which one can clearly see a mechanical hysteresis similar to those reported in Ref. [4]. This behavior indicates that our MD simulation results support the view that the MG is a viscoelastic solid. For a viscoelastic solid, if one assumes that the mechanical hysteresis originates from stochastic and reversible structural transitions occurring in local "soft" or "liquid-like" sites [inset of Fig. 2(b)], which can be associated with atomic hopping over the sub-basins on a ragged energy profile [2,4,30] [Fig. 2(b)], it could be derived that the uniaxial stress–-strain curve of MGs can be expressed in the following rate form regardless of the loading conditions [2,35,36]:

$$\dot{\gamma} + \frac{E_I E_{II}}{\eta(E_I + E_{II})}\gamma = \frac{\dot{\tau}}{E_I + E_{II}} + \frac{E_{II}}{\eta(E_I + E_{II})}\tau \tag{8}$$

where γ, τ, η, E_I and E_{II} is the total strain, the stress, the local viscosity of the "liquid-like" sites, the quasi-static elastic modulus and the "entropic" elastic (or complimentary) modulus [2], respectively. Note that the sum of E_I and E_{II} ($E_\infty = E_I + E_{II}$) is the elastic modulus of the "solid-like" regions or the unrelaxed elastic modulus of the MG, which, in principle, should be independent of the mechanical history. By fitting the MD simulation data to the rheological equation