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Direct atomic-scale evidence for shear–dilatation correlation in metallic glasses

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ABSTRACT

Direct atomic-scale evidence is presented for the shear–dilatation correlation in metallic glasses via molecular dynamics and first-principles calculations. A quantitative parabolic relationship is established between the atomic local shear and hydrostatic volumetric strains by carrying out statistical analysis on a deformed glass model. The correction is further verified by density functional theory. Our atomistic demonstration of shear–dilatation correlation collaborates with the experimentally observed a few percent volume change in shear bands. It brings quantitative insights into the unique correlation between shear transformation and cavitation in metallic glasses.

Metallic glasses (MGs) are a category of promising high strength structural materials with many other superior physical and chemical properties [1]. The deformation mechanisms of such amorphous solid state are in sharp contrast with their crystalline counterparts since there are no long-range atoms packing pattern in MGs [2,3]. No conventional mechanisms, such as ordinary dislocation plasticity or deformation twinning in crystals, exist in MGs which can carry plastic deformation. Therefore MGs usually suffer from the notorious catastrophic failure with a strong strain localization (shear banding) phenomenon [4,5].

Several models have been proposed to rationalize the inelastic deformation of MGs, which include free volume [6], shear transformation zone (STZ) [7–9], cooperative shear model (CSM) [10,11], flow unit [12], vibrational soft spot [13], shear-diffusive transformation [14,15], and our recently proposed tensile transformation zone (TTZ) [16–18]. All of these models are based on the local structural rearrangement of atoms via the interplay of atomic-scale shear and dilation/contraction in MGs [19–24]. Among them, Argon's STZ model involves local rearrangement of a cluster of atoms undergoing a stress-driven, and thermally activated shear distortion [25,23,24]. Whereas Spaepen's free volume model is based on a dynamic equilibrium between the stress-assisted creation and annihilation of free volume [6]. The free volume behaviors can be regarded as dilation and contraction of local atomic environments. Since both models have been successfully adopted to describe the homogeneous and inhomogeneous flows in MGs, there should be some intrinsic correlation between shear and dilatation/compaction during deformation of glasses [21,26].

Generally, shear–dilatation correlation is an intrinsic nature of deformation in amorphous alloys although local compaction is also allowed [27,28]. For example, intuitively derived law between shear strain and local dilatation has been used in constitutive modelings of MGs [29]. Shear is not necessarily the only deformation mode accommodating the local atomic rearrangement. The microscopic scenario is that the STZ operations redistribute stress spatially which usually leads to the creation of free volume via atomic-scale dilatation [21,1]. So that local structural dilatation [19,30,31], density change [27,28], and even nanovoids [32,33,21,34] have been observed within the shear bands of MGs. Although the concept of shear–dilatation correlation is widely accepted in the glass community, and various experiments and simulations have indicated STZ and cavitation as important deformation and fracture mechanisms of glassy alloys [33,35,31,18,17,34], there still lacks a direct microscopic evidence and no quantitative relationship established for such an intimate correlation. Whereas a direct observation and derivation of such a quantitative correlation [19] down to atomic-scale is usually an extreme challenging task in experiments [36].

To this end, we conduct combined molecular dynamics (MD) and density functional theory (DFT) calculations to confirm the shear–dilatation correlation in MGs. By statistical analysis on the atomic-scale strains, we establish a parabolic relationship between the atomic shear and volumetric strains in MGs both spatially and temporally. The atomic information provides quantitative insights into the intrinsic deformation and fracture characteristics of MGs.

To establish the shear–dilatation correlation, we conduct statistical analysis on a deformed $Cu_{50}Zr_{50}$ model glass described by a Finnis–Sinclair type potential [37]. The model contains 100,000 atoms which allows a reliable statistical analysis on the atomic strains. It is prepared by a heating–quenching technique from liquid to glass state with a cooling rate of 10^{10} K/s. The MD is performed by LAMMPS code [38].

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Pure shear deformation is applied to induce the atomic strains. The strain rate is $\dot{\gamma}= 10^6$ s^2, and temperature is 50 K. Such simulation conditions allow sufficient structural relaxation which eventually yields shear banding. The DFT calculations are carried out by VASP code [39] with a model containing 256 atoms. The generalized gradient approximation (GGA) of projector augmented wave (PAW) is adopted for parametrization of the exchange-correlation functional [40]. Athermal quasi-static shear is utilized to distort the atoms. During shear, all the components of stress tensor are relaxed to a negligible values except the shear direction [41]. The atoms are fully relaxed until the Hellmann–Feynman force is smaller than 0.01 eV/Å. The visualization is done by OVITO software [42].

To characterize the local distortion at atomic-scale, we use three definitions of atomic strains. First, the atomic local shear strain (local von Mises strain) is defined as [43]

$$\eta^{\text{Mises}} = \sqrt{\eta_{yz}^2 + \eta_{xz}^2 + \eta_{xy}^2 + \frac{\left(\eta_{yy}-\eta_{zz}\right)^2 + \left(\eta_{xx}-\eta_{zz}\right)^2 + \left(\eta_{yy}-\eta_{yy}\right)^2}{6}}, \tag{1}$$

where η_{xx}, …, are the components of local Lagrangian strain matrix. Then, the atomic hydrostatic volumetric strain is consequently written as [43]

$$\delta = \frac{\Delta V}{V} \approx \eta_{xx} + \eta_{yy} + \eta_{zz}, \tag{2}$$

which is used to denote atomic-scale dilatation. V denotes the volume of the simulation box, and ΔV is the variation. Finally, the local minimum non-affine squared displacement

$$D^2_{\text{min}} = \frac{1}{N}\sum_j \left\{ \vec{r}_j(t) - \vec{r}_i(t) - \boldsymbol{J}_i\left[\vec{r}_j(t-\Delta t) - \vec{r}_i(t-\Delta t)\right]\right\}^2 \tag{3}$$

defined by Falk and Lager [8] is also a good measure of inelastic deformation. Here the atom i is surround by $j \in N$ atoms. $\vec{r}$ is the position of atoms. J_i is the local deformation gradient. t and Δt denote time and time interval.

Fig. 1 shows the analysis of spatial strain distribution on a deformed MD model at macroscopic shear strain of $\gamma = 0.12$. The stress–strain curve shown in Fig. 1(a) indicates the appearance of shear localization at such strain magnitude. Fig. 1(b) plots the distributions of η^{Mises}, D^2_{min}, and δ for all 100,000 atoms, respectively. Most of the atoms have experienced atomic shear strain less than 0.1 with the peak at $\eta^{\text{Mises}} \sim 0.06$. Whereas there is a very wide distribution of D^2_{min}. Most of them are less than 1 Å^2. Because we apply pure shear deformation, the atomic volumetric strain distributes almost symmetrically around $\delta = 0$. If all the atoms are colored according to their atomic strains, as shown in Fig. 1(c), we can observe good spatial correspondence among them. It indicates that there is indeed strong correlation between shear, non-affine displacement, and dilatation at atomic-scale. It is also interesting to notice both atomic dilatation and contraction if one carefully check the volumetric coloring scheme, which agrees with latest experimental observations [27,28]. In Fig. 1(d) we bin and reduce the atomic strain along the y direction. It is noticed that the mostly strained atoms locate at around $y \sim 10$ Å, which is actually the location of shear banding. Again, the good correspondence illustrates the spatial shear–dilatation correlation in this model glass. Note that in Fig. 1(b), we plot the distribution of local dilation for all the atoms which seems to be symmetric about 0.0 but with slight deviation to the positive strain. It indicates that compaction also occurs at some regions. However, if we coarse-grain the volumetric strain spatially with 10 atoms in one unit, as shown in Fig. 1(d), the global effect is dilatation.

To further establish a quantitative relationship between shear and dilatation, we provide a statistical analysis on the atomic strains with all the 100,000 data points. The results are summarized in Fig. 2, in which Fig. 2(a) demonstrates the key results. For a first approximation, all the raw MD data (gray crosses) indicate some positive correlation between

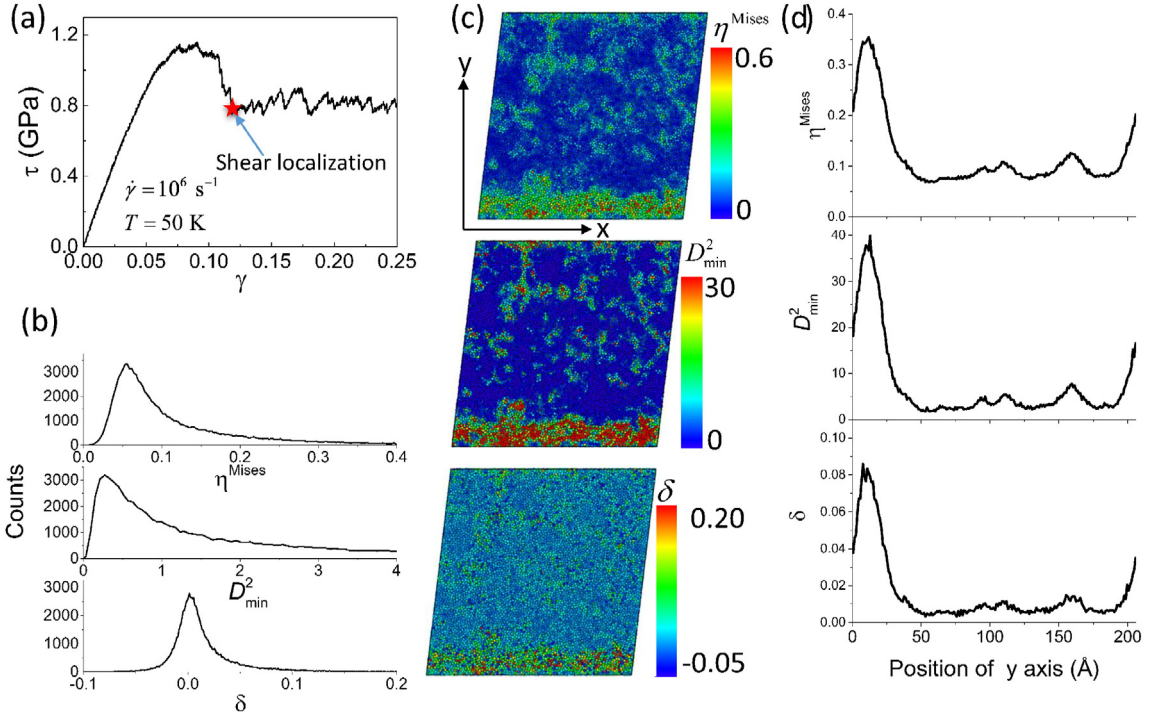

Fig. 1. Analysis on atomic strains and their spatial correlation. (a) MD shear stress–strain curve. (b) Distribution of atomic strains for all 100,000 atoms after yielding. (c) Color coding according to η^{Mises}, D^2_{min}, and δ, respectively. (d) Spatial correspondence among different atomic strains η^{Mises}, D^2_{min}, and δ.

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