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Structural aspects of elasto-plastic deformation of a Zr-based bulk metallic glass under uniaxial compression

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ABSTRACT

The structural rearrangements occurring during compressive deformation of a plastically deformable $Zr_{52.5}Ti_5Cu_{18}Ni_{14.5}Al_{10}$ bulk metallic glass have been investigated in situ using high energy synchrotron X-rays. It was found that in the elastic regime, the atomic distances at both short and medium range order vary linearly with macroscopic stress where the atomic bonds in short range order appear significantly stiffer than medium range order. Upon elastic loading, a small fraction of bonds in the first shell is broken in the loading direction whereas some new bonds are formed in the transverse direction. Atomic strain–stress correlation at medium range order deviates from linearity at the onset of plastic deformation which was correlated to the activation of irreversible STZs. This was confirmed by quantifying the amount of atomic shear strain value during loading. The length scale of 12.5 Å indicated the largest shear strain and is thought to be the most effective length scale in the formation of STZs. The typical fracture angle of this BMG was explained by the orientation of maximum atomic shear strain at the onset of major shear band formation.

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1. Introduction

Due to the amorphous structure and lack of long-range order, bulk metallic glasses (BMGs) do not experience any of the plastic deformation mechanisms of their crystalline counterparts, such as dislocation gliding or twinning [1]. Alternatively, the formation and propagation of localized shear bands nucleated from shear transformation zones (STZs) is the most accepted mechanism of room temperature plastic deformation in BMGs [1]. The proposed atomic-scale mechanisms of plastic deformation in BMGs are mainly based on simulations, but solid experimental evidences are still missing. High energy synchrotron X-ray diffraction (XRD) is a very effective tool to disclose the details of the atomic structure of amorphous materials [2–4]. High photon energies have a high penetration power enabling investigations of bulk samples in transmission geometry and the high momentum transfer gives access to a large reciprocal space allowing to study the pair distribution function (PDF). Moreover, the high brilliance of third generation synchrotron enables micro size focusing with high

photon flux and low background [3,4] which is ideal for precise structural characterization of BMGs during in situ mechanical tests [5,6].

So far, structural studies of BMGs during mechanical tests via high energy XRD have been performed following two different approaches. The first approach [7–9] assumes that the deformation of the BMGs is anisotropic at short length scales and involves non-affine atomic displacements created by strong shear stresses. By using spherical harmonics, this approach can qualitatively illustrate that the deformation induces significant changes in the anisotropic component of the atomic density function, while the isotropic component remains almost unchanged [9]. The second approach proposed by Poulsen et al. [5] assumes that BMGs deform isotropically at small strains and provides a more quantitative estimate of the atomic strains by considering the shift of the peak positions of the pair distribution functions (PDF) as atomic displacements. Using this approach, it has been shown by several authors that, in the elastic regime, the atomic displacement at the short (SRO) and medium (MRO) range scales in BMGs under uniaxial loading varies linearly with applied stress [10–14]. The atomic elastic strain is length scale dependent: the displacements increase with increasing distance from short to large length scales [10–12,14,15]. Vempati et al. [16] have shown that despite the

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different assumptions of the two approaches, they give very similar results for small displacements.

It has been shown that the atomic strain versus macroscopic compressive stress deviates from linearity at the onset of macroscopic flow [13,17]. Das et al. [13] attributed this to the activation of STZs. However, the details of this phenomenon and its correlation with the evolving shear strain have not been completely addressed, yet. The atomic scale events occurring upon elastic deformation are reversible upon unloading [10]. Also, it has been suggested that the average interatomic distances in a glass are not affected by room temperature plastic deformation since it proceeds via macroscopic events of shear banding [18]. Consequently, the majority of the reported atomic scale analyses of BMGs using high energy XRD have been focused on the in situ characterization of the elastic deformation.

This study uses high energy X-rays to characterize the atomic displacements and rearrangements within both the elastic and plastic deformation of the $\text{Zr}_{52.5}\text{Ti}_5\text{Cu}_{18}\text{Ni}_{14.5}\text{Al}_{10}$ BMG under uniaxial compression. The investigation is based on the approach of Poulsen et al. [5] as it permits to quantitatively measure the strain induced by plastic deformation. We have indicated that the shear strain component reaches a critical value needed to activate the STZs at the beginning of yielding and determines the major shear band orientation before fracture.

2. Experimental procedures

In situ X-ray diffraction during uniaxial compression of $\text{Zr}_{52.5}\text{Ti}_5\text{Cu}_{18}\text{Ni}_{14.5}\text{Al}_{10}$ (at.%) bulk metallic glass was performed at the P07 beam line at PETRA III (DESY, Hamburg, Germany) at ambient temperature using a Kammrath & Weiss GmbH mechanical test system with a maximum load of 5 kN at a nominal displacement rate of 1 $\mu\text{m/s}$. The XRD measurement was carried out in transmission mode with a photon energy of 100 keV and a beam size of $250 \times 250 \mu\text{m}^2$. A sample with dimensions of $1.2 \times 1.15 \times 2.27 \text{ mm}^3$ was cut from a glassy plate obtained by centrifugal casting (for details on sample preparation see [19]). Sides of the sample were ground to remove surface defects. Both ends of the sample were carefully polished to make them parallel to each other prior to the compression tests. To support the plastic deformation, an Al foil was used as lubricant material between the loading plates and the sample (for details see [20]). The measured force–displacement curve was corrected for the effect of foil and machine displacement. XRD patterns were recorded every 5 s. The patterns were calibrated using CeO_2 measured at the sample position and then integrated in 10° azimuthal slices between 0 and 360° using the Fit2D software [21]. The integrated data were processed using the PDFgetX3 package [22] to obtain the reduced PDFs. The plane-parallel geometry of the sample enabled using the same data-treatment procedure for all azimuthal directions. Due to rather small sample thickness, the absorption of the high-energy radiation was very small.

3. Results and discussions

3.1. Macroscopic stress–strain behavior

The room temperature macroscopic stress–strain behavior of the $\text{Zr}_{52.5}\text{Ti}_5\text{Cu}_{18}\text{Ni}_{14.5}\text{Al}_{10}$ BMG is shown in Fig. 1. The sample displays an elastic strain of about 2% and yields at $\sim 1450 \text{ MPa}$. The stress then increases with increasing strain to $\sim 1650 \text{ MPa}$. The strain hardening-like regime is followed by a stress plateau up to about 22% strain, where strain softening occurs due to formation of a dominant shear band. As illustrated in the inset of Fig. 1, the surface of the sample after fracture includes a high number of

Fig. 1. Macroscopic engineering compression stress–strain curve of the $\text{Zr}_{52.5}\text{Ti}_5\text{Cu}_{18}\text{Ni}_{14.5}\text{Al}_{10}$ BMG under elastostatic uniaxial compression. Inset is the image of the sample side after fracture, revealing the formation of a high density of shear bands.

shear bands as the main cause of the large plastic deformation of this BMG [1].

3.2. Short-range order characterization

Principally, pair distribution function obtained by Fourier-transformation of a normalized scattering intensity gives information on the distribution of atoms around a given atom in real space in only one-dimension. However, by structural studies of isotropic non-crystalline materials, PDFs are used for description of the spatial atomic distribution considering it as spherically symmetrical. Therefore atomic order in non-crystalline materials is characterized in terms of co-ordination shells, their radii and co-ordination numbers. This way, the short-range order is identified as composed by the atoms in the first nearest neighbor shell and is reflected by the main peak with a maximum probability in the PDFs at small r [23]. The higher coordination shells represent so-called medium range order (Fig. 2(a)). Details of atomic arrangement and chemical order at SRO for multicomponent Zr-based BMGs have not yet been fully understood. The direct observations with high resolution transmission electron microscopy (HRTEM) report that icosahedral-type atomic clusters exist in the structure of Zr-based BMGs [24,25]. These observations were also confirmed by analysis of partial coordination numbers obtained via neutron and X-ray diffraction [26,27] and simulations [28,29] who suggested densely packed icosahedral clusters with solute atoms in the center as a model of atomic arrangement in multi-component BMGs. A part of the PDF corresponding to the SRO of the present BMG at $\sigma = 0$ is shown in Fig. 2(b). After fitting, it is evident that there are two sub-peaks with positions at 2.67 Å and 3.13 Å contributing to the main peak. A similar splitting of the first peak has also been reported by for multi-component Zr-based BMGs [14,30] and binary systems [11]. Since this BMG contains five different elements (Zr, Cu, Ni, Ti and Al), ten types of atomic pairs between dissimilar atoms and five types of atomic pairs between similar atoms exist. Al and Ti (metallic atomic radii of 1.43 and 1.46 Å, respectively, [31]) as well as Cu and Ni (1.28 Å and 1.25 Å, respectively, [31]) cannot be distinguished due to their very similar atomic radius. Due to the low scattering of Al and Ti [32], the (Cu,Ni)–Zr, Zr–Zr, and (Cu,Ni)–(Cu,Ni) atomic pairs make the dominant contribution to the PDF. The value of $r_{1-1} = 2.67 \text{ Å}$ is close to the average distance expected for (Cu,Ni)–Zr and (Cu,Ni)–(Cu,Ni) atomic pairs (2.69 Å). This means that (Cu,Ni)–Zr and (Cu,Ni)–(Cu,Ni) atomic pairs might contribute to the peak at r_{1-1} . The second sub-peak on the PDF at $r_{1-2} = 3.13 \text{ Å}$ is in good

Fig. 2. (a) Total reduced PDF for undeformed $\text{Zr}_{52.5}\text{Ti}_5\text{Cu}_{18}\text{Ni}_{14.5}\text{Al}_{10}$ metallic glass. (b) The first main maximum of the PDF with fitted sub-peaks.

agreement with the length of the Zr–Zr bond, 3.10 Å [31] and it obviously reflects the Zr–Zr pairs.

3.3. Variation of atomic packing density in the loading and transverse directions

The first coordination number (CN) is a quantitative characteristic of atomic packing in a non-crystalline material. It is defined as the number of nearest neighbors around a central atom and is determined as the area under the first peak of the radial distribution function (RDF) [23]:

$$\text{RDF}(r) = r \cdot G(r) + 4\pi r^2 \rho_0 \quad (1)$$

where r is the atomic distance, $G(r)$ is the reduced PDF, and ρ_0 is the average atomic number density. It is clear that the coordination number cannot be calculated by integration of the RDF function for an anisotropic material as the assumption of spherical symmetry is not valid there. This is also true for uniaxially-deformed metallic glasses. However, the area under the first peak of a RDF might give useful information on the atomic packing in a corresponding direction. Fig. 3 shows the relative change of atomic packing for the present BMG as a function of the macroscopic strain along the loading and transverse directions. In the transverse direction it increases by about 0.7% within the elastic regime and then continues to increase with a slower rate up to the beginning of the macroscopic softening (compare with Fig. 1). Afterward, it starts to decrease until the fracture occurs. In contrast, at loading direction the atomic packing indicates a linear decrease of about 2% up to the elastic limit, followed by a moderate decrease until macroscopic strain of 7%. Afterward, it stays constant until the beginning of softening and finally increases upon approaching fracture.

Fig. 3. Variation of the area under the first peak of the radial distribution function versus macroscopic strain in the transverse and loading directions.

Although the changes in the atomic packing values are small, they clearly indicate atomic rearrangement during deformation. Since the values start to approach to the initial points after the beginning of softening, these rearrangements seem to be mainly reversible. The opposite trend of the changes in two directions in the elastic regime indicates that upon compressive deformation, a small fraction of bonds in the first neighborhood atoms are broken at the loading direction and inversely, some new bonds are formed in the transverse direction. This is in agreement with structural rearrangements reported in two directions for the Cu–Zr BMGs under compressive loading [10,33]. It is also worth to note that this experiment does not measure the atomic rearrangements in the direction parallel to the beam. However, it is reasonable to suppose that the changes in the plane perpendicular to the loading direction are isotropic. Considering this point, one can realize that the atomic packing changes in the transverse direction are smaller than in the loading direction.

3.4. Atomic displacements during elasto-plastic deformation

The peak positions in the reduced PDFs (as observed in Fig. 2(a)) corresponding to the different loads were extracted by fitting corresponding part of PDFs with a Gaussian function. The strain values, ϵ_{σ}^i , for the different shells were calculated according to the following equation:

$$\epsilon_{\sigma}^i = \frac{r_{\sigma}^i - r_{\sigma=0}^i}{r_{\sigma=0}^i} \quad (2)$$

where r_{σ}^i and $r_{\sigma=0}^i$ are the peak positions of the i th shell in reduced PDF at stress σ and 0, respectively. In order to calculate the components of the strain tensor, the angular variation of the strain, ϵ_{θ}^i , was fitted to the following equation [34]:

$$\epsilon_{\theta}^i = \epsilon_{xx}^i \cos^2 \theta + \gamma_{xy}^i \cos \theta \sin \theta + \epsilon_{yy}^i \sin^2 \theta \quad (3)$$

where ϵ_{xx}^i , ϵ_{yy}^i , and γ_{xy}^i are the transverse, loading and in-plane shear strains, respectively. The maximum shear strain of each shell, $\gamma_{\max}^i$, and its angle with the x axis, $\theta_{\gamma_{\max}^i}$, were calculated according to the equations [35]:

$$\gamma_{\max}^i = 2 \cdot \sqrt{\left(\frac{\epsilon_{xx}^i - \epsilon_{yy}^i}{2}\right)^2 + \left(\frac{\gamma_{xy}^i}{2}\right)^2} \quad (4)$$

$$\theta_{\gamma_{\max}^i} = \theta_{\epsilon_p} \pm 45^\circ \quad (5)$$

where θ_{ϵ_p} is the principal strain angle, obtained via the following equation [35]:

$$\tan 2\theta_{\epsilon_p} = \frac{\gamma_{xy}^i}{\epsilon_{xx}^i - \epsilon_{yy}^i} \quad (6)$$

In Fig. 4(a), the atomic strain values extracted from r_{1-1} and r_{1-2} (i.e. the SRO) and r_5 as a representative peak of the MRO are displayed versus macroscopic engineering stress for the loading and transverse directions. In addition, in order to show how the atomic strains are changing in the different stages of elastic and plastic (hardening, plateau and softening) deformation, the evolution of atomic-scale strain along the loading and transverse directions are plotted in Fig. 4(b) versus the macroscopic strain for the r_{1-2} and r_5 shells as representatives of SRO and MRO, respectively.

3.4.1. Elastic deformation

From Fig. 4(a), one can observe for both SRO and MRO that in the elastic regime up to ~ 1450 MPa the compressive strain (negative) in the loading direction and tensile strain (positive) in the transverse direction increase linearly with increasing stress. The linear correlation between atomic strain and applied stress for the SRO and MRO is in agreement with the findings of several groups studying the deformation of BMGs via high energy X-ray diffraction [10,13,14,36,37].

The loading ϵ_{yy} strain at the elastic limit is about -0.7% for r_{1-1} and -1.1% , for r_{1-2} . This indicates a higher stiffness of the (Cu,Ni)–Zr and (Cu,Ni)–(Cu,Ni) atomic pairs, resulting in the least contribution to the observed elastic deformation of the SRO. This is in agreement with the model proposed by Ma et al. [26,38], where the Zr–(Cu,Ni) pairs are highly rigid against external forces with respect to the more compliant Zr–Zr pairs.

The strain value of r_5 at the macroscopic elastic limit is about -1.4% . Similar results are obtained for the other MRO shells, i.e. r_2 , r_3 , r_4 and r_6 (not shown here). The calculated averaged Poisson's ratio of the shells from r_2 to r_6 supports this idea. The average Poisson's ratio of MRO shells is about 0.42, which is considerably higher than that of the SRO shells (0.36). Furthermore, the average Young's modulus of the MRO is 105 GPa, whereas it

is 197 GPa for r_{1-1} and 127 GPa for r_{1-2} . These observations clearly indicate that the SRO bonds are much stiffer against external loading compared to MRO. The easier deformation of MRO shells can be attributed to the free volume sites distributed mainly between clusters, while the atomic arrangement inside the clusters is efficiently packed and rigid [38]. Compared to the macroscopic Young's modulus of this BMG, 88 GPa [39], both the SRO and MRO shells are considerably stiffer. Coupled with the observed atomic density variations, such a large discrepancy confirms the point mentioned by other groups [10,11] that the elastic behavior of BMGs is not only governed by simple compression of the atoms/clusters but also other structural mechanisms like rearrangement of atoms/clusters might contribute to the elastic atomic displacement of the BMGs.

3.4.2. Plastic deformation

The stress–strain correlation of the MRO shells (e.g. r_5) along the loading and transverse directions starts to deviate from linearity at 1.4% (Fig. 4(a)) which corresponds to the macroscopic elastic limit of this BMG occurring at 2%. This suggests that yielding may be correlated with structural changes involving atomic displacements in the MRO. The non-linear correlation of the atomic strain versus stress beyond the elastic limit has also been reported by other groups [13,17]; however, so far it has not been addressed in detail. It is known that the main mechanism of plastic deformation in BMGs occurs by propagation of shear bands that have been nucleated from topologically unstable STZs [40]. Such STZs are found mostly in the high free volume regions [41]. Theoretical calculations [42], molecular dynamics simulations [43] as well as experimental nano-indentation test analysis [44,45] suggest that the size of STZ ranges from tens of atoms to several hundred atoms. This implies that the STZs may nucleate in both SRO and MRO. In order to interpret the deviations of the MRO strain observed at the macroscopic yielding, one can imagine the arrangement of clusters with a free volume region between them, as illustrated in Fig. 5(a). The MRO spacing in two perpendicular directions have been depicted with arrows between the clusters. As indicated in Fig. 6(a), with onset of the elastic deformation, the maximum shear strain $\gamma_{\max}$ starts to increase for all length scales (SRO and MRO). The resolved maximum shear stress/strain acts normally in the plane oriented at 45° with respect to the loading direction [34]. $\gamma_{\max}$ of the MRO reaches about 0.020 at the yield point and then it saturates at 0.026 (Fig. 6(a)), which is in very good agreement with the value reported by Johnson and Samwer for the critical value of shear strain for an individual STZ (0.0267 ± 0.0020) [46].

Fig. 4. (a) Loading ϵ_{yy} and transverse ϵ_{xx} strains for the peaks at r_{1-1} , r_{1-2} (SRO) and r_5 (MRO) versus macroscopic compressive stress, (b) Macroscopic stress–strain curve and atomic strains versus macroscopic strain in the two directions for SRO and MRO.

Fig. 5. Schematic illustration of how the inter-cluster distances are changed when an STZ in the MRO is formed by the induced shear stress.

Fig. 6. (a) Variation of $\gamma_{\max}$ and $\theta_{\gamma_{\max}}$ at different length scales against macroscopic strain, the dashed line indicates the beginning of macroscopic softening. (b) Schematics of $\theta_{\gamma_{\max}}$ occurring between two principal strains and is supplementary to the fracture angle, θ_f .

This suggests that a deviation of atomic strain–stress curve from linearity can present a qualitative measure of STZ formation in the beginning of plastic deformation. Nevertheless, the current method averages the information on a scattering volume of $250 \times 250 \mu\text{m}^2$ which is large enough to include thousands of STZs. Thus, extracting the mean size or distance between nucleated STZs requires knowledge on at least the number of activated STZs in the scattering volume

According to Fig. 5(b), the corresponding shear stress acting in the maximum shear strain plane will rotate and slide a layer of the clusters in this direction to rearrange them from topologically unstable positions into a more stable position with decreased inter-cluster distances in the loading direction and increased in the transverse direction, as illustrated by the length of perpendicular arrows, in agreement with the observations in Fig. 4(a). The increasing rate of $\gamma_{\max}$ is weaker with increasing stress and becomes almost saturated before softening (Fig. 6(a)), probably because the STZs are combined to form shear bands acting as a source for triggering next shear bands which will drive further plastic deformation.

Considering the different values of $\gamma_{\max}$ for different coordination shells in the plastic deformation regime, it is clear that $\gamma_{\max}$ of SRO is considerably smaller compared to MRO indicating that SRO has the least contribution to the shear transformation. It is also evident that $\gamma_{\max}$ is significantly smaller for $r_{1,1}$ compared with $r_{1,2}$ (Fig. 6(a)). Correspondingly, the amount of the deviation of ϵ_{xx} and ϵ_{yy} after the elastic limit is considerably smaller for the $r_{1,2}$ than for the $r_{1,1}$ (Fig. 4(a)). This can be an indication that Zr–Zr pairs have a larger contribution to the shear transformations compared to the Zr–(Cu,Ni) or (Cu,Ni)–(Cu,Ni) pairs. It is also worth to note that among the all MRO coordination shells, r_5 has the largest $\gamma_{\max}$ implying that the clusters at this length scale have the largest contribution to the STZs.

In Fig. 6(a), the change of the angle $\theta_{\gamma_{\max}}$ for the MRO is plotted versus the macroscopic strain. While $\theta_{\gamma_{\max}}$ oscillates around 45° in the elastic regime, it deviates from this value with starting of macroscopic plastic deformation, reaching about 48.5° at the beginning of softening (indicated by an arrow in Fig. 6(a)), i.e. at the formation of the major shear band. Therefore, according to the schematic representation in Fig. 6(b) the potential fracture angle (θ_f) deviates from 45° toward smaller angles, reaching a value of $90 - 48.5^\circ = 41.5^\circ$. This value is in very good agreement with the macroscopic observations for the fracture angle of this BMG under uniaxial compression, which occurs at about 42° [47]. It is also worth to note that, the calculated $\theta_{\gamma_{\max}}$ increases also after the beginning of softening up to the fracture. This is due to a higher decreasing rate of ϵ_{xx} (consequently $\epsilon_{xx} - \epsilon_{yy}$) compared to γ_{xy} (Fig. 4(b), Eq. (6)). However, once $\gamma_{\max}$ determines the formation

of the major shear band at $\theta_{\gamma_{\max}} = 48.5^\circ$, the deformation proceeds along this direction and the $\theta_{\gamma_{\max}}$ cannot alter the direction of the major shear band.

3.4.3. Softening

The beginning of the macroscopic softening of the BMG is due to the formation of one major shear band that localizes the entire macroscopic deformation, reduces the required deformation force, propagates slowly [48] and finally results in the fracture of the BMG. In order to understand the details of the softening, one should consider that the X-ray beam passes from the whole scattering volume of the sample and the diffraction patterns reflect structural information of the volume which includes the major shear band and the two detaching parts. Considering that the thickness of the shear band is negligible compared to the thickness of the detaching parts, the diffraction data include mainly structural information occurring in the two detaching parts. When a major shear band forms, the compressive force is essentially localized by a very thin ($\sim 10 \text{ nm}$) shearing region and the two detaching parts of the sample experience a decrease of the macroscopically induced load. This means that as the softening continues, these parts may reverse the elastic and anelastic structural changes that have occurred during the preceding deformation. This is well illustrated in the behavior of the SRO and MRO strains versus macroscopic strain beyond $\sim 22\%$ in Fig. 4(b), where both ϵ_{xx} and ϵ_{yy} are approaching zero with an increase of the macroscopic strain in the softening stage. This phenomenon can be also observed in Fig. 4(a) where the softening stage in the loading and transverse directions is indicated by downward arrows. In the loading direction, in particular for the MRO, the slope of the stress–strain curve in the softening stage is very similar to that of the elastic loading (indicated with an upward arrow). This suggests that the structure of the detaching parts is not irreversibly altered during plastic deformation of the glass. On the other hand, the rate of softening of the MRO in the transverse direction (Fig. 4(a)) is much smaller than that of the corresponding elastic loading part. This can be attributed to some irreversible structural changes that have occurred in this direction during deformation, irreversibly altering the structure.

3.4.4. Length scale dependence of atomic strains

In Fig. 7(a) and (b), ϵ_{xx} and ϵ_{yy} have been plotted at several values of stress in the elastic and plastic deformation regimes versus the length scale, r . It can be observed that there is a steep increase of atomic strain from SRO to MRO in both elastic and plastic regimes of deformation, in agreement with other reports [49,50]. In the different MRO shells, the atomic strains are almost similar in the elastic regime. However, at the stress level near the yield

Fig. 7. (a) ϵ_{yy} and (b) ϵ_{xx} at several stress levels as a function of interatomic distance (r), revealing the length scale dependence of the strain.

strength, (1418 MPa), as well as in the plastic deformation regime, (1671 MPa), one can observe that the strain extracted from r_5 at 12.5 Å is higher compared to the other MRO shells. A characteristic MRO length scale with higher strain was also reported by Hufnagel et al. [50] at 12–13 Å for $Zr_{57}Ti_5Cu_{20}Ni_8Al_{10}$ BMG under compressive loading and attributed to the reported STZ size of about 10 Å [51]. Our observation in Fig. 6(a), where the peak of r_5 indicated the largest γ_{max} supports the idea that this length scale has the highest contribution to the shear transformations underlying the main mechanism of plastic deformation of BMGs.

4. Conclusions

The elastic and plastic deformation of the $Zr_{52.5}Ti_5Cu_{18}Ni_{14.5}Al_{10}$ BMG was correlated to the structural changes at SRO and MRO scales. In the elastic regime, the atomic distances at SRO vary linearly with macroscopic stress. Analysis of the area under radial distribution function indicates that a small fraction of bonds in the first shell is broken in the loading direction whereas some new bonds are formed in the transverse direction. Atomic bonds at SRO appeared significantly stiffer than the MRO shells. Compared to the macroscopic values of elastic strain, Young's modulus and Poisson's ratio, both SRO and MRO appeared significantly stiffer implying that the elastic behavior of the BMG is not only governed by simple compression of the atoms/clusters but also is aided by rearrangement of atoms/clusters. The deviation of MRO atomic strain–stress correlation from linearity at the onset of plastic deformation was attributed to the activation of irreversible STZs as illustrated by strong shear strain value at the onset of yielding. This value is in a good agreement with the reported value of the critical shear strain needed for activation of an irreversible STZ. The length scale of 12.5 Å indicated the largest shear strain and is thought to be the most effective length scale in the formation of STZs. On the other side, the atomic pairs at SRO with smallest shear strain have the least contribution to the STZs. It is also indicated that the typical fracture angle of this BMG can be explained by the orientation of maximum shear strain at the onset of major shear band formation.

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