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# Mapping of residual strains around a shear band in bulk metallic glass by nanobeam X-ray diffraction

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ABSTRACT

Despite recent progress in understanding the outstanding role of shear bands in plastic deformation of metallic glasses, the details of structural changes in the shear-induced zone is not yet known. In order to probe such changes, we determined the distribution of residual strains at short- and medium-range order around a single shear band in cold-rolled Vit105 bulk metallic glass using a nano-focused high energy X-ray beam. Plastic deformation results in significant residual normal and shear strains at distances of more than 15 μm around the shear band. Based on a detailed analysis of the distribution profile, the magnitude and the direction of the residual shear strain, it is suggested that the shear strain plays a dominant role, compared to the normal strains, for triggering nucleation of further shear bands from a mature shear band.



## 1. Introduction

Shear banding is known as the main mechanism of plastic deformation in metallic glasses at ambient temperature. A shear band is a very thin (10–20 nm) localized sheared region which nucleates by cooperative action of numerous shear transformation zones (STZs) formed by sliding of energetically favored atomic clusters under shear stress [1,2]. The overall plastic deformation behavior of bulk metallic glasses (BMGs) at ambient temperature is a consequence of several characteristics of shear bands including the number, distance, direction, temperature, shear offset, propagation speed and their mutual interactions [1–3]. This outstanding role of shear bands has appealed almost all attempts aiming to resolve the biggest Achilles heel of metallic glasses – their rather limited room temperature ductility. An unique outcome of these studies is that the higher the number of intersecting shear bands with small shear offsets, the larger is the overall plastic deformation [1]. It has been suggested that shear banding localizes a large amount of shear strain in a very narrow planar band and results in softening due to disordering or heat generation [1,4,5]. When considering a network of intersecting shear bands, it is believed that the whole monolithic structure turns into a heterogeneous array of sheared and un-deformed regions which can result in a remarkable change in the macroscopic mechanical behavior of the BMGs [6–9]. The appearance of such heterogeneous structures in plastically deformed BMGs has been highlighted in terms of hardness gradients [10–13], residual strain/stress domains [9,14–20], and free volume changes [21,22]. These studies have well succeeded to draw a macroscopic image of a heterogeneous structure in BMGs. There have also been a limited number of computer simulations [23–25] and experimental studies [26–28] revealing the structural scale changes within or around shear bands. The measurement of the temperature profile along a shear band via in-situ thermographic observation [26,27] revealed that plastic

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deformation can cause a very high temperature increase at the core of the shear band resulting in premature failure of the deforming BMG. Nano-indentation studies [28–30] at directions perpendicular to a shear band have identified a wide shear-induced region where the shear band has the lowest hardness and elastic modulus compared to other regions.

The above mentioned experimental studies had a spatial resolution of several microns and could not provide detailed knowledge on localized structural features like residual strains at the area around an individual shear band. To overcome this problem, we have performed a X-ray nano-beam diffraction study of single shear bands formed by cold-rolling of $Zr_{52.5}Ti_5Cu_{18}Ni_{14.5}Al_{10}$ (at.%) (Vit105) BMG. This enabled us to reveal the changes of the short- and medium-range atomic order in plastically deformed metallic glass on the nanoscale. For the first time, we have mapped fluctuations of the inter-atomic distances across and around a shear band and established that plastic deformation results in a strong residual elastic shear strain extending far beyond the localized region of shearing. It is shown that the magnitude and orientation of the residual shear strain trigger the nucleation of further shear bands.

### 1.1. Experimental details

Bulk metallic glass with nominal composition $Zr_{52.5}Ti_5Cu_{18}Ni_{14.5}Al_{10}$ (at.%) was prepared as a plate with a thickness of 1.4 mm and a width of 3 mm by centrifugal casting. The glassy plate was rolled in very small steps to reach a 5% of reduction in thickness. Before rolling, one transverse side of the plate was mirror-polished. After rolling, the plate was ground from the opposite side to a thickness of ~100 μm with twofold aim: i) to make it transparent for the nano-focused X-ray beam and ii) to have just one shear band on the X-ray passway. A detailed microstructure analysis of the cold-rolled and grounded plate using scanning electron microscope (SEM) proved presence of the shear bands and absence of cracks. An area of $25 \times 45\ \mu m^2$ with a single shear band was selected for the X-ray diffraction investigations and marked with platinum dots of about 5 μm size deposited by a Focused Ion Beam (FIB). These dots were found with a florescence detector and used as guide points to limit the area of the XRD scans. The X-ray beam had a wavelength of 0.189 Å and a size of 150 nm height and 5 μm width, measured as the full width at half maximum of a fluorescent peak from the deposited platinum dot. The selected area across a shear band was scanned with sample holder movements of 1.0 and 0.5 μ in the directions parallel and perpendicular to the shear band, respectively. The exposure time for each diffraction pattern was 5 s. A total number of 4538 diffraction patterns was recorded. The XRD patterns were integrated in 10° azimuthal slices between 0 and 360° with the Fit2D software [31]. The integrated data were processed using the PDFgetX3 package [32] to obtain the reduced pair distribution functions (PDF).

The position of the first shell in the structure function, $q_1$, was obtained by fitting to a Gaussian peak. In order to characterize the structural changes at SRO (Short Range Order) and MRO (Medium Range Order) scale in real space, the center of mass (CoM) of each coordination shell in the PDF was determined according to following equation:

$$CoM = \frac{\int_{root_{min}}^{root_{max}} rG(r)}{\int_{root_{min}}^{root_{max}} G(r)}, \quad (1)$$

in which G(r) represents reduced PDF, $root_{min}$ and $root_{max}$ indicate intersection of G(r) with the line G(r) = 0 at SRO region. The strain values, $\varepsilon^i$, for the different coordination shells were calculated according to the following equation:

$$\varepsilon^i_{deformed} = \frac{r^i_{deformed} - r^i_{undeformed}}{r^i_{undeformed}}, \quad (2)$$

where $r^i_{deformed}$ and $r^i_{undeformed}$ are the centers of mass of the $i$th shell in reduced PDF for a deformed and undeformed state, respectively. The scanned area in the cross section of this BMG includes regions between the shear bands which are far enough from two shear bands and thus are not affected by shearing. The peak positions of the diffraction patterns of several subsequent points in this region were the same. Thus the peak positions in the diffraction patterns of these points were chosen as the reference point to calculate the strain values. In order to calculate the components of the strain tensor, the angular variation of the strain, $\varepsilon^i_\theta$, was fitted to the following equation [33]:

$$\varepsilon^i_\theta = \varepsilon^i_x \cos^2\theta + \gamma^i_{xy} \cos\theta\sin\theta + \varepsilon^i_y \sin^2\theta, \quad (3)$$

where $\varepsilon^i_x$, $\varepsilon^i_y$ are the directions parallel and perpendicular to the shear band, respectively and $\gamma^i_{xy}$ is the in-plane shear strains. The maximum shear strain of each shell, $\gamma_{max}$, and its angle with the $x$ axis, $\theta_{\gamma max}$, were calculated according to the equations [34]:

$$\gamma_{max} = 2\sqrt{\left(\frac{\varepsilon_x - \varepsilon_y}{2}\right)^2 + \left(\frac{\gamma_{xy}}{2}\right)^2}, \quad (4)$$

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

where $\theta_{\varepsilon_p}$ is the principal strain angle, obtained via following equation [34]:

$$\tan 2\theta_{\varepsilon_p} = \frac{\gamma_{xy}}{\varepsilon_x - \varepsilon_y}, \quad (6)$$

## 2. Results and discussions

Fig. 1(a) presents a schematic of the X-ray diffraction investigations of the shear-zone in cold-rolled Vit105 bulk metallic glass. The rolled sample contains a sequence of parallel shear bands oriented at an angle of ±45° with respect to the rolling direction. The scanning electron microscopy (SEM) image in Fig. 1(b) shows a single shear band and a scanned area marked with a red rectangle. The X-ray intensities, as illustrated in Fig. 1(c), indicate a fully amorphous structure with no trace of crystallinity, implying that the studied region is free from deformation- or heating-induced crystallization.

It is known that the first maximum of the X-ray intensity or structure function taken from a metallic glass, and in particular the position of the first peak $q_1$, carries significant information on amorphous structure [35]. Recently, Poulsen et al. [36] showed that the components of the strain tensor in uniaxially deformed metallic glass can be determined from the positions of $q_1$ measured over all azimuthal directions with respect to the incident beam. We have determined the variation of the first peak on the XRD intensities over the whole scanned area across the shear band in cold-rolled Vit105 metallic glass. The corresponding maps for the fully integrated diffraction patterns and the XRD intensities measured in the planes along and perpendicular to the shear band are plotted in Fig. 2(a). The map of $q_1$ extracted from fully integrated patterns reveals an asymmetric gradient with respect to the shear band