Effects of sample geometry on deformation modes of bulk metallic glasses at the nano/micrometer scale

Jianchao Ye, Jian Lu, and Yong Yang[a)]

The Department of Mechanical Engineering, the Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, People's Republic of China

Peter K. Liaw

The Department of Materials Science and Engineering, The University of Tennessee, Knoxville, Tennessee 37996-2200

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Intense debates have been prompted concerning whether homogeneous deformation can be achieved in bulk metallic glasses at room temperature through the suppression of shear bands at the submicron scale. In this short communication, we demonstrate that multiple shear banding can be successfully attained via a proper modification of the microsample geometry, resulting in the appearance of a homogeneous deformation mode at the submicron scale. However, the apparent deformation homogeneity in our microcompression experiment is a manifestation of the sample geometry effect on the propagation rather than nucleation of shear bands.

Understanding the behavior of shear bands in bulk metallic glasses (BMGs) is critical in the design of a new class of BMGs with superior mechanical properties. In BMG bulk samples, shear bands tend to propagate in a catastrophic way, resulting in the subsequent brittle-like fracture, which renders the BMGs with limited ductility at room temperature.[1] However, at the micrometer scale, shear bands were found to behave in a ductile manner, propagating without causing the sudden fracture of the microsample throughout a large plastic deformation process.[2] Moreover, it was reported that shear bands could even be completely suppressed by reducing the sample size into the submicron scale, which led to a homogeneous deformation mode at room temperature.[3,4]

However, the idea of the shear-band suppression is controversial and was later challenged by a few researchers based on their results of the microcompression experiments,[5–7] in which no homogeneous deformation mode was observed on the micropillars even though their diameters were reduced to a level less than that observed in the homogeneous deformation mode. It can be argued that the difference of the experimental results originates from the chemical composition of the microsamples, i.e., different BMGs have different critical length scales below which the shear bands cannot be nucleated. Thus, the homogeneous deformation is still an intrinsic effect, reflecting the shear-banding behavior at the small size scale. However, there is another extrinsic effect that could also cause the apparent deformation homogeneity, but was somehow ignored in previous studies,[2–4,6] which is derived from the sample geometry and the associated boundary conditions.

In mechanical testing of single crystals, it is known that the grips play an important role in determining the deformation morphology of a tensile specimen. If the lateral translations of both grips are constrained, a dislocation single slip is not favored, and, thus, the resulting deformation morphology is a reflection of the combined effect of the sample geometry and dislocation dynamics. Likewise, although shear banding is essentially heterogeneous in BMGs, an apparent homogeneous deformation mode is still possible as long as the shear offset resulting from the propagation of the small shear band is insignificant in changing the structural integrity of the microsample. In such a case, the deformation morphology of the microsample is greatly influenced by its geometry and boundary conditions. In other words, a seemingly homogeneous deformation mode can be triggered by suppressing the severe shear offset resulting from the propagation of a dominant shear band. In what follows, two different strategies are discussed to facilitate a seemingly homogeneous deformation mode in the microcompression experiments by properly modifying the sample geometry.

The first strategy is to increase the degree of tip rounding of the micropillar, which mitigates the stress concentration at the top surface and leads to the activation of a population of shear bands rather than the one at the stress-concentration site. The second strategy is to make the micropillar hollow, which defies the propagation of

[a)]Address all correspondence to this author.
e-mail: mmyyang@polyu.edu.hk
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a dominant shear band by cutting into its pathway. Both strategies have the same effect of encouraging a multiple shear-banding phenomenon. However, it is expected that the latter could have a larger impact on the overall deformation mode of the microsample because the whole structure of the microsample is thereby modified.

After the microfabrication procedure described in the literature,[4,8–10] micropillars were carved out using the focused-ion beams on the surface of a $Zr_{50}Cu_{37}Al_{10}Pd_3$ (in at.%) disk 3 mm in diameter. For the solid ones, the diameters ranged from ~0.7 to ~6 μm, and the aspect ratio ranged from 2:1 to 9:1. For the hollow ones, the outer diameter and aspect ratio were fixed at 4 μm and 3:1, respectively, and the thickness ranged from ~0.3 to 1.3 μm. Microcompression experiments were then conducted on a Hysitron nanoindentation system, outfitted with a ~10-μm flat-end nanoindenter, at the displacement controlled mode. Due to the ion-beam divergence, all of the micropillars were tapered and the taper angle was approximately ~3° on average. For simplicity, the nominal strain rate was fixed at approximately $\sim 6 \times 10^{-4}\ s^{-1}$.

For the solid micropillars, plastic deformation commenced with shear banding for the top diameters larger than 1 μm (data not shown). An apparent homogeneous deformation mode was only evidenced on the micropillar with a diameter of ~0.72 μm at the compressive displacement of 0.4 μm, which was equal to 5% of the height of the micropillar [Fig. 1(a)]. It was noticed that the micropillar exhibited an appreciable tip rounding before deformation, as shown by the inset in Fig. 1(a). However, as the plastic deformation process continued, a shear band emerged right below the homogeneous deformation region, and the subsequent deformation was then accommodated by the gliding of the shear band [Fig. 1(b)]. As discussed above, in the absence of lubricants, the tip rounding of a micropillar effectively reduces the stress concentration on the top surface and promotes the process of multiple shear banding. The tip-rounding effect is amplified in cases in which the radius of curvature at the micropillar's tip is comparable to the top diameter. Therefore, the appearance of the homogeneous deformation mode does not necessitate the complete suppression of shear bands. When the rounded tip is flattened with further plastic deformation, a single and dominant shear band is thus formed from the stress concentration site [Fig. 1(c)]. Before proceeding, it should be noted that the micropillar tapering can help to stabilize the shear-banding process. Through the rigorous analysis,[11] it can be shown that, in the tapered micropillar geometry, the angle of the shear band relative to the loading axis deviates from that in the nontapered one. Such a deviation implies that shear band may be more stable running in a less favorable shear direction. However, the resultant angular difference is small and approximately ~1° in a 3°-tapered micropillar. In such a case, the micropillar's tapering only plays a secondary role here compared with the other geometrical factors.

To check the validity of the above theories, the hollow micropillar compression experiments were carried out. In Figs. 2(a)–2(d), a clear trend can be seen illustrating that the formation of a dominant shear band was delayed with the decreasing top thicknesses of the hollow micropillars.

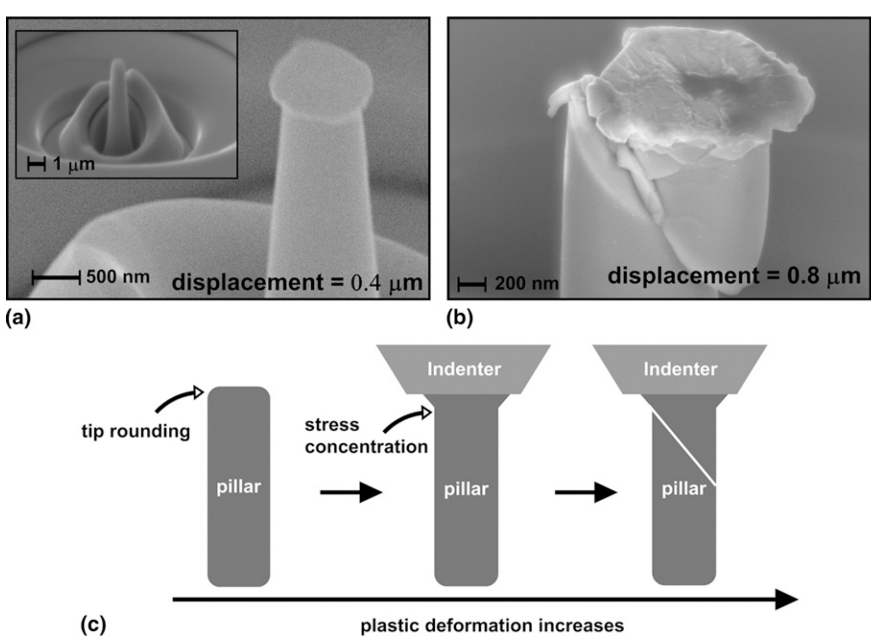

FIG. 1. (a) The deformation morphology of the micropillar 720 nm in diameter at the displacement of ~0.4 μm (the inset shows the original configuration of the micropillar); (b) the deformation morphology of the same micropillar at the displacement of ~0.8 μm; and (c) the sketched deformation process of a tip-rounded micropillar.

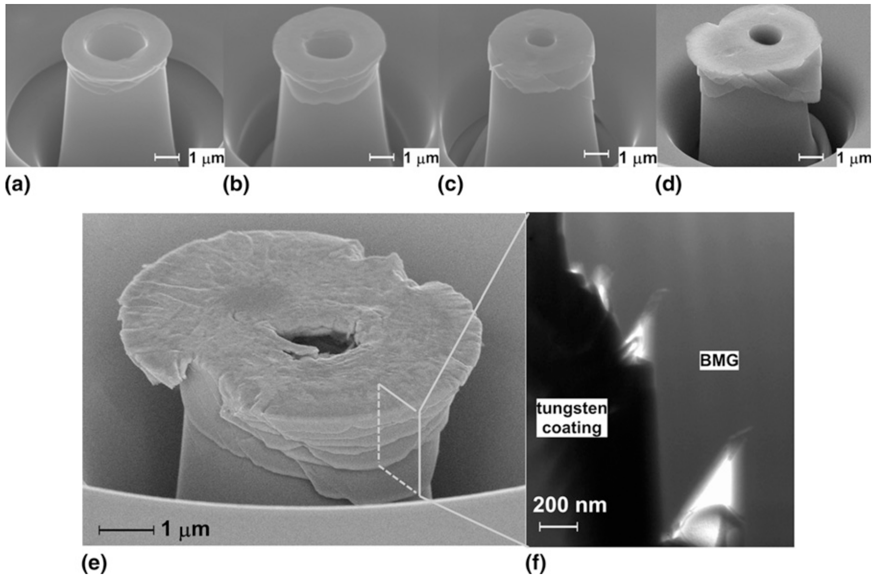

FIG. 2. The deformation morphologies of the micropillar with the top thickness of (a) 0.34 μm, (b) 0.47 μm, (c) 0.97 μm, and (d) 1.33 μm at the displacement of ~0.8 μm; (e) the severely deformed configuration of the micropillar with the top thickness of 0.34 μm; and (f) the transmission-electron microscopy (TEM) cross-sectional image of (e).

A peculiar "mushroom"-type deformation mode finally occurred in the micropillar when its top thickness was reduced below 0.47 μm. However, shear bands can still be observed right below the homogeneous deformation regions where the local thickness is approximately ~0.5 μm, which indicates that, despite the appearance of homogeneous plastic flows, shear bands still prevail at the submicron scale and the previous "homogeneous" deformation mode is simply a geometrical effect on the propagation rather than nucleation of the shear bands. Figure 2(e) presents the severely deformed configuration of the micropillar with the initial top thickness of 0.34 μm. Through the focused ion-beam cross-sectioning, the shear offsets along the edge of the hollow micropillar were examined by using the transmission electron microscopy. As shown in Fig. 2(f), it is evident that the shear offset scales with the local thickness of the hollow micropillar. At the top part, the shear offset becomes less pronounced compared to those at the bottom part.

In the literature, the size effect on the room temperature-deformation mode of bulk metallic glasses has attracted a great deal of interest. Other than in the microcompression experiments, the homogeneous deformation modes were also reported in the tensile experiments of BMG/crystal nanolaminates.[12] However, the homogeneous plastic flows occurred at a much smaller length scale, say, at approximately a few tens of nanometers, rather than a few hundreds of nanometers.

In theory, there are two length scales that have been proposed to rationalize the growth behavior of a shear band. The first one is the nucleation length, which is approximately 10 to 20 nm and comparable with the shear-band width reported so far.[13,14] The other one is the incubation length of a shear band,[15] which is derived from the transition of the shear-band local temperature from the ambient temperature to the glass-transition point and scales with $(T_g - T_0)^2/c$, where c is the shear-band speed, and T_g and T_0 denote the glass transition and ambient temperature, respectively.

Despite the current debate on the origin of the shear-band instability,[16] the incubation length provides a simple way to estimate the length over which the shear band becomes a runaway defect with significant materials softening inside. Assuming an adiabatic shear-banding process, the incubation length can be estimated ranging from ~10 to ~1000 nm on the order of magnitude, depending on the speed of the shear band at room temperature.[15] In such a case, it is not surprising that the propagation behavior of the micrometer-sized shear band shall differ from that of the mm-sized shear bands and the other factors; for instance, the sample geometry and the boundary conditions may become influential in the shear-banding dynamics at the small size scale.

It should be mentioned that our recent work on the Mg-based BMG micropillars shows that the stability of the shear band correlates with the shear offset and strongly depends on the elastic energy release rate at the outset of shear banding, whereas the latter scales with the characteristic dimension of the microsample.[17] The general result is that the longer the shear band, the larger the shear offset and the less stable the whole shear-banding process, which is also consistent with the experimental findings observed on the present hollow micropillars. It is expected that the current Zr-based BMG micropillars may also behave in the similar way, and the related research work is now in progress.

In summary, we devised a new method, in conjunction with the existing micropillar compression experiments, to facilitate the revelation of the transition in the BMG deformation mode at the small size scale. Based on our experimental results, it was found that multiple shear banding resulted in the seemingly homogeneous deformation mode in the microcompression experiments. The apparent deformation homogeneity is a reflection of the sample geometry effect on the propagation of shear bands in the current BMG system.

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