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Micromechanical mechanism of yielding in dual nano-phase metallic glass

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ABSTRACT

Through detailed experimental and theoretical analyses, here we uncover the mechanism of plasticity initiation in the Ni-P nano-grained metallic glass (NGMG) which contains nano-sized hard amorphous inclusions and soft amorphous inter-granular regions. In this dual nano-phase amorphous structure, plasticity is mainly initiated through the elongation and coalescence of the amorphous nano-grains, resulting in a shear band much wider than in its monolithic counterpart. Consequently, the NGMG turns out to be softer at the microscopic scale. At the fundamental level, our finding provides a universal mechanism which explains the unusual strength weakening observed in a variety of dual nano-phase amorphous systems.

Metallic glasses (MGs) are a typical disordered material with superb strength but poor plasticity due to the catastrophic failure along unhindered shear bands [1, 2]. In theory, shear banding in MGs is a multi-scale deformation process, entailing nucleation and growth of local shear intensified regions (LSIRs) towards the formation of a sample-spanning shear band [2, 3]. In the literature [4–9], shear banding in MGs, as a highly localized plastic flow, is commonly believed to possess a thickness of 10–20 nm. In contrast, Liu et al. [10] recently reported that the thickness of a shear band in a MG bulk sample could vary from 10 to 200 nm. This interesting finding suggests that shear band thickness could still be an open issue or it is possible that the thickness of a shear band widens when it grows as discussed in Refs [7, 11–13].

To mitigate the issue of shear localization and the resultant brittleness, micro-sized secondary phases were usually introduced into monolithic MGs to form MG matrix composites [14]. Plasticity in MGs can be thus enhanced by carefully controlling these secondary phases [15–17]. In most of the prior works, the size of the inclusions were usually varied from ~1 μm to ~50 μm [14] and their spacing was even greater, leading to a relatively low volume fraction of the secondary phases. Recently, it was shown that one can obtain nano-grained metallic glasses (NGMG) through various methods, such as inert-gas condensation (IGC) [18, 19], magnetron sputtering [20] and electrodeposition [21]. Compared to conventional MG matrix composites, both hard and soft phases in the NGMG are amorphous with their size ranging from 1 to 10 nm, being comparable to or even smaller than the typical thickness of a shear band [20, 22, 23]. Therefore, it could be naturally expected that the strength of these NGMG could be very high due to the effective blocking of shear bands. Nevertheless, it was noted recently that various NGMGs exhibit an abnormally low strength compared to their monolithic counterparts [18, 19, 24–29]. Now the questions arise: how does a shear band initiate in these NGMGs and why their yield strengths are weakened? These are issues attracting considerable interest [22, 23, 30, 31], but yet to be fully unresolved.

In this Letter, we intend to address the above issues through the systematic study of a NGMG with the composition of $Ni_{78}P_{22}$ (in atomic percent). The NGMG samples were prepared using the multi-phase pulsed electrodeposition technique [21]. By carefully controlling the deposition voltage, current density and time duration at different deposition stages (see Ref [21] for details), a dual-phase amorphous nanostructure was obtained. For comparison, a monolithic Ni-P MG with the same composition was also prepared with melt spinning. As seen in Fig. S1(a), the X-ray diffraction (XRD) patterns of both samples indicate that their structures are amorphous. Nevertheless, it appears that the NGMG contains two distinctive regions of different densities, which contrasts the uniform atomic structure in the MG, as one can infer from the differential scanning calorimetry (DSC) results [Fig. S1(b)]. Transmission electron microscopy (TEM) analyses were subsequently performed on both samples. As clearly seen in Fig. 1(a), the NGMG possesses a nano-grained amorphous structure with the average size of the amorphous grains 4 ± 2 nm and the inter-granular spacing 2 ± 0.5 nm. Note that both the intra- and inter-granular regions

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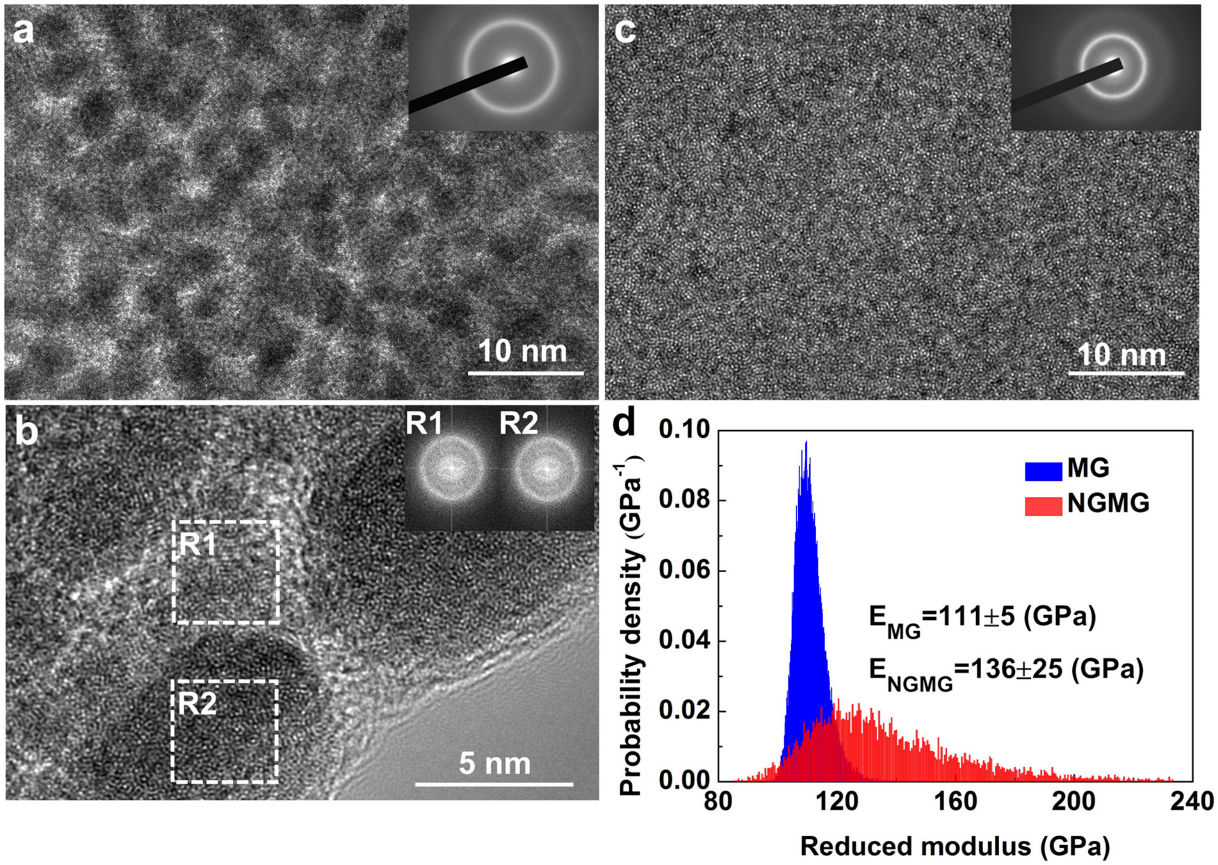

Fig. 1. (a) The TEM image of the $Ni_{78}P_{22}$ NGMG (the inset shows the corresponding selected area diffraction pattern), (b) the HRTEM image of the $Ni_{78}P_{22}$ NGMG (the insets show the selected area diffraction patterns of both grain and inter-granular regions), (c) the TEM image of the $Ni_{78}P_{22}$ MG (the inset shows the corresponding selected area diffraction pattern), and (d) the reduced modulus distribution of both $Ni_{78}P_{22}$ NGMG and MG.

are fully amorphous, as shown in Fig. 1 (b). Consequently, the volume fraction of these amorphous grains can reach over 50%. By comparison, the monolithic MG exhibits a typical uniform maze-like amorphous structure without any visible nano-scale structural heterogeneities, as shown in Fig. 1 (c). Furthermore, dynamic modulus mapping were carried out on the Hysitron™ nanoindentation platform. As seen in Fig. 1(d), the reduced modulus of the NGMG exhibits a distribution much wider than that of the MG. The average reduced modulus of the NGMG is around 136 ± 25 GPa, about 20% higher than that (111 ± 5 GPa) of its monolithic counterpart. Fitting the distribution to the Gaussian curves shows that the modulus distribution for the NGMG indeed has two peaks, one at 118 GPa and the other at 146 GPa [Fig. S1(c)], which is in line with the two-phase structure. Furthermore, chemical analyses were performed on the NGMG with energy dispersive x-ray spectroscopy (EDX) under the scanning transmission electron microscopy (STEM) mode. No obvious chemical heterogeneities were detected [Fig. S1(d)].

To investigate yielding in both the MG and NGMG samples, a series of microcompression experiments were carried out. The micropillars were fabricated using the ion-milling method [32], which had the diameter ranging from 500 nm to 5 μm. Subsequently, microcompression was performed at the constant strain rate of $5 \times 10^{-3}\ s^{-1}$. As demonstrated in Figs. 2(a)-(b), nearly all MG and NGMG micropillars show a pronounced displacement burst upon yielding, which can be keyed to the formation of a major shear band [the insets of Figs. 2(a)-(b)]. Following the methods in Refs [33–35]., we extracted the yield strengths of the MG and NGMG at different pillar diameters from the critical loads that result in a nominal strain jump greater than 2%. As shown in Fig. 2(c), it is striking to see that, despite the high modulus, the yield strength of the NGMG is however lower than that of its monolithic counterpart, particularly so when the micropillar diameter is below 2 μm. Meanwhile, the yield strength of the MG micropillars becomes strongly scattered for the pillar size less than 2 μm. However, such strength scattering is significantly reduced as the pillar size increases above 3 μm. A similar finding was also reported in Refs [34, 36, 37]. Recently, we systematically studied this sample size on strength scattering in microcompression, which could be attributed to the randomness in the shear band initiation site in tapered micropillars [33]. In contrast, the yield strength of the NGMG micropillars remains almost to be constant. Fig. 2(d) compares the yield strengths of the MG and NGMG normalized by the corresponding average elastic modulus. In such a case, the strength softening becomes evident for the NGMG. Notably, a similar phenomenon of strength weakening was also reported in the atomistic simulations of various NGMGs [25–27]. At first sight, this behavior may appear "counterintuitive" since it has been shown by many previous studies [38–40] that the presence of hard particles or phases in an amorphous matrix can lead to yield strengthening due to shear band blocking or branching.

To unravel the deformation mechanisms, the deformed MG and NGMG micropillars were FIB-cut along the pillar heights and the shear-banded regions were examined under TEM. Fig. 3(a) shows the typical bright field (BF) TEM image of a local shear intensified region (LSIR) observed along the shear trace in the MG, which resembles a local shear band as reported by Zhang et al. [6] and has the thickness of 10–20 nm. In contrast, distributed LSIRs can be observed along the individual microscopic shear trace in the NGMG, which spreads over a distance of ~100 nm in the direction perpendicular to the shear trace [Fig. 3(b)]. More structural details of these LSIRs were revealed by high resolution TEM imaging [Fig. S2 (a)]. Within these LSIRs, we observed 5-nm wide elongated regions separated from each other