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Effects of strain and strain rate on the evolution of shear bands for room temperature rolled Pd₄₀Ni₄₀P₂₀ bulk metallic glass

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ABSTRACT

Room-temperature rolling experiments were performed on Pd₄₀Ni₄₀P₂₀ bulk metallic glass at two different strain rates. It is found that at each strain rate the shear band density increases with increasing strain for the deformed samples. However, for samples endured the same deformation strain, more amounts of shear bands (i.e., a higher shear band density) was introduced into the sample deformed at the higher strain rate. In addition, the higher strain rate also leads to the generation of more amount of free volume for samples endured a same deformation strain. The hardness change behavior investigation result suggests that the introduction of multiple intersected shear bands leads to hardening of Pd₄₀Ni₄₀P₂₀ bulk metallic glass.

1. Introduction

It has been recognized that at low temperature and high strain rates, metallic glasses will deform inhomogeneously via the formation of highly localized shear bands [1–3]. In a shear band, as a region accommodating the plastic strain, the atomic density is lower than that in the undeformed metallic glassy matrix and this indicates that a shear band has enhanced free volume [4,5]. However, some recent investigation results indicate that shear bands showed alternatively both, an increase and decrease in density relative to the undeformed glassy matrix [6–8]. In addition, the atomic structure of shear bands was studied further by Feng et al. using molecular dynamics simulations and the structure inside shear bands was found to change in both the SRO (atomic short-range order) and MRO (medium-range orders) in comparison with that in the undeformed metallic glassy matrix [9]. Moreover, the structure has also been pointed out to change in the glassy matrix around shear bands for inhomogeneously deformed metallic glasses [10]. The structural difference between shear bands and undeformed metallic glassy matrix as well as the structural change in the glassy matrix around shear bands suggests that the structure is changed accompanied by the formation of shear bands for metallic glasses endured inhomogeneous deformation. Obviously, such structural modifications should consequently affect characteristic properties for metallic glasses, especially when the number of introduced shear bands or the shear band density is high enough. In actual fact, in comparison to their undeformed metallic glass counterpart, many structural related properties such as thermal stability, corrosion resistance, strength and

plasticity, etc., have indeed been found to change for inhomogeneously deformed metallic glasses that contain shear bands. For example, due to the introduction of shear bands, the thermal stability decreased for an Au-based metallic glass after inhomogeneous plastic deformation, evidenced by the reduction of the crystallization temperature [11]. Recently, the pitting corrosion behavior has been investigated in a cold-rolled Zr_{64.13}Cu_{15.75}Ni_{10.12}Al₁₀ metallic glass and it is found that the pitting corrosion occurs more easily for the deformed samples [12]. Moreover, it is observed that the strong intersections between multiple shear bands can lead to a geometric hardening and enhanced plasticity in Cu_{47.5}Zr_{47.5}Al₅ bulk metallic glass [13]. Especially for the improvement of the limited plasticity, which has been an inherent obstacle for their application of metallic glasses, the introduction of multiple shear bands has been verified to be an effective method. For examples, by introducing pre-existing multiple shear bands into metallic glass using cold rolling, compression, etc., the room temperature compressive plasticity can be effectively enhanced and even a little tensile plasticity can be obtained [14–18]. Obviously, introducing multiple shear bands via inhomogeneous plastic deformation offers new opportunities to modify the properties or even to obtain new properties for metallic glasses. Therefore, it is of significant important to study the factors influencing the evolution of shear bands in metallic glasses during an inhomogeneous plastic deformation process.

So far, one of the most important factors impacting the amount of shear bands or shear band density is the plastic strain and it is usually considered that the shear band density increases monotonously with increasing plastic strain. In addition, some quantitative relations

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between the plastic strain and shear band density have been determined for several metallic glassy systems [19–21]. However, the quantitative proportional relation reported in these works mentioned above are usually deduced based on the corresponding shear band observation results for metallic glasses deformed at one certain strain rate. Will this proportional relation between the shear band density and the plastic strain still exist or change if a metallic glass deforms at a different strain rate has not been systematically studied. On the other hand, many investigation works, either based on experimental results or simulation results, have pointed out that the shear band nucleation rate, propagation and sliding rates, even the number as well as the size of shear bands are closely related to the strain rate. For example, some nanoindentation experimental results indicate that when metallic glasses were deformed under a slow indentations, serrated load-displacement (P-h) curves as well as large, widely spaced shear bands on the specimen surface can be observed, while more rapid indentations exhibited homogeneous flow and a high number density of smaller shear bands [22–24]. In addition, the dependence of shear banding on strain rate has also been focused for metallic glasses or metallic glass composite endured compressive deformation [25,26]. Moreover, some simulation investigation results also indicate that the number of shear band nuclei generated increases with increasing strain rate [27]. Hence, not only the plastic strain, but also the strain rate will significantly affect the shear band density for an inhomogeneously deformed metallic glass. Investigating systematically the evolution of shear bands with strain for metallic glasses deformed at different strain rates seems to be significantly important. However, focusing on the effect of both the plastic strain and strain rate on the evolution of shear bands for metallic glasses endured inhomogeneous plastic deformation has seldom been reported so far.

In the present work, a series of room-temperature rolling experiments were carried out on Pd₄₀Ni₄₀P₂₀ bulk metallic glass (BMG) at two different strain rates. The investigation on the evolution of shear band and free volume indicates that both the shear bands density and average free volume seems to increase with increasing strain for samples deformed at a certain strain rate. However, for samples endured the same deformation strain, shear bands with a higher shear band density and more free volume were introduced into the sample deformed at a higher deformation strain rate. The hardness change behavior investigation result suggests that the introduction of multiple intersected shear bands leads to hardening of Pd₄₀Ni₄₀P₂₀ BMG.

2. Experiments

Pd₄₀Ni₄₀P₂₀ (atomic percent) master alloy ingots with the nominal composition have been fabricated by arc-melting high purity of Pd (99.9%) and Ni₂P (99.5%) under a Ti-gettered argon atmosphere. Each ingot was inverted and remelted several times to ensure compositional homogeneity and subsequently suction casting into a water-cooled copper mold. Cylindrical rods with a diameter of 4 mm and a length of about 25 mm were obtained. Cylindrical disks with a thickness of about 1.1 mm were cut from the as-cast rods for room temperature rolling (RT-rolling) deformation. Both sides of the disks were mechanically polished to make them parallel to each other prior to rolling. After polishing, the thicknesses of the disks were about 1 mm. During rolling, many small deformation rolling steps were repeated with a reducing gap between two rollers so that constant strain rates could be kept. The details to evaluate the strain rate for a sample during the rolling process can be expressed as follows: (1) the rotation speed of the rollers as well as the change of the reducing gap between the two rollers is fixed during the whole rolling process for a certain sample; (2) the thickness before and after each rolling step were measured respectively and the thickness change as well as the strain during each rolling step was calculated for the sample; (3) the length of the sample along the rolling direction was measured after each rolling step and the time needed during each rolling step was calculated based on both the measured

sample length and the rotation speed of the rollers; (4) the strain rate during each rolling step was obtained based on the strain calculated from step (1) and the time obtained from step (3); (5) the average deformation strain rate was obtained based on the statistical average of the strain rates during each rolling step for a certain sample. The whole strain is expressed by the thickness reduction, i.e., $(h_0 - h) / h_0$, where h_0 and h represent the thicknesses before and after rolling, respectively. The used strain rates were approximately 4.0×10^{-1} and $4.0 \times 10^{-2} \text{ s}^{-1}$, respectively, in this work.

The as-cast samples and the RT-rolled samples with different strains were analyzed by X-ray diffraction (XRD) on a Panalytical X'pert X-ray diffractometer with monochromatic Cu K α radiation (wavelength 1.5405 Å) and transmission electron microscopy (TEM) observations on a Tecnai G2 F30 electron microscope working with an acceleration voltage of 300 kV. The side surface morphology of the RT-rolled samples was observed with a LEO 1530 scanning electron microscope (SEM). The differential scanning calorimetry (DSC) analyses were performed on the samples using a Perkin Elmer Pyris Diamond thermal analyzer at heating rates of 20 K/min under flowing purified argon. The microhardness of the as-cast and deformed samples was tested using a Buehler Micromet 5104 Vickers microhardness tester. 20 indentations were measured on each sample at a static load of 100 g and with a dwell time of 15 s.

3. Results and discussion

3.1. Structure of the as-cast and deformed samples

The Cu K α XRD pattern of the as-cast Pd₄₀Ni₄₀P₂₀ sample is shown in Fig. 1. Besides the two broad diffraction halos around $2\theta = 42^\circ$ and $2\theta = 74^\circ$, no diffraction peaks corresponding to any crystalline phases can be detected. In addition, a uniform featureless contrast can be observed from the bright-field TEM micrograph of the as-cast Pd₄₀Ni₄₀P₂₀ sample shown in Fig. 2a. The corresponding selected area electron diffraction (SAED) pattern of the as-cast sample shown in the inset of Fig. 2a is consisted of a broad diffraction halo and a faint large one and this is typical for amorphous materials. Moreover, a homogeneous maze contrast is seen in the corresponding high resolution TEM (HRTEM) micrograph and no obvious lattice fringes can be found (Fig. 2b). Therefore, the as-cast Pd₄₀Ni₄₀P₂₀ sample is completely amorphous.

To study the microstructural changes induced by RT-rolling deformation in the Pd₄₀Ni₄₀P₂₀ BMG, the XRD measurements were performed. Fig. 1a and b exhibit the XRD patterns for the RT-rolled Pd₄₀Ni₄₀P₂₀ BMG samples with strains of 30%, 60%, 80% deformed at 4.0×10^{-1} and $4.0 \times 10^{-2} \text{ s}^{-1}$, respectively. Similar to that for the as-cast sample, the XRD patterns for all these RT-rolled samples exhibit only two broad diffraction halos around $2\theta = 42^\circ$ and 74° without any crystalline peaks and this suggests that no obvious crystallization is detected within the resolution limit of X-ray diffraction. To investigate further the evolution of structure during the RT-rolling process for Pd₄₀Ni₄₀P₂₀ BMG, TEM observation were performed on the deformed samples and the bright-field TEM and HRTEM micrographs of the RT-rolled sample with a strain of 80% deformed at $4.0 \times 10^{-1} \text{ s}^{-1}$ are shown in Fig. 2c and d. No other strong contrast than the shear bands with a bright contrast can be observed. In addition, the corresponding SAED consists of a broad diffraction halo and a faint large one. Moreover, no obvious lattice fringes can be found in the HRTEM micrograph around the area of a shear band shown in Fig. 2d. Hence, the XRD as well as the TEM results indicate that the deformed Pd₄₀Ni₄₀P₂₀ BMG samples including shear bands have a characteristic of amorphous structure.

3.2. Shear band evolution in the RT-rolled Pd₄₀Ni₄₀P₂₀ BMG with strain and strain rate

To investigate the effect of deformation strain as well as strain rate

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