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Effect of crystal phase on shear bands initiation and propagation behavior in metallic glass matrix composites

H.Y. Song[a,b,*], S. Li[a], M.R. An[a], Q. Deng[b], Y.L. Li[b,*]

[a] College of Material Science and Engineering, Xi'an Shiyou University, Xi'an 710065, China
[b] School of Aeronautics, Northwestern Polytechnical University, Xi'an 710072, China

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ABSTRACT

The effect of crystal phase structure on the shear bands (SBs) initiation and propagation behavior of $Cu_{50}Zr_{50}$ metallic glass (MG) matrix composite with a pre-existing crack is studied using molecular dynamics (MD) simulation method. It is found that the crystal diameter has almost no effect on the peak stress of MG-matrix composites, because the change of crystal diameter not only influences the STZ coalesce around the crystal-amorphous interface (CAI) but also affects the magnitude of the repulsive force between CAI and SB. Namely, CAI plays two roles of generating the immature SB and hindering its propagation. The results also indicate that the behavior of SB initiation and propagation shows a stronger dependence on the CAI. Compared with monolithic MGs, the crystal layer changes the propagation path of the SB in the composite. Additionally, we introduce the disorder degree (i.e. entropy) method to analyze the formation process of SBs.

1. Introduction

Bulk metallic glasses (MGs) have attracted great research mainly originating from its outstanding strength, high hardness, and the ability to store high elastic strain energy [1–5]. In addition, MGs possess high wear resistance because of the lack of dislocation defects [6], which makes them an ideal structural material. It is noted that the plastic deformation of MG is easy to produce shear bands (SBs) [7]. Namely, plastic strain highly localized into nanoscale narrow regions. Because of the SB initiation and propagation, MGs are generally regarded as brittle materials. In order to design MGs with high strength and excellent plasticity, it is important to understand the fundamentals of SB initiation and propagation behavior are important for the MGs and MG-matrix composites widespread applications.

There has been a lot of study to improve the ductility of MGs. The strategy of improving the plasticity of MG has the reduction in size [8–11] and the introducing of defects [12,13]. The effort of improving the plasticity of MG is mainly concentrate upon the uniformly distributing the SBs. The improved ductility is generally ascribed to the increased number of SBs. The focus of the amorphous study has been on disclosing the nature of SBs initiation and propagation behavior [14–16]. A high-resolution TEM imaging combination molecular dynamics (MD) simulations method by Brink et al. [14] demonstrated that SBs can dissolve precipitates, can wrap around crystal obstacles, or can be blocked depending on the size and density of the precipitates. Zhou et al. [15] claimed that pre-existing SBs in a MG can suppress shear localization. They also indicated that the yield strength of the material is in competition with the critical stress required for the formation of mature SBs in the load-bearing materials. Sha et al. [16] elucidated that the plastic deformation is easy to start from the notch root. When the shear transition region (STZs) reaches the threshold value, the SB is propagating from the crack tip and causes the material failure. Through these studies, it is found that the plastic deformation of MG is affected by SBs initiation and propagation. And the question is hard to clarify SBs initiation and propagation behavior. At the present time, however, there is still no general consensus regarding the cracked and crystal-amorphous interface (CAI) affects the SBs initiation and propagation behavior. Here, the effect of crystal phase structure on the SBs initiation and propagation behavior of $Cu_{50}Zr_{50}$ MG matrix composite with a pre-existing crack is studied using molecular dynamics (MD) simulation method.

The paper is organized as follows. The simulation is given in Section 2. In Section 3 we describe the results and discussion. In Section 4 is the conclusion based on those observations.

2. Atomistic simulations method

Here, our aim is to investigate the SBs initiation and propagation behavior of $Cu_{50}Zr_{50}$ MG-matrix composites with a pre-existing crack under tension loading. The time integration step is chosen as 2.0 fs. The

* Corresponding authors at: College of Material Science and Engineering, Xi'an Shiyou University, Xi'an 710065, China.
E-mail addresses: gsfshy@sohu.com (H.Y. Song), liyulong@nwpu.edu.cn (Y.L. Li).

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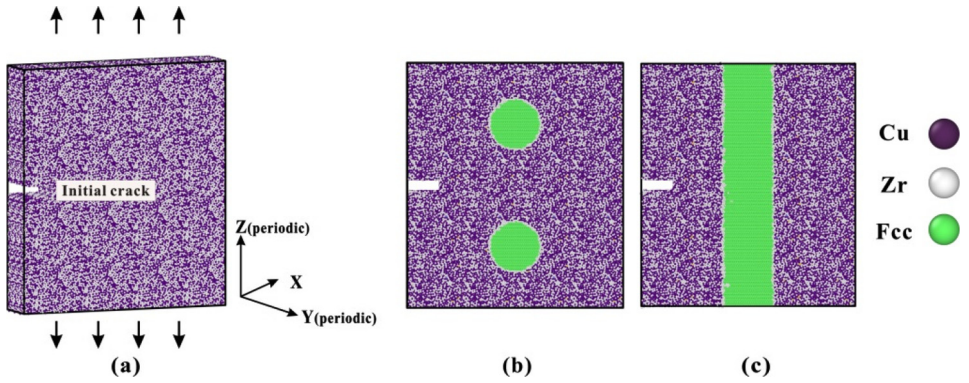

Fig. 1. The geometry of samples with a pre-existing unilateral crack.

$Cu_{50}Zr_{50}$ MG with dimension of 9.2–2.0–9.2 nm^3 and 9680 atoms are generated. After the sample melted at 2000 K and zero pressure for 2.0 ns to ensure homogeneity, during which periodic boundary conditions (PBC) are applied to all three dimensions. The cell was then cooled at quenching rate of 10^{12} K/s to 50 K. The melting temperature is far higher than the melting point [17]. In our simulation, the dimension we use by replicating the original $Cu_{50}Zr_{50}$ MG is 36.8–2.0–36.8 nm^3. After the MG is relaxed completely, the introduction of a crack by removing the atom from the amorphous phase, as delineated in Fig. 1(a). To control the initiation of the SB, a depth 5.52 nm, radius 0.80 nm crack is used. Two different configurations, as shown schematically in Fig. 1(b) and (c), are constructed for this study. The first sample was a cylindrical Cu crystal with a different diameter. The crystalline phase of MGs in two models of this study is single crystal Cu, which is similar to that used by Zhou et al. [31]. The Young's modulus of pure crystalline Cu is here 109 GPa, while that of pure amorphous $Cu_{50}Zr_{50}$ is 62 GPa. In addition, the Cu crystal particles are harder than the MG. As shown in Fig. 1(b), the cylindrical Cu crystal was introduced by removing the atoms from the perfect amorphous phase. The diameter of cylindrical Cu crystal is 8.0, 10.0 and 12.0 nm, respectively. The center distance between crystal phases is 18.4 nm. In the second structure, we combine $Cu_{50}Zr_{50}$ MG and single crystal Cu with a layer size of 8.0 nm to construct the nanolaminate structures, as shown in Fig. 1(c). To mainly investigate the impediment effect of crystal phase on the SBs propagation, the single crystal Cu and the $Cu_{50}Zr_{50}$ MG act as here hard phase and soft phase, respectively. The crystal orientation of single crystal Cu along the X, Y and Z axis were $[1\bar{1}0]$, $[11\bar{2}]$ and [1 1 1], respectively. Additionally, free surface condition along X axis, while PBCs were imposed in the Y and Z directions under tensile loading. A constant strain rate of 1.25×10^8/s along the Z-direction was used at temperature of 50 K.

In this work the embedded atom method (EAM) potential [18] is used to describe the interaction between Cu-Cu, Zr-Zr and Cu-Zr atoms. This potential has been verified to be successful in simulating some of important physical properties [8,19,20]. The crystal phases is identified by using the common neighbor analysis (CNA) [21] method. In our simulations, the local shear invariant [22] η^{Mises} in the glass matrix as implemented in the Open visualization tool OVITO[23]. Atoms, with a η^{Mises} value larger than 0.3, are illustrated to visualize the deformation process. In all the atomistic configurations presented in this paper, atoms are painted according to the following scheme: red for atoms in STZs, green for face-centered cubic (fcc).

3. Results and discussion

3.1. Shear band in MG-matrix composites with cylindrical crystal

Our aim is to investigate the cylindrical crystal phase size on SBs initiation and propagation behavior. Fig. 2 depicts the tensile stress-strain curves for $Cu_{50}Zr_{50}$ composites with cylindrical crystal and monolithic MG. Each of curves in Fig. 2 is divided into two stages, which are elastic and plastic stage, respectively. At the elastic deformation stage, the stress increases when increase of the strain. Meanwhile, the samples undergo purely elastic deformation. As shown in Fig. 2, the four curves show different slopes, and the slope of monolithic MG is the smallest among the four samples. This means that the introduction of single crystal Cu changed the elastic deformation behavior of the MGs. The slope of the stress-strain curves at the initial linear stage increases with the relative increase of crystal diameter, as shown in Fig. 2. This also means that different crystal diameter strongly influences the elastic deformation. During the plastic deformation, the stress drop of all samples is not abrupt but gradual, which eventually leads to the nucleation of SBs. For those samples, the stress has reached a platform, representing a homogeneous deformation situation [24]. To reveal the SBs initiation and propagation behavior in the $Cu_{50}Zr_{50}$ MG-matrix composites, it is important to shows a sequence of snapshots. Fig. 3 shows the deformation snapshots of samples with three different Cu crystal diameters under various strains. It should be noted that in all of our present simulations, a SB always initiates from the crack tip or the CAI and subsequently propagates, and then a drop in stress is observed. For MG-matrix composites with crystal diameter 8.0 nm, a striking observation is that the STZ is form at the crack tip and the CAI. On subsequent loading, the small STZ coalesce to form a larger STZ. And then, such super-sized STZs are connecting crack and the CAI to form two mature SBs. The SBs propagation is along maximum shear stress direction. Considering the PBCs along the Z direction, the MG-matrix composites only have two mature SBs. When the crystal diameter increases from 8.0 to 10.0 nm, the SB propagation deflects ~45°

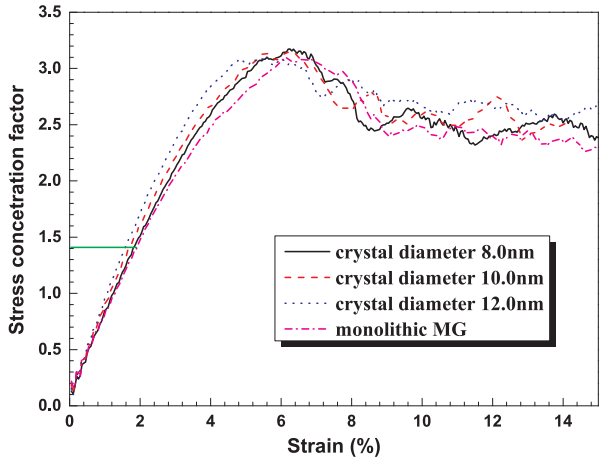

Fig. 2. Stress versus strain of MG-matrix composites with different crystal diameters and monolithic MG.