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Atomistic investigation of the intrinsic toughening mechanism in metallic glass

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ABSTRACT

Metallic glasses (MGs) can have high fracture toughness by carefully choosing chemical compositions. However, their intrinsic toughening mechanism is vital but mysterious. In this paper, large scale molecular dynamic simulations are conducted to study the fracture behavior and underlying mechanism of MGs from atomistic points of view. By changing the composition ratios, the fracture behavior of the MGs transits from void nucleation and coalescence to shear bands toughening. Uniformed local atomic number density is found to be responsible for the high toughness while highly fluctuated local atomic number density result in cavitation governed brittle fracture. The strength of the ductile MGs is more sensitive to the initial void compared with the brittle ones due to the different fluctuations in atomic structures. In the simulations, it is also found that the ductile MGs have a higher Poisson's ratio which may also improve the toughness. The obtained results shed light on the effect of chemical compositions upon the toughness of MGs.

1. Introduction

Metallic glass (MG) with long range disorder atomic structures is one of the most promising engineering materials with superior mechanical properties as high elastic limit, high hardness and good corrosion resistance, etc. [1–3]. Fracture toughness is important for metallic materials in real applications. Both scientific researchers and engineers have payed significant attentions to the crack growth resistance of MGs [4–6]. It has been reported that MGs have fracture toughness in a wide range of about 2–100 MPa $m^{1/2}$ [7–11]. Some MGs such as Zr-based ones possess fracture toughness as high as steels and Ti alloys [11,12]. There are also some MGs like Mg-based ones are as brittle as Si glasses [9]. Molecular dynamic simulations by Murali et al. [13] showed that brittle fracture in FeP was governed by intrinsic cavitation mechanism while ductile fracture in CuZr was controlled by intensive shear banding.

Intrinsic and extrinsic methods are proposed for improving fracture toughness in MGs. For example, crystalline phases were utilized to form metallic glass matrix composites which could be toughened by multiple shear band interactions and crack deflections [14,15]. But this extrinsic toughening method sometimes reduces the strength. MGs with high toughness can also be obtained by carefully choosing the chemical compositions. Inspired by the correlation between the local structural characteristics and the shear transformations propensity, Xu and Ma [12] obtained a record-breaking fracture toughness of $Zr_{61}Ti_2Cu_{25}Al_{12}$ MG using the extensive shear band interactions. Demetriou et al. [16] reported a MG of fracture toughness comparable to the toughest materials known and the high fracture toughness is a result of crack shielding induced by an extensive shear band sliding process. A number of experiments showed that Poisson's ratio affects the plasticity and toughness of MGs [17–21]. By changing the composition ratios one could get MGs with high Poisson's ratio which leads to ductile deformation [19,22]. Liu et al. [23] developed a criterion to reveal the correlation between the toughness and the Poisson's ratio and describe the various deformation modes. They claimed that the ductile to brittle transitions and different deformation modes were caused by the competition of shearing and cracking. However, Zheng et al. [24] showed that adding soft atoms improves the structural heterogeneity and ductility of MGs. From experiments, they found that the atomic-scale heterogeneity in MGs acts as the defects in crystalline alloys and is responsible for the plasticity in MGs rather than the Poisson's ratio.

To obtain MGs with high fracture toughness, the intrinsic toughening mechanisms must be fully understood. Rycroft and Bouchbinder [25] calculated the fracture toughness as a function

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of the degree of the structure relaxation, indicating that the elasto-plastic crack tip instability in fully relaxed MGs leads to the sharp drop in fracture toughness. Dai and his co-workers [26] suggested that the competition between shear transformation zones (STZs) and tension transformation zones (TTZs) dictates the fracture mechanisms. Li et al. [27] proposed a brittle to ductile transition map considering the STZ versus TTZ which was shown to depend on the strain rate, temperature and free volume. Zhao et al. [28] studied the composition effects on intrinsic plasticity or brittleness in MGs and found that the compositions at or near intermetallic compounds are extremely ductile whereas the ones at or near eutectics are brittle. However, an atomistic view for the intrinsic toughening mechanisms by changing compositions in MGs need further investigation.

Molecular dynamics (MD) simulation is a good method to study the atomistic mechanisms of fracture, fatigue and plastic deformation in metals [29–34]. Huang et al. [35] used MD simulations to study the ductile to brittle transition in spallation of MGs. They found that the transition is governed by interaction between void nucleation and growth which can be seen as the competition between TTZ and STZ. In this paper, the fracture mechanism of MGs with different composition ratios are investigated by molecular dynamics simulation. The crack growth behaviors and cavitation evolutions are studied. Intrinsic toughening mechanisms by changing the composition ratios in MGs are discussed in an atomistic view.

2. Materials and methods

The considered MgAl MGs with different composition ratios, i.e., $Mg_{80}Al_{20}$, $Mg_{50}Al_{50}$ and $Mg_{20}Al_{80}$ are studied by molecular dynamic simulations using Lammps [36]. The embedded atom method (EAM) potential is chosen to describe the interaction between atoms in the simulations [37]. The EAM potential describes the interatomic interactions of amorphous structure very well. To obtain the MG materials, melting and cooling are adopted to the MgAl crystalline metals. The fcc structure of MgAl alloys are melt at 2500 K for 100 ps, then cooled down to 1 K in 400 ps, corresponding to an effective cooling rate of about 6 K/ps. After cooling to 1 K, the MGs are relaxed for additional 100 ps. During the process, periodic boundary conditions were kept in all three directions. The melting and cooling methods are adopted to ensure amorphous structure.

The obtained $Mg_{80}Al_{20}$, $Mg_{50}Al_{50}$ and $Mg_{20}Al_{80}$ amorphous structures with size of $34 \times 34 \times 6$ nm^3 are duplicated and cut to form rectangle plates as shown in Fig. 1(a). The height H of the plate is 100 nm and the length W in the x direction is 50 nm. The thickness of the plate in the out of plane direction is 5 nm. For the plates, the boundary condition in the x direction is free and the other directions are periodic. Before loading, the MG plates are relaxed at 300 K for 150 ps and then cooled down to 1 K and relaxed for 50 ps again. This low temperature could eliminate the thermal effects during deformation. The pressure is kept at 0 bar during the relaxation. The relaxation process is to exclude the interface effect during the assembling. To investigate the fracture behavior of the MG models with different composition ratios, a notch is created by removing atoms in the plates. As shown in Fig. 1(a), the length of the notch is $a = 6$ nm and the width is $b = 2$ nm. The thickness of the crack keeps the same with the plate of 5 nm. Fig. 1(b) shows the radial distribution function (RDF) of the notched plates in the equilibrium state. The RDF of plates indicate that the materials have amorphous structures. Tensile loading is imposed in the y direction on the notched plates with a strain rate of 5×10^8 s^{-1}.

3. Simulation results

3.1. Fracture behaviors

The atomistic configurations of fracture processes in the $Mg_{80}Al_{20}$, $Mg_{50}Al_{50}$ and $Mg_{20}Al_{80}$ MG plates at different global tensile strains are shown in Fig. 2. The atoms are painted according to the local Von Mises shear strain η_{Mises} [38]. To clearly show the fracture mechanisms, the insets in Fig. 2 present the crack tip configurations. The whole process can be seen from the simulation movies in the Supplementary Materials.

Fig. 2(a)–(d) displays the fracture processes of $Mg_{80}Al_{20}$ at different global strains. At the beginning of the tensile loading (see Fig. 2(a)), STZ activations happen at the notch root due to stress concentration. Then two shear bands form and propagate along the ~45° directions of the loading axial. Nano void appears at the crack tip as can be seen in Fig. 2(b). Crack initiates and links with the voids, leading to fracture of the MG. Due to the cavitation nucleation and coalescence events, the fracture surface of $Mg_{80}Al_{20}$ is very rough as shown in Fig. 2(c) and (d). This intrinsic cavitation related mechanism is typical for brittle MGs [13].

The fracture processes of $Mg_{50}Al_{50}$ are shown in Fig. 2(e)–(h). When the global strain is $\varepsilon = 0.05$, there are STZ activations at the notch root. With the global strain increasing to 0.1, crack initiates at the site where the local strain is very large and shear bands start to form. As shown in Fig. 2(g) (i.e. $\varepsilon = 0.1955$), a formed dominant shear band affects the crack growth route. The facture surface becomes rough because of crack deflection. No pronounced cavitation appears until the global stain reaching 0.2 (see, Fig. 2(h)).

Different from $Mg_{80}Al_{20}$ and $Mg_{50}Al_{50}$, the fracture of $Mg_{20}Al_{80}$ is governed by shear band toughening. As shown in Fig. 2(i), the

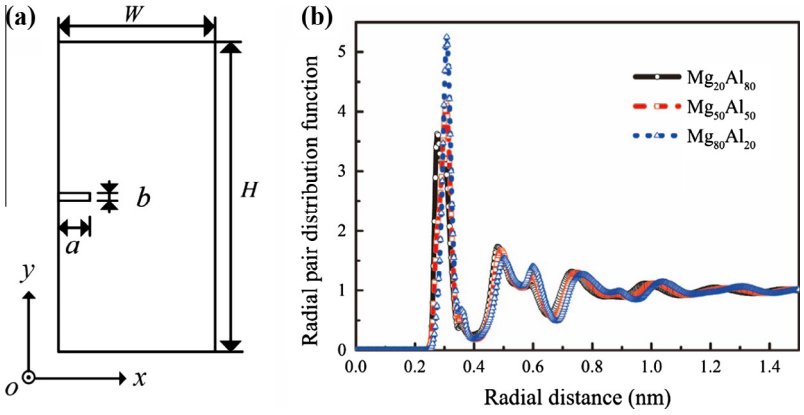

Fig. 1. (a) Schematic of a metallic glass sample with notch. (b) The radial distribution function for MG samples in equilibrium.