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Effect of aspect ratio on the mechanical properties of metallic glasses

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To examine the effect of aspect ratio, atomistic simulations are performed on the tensile failure of $Cu_{50}Zr_{50}$ metallic glasses (MGs) with aspect ratios from 2:1 to 12:1. All samples fail via a single shear band (SB), and the Young's modulus and the tensile strength are independent of the aspect ratio. For long MGs, however, an abrupt unstable shear banding failure is observed, while a combined abrupt unstable shear banding and slow stable SB sliding is observed for short MGs.

Keywords: Metallic glasses; Aspect ratio; Mechanical properties; Failure mode

The effect of aspect ratio (height to diameter ratio) on mechanical properties is a major focus of research in the field of materials science and engineering [1]. For example, Wu et al. reported that short Cu nanowires fail via a ductile mode, while long wires exhibit extreme shear localization and abrupt failure [2]. Metallic glasses (MGs) have revolutionized structural materials due to their superior mechanical properties [3–11]. In the past 10 years, although great efforts have also been made to comprehend the effect of aspect ratio on the mechanical properties of MGs [12–15], several key issues still remain to be convincingly explained from an atomic-scale perspective.

First of all, one of the major difficulties in understanding the intrinsic effect of aspect ratio on the mechanical properties of MGs is to exclude the extrinsic effects from experimental measurements, such as tapering, testing machine stiffness, geometry constraints and some other geometric imperfections [1,13,15,16]. For example, Zhang et al. [15] reported a large compressive ductility and the formation of multiple shear bands (SBs) in MGs with an aspect ratio of 0.67; this experimental finding was attributed to the lateral stress induced by friction between the end of the MG samples and the crosshead of the testing machine. Mondal et al. [17] reported that geometry-constrained SB interaction, lateral force and mechanical interlocking of crack can all lead to large plasticity of MGs. Thus to understand the inherent ductility of MGs, it is important and necessary to get rid of the constrained plasticity. Secondly, because several key issues regarding the fundamental mechanisms of shear banding in MGs remain to be understood [13,14], the understanding of the effect of aspect ratio on the mechanical properties of MGs remains a subject of active debate. For example, based on the concept of the SB instability index, Han et al.'s experimental results showed that a MG sample with a small aspect ratio of 1:1 exhibits larger plasticity with multiple SBs than that with a large aspect ratio of 2:1, which has a larger SB instability index [13]. In Liu et al.'s experimental work [14], compression tests were conducted on MG samples with different aspect ratios from 2:1 to 4:1, and the MG with the middle aspect ratio of 2.5:1 showed the largest plasticity. Therefore, they concluded that the largest plasticity may appear at an optimal aspect ratio as the aspect ratio affects not only the SB stability index but also the critical SB length.

It appears that great efforts are needed to eliminate artifacts from experimental measurements in order to investigate the intrinsic effects of aspect ratio on the mechanical properties of MGs [1,13,15–17]. It is intriguing to know whether the plasticity of MGs is an inherent property of these materials or originates from geometry constraints. Moreover, the conclusions on the effects of aspect ratio on MGs based on the SB model are inconsistent [13,14]. It is also intriguing to know whether the aspect ratio affects the nucleation/formation, or propagation, of SBs [1].

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Recent experiments on MGs by reducing sample size reveal a brittle-to-ductile transition [18,19]. To examine the aspect ratio effects on MGs at the nanoscale is also a topic of research and practical interest. Advantages of molecular dynamics (MD) simulations include the ability to exclude the extrinsic effects from experimental measurements, and the ability to investigate the initiation and propagation of SBs at the atomic scale. However, there are few relevant MD simulations reported in the literature as the simulation of MG sample with a large aspect ratio requires many millions of atoms. In the present work, our MD simulations span a sufficient range of aspect ratio from 2:1 (commonly used experimentally) to 12:1. The maximum number of atoms in the MG sample with the aspect ratio of 12:1 is ~3.32 million. Uniaxial tensile loading tests of $Cu_{50}Zr_{50}$ MGs with different aspect ratios are performed using very large-scale MD simulations. We attempt to systematically reveal the intrinsic effect of aspect ratio (2:1–12:1) on the tensile strength, plasticity as well as the corresponding SB deformation and fracture mechanisms for MGs. Our simulations show that there is no change in the failure mechanism, i.e. all samples fail via a single SB, and the tensile strength maintains almost a constant value. However, the aspect ratio plays a role in determining the tensile failure modes of the MGs. Long MGs show an abrupt failure, which is attributed to the unstable propagation of SBs. In contrast, short MGs fail in a combined unstable and stable propagation of a single SB. This change in failure mode can be explained by the elastic energy stored in specimens and the tensile stress in the sliding region. The present work sheds light on a possible way to extract the intrinsic mechanical properties from experimental measurements by excluding extrinsic effects and provides a useful atomic understanding of the mechanical properties of MGs as a function of the aspect ratio.

Our MD simulations were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [20–22]. The $Cu_{50}Zr_{50}$ MGs samples have fixed Y and Z dimensions of 28.0 nm × 6.24 nm. By changing the X dimension, the aspect ratio is varied from 2:1 to 12:1, and the samples contain 0.55–3.32 million atoms. A constant integration time step of 2 fs was used in all the simulations. The interatomic interaction is described by the embedded atom method (EAM) potential [23]. In constructing the sample, a small cube (~13,000 atoms) with periodic boundary conditions (PBCs) along all three dimensions was first equilibrated at 2000 K for 2 ns, and then cooled at a quenching rate of 10^9 K s^{-1} to 50 K, at zero external pressure (NPT ensemble). The simulation samples were then constructed by replications of the small cube, then annealed for 0.5 ns at 800 K, and finally brought back to 50 K [24,25]. For uniaxial tensile tests, PBCs were imposed along the X- and Z-directions, while free surface condition was used along the Y-direction. A constant strain rate of 4×10^7 s^{-1} (slower than that typically used in MD simulations [24–26]) was used along the X-direction.

Figure 1a depicts the tensile engineering stress–strain curves for $Cu_{50}Zr_{50}$ MGs with aspect ratios of 2:1, 4:1, 8:1 and 12:1. From the curves, it can be seen that the initial elastic behavior and the subsequent non-linear behavior before reaching the peak strength are the same for all MGs despite the different aspect ratios. In addition, it is noted that all MG samples show the same peak strength of ~3.23 GPa at ~7.52% strain. These indicate that both Young's modulus

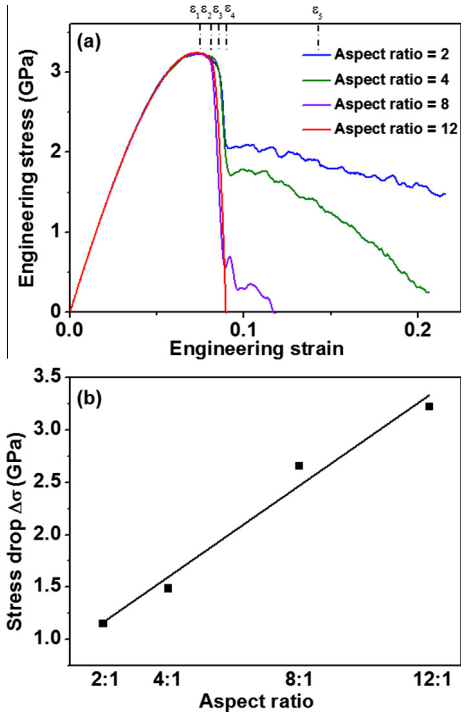

Figure 1. (a) The tensile engineering stress–strain curves for $Cu_{50}Zr_{50}$ MGs with aspect ratios of 2:1, 4:1, 8:1 and 12:1. The five dotted lines correspond to the strains of the snapshots shown in Figure 2. (b) The level of stress falls as a function of aspect ratio.

and the maximum strength are independent of the aspect ratio. After reaching the peak strength, all samples suffer a sudden and rapid drop in stress, corresponding to spontaneous shear localization into a narrow band [24,27]. However, the size of the stress drop in these four samples is substantially different. Figure 1b shows the size of the stress drop as a function of aspect ratio, which appears to be a nearly linear function of aspect ratio. With increasing the aspect ratio, the stress drop becomes more obvious. The MG with the largest aspect ratio fails after the first stress drop, suggesting that it fails in an abrupt (brittle) manner. However, for the MGs with smaller aspect ratios, stable plastic flow then occurs after the initial abrupt stress drop. For these short samples, the stress drop to zero is not abrupt but gradual, and an extensive plastic deformation is observed. Our results reveal that the aspect ratio of MGs plays a key role in determining MGs failure modes. By comparing the failure mechanism for all the samples studied here, we find that there is no change in failure mechanism: all the samples fail by the nucleation and propagation of a single SB.

To reveal the deformation and failure behavior in the MGs with different aspect ratios, we further investigate the atomic deformation processes by examining the atomic local shear strain [28,29] with reference to the relaxed samples prior to the tensile loading. Figure 2 shows a sequence of snapshots that capture SB initiation and propagation for $Cu_{50}Zr_{50}$ MGs with different aspect ratios at strains of 7.52%, 8.12%, 8.52%, 8.92%, and 14.12%. At a strain of 7.52%, corresponding to the peak strength, there is no difference between any of the MGs samples. However, thereafter it can be seen that the SB formation in long MGs is ahead of that in short MGs. Furthermore, once the SB formation