



Strengthening and toughening mechanisms of amorphous/amorphous nanolaminates



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ABSTRACT

Bulk amorphous alloys are in general strong, but brittle. Properly introduced interfaces can effectively improve their ductility. In this paper, the tensile behavior of amorphous/amorphous (A/A) nanolaminates is investigated by atomistic simulations. Upon loading, multiple shear bands transmit through the A/A interfaces and interact with each other. As a result, plastic plateaus are presented in the simulated tensile stress–strain curves of the nanolaminates with small layer thickness. Moreover, the strength of the A/A nanolaminates increases with the layer thickness decreasing, due to the interface obstruction to the shear band motion. It is also found that the plastic deformation mechanisms transit from localized shearing in the soft amorphous layers to multiple shear band interactions in the whole sample at a critical size. An analytical model considering shear band motion is proposed to predict the critical layer thickness for the localized to homogenous deformation transition in A/A nanolaminates.

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1. Introduction

Amorphous alloys have long range disordered atomic structures (Klement et al., 1960; Chaudhari et al., 1980) and possess unique mechanical properties including high strength, high hardness, good corrosion resistance, and so on (Schuh et al., 2007). However, amorphous alloys usually deform in localized shear band and undergo brittle failure at room temperature (Wang et al., 2004; Schuh et al., 2007), which is the main obstruction for them to become one of the most promising materials for engineering applications (Ashby and Greer, 2006). Unlike crystalline materials, amorphous alloys do not have microstructures like dislocations, grain boundaries and twin boundaries. As a result, they cannot restrict individual shear band motion and suffer from strain softening and catastrophic failure (Jiang et al., 2008; Greer et al., 2013). Therefore, a long-standing goal for amorphous alloys is to improve the tensile ductility.

Numerous of methods were proposed to overcome the brittleness of amorphous alloys (Schroers and Johnson, 2004; Wang et al., 2007; Hofmann, 2010; Chen, 2011; Nieh et al., 2012; Zhang et al., 2012; Kim et al., 2013; Kim and Kim, 2015). For instance, crystalline particles were added to amorphous matrix to form amorphous crystalline composites (Eckert et al., 2007; Hofmann, 2013). The crystalline phase can impede shear bands propagation (Hays et al., 2000; Hofmann et al., 2008) and deflect them (Hajlaoui et al., 2006), resulting in improved plasticity and toughness. Initiation and absorption of shear bands at the crystalline inclusions are responsible for the enhanced plasticity in the composites. The shape, orientation and

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fraction of the crystalline inclusions were also found to affect the ductility enhancement (Fan et al., 2007; Jia et al., 2015). Experimental results showed that shear band formation is inhibited by reducing the sample size under 100 nm, leading to remarkable plasticity via homogenous deformation (Guo et al., 2007; Shan et al., 2008; Volkert et al., 2008; Jang and Greer, 2010; Luo et al., 2010; Jang et al., 2011; Zhou et al., 2015). Wu et al. (2015) claimed that factors like sample size, pre-strains and loading conditions may affect the initiation and evolution of local strain heterogeneity and hence can affect the ductility of bulk amorphous alloys. Another effective means to enhance plastic deformation is to improve the structural heterogeneity. It was shown that adding soft atoms to amorphous alloys could change the micro-scale inhomogeneity and stimulate multiple shear bands to improve plasticity (Das et al., 2005; Zheng et al., 2012). By conducting statistical nanoindentation and three-point bending tests, the plastic deformation as well as the fracture behavior of MGs were found to be governed by the structural heterogeneity through interactions between defect density and crack tip (Li et al., 2013, 2015). Liu et al. (2007) obtained amorphous materials with soft and hard components surrounding with each other and achieved a remarkable fracture strain of 160%. In the experiment of Liu et al. (2007), extensive shear bands were found to start to form from the interfaces and interact with each other. The phase separation in amorphous alloys result in enhanced plasticity and has been reported in various experiments (Park and Kim, 2006; Du et al., 2007; Chen et al., 2014; Chen and Todd, 2015). Nanoglass synthesized by nanometer sized amorphous grains (Gleiter, 2013) was proved to be beneficial for the ductility of amorphous alloys (Adibi et al., 2013; Albe et al., 2013; Franke et al., 2014). Note that the densities of atoms are different in the interior regions of grains and the interfaces between grains (Fang et al., 2011). Usually, shear bands are easier to initiate at the interfaces, followed by going through the grains then interacting with each other.

Amorphous alloys with interfaces exhibit enhanced plastic deformation so that amorphous/amorphous (A/A) nanolayered composite could be a new kind of materials to overcome the brittleness of amorphous alloys. Sharma et al. (2009) reported experimental evidence that brittle La-based amorphous alloy deformed plastically when in the form of multilayers with other amorphous alloys. Kuan et al. (2010) showed that amorphous nanolaminates deform more homogeneously than monolithic amorphous alloys. It was also observed in the experiment that the deformation mode and failure mechanism of the nanolayered composites depend upon the modulus mismatch and the loading type. Ma et al. (2013) synthesized multilayered Pb-based amorphous alloy by the thermoplastic bonding method and found that the blocking effect of the bonding interface improves plasticity. To further explore the enhanced plasticity of A/A nanolayered materials, the underlying responsible mechanism has to be elucidated, especially for the influence of A/A interfaces on shear band motion. Atomistic simulation is effective to study the microstructure evolutions during the deformation of nanolayered materials (Abdolrahim et al., 2014). The tensile behavior of amorphous alloy matrix composites (Zhou et al., 2013) and metallic alloys with amorphous structure (Zhou et al., 2014) have been studied by atomistic simulations. The revealed atomic mechanisms are helpful to design amorphous materials with good mechanical properties. Adibi et al. (2013) showed the transition from localized shear banding to homogenous superplastic flow in nanoglass by atomistic simulations. To the author's knowledge, atomistic investigation of A/A nanolayered composites has yet to be reported. To clarify the A/A interface effects on the plastic mechanisms and strength, the tensile deformation of A/A nanolaminates are studied by large-scale molecular dynamic simulations in this paper. The strengths, ductility and underlying dictating mechanisms of A/A nanolaminates with different layer thickness are analyzed.

The paper is organized as follows. Details of the atomistic simulations including method and models are presented in Section 2. Also, simulated typical tensile stress–strain curves and the corresponding plastic deformation patterns are discussed. In Section 3, the strength, plasticity and failure modes of the A/A nanolaminates are discussed. An analytical model considering the shear bands motion is proposed. The model predicts the critical size of layer thickness for the localized to homogenous deformation transition in A/A nanolaminates. The paper is concluded in Section 4.

2. Atomistic simulations

2.1. Method and models

To elucidate the interface effect in A/A nanolaminates, the tensile behavior of $\text{Mg}_{80}\text{Al}_{20}/\text{Mg}_{20}\text{Al}_{80}$ nanolaminates is studied by molecular dynamic simulations using Lammmps (Plimpton, 1995). The embedded atom method (EAM) potential is adopted in the simulations to describe the interatomic interactions (Mendeleev et al., 2009). Firstly, two monolithic amorphous alloys, i.e., $\text{Mg}_{80}\text{Al}_{20}$ and $\text{Mg}_{20}\text{Al}_{80}$, were formed. To obtain the amorphous structures, fcc MgAl alloys were melt at 2500 K for 100 ps, then cooled down to 1 K with an effective cooling rate of about 6 K/ps. During the process, the models were maintained to be periodic in all directions and the pressure was fixed at 0 bar. The constructed monolithic amorphous alloys were then cut to form the $\text{Mg}_{80}\text{Al}_{20}/\text{Mg}_{20}\text{Al}_{80}$ nanolaminates with equal thickness for each layer. Tensile deformation of the nanolaminates with various layer thicknesses ranging from 1 nm to 50 nm were simulated to investigate the size effects. The length and the height of the nanolaminates in the x and y directions were 50 nm and 100 nm, respectively. The thickness of the nanolaminates along the z direction was 5 nm. Periodic boundary conditions were enforced in the y and z directions while the x direction kept free. Before loading, the $\text{Mg}_{80}\text{Al}_{20}/\text{Mg}_{20}\text{Al}_{80}$ nanolaminate was relaxed at 300 K for 150 ps and cooled down to 1 K with an additional 50 ps relaxation. During the relaxation, the pressure along the y and z directions were controlled at 0 par using NPT ensemble. Fig. 1 shows the equilibrium atomic configurations of three nanolaminates with different layer thicknesses of $t = 1$ nm, 10 nm and 25 nm. The blue atoms refer to Mg while the orange atoms denote Al atoms. After equilibrium, the nanolaminate was stretched along the y direction with a strain rate of $5 \times 10^8 \text{ s}^{-1}$.

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