Computational Materials Science 141 (2018) 375–387

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Orientation dependent plasticity of metallic amorphous-crystalline interface

Ehsan Alishahi, Chuang Deng *

Department of Mechanical Engineering, University of Manitoba, 75A Chancellors Circle, Winnipeg, MB R3T 5V6, Canada

ARTICLE INFO

Article history:
Received 28 July 2017
Received in revised form 26 September 2017
Accepted 29 September 2017

Keywords:
Amorphous-crystalline interface
Molecular dynamics simulation
Dislocation nucleation
Shear localization

ABSTRACT

In this study, the influence of crystalline orientation on the plasticity of metallic amorphous-crystalline interface (ACI) has been investigated in a model system of crystalline Cu-amorphous CuZr multilayers by molecular dynamics simulations. It is found that the ACIs with various crystalline orientations all show similar structure with a gradual transition from crystalline to amorphous. As a result, the energy of ACIs shows only a weak dependence on the crystalline orientation. Additionally, the ACI shows no stress concentration or area of high energy than the rest of the materials. Those findings are in contrast to other types of planar defects such as grain boundaries or free surfaces. However, the strength and the yielding behavior vary significantly among the different amorphus-crystalline (A-C) multilayers. Specifically, it is found that the yielding mechanism, e.g., through dislocation nucleation in the crystalline Cu or through shear localization in the amorphous CuZr layer, is mainly determined by the crystalline orientation. What is more, the simulations on ACIs with polycrystalline Cu suggest that the plasticity of A-C multilayers strongly depends on the texture orientation of the columnar grains in the Cu layer, which can be used to explain some of the experimental observations on similar materials.

1. Introduction

Amorphous metallic alloys, also known as bulk metallic glasses (BMGs), have attracted significant attention among researchers since 1990s due to their outstanding properties such as high mechanical strength and corrosion resistance [1–5]. However, sudden brittle failure was one of the main drawbacks that imposed restrictions on commercialization of BMGs [6,7]. To enhance the ductility of these amorphous alloys and then, extend their applications for industrial purposes, the idea of amorphous-based composites reinforced with secondary crystalline phase was extensively followed by researchers [8–10]. Various types of metallic amorphous-crystalline (A-C) composites, e.g., A-C nanolaminates [11–13], have been synthesized and shown to exhibit a combination of both high strength and ductility, which has been mainly contributed to the interaction of plasticity between the crystalline and amorphous phases at the amorphous-crystalline interfaces (ACIs).

It is well-known that dislocations are responsible for plastic deformation in crystal metals. On the other hand, deformation mechanism in amorphous alloys is usually accommodated by local high shear areas known as shear transformation zones (STZs) [14]. These STZs can propagate and join each other to form shear bands. The interaction between these two mechanisms, i.e., dislocation and STZ activities mainly at the ACI, plays a vital role in the deformation behavior of A-C composites. As a result, the capability of ACIs in absorbing dislocations or blocking shear band propagation is the key to improve the mechanical properties of metallic A-C composites. For instance, it has been reported that homogeneous deformation [15,16] or suppression of shear banding at the ACIs of A-C multilayered structures [7,16,17] can lead to enhancement of ductility in those materials.

Some experimental studies have been carefully designed to investigate the interaction between dislocation and shear bands at ACIs. For instance, Zhang et al. [11,18] investigated the CuZr-Cu nanolaminates through micro-compression test. Their results indicated nucleation of some nanocrystalline zone in amorphous layers and then, absorption of dislocations at the interfacial region which was responsible for the improvement of plasticity. In a different study, Guo et al. [19,20] reported coincidence of dislocation and shear banding at the interface of CuZr-Cu A-C multilayers by performing nanoindentation and microstructural analysis through transmission electron microscopy (TEM). In addition to various experiment techniques, molecular dynamics (MD) simulation has also been widely used to investigate the A-C composites. Pan and

* Corresponding author.
E-mail address: Chuang.Deng@umanitoba.ca (C. Deng).

https://doi.org/10.1016/j.commatsci.2017.09.057
0927-0256/

Rupert [21] have studied the potential role of amorphous film in the absorption of dislocations by performing MD simulations on a sandwich structure with an amorphous intergranular film between crystalline layers. The main findings were that both crack nucleation and propagation was retarded, leading to higher ductility and fracture toughness. These results were in good agreement with Wang et al. [12] who showed triggering of shear bands at the interface of A-C multilayers upon dislocation absorption under tensile loading. Additionally, MD simulation of Cu-CuZr multilayer under shear deformation performed by Brandl et al. [22] revealed co-existence of dislocation activity and STZs at the ACI. Similarly, interfacial sliding that was caused by STZ plasticity accommodated by dislocation nucleation and propagation at the ACI was also studied by Chen et al. [23]. Furthermore, Cui et al. [24] studied the size effects on the failure mechanisms of Cu-$Cu_{50}Zr_{50}$ A-C composites under pure shear loading. Their results indicated a transition from pure shear banding in amorphous layer to the co-existence of dislocations STZs in the crystalline and amorphous layers respectively by changing the thickness of the crystalline layer.

In spite of the aforementioned researches on metallic ACI from both experiments [11,19,20,25–27] and MD simulations [21–24,28,29], there are still many issues to be explored due to the complex characteristics of such an inhomogeneous interfacial region as well as its sensitivity to geometry, temperature, loading states, relaxation procedure, etc. In particular, while structure-property relationship has been widely studied and well-established for common interfacial defects such as free surfaces and grain boundaries, such correlation is yet to be established for metallic ACI. It is thus the goal of this research to build a link between some of the most fundamental properties of ACI, e.g., the interfacial energy and strength, and their structure, e.g., the crystalline orientation. A model system based on crystalline Cu-amorphous CuZr multilayer was thus constructed and studied in this research based on MD simulations.

The paper is organized as follows: In Section 2, the methodology and the models used for this research were introduced. The stress and energy at ACIs were then analyzed and correlated with the structure in terms of atomic density, composition, radial distribution function, and Voronoi analysis in Section 3. Following that, the deformation behavior of both the crystalline and amorphous phases as well as the effects of crystalline orientation and loading conditions on the failure mechanisms were investigated and discussed. Finally, the conclusions of this study were made in Section 4.

2. Methodology

2.1. MD simulation model and procedure

All MD simulations in this work were performed using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [30]. Embedded Atom Method (EAM) potential developed by Mendelev et al. [31] was employed to characterize the inter-atomic interactions for both the crystalline Cu and amorphous CuZr. This potential has been carefully calibrated based on experiment data on liquid and amorphous $Cu_{64.5}Zr_{35.5}$ alloy and has been widely adopted for modeling the mechanical deformation of amorphous CuZr in the past, for example, [32–34]. The composition of amorphous CuZr layers in all models of this study was $Cu_{63}Zr_{37}$, which is similar to that used by Mendelev et al. [31]. The amorphous CuZr was created through a melting and quenching process. The desired atomic composition was first created by randomly replacing Cu atoms in a crystalline model with Zr atoms. Then, the model was heated up to 2000 K and held in this temperature for 250 ps. Following that, a three-step cooling process was applied to make sure that an amorphous structure was achieved. Firstly, the model was cooled rapidly to 1000 K at a cooling rate of 4 K/ps. After that, a slow cooling rate of 0.12 K/ps was used in the temperature range of 1000–700 K during which the glass transition occurred (near 750 K [31]). Finally, the model was cooled down to 10 K at an intermediate rate of 1.38 K/ps. The well-quenched amorphous sample was then cropped into different sizes to construct the various A-C composites in this research.

Three different configurations, as shown schematically in Fig. 1, were constructed for this study. Fig. 1(a) shows a representative A-C model. This model is relatively small (thus requiring less simulation time and processors) which was mainly used to calculate the interfacial energy (γ_{int}) and critical resolved shear stress (*CRSS*) for dislocation nucleation at the ACI. The size of the A-C models was $\sim 20 \times 2.6 \times 20$ nm in *X*, *Y* and *Z* direction respectively as defined in Fig. 1(a) although there was a slight variation along the Z direction due to different crystalline orientations. The number of atoms was in the range of 76,000–79,000 based on the orientation of the crystalline layer. The amorphous-crystalline-amorphous (A-C-A) model, shown in Fig. 1(b), is larger in all dimensions than the A-C models and was mainly used to investigate the failure mechanisms in those models with free surfaces. The number of atoms in A-C-A models was around 2,000,000. The size of the A-C-A models also varied with different crystalline orientation and was $\sim 27 \times 23 \times 50$ nm along *X*, *Y* and *Z* axis, respectively. In both A-C and A-C-A models, the single crystalline Cu layer was constructed in such a way that the *Y* axis was orientated along [1 −1 0] direction in all models and the other two orientations (*X* and *Z*) were varied systematically between [1 1 0] and [0 0 1]. Additionally, in order to capture the failure mechanisms in the presence of grain boundaries and study the effects of texturing, two A-C-A models with a columnar polycrystalline Cu layer with average grain size of 7 nm and the *X*-dimension oriented along ⟨0 0 1⟩ and ⟨1 1 1⟩ respectively were also constructed based on Voronoi tessellation method [35]. The thickness of the polycrystalline Cu layer was ~10 nm, which varied slightly between the two models due to the different periodic length along ⟨0 0 1⟩ and ⟨1 1 1⟩ directions. The cross section of the polycrystalline A-C-A model with *X* oriented along ⟨0 0 1⟩ is shown in Fig. 1(c) as a representative. In these polycrystalline models, the total number of atoms was ~1,600,000 and the size of the model was $\sim 28 \times 20 \times 40$ nm in the Cartesian coordination system.

All models were relaxed using the heating-and-quenching technique under zero pressure and the isothermal-isobaric (NPT) ensemble. Firstly, each model was heated up to 1000 K and kept at this temperature for about 1 ns. Then, the model was cooled to 10 K at the cooling rate of 0.5 K/ps. Finally, the model was relaxed at 10 K and zero pressure for 100 ps. Periodic boundary conditions were applied in the relaxation process for all models. The boundary conditions were also set as periodic in all three directions in the A-C models when measuring the interfacial energy and *CRSS*. However, free surface (shrink-wrap) condition along *X* axis was applied in tensile simulation of A-C-A models with single crystalline Cu layer. In both cases, the simulation cell in the *Y* direction was kept constant while allowing shrinkage along the *X*-direction to simulate the tensile loading in a thin film along the *Z*-direction. Additionally, both periodic and free surface boundary conditions were applied to the simulation cell along the *X*-direction during the tensile simulation of the A-C-A model with polycrystalline Cu to capture its deformation behavior under different conditions. The tensile loading was applied with a constant strain rate of 10^{-4}/ps along *Z* direction in all models. All tensile simulations were performed at 10 K by using the Noose-Hoover thermostat under canonical ensemble (NVT), during which the lateral directions will contract accordingly to maintain a