



Full length article

Interdiffusion cross crystal-amorphous interface: An atomistic simulation

Yiying Zhu^a, Guanglan Liao^{a, **}, Tielin Shi^a, Zirong Tang^a, Mo Li^{b, *}^a State Key Laboratory of Digital Manufacturing Equipment and Technology, Huazhong University of Science & Technology, Wuhan 430074, China^b School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332, United States

ARTICLE INFO

Article history:

Received 26 February 2016

Received in revised form

13 April 2016

Accepted 14 April 2016

Available online 6 May 2016

Keywords:

Interdiffusion

Amorphization

Diffusion bonding

Metallic glass

ABSTRACT

Interdiffusion cross the interface between metallic glass CuZr and crystal Al is investigated using molecular dynamics simulation. We show that the interdiffusivity is highly asymmetric in the adjacent amorphous and crystal phases and strongly concentration dependent. Anomalous interdiffusion is observed in the interdiffusion zone grown from the initial interface. The underlying mechanisms of the mass transport phenomenon in the heterogeneous media involve interplay of simultaneous structural transformation from crystal to amorphous and then to liquid phase with subtle changes in local atomic bonding and packing and the difference in the intrinsic diffusivity of the alloy elements. The complexity is a natural consequence of the heterostructure evolving toward equilibrium. The significance and application of the interdiffusion and resulting bonding for metallic glass and crystals are discussed.

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1. Introduction

Interface formed by different materials is omnipresent through natural or artificial processes. When two or more different materials are in contact, diffusion often sets in, resulting in atomic transport from one material to another, or interdiffusion, driven by the chemical potential difference across the interface [1]. Interdiffusion plays important roles in many material synthesis, properties and applications, such as coating, composite, gas or liquid permeation, and microelectronic or structural materials [2–4]. For example, multilayer structure is often used in microelectronic materials where interdiffusion is a key to achieve desired functionality [4]. In mechanical alloying, different elemental metals or alloys are mixed while under repeated plastic deformation; the final products are metastable alloys with extended solute solubility resulted from interdiffusion that have extraordinary strength or magnetic properties [5]. Interdiffusion is also the key mechanism of coating or welding in forming composites made of different materials. The quality of the bonding depends crucially on diffusion cross the interface.

In this work, we shall focus on interdiffusion in the heterostructure made of metallic glass (MG) and elemental metal for the following reasons: First, while much is known about crystal-crystal interdiffusion, amorphous-crystal interdiffusion has not been widely studied [6], except for some crystal-crystal interdiffusion couples, such as Ni/Zr [7], Co/Zr [8] and Si/Ge [9] and subsequent amorphization between the crystalline phases. Although interdiffusion between the formed amorphous interlayer and the remaining crystals is a key process in amorphization that not only limit the growth of the amorphous phase but also crystal stability, the small size and the transient nature make the investigation difficult of the detailed atomic mechanisms and quantitative characterization of interdiffusion between the transient amorphous phase and crystals. Interdiffusion in crystalline materials is dominated by either the thermodynamic driving force that is behind the formation of the equilibrium phases such as in phase diagrams, or various defects in interface and bulk. When the structurally heterogeneous phases such as MG and metal come in contact, we may expect not only more complex but also different mechanisms to emerge: Since the alloy elements in amorphous phase are quenched in by nonequilibrium process, it is not entirely clear yet how the chemical species redistribute and the structures change in interdiffusion when the metastable phase outside of thermodynamic equilibrium solubility is joint with one of the glass forming crystal phases. In addition, there are no extended structural defects such as grain boundary, dislocation and stacking fault

* Corresponding author.

** Corresponding author.

E-mail addresses: guanglan.liao@hust.edu.cn (G. Liao), mo.li@gatech.edu (M. Li).

in amorphous materials, which are known to facilitate the kinetic process in crystals. Shear band and void may contribute to interdiffusion but usually in special circumstances such as under high external stress or severe plastic deformation. How diffusion occurs across the interface and in the adjacent amorphous and crystalline phases remains open. These unique features and questions warrant an in-depth investigation of the fundamental processes and underlying mechanisms.

Second, MG is a technologically new class of solid metallic materials with many excellent properties, such as high strength, hardness, wear resistance, and corrosion-resistance as compared with crystalline materials [10]. These properties make it a special and potentially game changing material in many fields. However, MGs are in general brittle, which seriously limits the applications [11,12]. Attempts to improve the plasticity of MGs have been made via compositing [13] by introducing *in situ* and *ex situ* reinforcement [14–16]. Direct bonding with other materials is the method of choice in MG composites by introducing other phases so as to obstruct shear bands spread and improve the strength-plasticity performance, such as diffusion bonding [17], friction bonding [18], explosion bonding [19] and laser beam bonding [20], etc. Diffusion bonding, which is conducted under low temperature, has a unique advantage in avoiding crystallization [21]. Besides making composite, joining different types of materials including crystals to MGs may be necessary in certain critical applications such as aerospace, nuclear energy and microelectronics [22]. In all above cases, interdiffusion is a key step in determining the properties and performance: a good bonding formed by sufficient interdiffusion can significantly reduce fracture initiation and delamination; and in special circumstances, the interface formed with particular alloy composition and atomic structure can function independently, such as in corrosion-coating and thermal or irradiation barrier.

In this work we will focus on this type of heterogeneous materials with a particular emphasis on the atomistic process of interdiffusion in the narrow regions around and in the interface. Experiment using neutron, synchrotron, or tracers has been widely employed in crystalline materials. But due to the amorphous nature, the effectiveness of the scattering methods may be greatly reduced. In contrast, atomistic simulation can provide atomic level information of the diffusion process and related structural, thermodynamic and kinetic factors, and thus detailed understanding of the atomic mechanisms. Indeed, through this particular angle we found the diffusion in the heterostructure is highly asymmetric with the faster diffusion made by one of the glass-forming elements Cu from the metastable metallic glass into the crystalline Al. As a result, the sharp interface gradually grows into a broad interdiffusion zone, part of which is transformed from stable crystal to metastable amorphous phase first and then the amorphous solid to undercooled liquid. The Boltzmann-Matano analysis gives an anomalous high interdiffusion constant within the interface diffusion zone that is the result of glass transition caused by the interdiffusing Al left behind the diffusion front. Our further analysis also provides insights into the role played by the local atomic packing in the interdiffusion process. We show that the topological packing such as the icosahedral and non-icosahedral packing exhibit different mobility, the former is slower than the latter; and its role is complicated by the chemical effect, i.e. the presence of Al, which can effectively change the local bonding energy of icosahedra and destabilize them. This subtle change explains partly the asymmetric diffusion across the interface.

This paper is organized as follows. In the next section, we present the methods used in sample preparation and the atomistic simulation of interdiffusion. In Section 3, we give the results obtained from the simulation, in particular the interdiffusion constant obtained from the Boltzmann-Matano method from the

concentration profile, the amorphization and glass transition induced by the excessive Al concentration, and the icosahedral packing and its role in diffusion. In Section 4, the effect of stress on the interdiffusion and phase transitions mechanisms is analyzed. In Section 5, we discuss and summarize our results. We should mention that although amorphization is a key process in the observed interdiffusion, due to limited space, here we shall focus primarily on the latter; a detailed description of the former shall be given elsewhere.

2. Simulation methods and sample preparation

In this work, we use molecular dynamics (MD) simulation, specifically, the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS), to simulate diffusion and related structural change. To create a diffusion couple made of amorphous phase and pure metal, we use $\text{Cu}_{46}\text{Zr}_{54}$ binary metallic glass and Al single crystal. The interatomic interaction between the atoms are described by the embedded atom method potentials [23,24], $E_i = F_\alpha(\sum_{j \neq i} \rho_\beta(r_{ij})) + 1/2 \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij})$, where F is the embedding energy, ϕ is a pair potential interaction, and α and β are the type of the atoms labeled by i and j [25]. We should mention that CuZr MGs dictated by these potentials should be best considered as “model” system to the real ones. Nevertheless, the trend and general behaviors obtained from the simulation can serve the purpose for further exploration of the real systems and our conceptual understanding of the kinetic properties and MGs.

The choice of the Cu–Zr MG and Al as a model system is based on two considerations: (1) Al is a glass forming enhancing element – its addition to Cu–Zr binary glass forming system leads to bulk Cu–Zr–Al bulk metallic glass [26,27]. The negative heat of mixing between Al and Cu and Zr provides the driving force for mixing and forming more stable liquid. (2) For this reason, Al would be a natural choice as a wetting layer in making MG-metal laminates such as MG–Al–Cu or MG–Al–W where sufficient diffusion is needed to form strong bonding between MG and other metals.

The samples used for diffusion couple are made of the $\text{Cu}_{46}\text{Zr}_{54}$ MG sandwiched between two blocks of single crystal Al (Fig. 1). The typical dimension of the sample used in the MD simulation is $121 \text{ \AA} \times 121 \text{ \AA} \times 100 \text{ \AA}$ for $\text{Cu}_{46}\text{Zr}_{54}$ MG and $121 \text{ \AA} \times 121 \text{ \AA} \times 80 \text{ \AA}$ for Al. The model contains the total number of 220 242 atoms. A few larger systems are used to check size effects. The MGs are prepared by cooling the liquid at the cooling rate of 2 K/ps to 300 K; and the Al single crystal is also prepared at 300 K. Similar to experiment, blocks of MG and Al are brought together to form diffusion couple. In atomistic simulation, the MGs are cut into the size that is commensurate with that of Al since Al has the ordered structure and the shape/size of the crystal block can only be varied in the multiple of crystalline lattice parameter. So the block of MGs are “cut” and matched to the pre-cut Al block with the minimum “size mismatch” in the initial diffusion couple. We assemble MGs with Al by adjusting carefully their positions to avoid any severe deformation, i.e. overlapping or excessive separation at the interface with the smallest initial internal stress. Three typical orientations, (100), (110) and (111), of the Al are used; in this work we only present the results from (100) orientation; the results from others, which are not qualitatively different, will be presented elsewhere.

We use the isothermal-isobaric (NPT) ensemble MD with time step of 1 fs and the periodic boundary conditions in three directions of the sample. The initially setup diffusion couple is relaxed at 300 K to allow the atoms in the sample to reach equilibrium for 20 ps. The samples are then heated to 700 K at the heating rate of 20 K/ps. The pressure of the system during heating is set as 0 MPa

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