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Effect of amorphous phase on the plastic deformation mechanism of Mg: A molecular dynamics study

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ABSTRACT

Improving the plasticity of Mg alloys is an important frontier topic in the field of mechanics and materials. The influence of introduction of amorphous phase, grain size and temperature on the deformation mechanisms of nano-polycrystal Mg under tensile loading here is studied by molecular dynamics simulation method. The results indicate that the introduction of amorphous grain can improve the plasticity of the nano-polycrystal Mg due to cooperative movement of atoms in crystalline and amorphous phases. With the decrease of grain size, the plastic deformation of crystal phase in crystal-amorphous Mg-MgAl nanocomposites change from the nucleation of dislocations and growth of tensile twins to the grain boundaries glide and grains rotation, and the plastic deformation mode of amorphous phase change from the shear band dominated deformation to the homogeneous plastic deformation. The results also show that the amorphous grain plays a more and more important role during plastic deformation of Mg-MgAl nanocomposites as grain size decreases, and the deformation behavior of nanocomposites obviously depends on temperature. In addition, some quantified analysis about the deformation mechanism of nanocomposites is also presented.

1. Introduction

Researches of nanocrystalline metals are attracting wide attention due to their exceptional and unique mechanical properties compared to traditional metals [1–5], for example, high strength and high ductility. However, the studies on the mechanical properties and deformation mechanisms of nano-polycrystalline metals are mainly focused on face-centered cubic (fcc) metals, especially copper and its alloys [1,3,5]. Achievement about the hexagonal close-packed (hcp) metals is still relatively rare. The deformation mechanism of hcp metal is extremely different from the fcc one. Due to the finite number of slip systems [6], twinning activities play an important role in the plastic deformation of hcp metals. As a typical example of all hcp metals, Mg and its alloys are becoming more significant in recent years. Mg is the lightest of all metals constructional materials. As a result, it is regarded as the primary potential candidate which will reduce the weight of structure and components [7–11]. At present, Mg alloys have been widely used in the fields of automobile [7–9] and aerospace [10,11] products. However, the limited ductility of hcp crystals has brought challenges to the wide application of Mg alloys in industry [12]. Accordingly, it is crucial to find a method to increase the plasticity of Mg and its alloys, for the design and applications of high-performance Mg-based composite materials.

Controlling the interface structure to enhance the corresponding mechanical properties of the material, this major tactics of material science has also been applied to the design of Mg and its alloy. Amorphous alloys are also known as metallic glasses (MGs), which have been applied in many fields due to their outstanding properties [13,14], such as mechanical, physical and chemical characterizations. Different from the periodic arrangement of atoms and its long-range structural order in crystalline materials, the atomic arrangement in amorphous alloy is short-range order and long-range disorder. The plastic deformation of amorphous alloys is related with the formation of shear transformation zone (STZs), which is distinct from the slip of dislocations and the growth of twins dominated deformation in crystal materials. Once the MGs yielded, the plastic deformation started and the STZs linked quickly in a narrow shear band (SB) [15,16]. Fortunately, homogeneous superplastic flow behavior occurs when grain size of nanoglass (consisted of nanometer-sized MGs grains separated by interfaces) is reduced to the critical average size [17]. And it is well known that introducing a crystalline phase into amorphous can significantly improve amorphous' plasticity [18,19], and the crystalline-amorphous composite can exhibit a combination of both high strength and ductility. In the composite metal containing amorphous and

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crystalline phase, amorphous particles can both act as a sink and source of dislocations [20]. At the same time, the crystal phase may also impede the rapid growth of SB at the amorphous phase. Wang et al. [21] studied the deformation behavior of crystalline-amorphous nanolaminates, and indicated that the addition of CuZr amorphous phase can considerably elevate the tensile ductility of nanocrystalline Cu. Whether the introduction of amorphous phase within hcp metals can improve their mechanical properties synchronously? Recently, we [22] firstly proposed a dual-phase nanostructure model to improve the plasticity of Mg. The results showed that the plasticity of nano-polycrystal Mg can be enhanced with the introduction of amorphous phase. When amorphous phase thickness is 5.2 nm and larger, the superior tensile ductility and nearly perfect plastic flow behavior occur during plastic deformation due to cooperative interactions between crystalline and amorphous. Subsequently, Wu et al. [23] used magnetron sputtering to fabricate a high-strength Mg alloy with an amorphous/nanocrystalline dual-phase structure. This structure also showed a near-ideal strength of 3.3 GPa. And its hardness reached to 6.5 GPa, which is higher than that of most magnesium-based metallic thin films. However, the amorphous phase in the above studies is in the form of shell liked grain boundary, and the deformation mechanisms of dual-phase Mg alloys are still relatively poorly understood. If amorphous is embedded as a grain into nano-polycrystal Mg, will the plasticity of nanocomposites be better? Relative research still has not been reported. Here, we investigate the influence of the introduction of amorphous grain, grain size and temperature on the deformation mechanism of crystal-amorphous (Mg-MgAl) nanocomposites under tensile loading using our parallel MD simulation code.

The rest of the paper is organized in the following way. In Section 2, we describe the simulation model and method for MD simulation. Section 3 provides results and discussion. Finally, some concluding remarks are given in Section 4.

2. Simulation model and method

Here, the simulated samples contain four grains with the columnar structure. Compare with the practical condition, the columnar structures used in our simulation are simpler, and the larger grain size can be simulated when sample cell contains the same number of atoms. Fig. 1(a) shows the initial configuration of nano-polycrystal Mg. Hexagonal grains initially have the same crystallographic orientation in the structure, the $[11\bar{2}0]$ texture axis is defined as *Z*-axis. Each grain rotates a certain angle around Z-axis and is separated from each other by grain boundary. To avoid twinning at an angle of 86.3° in the original structure, the misorientation angles of 11.25°, 33.75°, 56.25° and 78.75° are chosen for the four grains (from grain 0 to grain 3), respectively. The selected columnar microstructure is identical to the one used by Kim et al. [24]. To investigate the deformation mechanism of Mg-MgAl nanocomposites, the sample used in our simulation consists of one amorphous grain and three crystalline grains, as shown in Fig. 1(b). Atoms are shown in different colors according to the local structural environment of atoms calculated by common neighbor analysis (CNA) [25]. In CNA method, the characteristic signature of local structural environment is computed from the topology of bonds that connect the surrounding neighbor atoms [26]. This is performed in the Open Visualization Tool (OVITO) [27]. The hcp, fcc and non-structured atoms are colored red, green and gray, respectively. In the past reports, it is mentioned as a generic model that nanocrystalline and nanoglasses materials can be produced by cold compaction of single crystalline nanoparticles and nanometer-sized glassy particles, respectively [28–30]. So the amorphous/nanocrystalline dual-phase nanocomposites are also produced by cold compaction of single crystalline nanoparticles and amorphous nanoparticles, the process is shown in Fig. 1 (c).

In present work, the interaction between Mg-Mg, Al-Al and Mg-Al atoms are described according to the embedded atom method (EAM) potential developed by Liu et al. [31]. The samples thickness in *Z*-axis is 1.92 nm, slightly smaller than thrice of the potential cutoff radius. The nominal grain size *d* (i.e., the distance between two parallel grain boundaries) ranges from 5.8 nm to 23.1 nm. The periodic boundary conditions (PBCs) are applied in all three spatial directions without free surfaces. The equations of motion are integrated by the Verlet algorithm. A constant strain 0.0005 is applied to the models in Y-axis and 0 bar pressure is kept in the X- and *Z*-axis. And a 1.0 fs time step is used in simulation process. To investigate the effect of temperature on the deformation mechanism of Mg-MgAl nanocomposites, the simulation temperature of 50 K and 300 K are performed.

3. Results and discussion

3.1. Effect of amorphous grain

We firstly investigate the effect of the introduction of amorphous grain on the deformation behavior of nano-polycrystal Mg. Fig. 2 presents the typical stress-strain curves of the nano-polycrystal Mg and the Mg-MgAl nanocomposite with grain sizes of 23.1 nm at 50 K. The stress-strain relationship can be used to describe the overall mechanical response of the sample under mechanical loading. Here, the tensile stress can be calculated from the virial theorem. The Young's modulus is equivalent to the slope in the stress-strain curve in the linear elastic regime. It can be observed from Fig. 2 that the Young's modulus of the Mg-MgAl nanocomposite and that of the nano-polycrystal Mg are almost the same. However, the peak stress of Mg-MgAl nanocomposite is lightly less than that of nano-polycrystal Mg. As shown in Fig. 2, the tensile stress increases linearly until the strain reach 2.5% and 4.1% for Mg-MgAl nanocomposite and nano-polycrystal Mg (shown the “a” and “a′” point at Fig. 2). Then the curve deviates from the straight line, representing the beginning of the plastic deformation of samples. It is observed from snapshots (a) and (a′) that basal dislocations nucleate and slip from this point at the intersection of grains for Mg-MgAl nanocomposite and nano-polycrystal Mg, respectively. It is clear that the stress firstly concentrates at the intersection of grains. It can be seen from Fig. 2 that the stress reaches the first peak point at strain of 4.4% in Mg-MgAl nanocomposite and 5.6% in nano-polycrystal Mg. The insets (b) and (b′) show that the prismatic dislocations nucleate and slip at grain boundaries. This indicates that the Mg-MgAl nanocomposite enters the plastic deformation stage more earlier than the nano-polycrystal Mg, the reason may be that the interface energy of amorphous-crystalline interface (ACI) is higher, and the stress is preferential to concentrate upon the intersection of crystals and amorphous grains. That is to say that the amorphous grain promotes the nucleation and slip of basal dislocations and prismatic dislocations within crystal grains. It can be also seen from Fig. 2 that with the increase of strain, the stress of nano-polycrystal Mg decreases slowly after the strain of 14.0% and drops suddenly when the strain reaches 19.7%. However, for the nanocomposite with amorphous grain, the stress maintains a horizontal line even the strain reaches 23.0%. In other words, although the strength of polycrystalline Mg is slightly reduced, its plasticity is obviously improved with the introduction of amorphous grain.

The insets (c′) and (d′) show that the grain boundary crack of nano-polycrystal Mg nucleates when strain lies near 14.0%. As the strain increases to 19.7%, the grain boundary crack begins to expand quickly, accompanied by a sudden drop of stress, as shown in Fig. 2. The formation of cracks during the tensile process is a main reason for the worse plasticity of the nano-polycrystal Mg sample with a large grain size. However, there is no grain boundary crack in the nanocomposites with amorphous grain, even when the strain reaches 23.0%. To further analyze the role of amorphous grain in the process of crack formation, the atomic displacement vectors of nano-polycrystal Mg and Mg-MgAl nanocomposites are calculated and their color is set as green. Fig. 3 depicts the snapshots and local atomic displacement vectors of two samples at strain of 14.0%. As shown in the local enlarged drawing of

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