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Effect of precipitate orientation on the twinning deformation in magnesium alloys

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ABSTRACT

In magnesium alloys, the precipitate orientation was observed to play an important role in the precipitation hardening effects. In this work, molecular dynamics (MD) simulations were employed to study the interaction of {10–12} extension twin boundaries (TBs) with plate-like $Mg_{17}Al_{12}$ precipitates having different orientation angles with respect to the TB at room temperature and strain rate of 1.25×10^8/s. The results show that the precipitation hardening effect on twinning is strong when the plate-like precipitate is parallel to the TB, while decreases as the precipitate deviates from the TB, and is minimized for the perpendicular precipitate. An analytical model capable of predicting the precipitate orientation effect was further developed, which is in good agreement with the MD simulations. The orientation effect was found to be controlled by the travelling distance of TB during the full interaction with precipitate.

1. Introduction

Precipitation or aging is a feasible method used commonly to treat metallic materials due to the considerable strengthening effects. Although the precipitation hardening was studied extensively in the past century [1] and many strengthening models were revealed in steels and aluminium alloys [2–4], it is still essential to explore new strengthening mechanisms since the precipitation hardening effect is very weak in magnesium (Mg) alloys. For example, 5% precipitate volume fraction is able to increase the strength by 0.3*G* in aluminium alloys (*G* is the shear modulus), whereas the strength of Mg-9Al-1Zn alloys with a precipitate volume fraction of 15% is only improved by 0.067*G*. This weak precipitation hardening effect in Mg alloys was found to be a result of various dislocation slip modes, deformation twinning, the precipitate orientations and shapes [5].

In Mg, numerous deformation modes were observed, such as dislocation slip (basal, prismatic and pyramidal dislocations) and twinning (extension and contraction twinning). The mechanical behaviour exhibits strong anisotropy and, as a result, the precipitate orientation plays an important role in the hardening effects. As aforementioned, the precipitation hardening effect in AZ alloys is much weaker than that in Al alloys, which is mainly because the plate-like precipitates cannot effectively impede basal slip [6]. Nie [7] studied the effects of precipitate orientation and predicted the prismatic/pyramidal plate-like precipitates have a strong blocking effect on basal slip. However, such prismatic precipitates were observed to be weak in blocking prismatic slip and twinning [8]. Although the blocking effect from basal precipitates is weak on basal slip, it becomes strong on twinning and prismatic slip [9]. In addition, rod-like precipitates have a reasonable blocking effect on prismatic slip and basal slip, but a negligible effect was observed on pyramidal slip and twinning deformation [10,11].

Although the precipitation hardening was studied in experiments, the precipitate orientation effect is not well understood by theoretical model. Nie [7] developed a physical model to study the precipitate shapes and orientations based on the Orowan model. Nevertheless, this model cannot be used for twinning deformation because the Orowan model was shown to underestimate substantially the precipitation hardening effects on twinning [9,12,13]. Recently, Fan et al. [14] developed a physical model to describe the precipitation hardening effects on twinning deformation, which was observed to be in good agreement with molecular dynamics simulations and experiments. However, the effect of precipitate orientation was not predicted.

2. Methodology

Aiming at the precipitate orientation effects, we firstly performed molecular dynamics (MD) simulations to study the TB interactions with plate-like precipitates having different orientations. All MD simulations

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Table 1
Properties of magnesium from the potentials and experiments.

	Liu potential	Sun potential	Kim potential	Experiments
Lattice constant a (Å)	3.206	3.184	3.209	3.196
c/a ratio	1.623	1.628	1.620	1.623
Cohesive energy E_c (eV/atom)	1.516	1.529	1.5502	1.51
Bulk modulus B (Mbar)	0.367		0.369	0.369
Stacking fault energy E_{sf} (mJ/m^2)	54		30	60

were performed using the open source code "LAMMPS" [15], and the Liu et al. embedded atom method (EAM) potential was used for MgAl alloys [16]. In fact, other two potentials are also available for Mg simulations, such as Sun et al. EAM potential [17] and Kim et al. MEAM potential [18]. Our preliminary simulations show that the Sun potential cannot predict a perfect TB structure. This is probably because in Sun potential, the lattice constant of a axis is small, while the lattice constant of c axis is large, as shown in Table 1. The Kim potential has identical predictions to the Liu potential, as seen in Table 1, but it is very expensive computationally. As a result, the latter two potentials were not used here.

Fig. 1 shows the initial configuration of the MD simulations. The simulation cell dimensions are $L_x = 48$ nm, $L_y = 41.136$ nm and $L_z = 40$ nm. About 3.4 million atoms are created in the simulation cell. Firstly, a horizontal {10–12} extension TB is introduced into the simulation cell, as shown by the crystal orientations in Fig. 1. This TB is the most common TB type observed in pure Mg and Mg alloys [19]. Periodic boundary conditions are used in the x and y directions, while free surface boundary conditions are used along the z direction so as to apply the shear stress. The plate-like precipitate is then introduced by deleting Mg atoms in the precipitate zone and filling it with $Mg_{17}Al_{12}$ atoms. The precipitate volume is L (length = 20 nm) × W (width = 15 nm) × T (thickness = 1.5 nm), as shown in Fig. 1. The $Mg_{17}Al_{12}$ precipitate has a body-centred cubic structure with 58 atoms per unit cell [20], which is typically observed in the MgAl alloys. The lattice orientation relationship between the precipitate and matrix was clearly revealed, as follows,

$$(0\,0\,0\,1)_M//(1\,1\,0)_P, \quad [-2\,1\,1\,0]_M//[1\,-1\,1]_P, \quad [0\,-1\,1\,0]_M//[-1\,1\,2]_P \tag{1}$$

The precipitate has an orientation angle of θ with respect to the TB. In order to observe the precipitate orientation effects, we vary the orientation angle in the range of (0°, 180°) by an increment of 15°. During the variation of the orientation angle, the three typical plate-like precipitates are covered, i.e. basal plate at ~135°, pyramidal plate at ~75° and prismatic plate at ~45°. It should be noted that the precipitates in Mg alloys usually have a specific orientation, such as the $Mg_{17}Al_{12}$ plate precipitate resides on the basal planes in Mg-Al alloys, and the orientation angle is not quite controllable for a specific alloy system. However, if we consider all the alloy systems together, we can see various orientations, such as prismatic plate-like precipitate in WE54 alloy and Mg-In-Ca alloys, {31–40} plate-like precipitate in Mg-Y alloys, as well as pyramidal precipitate in Mg-Sn-Zn alloy [5]. Therefore, current work is capable of predicting precipitation hardening effects in various alloy systems although here we only took $Mg_{17}Al_{12}$ precipitate as a sample.

After the introduction of TB and precipitate, an energy minimization step is performed on the entire simulation cell. Then the NPT ensemble is employed to increase the temperature to 300 K in 500 ps and relax the system again to realize a zero-pressure state. A pure shear strain ε_{yz} is imposed on the free surfaces at the shear strain rate of 1.25×10^8/s. To apply the shear strain, two rigid surface layers are created by freezing the atoms 1 nm from free surfaces. Then opposite in-plane displacements are applied on the two surface layers. The time step in LAMMPS simulations is 0.001 ps. Previous MD simulations of Mg crystals showed that the twinning deformation is insensitive to strain rates less than 10^9/s [21]. Therefore, the current strain rate would weakly influence the predicted TB-precipitate interactions. Since the shear strain is along the twinning shear direction, the TB would be moved and interact with the precipitate. In post-processing, the software OVITO [22] is used to export all the atomic figures in this work. Since current MD simulations were performed at 300 K, thermal fluctuation is observed on each atom and leads to difficulty in observing the defect structures. Here, conjugate gradient relaxation is performed for 50 steps in LAMMPS before exporting each atomic configuration [23].

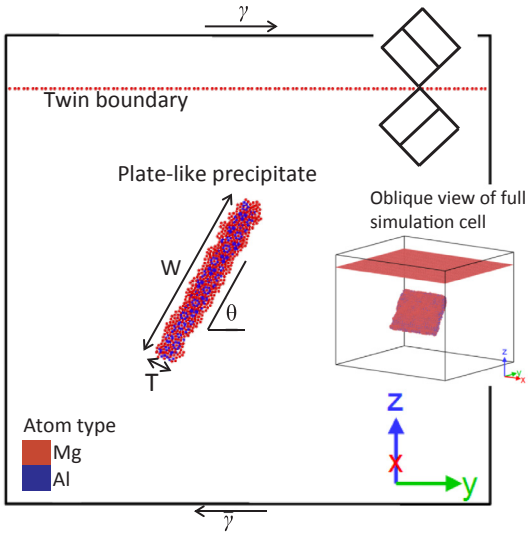

Fig. 1. MD simulation cell showing a horizontal TB and a plate-like precipitate having an angle θ with the TB. The matrix is pure Mg, and the precipitate is $Mg_{17}Al_{12}$. Periodic boundary conditions are imposed in the x and y directions, while free surface boundary conditions are used along the z direction so as to apply the shear stress.

3. Results and discussions

The shear stress-strain curves predicted by the MD simulations are shown in Fig. 2 for different precipitate orientation angles. The precipitate-free case is shown as well. In all simulations the material yields

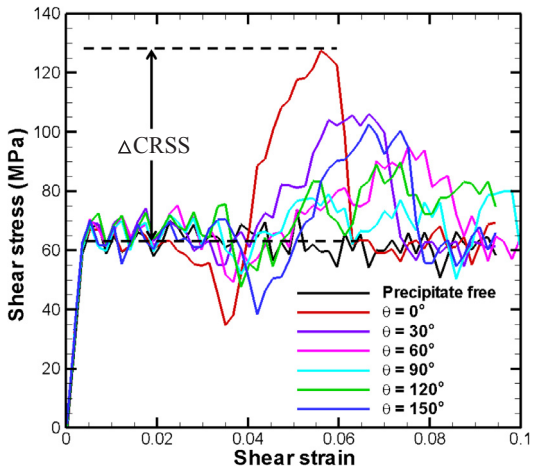

Fig. 2. Shear stress-strain curves for plate-like precipitates having different orientation angles.