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Origin of deflection of precipitates during interaction with a migrating twin boundary in magnesium alloys

F.X. Wang, B. Li*

Department of Chemical and Materials Engineering, University of Nevada, Reno, NV 89557, USA
Nevada Institute for Sustainability, University of Nevada, Reno, NV 89557, USA

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ABSTRACT

During interaction between a $Mg_{17}Al_{12}$ precipitate and a migrating $\{1\,0\,\bar{1}\,2\}$ twin boundary, a deflection on the precipitate has been reported and interpreted as a result of twinning shear. However, in the experimental reports, important features of twin boundaries that deviate from classical twinning behavior have been neglected. To better understand how such deflection is produced, in this work we performed atomistic simulations on interaction between precipitates and a moving twin boundary. Detailed analyses of lattice transformation during twinning, the evolution of the precipitate-matrix interfacial structure and the evolution of displacement of selected atoms of the precipitate were conducted. The results show that although the magnitude of twinning shear equals zero, deflection can still occur when the twin boundary is passing the precipitate. Such deflection is inversed during interaction as a result of relaxation to the precipitate caused by basal-prismatic transformation which generates a tensile strain along the *c*-axis of the parent. When the precipitate is partially engulfed by the twin, the portion in the parent and the portion in the twin experience different strain state, giving rise to the deflection which has nothing to do with the theoretical twinning shear.

1. Introduction

Magnesium (Mg) is the lightest structural metal which has a high specific strength due to its low density. Mg and its alloys have huge potential for engineering applications, for example, automotive industry to reduce the energy consumption [1–4]. Mg-Al-Zn alloys are the most common commercial materials, in particular, Mg-3Al-1Zn (AZ31) alloys have frequently been used as model alloys for fundamental research [5,6]. To increase the strength of these alloys, precipitation hardening is a main approach. Precipitates of metallic compounds produced through aging from solid solutions impede the movement of dislocations in the crystals [4,7–9]. Mg has a hexagonal close-packed (HCP) structure in which basal slip and $\{1\,0\,\bar{1}\,2\}\langle 1\,0\,\bar{1}\,1\rangle$ extension twinning are the two easy deformation modes in Mg [6,10–14]. Therefore, precipitates strengthening for Mg should consider the interactions of precipitates with both dislocations and migrating twin boundaries. However, precipitate hardening of Mg alloys is far less effective than that of Al alloys which has face center cubic (FCC) structure. This has been attributed to two possible reasons: (1) the dislocations do not effectively shear the precipitates because of the spacing is not small enough between the precipitates, thus, the strengthening effect is limited [15]; (2) The morphology of both discontinuous and continuous precipitates in Mg-Al-Zn Mg alloys are plate-like $Mg_{17}Al_{12}$ β-phase, and the primary orientation relationship with the matrix is the Burgers orientation relationship (OR), which is $(0\,0\,0\,1)_{Mg}\|(0\,1\,1)_P$, $[2\,\bar{1}\,\bar{1}\,0]_{Mg}\|[1\,\bar{1}\,1]_P$ [7,16–19]. The precipitate plates are parallel to the basal plane of the matrix, and thus less effective to block the basal slip which is the easiest deformation mode in Mg alloys [20].

Interactions between precipitates and dislocation slip have been studied through both computational simulations and experiments. Liao et al. [21,22] studied the interactions of $Mg_{17}Al_{12}$ β-phase with basal and prismatic slip in Mg using molecular dynamic (MD) simulations. They found that when a basal dislocation impinges on a precipitate, it can pass the precipitates without generating a dislocation loop or cutting into the precipitate. In contrast, a prismatic dislocation can shear through the particles. By using the Orowan looping mechanism, Robson et al. [8,9,23] calculated the hardening effect from precipitation [20]. They showed that the shape and habit plane of the precipitate have an effect on the mechanical asymmetry in Mg alloys. Rod-like precipitates along the *c*-axis are more effective impeding dislocation slip by increasing the critical resolved shear stress (CRSS) of dislocation slip, than plate-like plates that are parallel to the basal plane.

In addition to precipitate/dislocation interaction, interaction

* Corresponding author at: Department of Chemical and Materials Engineering, University of Nevada, Reno, NV 89557, USA.
E-mail address: binl@unr.edu (B. Li).

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between precipitates and TBs may play another important yet less understood role in the hardening behavior of Mg alloys and other HCP metals. In classical twinning theory, TB migration is generally mediated by twinning dislocations on the twinning plane [11,12]. The twinning dislocations generate the required simple shear which is homogeneously distributed over consecutive twinning planes, resulting in a shape change. It can be expected that precipitates will interact with migrating TBs [8,24,25]. Gharghouri et al. [25] performed transmission electron microscopy (TEM) observations on interaction between a $\{1\,0\,\bar{1}\,2\}\langle 1\,0\,\bar{1}\,1\rangle$ twin and $Mg_{17}Al_{12}$ precipitates. They found that the $Mg_{17}Al_{12}$ particles can be totally engulfed by the twin without being sheared. Experiments also observed that large precipitate can entirely arrest twin growth [25], and a precipitate can be sheared inside a twin [26,27]. Recently, Liu et al. [28] studied twin-precipitate interaction using in-situ TEM on micro-pillars. They observed that the dispersed particles (rods or basal plates) are ineffective in suppressing TB migration. Wang et al. [29] also observed similar behavior that precipitates in a Mg-5Zn alloy cannot suppress twinning during micropillar compression. Li et al. [30] simulated interaction between a $\{1\,0\,\bar{1}\,2\}$ twin and a $Mg_{17}Al_{12}$ precipitate using atomistic simulations, and showed that the particle was not sheared as the TB passed through, and twin growth was not mediated by twinning dislocations. Recently, Li and Zhang showed that the magnitude of $\{1\,0\,\bar{1}\,2\}$ twinning shear cannot be any finite value but zero by using lattice correspondence analysis [31], which is able to account for the anomalous properties of this particular twinning mode.

Fig. 1 shows an example of twin-precipitate interaction reported by Geng et al. [32]. The TB is passing the precipitate and a deflection of the precipitate can be observed. This deflection was interpreted as a result of twinning shear. In this figure, the parent basal plane was indicated by the white dashed line. Although the misorientation angle is ~86°, if we add the trace of the $\{1\,0\,\bar{1}\,2\}$ twinning plane (the yellow line) to this micrograph, immediately, two important features can be observed. First, the TB is incoherent and departs from the twinning plane. Second, although the TEM micrograph was taken right on the zone axis, the TB appears to be a rather wide band of extinction of contrast which clearly indicates the TB is not edge-on as it should be. This implies that the TB is not sharing the same zone axis with the twinning plane, which should not happen in classical twinning theory. Thus, a homogeneous simple shear, which is required in classical twinning, cannot occur on the twinning plane or on the TB. Then a question arises: what causes the deflection of the precipitate?

To answer this question, in this study, we closely examine how a plate-like $Mg_{17}Al_{12}$ precipitate interacts with a moving $\{1\,0\,\bar{1}\,2\}\langle 1\,0\,\bar{1}\,1\rangle$ TB on the atomic scale when a tensile load is applied along the *c*-axis of the parent crystal. Lattice correspondence analysis is used to analyze the lattice transformation such that the interaction mechanism can be better resolved and understood. The results provide new insight on the deformation behavior of Mg-Al-Zn alloys.

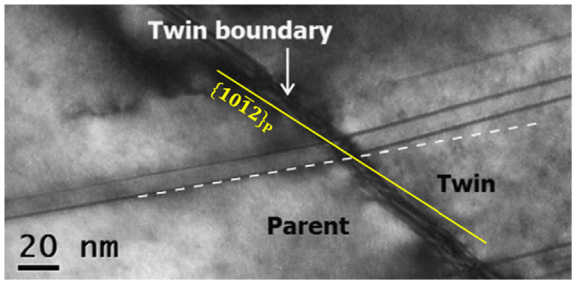

Fig. 1. The observed deflection of a precipitate when a twin boundary (TB) is passing (with permission of Elsevier) [32]. Notably the TB departs from the twinning plane (the solid yellow line) and not edge-on although the misorientation angle was ~86° and the TEM image was taken right on the zone axis. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

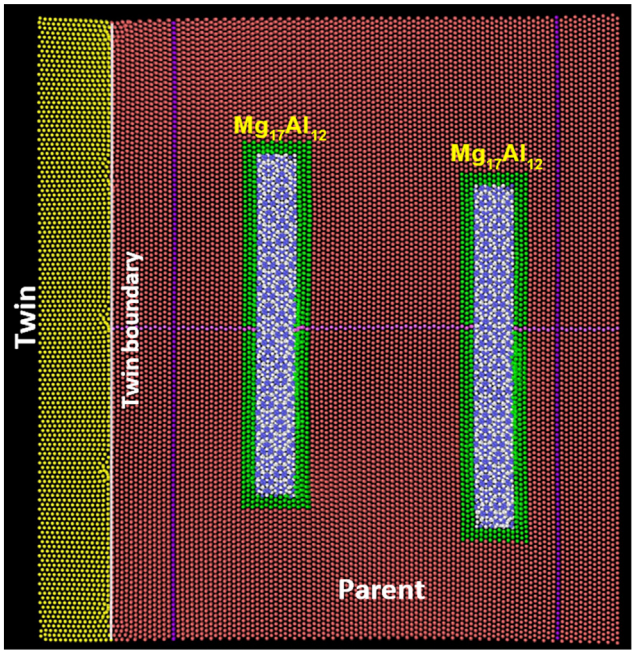

Fig. 2. The relaxed configuration of the atomistic simulations. Two plate-like $Mg_{17}Al_{12}$ precipitates (Mg in white; Al in blue) were embedded inside the Mg parent (in red). A $\{1\,0\,\bar{1}\,2\}$ twin shown in yellow. In the parent, a prismatic plane (in pink) and two basal planes (in purple) were pre-selected for structural analysis. Three layers of Mg atoms of the parent at the $Mg/Mg_{17}Al_{12}$ interface were colored in green. The color patterns were retained throughout the simulations such that structural evolution can be better analyzed. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

2. Simulation method

The atomistic simulation was performed by using XMD molecular dynamics simulation package. Embedded atom method (EAM) [33] interatomic potentials developed by Liu et al. [34,35] was used for the simulations. The visualization tool Ovito [36] was used for analyzing the simulation data.

The initial simulation system was constructed as shown in Fig. 2. The dimension of the system is 25 × 32 × 35 nm which comprises a total number of 1,237,500 atoms. A pre-existing TB was constructed. The atoms of the $\{1\,0\,\bar{1}\,2\}$ twin are colored in yellow, and those atoms of the parent are colored in red. The TB is a basal/prismatic interface that has been observed extensively in TEM and simulations [31,37]. In low magnification TEM observations [32], TBs tend to be close to the twinning plane due to their lower TB energies. But in high resolution TEM (HRTEM) observations [31], TBs are still composed of nanoscale basal/prismatic interfaces. Two plate-like β-phase precipitates were placed in the Mg matrix. Each precipitate has a thickness ~2.0 nm with an aspect ratio ~10. The plate plane of the precipitates is parallel to the basal plane of the parent. The left precipitate is located about 8 nm away from the TB. The distance between the bottom surface of the left precipitate and that of the matrix is about 8 nm. For the right precipitate, it resides about 20 nm away from the TB, and the distance between the bottom surface of the right precipitate and that of the matrix is about 6 nm. The orientation relationship between the precipitates and the matrix satisfies the Burgers OR. We color three layers of matrix Mg atoms which are at immediate vicinity to the precipitates. The structure of these interfacial layers will be analyzed in great detail such that a high clarity can be achieved.

Additionally, in the Mg parent, atoms on a double-layered or