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Effect of twin boundary on crack propagation behavior in magnesium binary alloys; Experimental and calculation studies

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ABSTRACT

The impact of alloying elements on crack propagation and atomistic phenomenon at {10$\bar{1}$2}-type twin boundaries in magnesium was investigated via both experiments and calculations. The alloying elements clearly affected the crack propagation behavior. Cracks were difficult to propagate along matrix-deformation twinning interfaces in alloys that had high fracture toughness. In such magnesium alloys, the solute atoms, e.g., silver, manganese and zinc atoms, create adhesive interactions between magnesium atoms. Closed-shell and covalent-like bonding of these types of solute atoms would influence strong adhesion, which impedes the nucleation of a new surface at the twin boundary.

Deformation twinning is known to be a required deformation mechanism for magnesium and its alloys at room and low temperature ranges, because of compensation for a lack of slip systems. In particular, the {10$\bar{1}$2}-type of deformation twinning, which forms at the beginning of plastic deformation, leads to crystal orientation along the <c>-axis direction; however, the interface between the matrix and its twin boundaries has been demonstrated to easily become the crack propagation site, when using a pre-crack induced sample in fracture toughness tests [1,2]. Hence, the fracture toughness of conventional magnesium alloys is lower as compared to that of well-known competing light metallic material, i.e., aluminum alloys. This low fracture toughness is a serious issue for the use of magnesium alloys as structural parts, due to their unsatisfactory safety and reliability.

It has been accepted that control of deformation twinning morphologies and deformation twinning characteristics is an important strategy for improving fracture toughness. In the former case, grain refinement is recognized as playing an effective role in decreasing the formation of deformation twinning [3]. This is due to the high activation of grain boundary (GB) induced plasticity, e.g., the operation of non-basal dislocation slips [4] and GB sliding [5], that prevents the formation of deformation twinning. As a result, the fracture toughness of fine-grained magnesium alloys is reported to be comparable to that of aluminum alloys [6]. The latter case is a practical use of matrix-twinning interface control via heat treatment or the addition of alloying elements [7,8]. The interface becomes coherent by short-time annealing, and changes into an ordered accumulation of an individual solid solution by the specific alloying element addition [7]. The fracture toughness of twin-induced and subsequent annealed binary alloys is also influenced by the alloying element [9,10]. This results from differences in the segregation energy of {10$\bar{1}$2}-type twin boundaries [9]. The segregation energy of the twin boundary in each alloy has been obtained from the first-principles calculation method [11]. The addition of an alloying element, e.g., silver or manganese, plays a role in the stabilization of twin boundary energy; thus they lead to increase in the fracture toughness. However, to the best of our knowledge, a systematic relation between the role of twin boundaries and the fracture behavior for various binary alloys has not yet been reported. Therefore, in this study, we investigated the impact of the alloying element on i) the crack propagation behavior and ii) the atomistic phenomenon at the twin boundary using both experiments and calculation methods.

Three kinds of twin-induced Mg-0.3 at.%X (X = Ag, Li and Pb) binary alloys, which had an average grain size of ~20 μm and a {10$\bar{1}$2}-type twin boundary fraction of ~20%, were used in this study. Details of the material procedures for the Mg-Ag and Mg-Pb alloys were reported in our previous study [9]. As for the Mg-Li alloy, it was also produced by casting, and then was extruded at a temperature of 373 K into a plate

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Table 1
Materials process conditions and microstructural information for each twin-induced alloy.

	T_{ext}, K	T_{ann}, K	t_{ann}, ks	d, μm	f, %	θ, deg
Mg-Ag	488	523	1.8	21.1	0.22	62.6
Mg-Li	373	523	0.5	21.5	0.20	57.9
Mg-Pb	448	473	1.8	20.0	0.18	61.3

Where T_{ext} is the extrusion temperature, T_{ann} is the annealing temperature for grain coarsening, t_{ann} is the annealing time for grain coarsening, d is the average grain size, f is the fraction of $\{10\bar{1}2\}$-type twin boundary and θ is the average misorientation angle.

shape. This extruded alloy was annealed at 523 K for 0.5 h to control the average grain size, and then was compressed at room temperature to induce $\{10\bar{1}2\}$-type deformation twinning into the matrix. After inducing deformation twinning, this alloy was annealed at 423 K for 2.5 h to stabilize the solute element at twin boundaries (to produce twin boundary segregation). The detailed initial microstructures of all alloys are summarized in Table 1. Using these twin-induced alloys, a three-point bending test was carried out to investigate the crack propagation behavior. The three-point bending specimen had dimensions of $5 \times 10 \times 50$ mm, and the V-notch was perpendicular to the extruded direction. A pre-crack with a length of ~1 mm was inserted by a fatigue test. Then, the specimens were polished and etched with acetic-based solutions to observe the microstructure before the bending state using an election backscatter diffraction (EBSD). After the three-point bending test, a deformed microstructure near the crack-tip region was observed via a laser microscopy and a scanning electron microscopy (SEM). The fracture toughness of the twin-induced Mg-Li alloy was also evaluated using the three-point bending specimen mentioned above. The conditions and method for obtaining the fracture toughness were the same as those in our previous study [9].

The microstructural evolutions near the crack-tip are shown in Fig. 1 for (a), (b) Mg-Li and (c), (d) Mg-Ag alloys. Figs. 1(a) and (c) are the image quality maps including boundary analysis before a three-point bending test observed by EBSD. These figures show the lenticular morphology into the matrix, which is recognized as $\{10\bar{1}2\}$-type deformation twinning. Although the results of the misorientation angle and texture obtained from EBSD analysis are not shown here, these alloys have similar average misorientation angles, as listed in Table 1, and have twin-induced texture, as reported in [9,12], irrespective of the alloying element. Figs. 1(b) and (d) are the deformed microstructures, which are in the same region as shown in Figs. 1(a) and (c) before the bending test, observed by laser microscopy or SEM. Strains exist near the crack-tip and crack-propagated regions; however, several sites, i.e., the grain interior, GBs and the matrix-twinning interface, are confirmed as paths of crack propagation. Each white arrow in Fig. 1 corresponds to a crack-propagated site. As compared with Figs. 1(b) and (d), these alloys exhibit different crack propagation behavior.

The fraction of the crack-propagated site in several twin-induced binary alloys is shown in Fig. 2(a). This figure includes the results of crack propagation behavior in twin-induced Mg-Mn and Mg-Al alloys, which had similar initial microstructures, i.e., grain size, texture, misorientation angle and twin boundary fraction. The initial and deformed microstructures of these two types of twin-induced alloys were reported in our previous study [9]. As expected, while the matrix-twinning interface is found to become the crack propagation site in all of the twin-induced alloys, the fraction of the crack propagation site varies with the alloying element. In the Mg-Pb alloy, the matrix-twinning interface has the largest fraction among them; on the contrary, the crack-propagated fraction of the matrix-twinning interface in the Mg-Ag alloy is reduced, which is interestingly noted to be smaller than that of the grain interior. The relationship between the fracture toughness (in Table 2) and the matrix-twinning interface fraction recognized as the crack propagation site is shown in Fig. 2(b). This figure reveals that crack propagation behavior is closely related to fracture toughness. When twin-induced magnesium alloys have high fracture toughness, the matrix-twinning interface has difficulty become the crack propagation site.

The effects of alloying elements on bonding against magnesium [13–15], vacancies [16–18], stacking faults [19–30] or dislocations [15,31,32] of magnesium alloys have been well investigated through several calculation methods. Although quite a few of reports have considered grain/twin boundaries, these studies have been examined only the specific alloying elements, i.e., rare-earth and zinc atoms [7,33]. Thus, focusing on the atomistic phenomenon at the $\{10\bar{1}2\}$-type twin boundary in various magnesium alloys, first-principles calculation was systematically performed to clarify the influence of the alloying elements. The unit cell for a $\{10\bar{1}2\}$-type twin boundary model was firstly prepared as shown in Fig. 3(a). Rectangular models, containing 248 atoms with $2 \times 2 \times 1$ aligned along the $<1\bar{2}10>$, $<\bar{1}011>$ and $<10\bar{1}2>$ directions of the unit cell, were used for the twin boundary segregation. Two magnesium atoms existing at the twin boundary were replaced by solute atoms (Ag, Al, Ca, Li, Mn, Pb and Zn, which are well known to be solute atoms into magnesium) to investigate the impact of the alloying element. Density functional theory (DFT) calculations were carried out

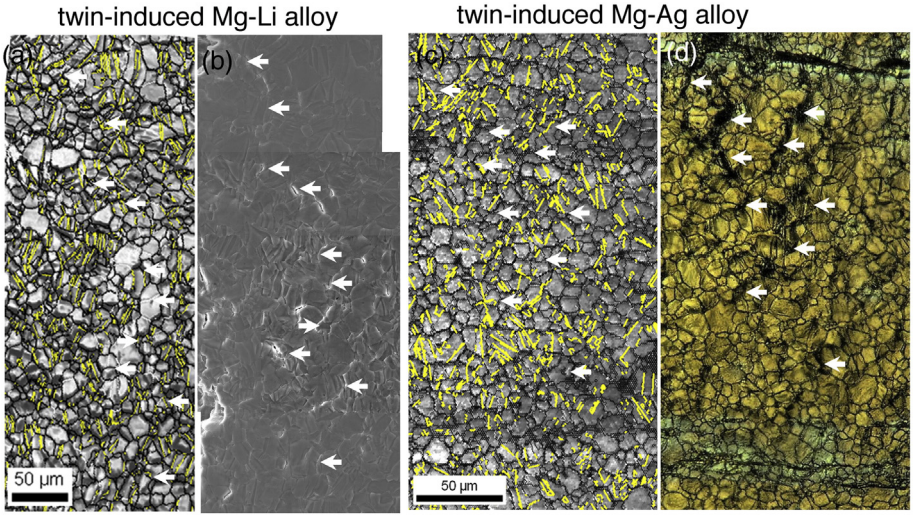

Fig. 1. The microstructural evolution near the crack tip region; (a), (c) initial microstructures observed by EBSD and (b), (d) deformed microstructures observed by SEM or laser microscopy. The black, white and yellow lines in image quality maps indicate high-angle ($\theta \geq 15°$), low-angle grain boundaries ($15° > \theta \geq 4°$) and $\{10\bar{1}2\}$-type twin boundaries, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)