Journal of Alloys and Compounds 692 (2017) 274–279

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: http://www.elsevier.com/locate/jalcom

Characteristics of cross grain boundary contraction twin pairs and bands in a deformed Mg alloy

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ARTICLE INFO

Article history:
Received 28 June 2016
Received in revised form
2 September 2016
Accepted 3 September 2016
Available online 6 September 2016

Keywords:
Mg alloys
Twinning
Plastic deformation
Grain boundaries

ABSTRACT

With the help of trace analysis, cross-grain boundary (cross-GB) contraction twin (CTW) pairs and bands can be identified more easily in a deformed Mg alloy. Cross-GB CTW pairs can form in two neighboring grains with misorientations from 5° to 60°. Schmid factor (SF) analysis reveals that the majority of them are high SF twin variants, indicating that the applied macro stress plays the most important role in their nucleation. Twinning shear compatibility over GB has been explicitly evaluated by a geometrical compatibility parameter (m′). It is found that nearly half of the cross-GB contraction twin pairs have high m′ values greater than 0.7, indicating that their formation is mainly due to twinning shear transmission over GBs. However, dramatically different from cross-GB extension twin pairs and bands reported before, the rest of the cross-GB contraction twin pairs have low m′ values smaller than 0.4. Their formation is due to the dominance of the applied macro stress near GBs.

1. Introduction

Twinning is an important deformation mechanism for Mg alloys with hexagonal close-packed (hcp) structure. During high strain-rate deformation, enhanced deformation twinning and dynamic recrystallization result in ultra-fine grained microstructure and enhanced ductility [1]. An applied contraction stress along the c-axis of a grain is possible to activate contraction twinning, of which {10-11}⟨10-1-2⟩ contraction twinning is widely observed [2–6]. Continued increase of the stress can activate secondary {10-12}⟨-1011⟩ extension twinning in the primary {10-11}⟨10-1-2⟩ contraction twins (CTWs), resulting in {10-11}-{10-12} double twins (DTWs) [7–9]. Due to reorientation of crystal caused by twinning, dislocation slipping will be greatly intensified in the DTW region, which results in early shear localization and trans-granular void and crack initiation [8,10].

Atomistic simulations and electron back-scattering diffraction (EBSD) analyses reveal that twin nucleation preferentially occurs at grain boundaries (GBs) [11,12]. The stress induced by a twin in one grain may influence the nucleation of another twin in its neighboring grain, resulting in the formation of a cross-GB twin pair [13–15]. Chain-reacting of this will form cross-GB twin bands consisting of several connected cross-GB twin pairs [14]. A geometric compatibility parameter of twinning shears (i.e., m′-factor) is found to be quite useful for analyzing cross-GB {10-12}⟨-1011⟩ extension twin (ETW) pairs. The m′-factor is defined as $m' = \cos\alpha \cdot \cos\beta$, where, for a pair of cross-GB twins, α is the angle between the two twinning plane normals while β is the angle between the two twinning shear directions [14,16–18]. When $m' = 1$, complete twinning shear compatibility is achieved over the GB. When $m' = 0$, the twinning shears are independent. When $m' = -1$, the twinning shears exactly oppose each other. For cross-GB extension twin pairs, it is found that the majority displays an m′ value grater than 0.7, especially for those of twins with high Schmid factors (SFs) [14,16]. For extruded Mg alloys with basal fiber texture, it is also found that more than half of cross-GB extension twin pairs have the first m′ rank and an m′ value grater than 0.6 [18]. However, such a rule completely fails when one of the twins in a cross-GB extension twin pair has a low SF. In such a case, statistical EBSD analysis reveals that less than 5% of them display m′ values grater than 0.7 [17]. This indicates that twinning shear transmission is blocked by the GBs, while strain accommodation plays the most important role in nucleation of low SF extension twins [17]. In-situ EBSD observations also confirm the role of local strain compatibility in twin variant selection of cross-GB ETWs [19].

Another criterion for cross-GB extension twin pairs is

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http://dx.doi.org/10.1016/j.jallcom.2016.09.024
0925-8388/

misorientation angle $\Delta\theta$, which is defined as $\Delta\theta = \theta_G - \theta_{Twin}$, where, for a pair of cross-GB twins, θ_G is the minimum misorientation angle between their host grains while θ_{Twin} is that between the twins [20]. Statistical EBSD analysis reveals that the majority of cross-GB extension twin pairs displays a $\Delta\theta$ value close to 0° [20]. Again, this rule cannot be applied to a cross-GB extension twin pair containing a low SF extension twin, which is also due to the dominance of strain accommodation for twin nucleation [17].

Probably due to difficulties encountered for the detection of thin lath-like contraction twins by EBSD [8,21,22], the characteristics of cross-GB contraction twin pairs have not been well investigated before, which will be done in this paper.

2. Material and methods

The material used was hot-rolled commercial AZ31 Mg alloy (Mg–3Al–1Zn in mass%) sheet with 2 cm in thickness. The rolling, transverse and normal directions of the sheet were designated as RD, TD and ND, respectively. Before compression tests, the sheet was annealed at 400 °C for 2 h and then cubes of 1 cm in length were cut from it for compression along ND, at room temperature with a strain rate of $1x10^{-3}$ s^{-1}. The tests were interrupted at engineering strains of 4%, 6% and 8%. The present analysis focused on the compressed samples with 6% engineering strain. The deformed samples were sectioned for EBSD microstructure analysis on the sectioned faces within the bulk. The faces for observation were ground using SiC papers with grits from 2000 to 5000, and then electrolytically polished in an electrolyte of 62.5% phosphoric acid and 37.5% ethanol at 1.5 V for 1 min, at −15 °C. The EBSD measurements were performed using a Zeiss Auriga field emission scanning electron microscope. The step size was set to be 0.1 μm in order to detect narrow contraction twins. The measured data were analyzed using the MATLAB™ toolbox MTEX (version 4.1.beta4) [23].

With the measured Euler angles of a contraction twin and its host grain, the twinning system corresponding to the twin can be identified according to Table 1. Then the angles α and β for calculating m′-factor can be calculated using the measured Euler angles of two neighboring grains and the identified twinning systems of two contraction twins in them respectively. When only Euler angles of a host grain are measured, the twinning system corresponding to a contraction twin can still be identified with the help of trace analysis. The ideal twinning plane traces of the six possible contraction twin variants in a grain (Table 1) on the EBSD measured surface can be determined by {10-11} pole figure of the grain. If the practical twinning plane trace of an observed twin is close to one of the ideal twinning plane traces, the twinning system corresponding to the twin can be identified, as demonstrated in Fig. 1c.

3. Results and discussion

A representative EBSD measured microstructure of a sample before compression is presented in Fig. 1a, in which the same area with inverse pole figure (IPF) color code and band contrast (BC) grey scale is shown on the left and on the right, respectively. The IPF color code is based on the indexed Kikuchi patterns. However, band contrast grey scale is based on the contrast of the Kikuchi bands, which is collected whether or not the Kikuchi pattern is indexed. Low band contrast corresponds to dark regions with a poor degree of lattice perfection, such as grain boundaries, twin boundaries, particles and regions of higher dislocation density [22]. Therefore, BC map is quite useful when the Kikuchi pattern indexing is low. In Fig. 1a, GBs with misorientations larger than 5° are outlined in black. Twins are not detected in the sample. The inserted pole figures indicates that most of the grains' c-axes are around ND, which is typical for hot-rolled AZ31 Mg alloy [17,24,25]. Therefore, the compression loading along ND favors the formation of contraction twins.

Fig. 1b shows the EBSD measured microstructure of a sample after 6% compression along ND, of which IPF and BC maps are put on the left and on the right, respectively. Boundaries with misorientations larger than 5° are outlined in black, including grain boundaries and twin boundaries. Thin lath-like regions in the IPF map correspond to contraction twins or double twins, which lie on the dark regions within the grains in the BC map. By comparison, it can be seen that only fractions of the twins are indexed. Such a problem of low indexing within narrow twinned regions has also been encountered in other studies [8,21,22]. However, trace analysis applied to the BC map can recognize the missing twins in the IPF map. An example is given in Fig. 1c, in which trace analysis is applied to twins within the Region 1 in Fig. 1b. For calculation, all the possible contraction twin variants (CVs) and extension twin variants (EVs) are defined in Table 1. There exist 36 possible double twin variants in a grain. They can be expressed explicitly by CVi-EVj (i, j = 1–6), in which CVi and EVj refer to the primary contraction twin variant and the secondary extension twin variant, respectively. The measured Euler angles of a twin and its host grain in Fig. 1c are (67°, 32°, 178°) and (157°, 17°, 210°), respectively. It can be calculated from the Euler angles that the twin corresponds to double twin variant CV6-EV6. The twinning plane trace of any contraction twin variant on the EBSD measured surface can be determined with the help of the calculated {10-11} pole figure of its host grain, which is normal to the line connecting the center of the pole figure and the pole of the contraction twin variant. Accordingly, the twinning plane trace of CV6 is drawn in Fig. 1c, which travels along the twinned region corresponding to CV6-EV6. This indicates that the secondary extension twinning does not change the twin boundary of the primary contraction twin, which agrees with other studies [26,27]. Clearly in the BC map in Fig. 1c, there also exists a not-indexed thin lath-like dark region along the twinning plane trace of CV6, which corresponds to CV6 or CV6-EV6. Trace analysis can identify contraction twin variants, though it cannot tell whether secondary twinning happens in contraction twins or not. In the present study, the advantage of trace analysis helps to determine characteristics of cross-GB contraction twin pairs and bands in the material.

Regions 2–6 in Fig. 1b, which contain cross-GB contraction twin pairs or bands, are analyzed in Fig. 2a–e, respectively. In Fig. 2a, the partly indexed G1-CV1-EV1 refers to the double twin in grain G1 whose primary contraction twin variant is CV1 and secondary extension twin variant is EV1 (Table 1). Logically, the partly indexed G2-CV4-EV4 refers to the double twin in grain G2 whose primary contraction twin variant is CV4 and secondary extension twin variant is EV4. Trace analysis identifies a not-indexed twin G3-CV1. The BC map in Fig. 2a shows that G3-CV1, G1-CV1-EV1 and G2-CV4-EV4 form a cross-GB twin band. SF, SF rank and SF ratio are calculated in order to study twin variant selection. In any grain, there exist six possible contraction twin variants. The SFs corresponding to them can be ranked decreasingly, i.e., rank 1 corresponds to the

Table 1
Definition of twin variants and twinning systems of ETW and CTW.

CTW variant	CTW system	ETW variant	ETW system
CV1	(10-11) [10-1-2]	EV1	(10-12)[-1011]
CV2	(01-11)[01-1-2]	EV2	(01-12)[0-111]
CV3	(-1101)[-110-2]	EV3	(-1102)[1-101]
CV4	(-1011)[-101-2]	EV4	(-1012)[10-11]
CV5	(0-111)[0-11-2]	EV5	(0-112)[01-11]
CV6	(1-101)[1-10-2]	EV6	(1-102)[-1101]