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# Variant selection of twins with low Schmid factors in cross grain boundary twin pairs in a magnesium alloy

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**Abstract.** Samples of magnesium AZ31 alloys are deformed in compression at room temperature under a strain rate of  $1 \times 10^{-3} \text{ s}^{-1}$ . The initial texture with respect to the loading direction is favorable for  $\{10\text{--}12\}\langle -1011 \rangle$  extension twinning during the deformation. At an engineering strain of 2.75%, many extension twins are found to be connected with each other at grain boundaries, forming cross grain boundary twin pairs. Some have low positive or even negative Schmid factors (SFs). The variant selection of them are interpreted in terms of shear accommodations. The observed twin variants require the least or no accommodation through deformation modes with high CRSSs, but the most or more accommodation through those with low CRSSs.

## 1. Introduction

Mg and its alloys have drawn much attention in recent years mainly because of their low densities, which renders them high specific yield strength critical for aviation and great potentiality of fuel saving and CO<sub>2</sub> emission reduction for car industry. Extended civil application of Mg alloy as light-weighted structure material depends on achieving ductility, simpler manufacturing and high processing qualities [1]. Twinning is an important deformation mode of wrought Mg alloys at low temperatures [2, 3], the study of which is necessary to predict their mechanical responses, and thereby benefits computational alloy design. When formed abundantly,  $\{10\text{--}12\}\langle -1011 \rangle$  extension twins (ETWs) contribute to significant strain softening [2, 4]. After they introduce sufficient interfaces, they lead to strain hardening due to impediment of continuous dislocation slip by the additional interfaces [4, 5].

ETWs are easy to form "cross grain boundary" twin pairs [6, 7]. A statistical study reveals that the minimum misorientation angle between two twins in a cross grain boundary pair is nearly equal to that between their host grains [6], which is an empirical rule. A geometrical factor ( $m$ ) is widely used to evaluate the shear compatibility between two twins in a cross grain boundary pair. This  $m$ -factor is described by  $m = \cos\alpha \cdot \cos\beta$ , where  $\alpha$  and  $\beta$  are the angles between the twinning planes and the shear directions, respectively [7, 8]. Previous studies find that the majority ETWs in cross grain boundary twin pairs have  $m$  factors close to 1, indicating high shear compatibilities [7, 8]. This paper studies on ETWs with low Schmid factors (SFs) in cross grain boundary pairs, which cannot be interpreted neither by  $m$ -factor nor by the empirical rule of misorientation angles.

## 2. Experimental procedure

The material is a hot rolled sheet of commercial Mg AZ31 alloy (Mg-3Al-1Zn, wt.%). Its rolling, transverse and normal directions are designated as RD, TD and ND, respectively. Uni-axial compressions along RD were performed on cubic specimens from the sheet, at room temperature and a strain rate of  $1 \times 10^{-3}/\text{s}$ . The microstructures of the specimens were measured by electron backscatter diffraction (EBSD). EBSD samples were grinded using SiC papers with grits from 2400 to 4000, and then electrolytically polished in an electrolyte of 62.5% phosphoric acid and 37.5% ethanol at 3 V for 30 s followed by at 1.5 V for 2 min, both



at  $-15\text{ }^{\circ}\text{C}$ . The instrument used was JEOL 6500F FEG SEM with Channel 5 analysis system (Oxford HKL).

### 3. Results and discussion

The rolled sheet exhibits a typical fiber texture with grains' c-axes around ND. The as-received material has been heat-treated without twins. After the compression along RD, ETWs are abundantly intruded, as shown in Fig 1. The (macro) SF of an ETW can be calculated, which is the external stress resolved along the shear direction on the twinning plane. The ETWs are then classified into two groups, i.e., low and high SF twins. Here, a low SF twin is defined by two criteria. One is that its  $\text{SF} \leq 0.3$ , the other is its SF ratio  $\leq 0.6$  when its  $\text{SF} > 0$ . The SF ratio (designated as  $\text{SF}_{\text{ratio}}$ ) is the ratio of the SF of a twin to the possible highest SF of the twins in a particular grain.  $\text{SF}_{\text{ratio}}$  is only applied to a twin with  $\text{SF} > 0$ , because a negative SF renders the appearance of a twin abnormal but a positive low SF may be the possible highest one in a particular grain so that its associated twin should be activated preferentially. The above criteria select a twin with not only a SF absolutely low, but also a SF relatively lower in a particular grain. Oppositely, a high SF twin can be defined. It is intuitive that high SF ETWs are easy to be activated, which indeed constitute the observed majority.

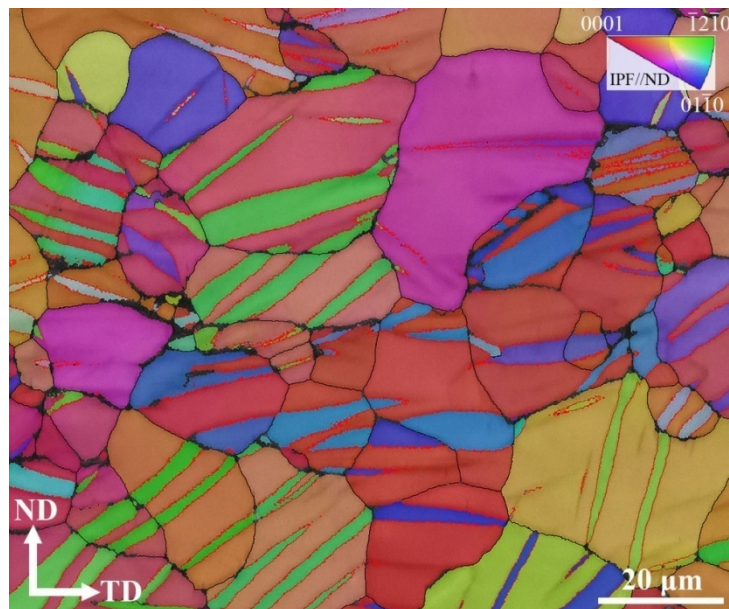


Fig. 1. An EBSD microstructure showing ETWs in the compressed sample with inverse pole figure (IPF) coloring component and band contrast (BC) component. Boundaries between the ETWs and matrices are outlined in red. Other boundaries with misorientation angles larger than  $5^{\circ}$  are outlined in black.

However, low SF twins are also detected. Fig. 2a shows a cross grain boundary pair of twins consisting of Twin 1 in Grain 1 and Twin 2 in Grain 2. Fig. 2b and 2c provide  $\{0001\}$  pole figures of the grains and the twins in Fig. 2a. From these figures, it is seen that Twin 1 has a negative SF of  $-0.08$ , while Twin 2 has a positive SF of  $0.22$  and the highest  $\text{SF}_{\text{ratio}}$  of 1. Therefore, the cross grain boundary twin pair contains low SF Twin 1 and high SF Twin 2. The m-factor mentioned in the introduction section is first applied to the twins in order to evaluate their shear compatibility. It can be calculated that their m-factor is  $0.32$ , indicating a low shear compatibility between the twinning systems of Twin 1 and Twin 2. The minimum misorientation angle between Grain 1 and Grain 2, and that between Twin 1 and Twin 2 are calculated to be  $26.2^{\circ}$  and  $35.4^{\circ}$ , respectively. The difference between them is  $9.2^{\circ}$  so that the empirical rule of misorientation angles mentioned above cannot be applied to this case. Next, we further explore the rule of variant selection governing low SF Twin 1.

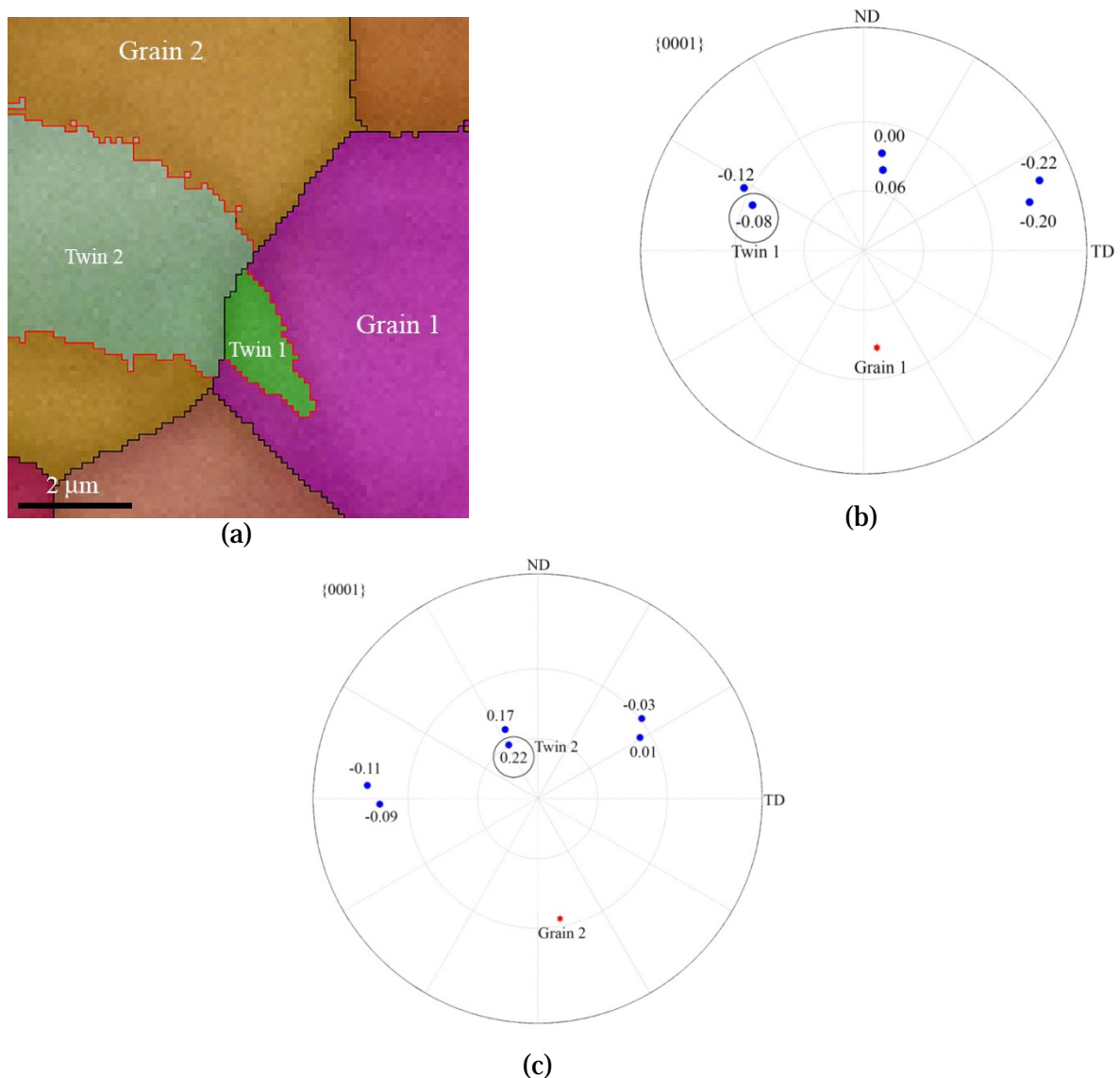


Fig. 2. (a) An EBSD microstructure showing a cross grain boundary twin pair, Twin 1 and Twin 2, with IPF coloring and BC components as contained in Fig. 1. (b) {0001} pole figure of Grain 1 and its 6 possible ETW variants with their associated SFs. (c) {0001} pole figure of Grain 2 and its 6 possible ETW variants with their associated SFs.

Since twinning produces shear deformation, the growth of a twin requires shear accommodations in its neighboring crystals, which could happen in its host grain, neighboring grain or twin. The accommodation abilities of the shear induced by one twin through different deformation modes in another twin can be evaluated by a method developed in reference [9]. For Mg alloys, 5 common deformation modes for accommodation are chosen to be studied, which are basal, prismatic and  $\langle c+a \rangle$  pyramidal slips as well as  $\{10\text{-}12\}\langle\text{-}1011\rangle$  and  $\{10\text{-}11\}\langle 10\text{-}1\text{-}2 \rangle$  twinings. The shear magnitude of Twin 1 along the shear direction on the twinning plane is 0.129 when the  $c/a$  ratio is 1.624 [3]. It can be resolved along the slip direction on the slip plane of a slip mode or along the shear direction on the twinning plane of a twinning mode in Twin 2, with the method provided in reference [9]. The resulted shear in Twin 2 is thus called as a geometric accommodation shear for Twin 1. There exists several variants of a deformation mode, e.g. basal slip mode has 3 variants, and thereby several corresponding geometric accommodation shears. The largest one of a deformation mode "i", designated as  $e^{i\max}$ , sheds light on twin variant selection.

Table 1. The  $e^{i\max}$  values associated with the 6 possible twin variants in Grain 1, where  $i$  = BS (basal slip), PR (prismatic slip), PY (<c+a> pyramidal slip), ETW ( $\{10\text{-}12\}\langle\text{-}1011\rangle$  twinning) or CTW ( $\{10\text{-}11\}\langle\text{-}10\text{-}1\text{-}2\rangle$  twinning). The observed Twin 1 is variant 3.

ETW variant in Grain 1	SF	BS	PR	PY	ETW	CTW
1	-0.20	0.0242	0.0685	0.0815	0.0280	0.0968
2	0.06	0.0278	0.0426	0.1145	0.0091	0.1226
<b>3</b>	<b>-0.08</b>	<b>0.0049</b>	<b>0.1138</b>	<b>0.0533</b>	<b>0.0367</b>	<b>0.0473</b>
4	-0.22	0.0823	0.0871	0.0672	0.0290	0.0682
5	0.00	0.0918	0.0434	0.0859	0.0095	0.0915
6	-0.12	0.0431	0.1064	0.0379	0.0352	0.0292

Table 1 lists the  $e^{i\max}$  values associated with the 6 possible ETW variants in Grain 1. Comparing the  $e^{i\max}$  values in each column of the table, one can find that variant 3 has the highest  $e^{\text{PR}\max}$  and  $e^{\text{ETW}\max}$  values, but the second lowest  $e^{\text{PY}\max}$  and  $e^{\text{CTW}\max}$  values, in the 6 ETW variants in Grain 1. In AZ31 Mg alloy, the critical resolved shear stresses (CRSSs) of the 5 deformation modes can be ordered increasingly as BS < ETW < PR < RY & CTW [10]. Therefore, variant 3 requires the most shear accommodations through prismatic slip and extension twinning with low CRSSs, but less those through pyramidal slip and contraction twinning with high CRSSs. This indicates that Twin 2 is readier to accommodate the strain induced by variant 3, which corresponds to the observed Twin 1 with negative SF. Analogous to Twin 1, statistical analysis reveals that over 70% of the low SF twins in 66 cross grain boundary twin pairs require the most or more shear accommodations through prismatic slip and/or extension twinning with low CRSSs, but the least or less through pyramidal slip and/or contraction twinning with high CRSSs. Due to the length of the paper, the statistical data is not included here.

#### 4. Conclusions

This paper focuses on the ETWs with low SFs in cross boundary twin pairs. The shear compatibility between two twins in such a twin pair is low, which is evaluated by the widely used m-factor. A newly developed method is used to calculate the shear accommodation of a deformation mode in one twin, which is generated by the shear induced by another twin. With this method, it is found that a low SF twin requires the most or more shear accommodations through prismatic slip and/or extension twinning with low CRSSs, but the least or less those through pyramidal slip and/or contraction twinning with high CRSSs, in the other twin in the twin pair.

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