Effect of initial texture on the \{10–12\} twinning variants selection mechanism in AZ31 magnesium alloy

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Abstract
The influence of the initial texture of the \{10–12\} twinning variants selection mechanism of the magnesium alloy was investigated using the compression test, the EBSD technology, the trace method, the orientation rotation method, and the Schmid’s law. Results show that various \{10–12\} twin patterns are observed in the AZ31 E90 sample subjected to compression. In the multi–twins inside a grain pattern, the high Schmid factor (SF) variant is activated first to coordinate the externally imposed strain, and the ortho–position (OP) variant with the best strain compatibility is activated. Typical case of paired twins in two neighboring grains usually have high SF, and the activation of corresponding variants follows the Schmid’s law. When E45 sample is compressed, the SF_{15}, of a pair of relative variants among the six twin variants in the crystal is very large and favorable for local strong basal texture formed by the two adjacent grains for the twin–transfer phenomenon. When E0 sample is compressed, the activation of the corresponding variants follows the Schmid’s law and is linked to the stress fluctuation at the grain boundary.

1. Introduction

The number of independent slip systems in HCP structures at room temperature is not enough. Thus, deformation twins often occur during the plastic deformation of magnesium. Studies show that the critical resolved shear stress (CRSS) of \{10–12\} tensile and \{10–11\} compression twins are 2.0–2.8 [1] and 76–153 MPa [2], respectively. The \{10–12\} twins are often active because of the small shear strain [3, 4]. In the HCP structure, each twin model has six possible variants [5, 6], and the initiation of different variants rotates the twin c-axis in different directions. Thus, the twin of magnesium alloy can promote the plastic deformation, refine the grains, adjust the texture by changing the texture of the grains [7], and improve the mechanical properties of magnesium alloys [8–11].

Researchers reveal that the variant selection in twinning nucleation usually follows the Schmid’s law [12, 13]. The twin variant with the largest SF is activated first. The Schmid’s law can explain the primary \{10–12\} twinning behavior of magnesium alloys under various deformation geometries, but many twinning activities that violate the Schmid’s law remain and are affected by the local strain coordination effect [14–16]. For example, under uniaxial deformation, the Schmid’s law of twinning behavior is treated in accordance with uniaxial stress, and all twinning activities can be well explained.

However, for the twinning behavior under slightly complicated stress, different researchers have different understandings and treatments of Schmid’s law [17–19]. Tucker [20, 21] and Dllilamorae [22] have used the equivalent SF of slipping under rolling deformation in the simulation of the rolling texture of aluminum alloy and considered that the shear stress acting on the slip system under rolling condition is synthesized by two independent forces, namely, the rolling tension along the rolling direction and the normal pressure along the plate. Luo [23] has improved the algorithm of the equivalent SF on the basis of this study and applied this SF to...
the twin deformation of magnesium alloy to explain the variant selection of the compression and the secondary twins in the warm rolling of AZ31 plate of the equivalent SFrolling. Barnett et al [24] have assumed that the rolling stress states along ND and TD are $\sigma$ and 0.5$\sigma$, respectively, and calculated the SF of twins. Molodov et al [25, 26] have used similar stress hypothesis to evaluate the activity and the variant selection of tensile twin in PSC. Xin et al [19, 27] has proposed the ‘Normalized Schmid factor’ to predict variant selection mechanisms and avoid the error in calculation of the SF.

In the present study, the equivalent SFrolling in the E45 sample is established to evaluate the effect of initial texture on variant selection. The compression of three different initial textures is designed. The compression directions are 0°, 45°, and 90° with the ED. The variant selection mechanisms for {10–12} multi-twins inside a grain, twin pair, and twin transfer crossing neighboring grains are investigated, and the microstructure after the deformation is tracked using EBSD.

2. Materials and methods

2.1. Sample preparation

The initial material selected in this study was a commercially extruded AZ31 magnesium alloy bar with a diameter of 40 mm. The cuboid compression samples (8 mm × 8 mm × 12 mm) (figure 1(b)) were cut from the directions of 0°, 45°, and 90° deflected along the ED. The corresponding samples were successively numbered as E0, E45, and E90 are displayed in figure 1(a). Compression tests at a strain rate of $10^{-3}$ s$^{-1}$ and loading direction along the long axis were carried out at room temperature. After compression, the EBSD was characterized on the inner side of the surface by throwing away along the longitudinal section (ED–ND surface).

The extrusion direction of the magnesium alloy was expressed using ED, and the transverse and normal directions perpendicular to the extrusion direction were expressed using TD and ND, respectively. The inverse pole diagram of the three faces of the magnesium alloy was measured using the EBSD technology and combined into a three-dimensional microstructure is displayed in figure 2(a). Most of the initial samples had an equiaxed crystal structure, and the average grain size was 38 $\mu$m. In addition, some elongated grains can be revealed due to the grain stretching along the ED during extrusion. The corresponding inverse pole figure is shown in figure 2(b). The original pole figure obtained by EBSD is shown in figure 2(c). Most of the c-axis of the grain was perpendicular to the ED, that is, the base was parallel to the ED, resulting in a strong basal texture in the initial
pole figure distribution of the magnesium alloy. The texture component was distributed homogeneously along the arc between [10–10]//ED and [2-1-10]//ED.

2.2. Schmid factor calculation
In the process of plastic deformation, each deformation mechanism can be activated if the shear stress $\tau$ along the slip direction of the external load on the slip surface reaches the corresponding CRSS. The formula of shear stress is as follows [28]:

$$\tau = \left( \frac{F}{A} \right) \times \cos \theta \times \cos \varphi = \left( \frac{F}{A} \right) \times SF,$$

where $F$ is the true external force load, $A$ is the cross-sectional area of the sample, $F/A$ is the macroscopic yield stress, $SF = \cos \theta \times \cos \varphi$ is the Schmid factor, and $\varphi$ is the angle between the normal direction of the slip plane and the stress axis. $\theta$ is the angle between the slip direction and the stress axis.

In this study, the algorithm of the equivalent Schmid factor under rolling condition was improved. The shear stress acting on the twin system in the E45 sample was considered to be synthesized by two independent forces, namely, the pressure along the ED and the pressure along the ND. The expression of the improved equivalent Schmid factor ($SF_{45}$) is as follows:

$$SF_{45} = -0.5 \times \cos \theta_{ED} \times \cos \varphi_{ED} - 0.5 \times \cos \theta_{ND} \times \cos \varphi_{ND},$$

where $\theta_{ED}$ (or $\theta_{ND}$) and $\varphi_{ED}$ (or $\varphi_{ND}$) are the angles between the normal direction of the twin surface and the twin shear direction in the ED (or ND), respectively. The SF is negative when the stress in the ED or ND is compressive. The equivalent Schmid factor in the E45 sample after compression is a simple weighting of the twin SF of two independent forces perpendicular to each other along with the ED and ND. In the equation, the weight was 0.5 to satisfy the normalization condition.

3. Results and discussion

3.1. Twinning behaviors
Figure 3 shows the pole figure, EBSD maps, grain boundary structure maps, and {10–12} twin volume fraction (TVF) when the compression of different samples is 0.08. In the EBSD maps, the grain boundary satisfying the orientation relationship of $86.3^\circ \pm 5^\circ$ is defined as the tensile twin grain boundary, which is represented by the red solid line. As shown in figure 3(d), the TVF of {10–12} increases nonlinearly with changing loading direction. E0 sample is compressed to 8%, the high activity of the tensile twins leads to the rotation of the grain $c$-axis to $\sim 90^\circ$ [29], which makes the pole density of the {0002} basal texture shift to the positive and negative directions of ED (figure 3(a)), and the TVF of the {10–12} (figure 3(d)) is about 3.5%. This finding is due to the twin growth and fusion behavior of the specimen in the later stage of deformation [30], resulting in a surface phenomenon wherein the TVF decreases due to the disappearance of twin boundaries. When E45 sample is compressed, the initial texture of all grains is rotated along the ED direction by $45^\circ$, and the resulting texture is shown in figure 3(b). After 8% compression of the E45 sample, the rotation of the {0002} base of the grain in the direction of the application of force, formation of less {0002} basal texture perpendicular to the squeezing axis and less tensile twinnings, and 11% TVF are observed. After 8% compression of the E90 sample, the grain orientation of these grains that has a $C$-axis nearly perpendicular to the compression direction changes abruptly (figure 3(c)). The $C$-axis of these grains is in a state of tensile stress, which is conducive to the activation of the stretched twins, and the TVF is 28% [31].

Table 1. The code, crystallographical indices and illustration of six {10–12} twin variants

| Twin variants | Twinning system   | Schematic diagram |
|---------------|------------------|------------------|
| V1            | (-1102)[1-102]   |                  |
| V2            | (1-102)[1-1101]  |                  |
| V3            | (-1012)[10-11]   |                  |
| V4            | (10-12)[1011]    |                  |
| V5            | (0-112)[01-11]   |                  |
| V6            | (01-12)[01-11]   |                  |
3.2. Analysis of the twinning variant selection mechanism

The \{10–12\} twin model corresponds to six possible twin variants due to the special HCP structure of the magnesium alloy. The crystal coordinate system of X//\{10–10\}, Y//\{12–10\}, and Z//\{0001\} based on HCP structure is established to facilitate this research, and the \{10–12\} planes of the six variants are successively marked as V1, V2, V3, V4, V5, and V6 in accordance with the crystal surface (Table 1). Table 1 shows three theoretical orientations among the six twin variants. The twin variants V1 and V3 (or V6) are in the

![Figure 3. Pole figure (initial and compression 8%), EBSD and boundary structure maps of the sample: (a) E0, (b) E45, (c) E90, and (d) twin volume fraction (TVF) in the three samples during compression of 0.08.](image-url)
ortho-position (OP; 60.0° (10–10)), V1 and V4 (or V5) are in the meta-position (MP; 60.4° (8–1–70)), and V1 and V2 are in the para-position (PP; 7.4° (1–210)) [32]. The typical twin features A, B, C, and D (figure 4) under different initial orientations are considered for convenience. The superposed pole figures of {0001} and {10–12} planes are collected using EBSD, which include the parent, the actual variant {0001} plane poles, and the six twin variant {10–12} plane poles.

Figure 4 shows the identification results of a typical case of variants activated in grain of E0 sample after compression. In figure 4(a), the EBSD detection plane is the ED–ND plane, and the Ta1 is the intragranular twin formed in the grain Ma. Figure 4(b) is the superposition pole figure of the {0001} and the {10–12} planes of Ma and Ta1. Figure 4(c) is the crystallographic relationship between parent grains and twin variants. Figure 4(d) is the result of identifying the Ta1 variant by the orientation rotation method [33]. Figure 4(e) is the SF of six possible twin variants of parent grain Ma.

| Misorientation angle /° | Ma (66.4,137.8,18.8) |
|-------------------------|----------------------|
| V1                      | 61.6                 |
| V2                      | 62.4                 |
| V3                      | 58.8                 |
| V4                      | 57.9                 |
| V5                      | 9.7                  |
| V6                      | 2.8                  |

(d) 20μm

Figure 4. Typical twin case in E0 sample grain Ma: (a) EBSD map; (b) Superposed {0001} (green orientation) and {10–12} (blue orientation) pole figure of the parent grain Ma. The blue dash lines are twin plane traces of the corresponding variants. (c) Crystallographic relationship between parent grains and twin variant; (d) Misorientation angles between Ta1 and six possible variants of Ma; (e) SF of six possible twin variants of parent grain Ma.

Figure 5 shows the identification results of typical twin transfer crossing neighboring grains of E45 sample after compression. Analyzing the variant of Tb1 by using the trace method is difficult. Figure 5(d) shows that the misorientation angle between Tb1 and variant V1 is 0.6°. Thus, Tb1 is accurately identified from V1, and Tc1 is from variant V3. Figure 5(b) shows that the (0001) poles of the grains Mb and Mc are distributed in the third quadrant very close to the ND, which indicates a close orientation relationship between them and may indicate the twin transfer between them. Scientists have revealed the slip and twin transfer phenomenon in Zn [39] and Ti [40] of the HCP metal. The crystallographic analysis shows that the misorientation angle of Mb and Mc is 5°,
forming a strong local basal texture. Guo [33] believes that the strong basal texture is a favorable condition for the formation of twin transfer crossing neighboring grains. This strong basal texture results in at least one pair of very large SF variants in each grain (figure 5(e)), and high-SF variants in neighboring grains have high matching. Figure 5(e) shows that variants V1 and V3 have the first high SF. Thus, the variants V1 and V3 are activated following Schmid’s law and form the twin transfer crossing neighboring grain phenomenon.

Figure 6 shows the identification results of typical multi-twins inside a grain of E90 sample after compression. Figure 6(a) shows that twins Te1 and Te2 are delivered to each other in grain Me, forming a high twin boundary angle. The orientation rotation method analysis (figure 6(d)) shows that Te2 is from variant V3 and that Te1 is from variant V5. Therefore, Te1 and Te2 are OP relations, and the activation is in the same grain with a theoretical misorientation angle of 60.0°. Figure 7(e) shows that the two variants have the first and third high SF. Therefore, variant V5 is considered activated first following the Schmid’s law in compression to form twin Te1. Other variants need to be activated in grain Me to fully coordinate the externally imposed strain.

Variants V3 and V2 have the best strain compatibility with V5 in the OP [41]. However, considering that V3 (Te2) has higher SF than V2, V3 is activated together with V5. Moreover, the SF of twin Te2 is less than 0.6,
which is a typical non-Schmid twin [42]. From the area and morphology shown in figure 6(a), Te2 and Te1 are wide at one end of the grain boundary and form a tip at the delivery. Therefore, when the deformation geometry makes the SF of the two variants meet Schmid’s law and the strain coordination effect, Te2 and Te1 are first activated inside the parent grains. These primary twin variants grow and impinge, forming boundaries with 60° 011̅ orientation relationship and meet each other through historical growth [43].

Figure 7 shows the identification results of a typical case of paired twins in two neighboring grains of E90 sample after compression. As shown in figure 7(a), the twins Tf1 and Th1 are formed in the grains of Mf and Mh, respectively, and are connected at the grain boundaries. The analysis of the orientation rotation method (figure 7(d)) shows that Tf1 and Th1 come from the variants V6 of Mf and V5 of Mh, respectively. The strain transfer efficiency between Tf1 and Th1 is relatively high, forming twin pair in to neighboring grains. Figure 7(e) shows that both variants have a first SF, which is significantly higher than those of other variants. Therefore, the two variants are activated because they can coordinate the external strain to the maximum and conform to Schmid’s law. Figure 7(f) shows the twin pairs with high SF are inferred to have high geometrically compatible (~0.8) [16] and easily form twin pair in two neighboring grains. Researchers reveal two possible paths for the formation of twin pairs [42]. (1) The twins in one grain grow longitudinally to the grain boundary and induce twinning of adjacent grains at the delivery point. (2) Two twins nucleate from the same site of the grain boundary and grow to the inner part of their respective parent. In figure 7(a), twin Tf1 has a tip, and the twin grows at 45° and ends at the inside of Mf, whereas the other end is quite wide at the grain boundary of Mf–Mh. The twin Th1 has similar characteristics. This twin morphology indicates that the twins Tf1 and Th1 are formed through the second path and twin transmission cannot occur [44].
4. Conclusion

(1) In uniaxial compression, the activity of the \(\{10\text{--}12\}\) twin increases nonlinearly as the loading direction shifts from perpendicular to the grain C-axis to parallel to the grain c-axis.

(2) When E0 sample is compressed, the essence of less TVF is the growth and fusion of twins. The twin excitation at the grain boundaries is affected by the stress fluctuations, and the activation of the corresponding variants follows the Schmid’s law.

(3) In accordance with the improved twin selection parameter ‘SF\(_{15}\)’ in the E45 sample, the twin selection also follows Schmid’s law, and the local strong basal texture is the favorable condition for the formation of twin transfer crossing neighboring grains.

(4) Various \(\{10\text{--}12\}\) twin patterns, such as multi-twins inside a grain and twin pair in two neighboring grains, are observed in the E90 sample after compression. In the multi-twins inside a grain pattern, the high-SF variant is activated first to coordinate the externally imposed strain, and the OP variant with the best strain
compatibility is activated and can activate a certain amount of non-Schmid twins. Twin pair in two neighboring grains usually have high SF, and the activation of corresponding variants follows Schmid’s law.

Acknowledgments
This research was funded by National Key Research and Development Program of China (No. 2018YFB1307902), National Science Fund Subsidized Project (No. U1710113), Shanxi Province Joint Student Training Base Talent Training Project (No. 2018JD33), Shanxi Excellent Youth Fund (No. 201901d211312), Transformation and cultivation project of scientific and technological achievements in Colleges and universities of Shanxi Province (No. 2019KJ028), Shanxi Graduate Education Innovation Project (No. 2019YF482).

Conflicts of interest
The authors declare no conflict of interest.

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