Law of Atomic Motion during {1011} Twinning in Magnesium Alloys

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Twin types in a room-temperature compressed magnesium alloy (Mg-3Al-1Zn) sample were identified by using electron backscattered diffraction (EBSD) technique, and the results indicate that most of the twins are $\{10\bar{1}2\}$ twins and only a few of them are $\{10\bar{1}1\}$ twins. In order to study the law of atomic motion in the $\{10\bar{1}1\}$ twinning, we calculated the displacement vectors of the twinning atoms in the $\{10\bar{1}1\}$ twinning and found that the atomic motion can be explained through a model named quadrangular prism-shaped atomic group (QPAG). In the QPAG model there exist two types of alternately distributed QPAG units totally. Though the rotational angle of the two types of QPAG units in the $\{10\bar{1}1\}$ twinning is smaller than in the $\{10\bar{1}2\}$ twinning, the relative displacement magnitude in the $\{10\bar{1}1\}$ twinning is larger than in the $\{10\bar{1}2\}$ twinning due to its more complicated atomic motion, and this should be the reason that the $\{10\bar{1}1\}$ twinning is harder to occur than the $\{10\bar{1}2\}$ twinning. [doi:10.2320/matertrans.MC201022]

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1. Introduction

Magnesium alloys have been the focus of a number of researches for their potential engineering applications and important significance in basic science researches.^{1,2)} However, technically speaking, a key factor impeding the practical applications of magnesium alloys is the poor plasticity and limited toughness of the materials at room temperature.³⁻⁵⁾ Theoretically, the poor deformation capability of magnesium alloys at room temperature is rooted in the hexagonal close-packed (HCP) structure. Because the non-basal slip systems in the HCP structure materials are hard to be activated for the high critical resolved shear stresses (CRSSs), thus the HCP structure materials can not satisfy the Von-Mises criterion.⁶⁾ Nonetheless, it is of special significance for the room-temperature deformation of magnesium alloys to improve their yield strengths and gain the required anisotropy for practical applications. Due to the existing disputes on deformation mechanism of magnesium alloys and the increasing demands of actual production of magnesium, a number of researches on the deformation of magnesium alloys at room temperature have been carried out.^{7,8)} Twinning is an important deformation mode for the HCP structure materials,^{9,10)} because it makes the materials meet the requirement of five independent sliding systems for arbitrary deformation.^{11,12)}

It is generally considered that the deformation of magnesium alloys is primarily dominated by the twinning and basal slip at room temperature whereas governed by grain boundary sliding at elevated temperatures.^{13–16} Deformation twinning in magnesium alloys is approximately divided into two types: one is { $10\overline{1}2$ } extension twinning which requires a tensile stress component along the c axis; the other is { $10\overline{1}1$ } contraction twinning which requires a compressive stress component along the c axis.^{17–19)} In addition, the extension twins are often formed within the former-formed contraction twins, which are called "double twins" or "secondary twins".²⁰⁾ Some formed twins can also disappear or turn thinner under the reversible stress, and this phenomenon is known as "detwinning".^{11,21)}

Nowadays, most of the researches are focused on the $\{10\overline{1}2\}$ twinning for its frequent emergences, whereas the researches on the $\{10\overline{1}1\}$ twinning are much fewer.²²⁾ In a sense, the $\{10\overline{1}1\}$ twinning is of important significance for the deformation in magnesium alloys, because it contributes to the contraction of grains along the c axis. It also has a close relation to the fracture behavior of the materials.²³⁾ The purpose of this study is to clarify the mechanism of the contraction twinning in magnesium alloys from a microscopic angle. We have constructed a model to describe the law of atomic motion in the $\{10\overline{1}2\}$ twinning.²⁴⁾ In this paper we calculated the displacement vectors of the twinning atoms in the $\{10\overline{1}1\}$ twinning and applied the above model to explain the law of atomic motion in the {1011} twinning. At last, we contrasted the two types of twinning modes to reveal the reason that the {1011} twinning is harder to occur than the {1012} twinning.

2. Experimental Procedures

A cuboid sample with the size of $10 \times 10 \times 20 \text{ mm}^3$ was cut from an as-cast AZ31 magnesium alloy (2.5–3 mass% Al, 0.7–1.3 mass% Zn, Mn, Fe $\leq 60.02 \text{ mass}\%$, others $\leq 0.01 \text{ mass}\%$, and Mg balance) using wire-cutting technology. The sample was homogenized at 673 K for 5 h. The compression test was conducted by using CMT25150 universal testing machine at the strain rate of 0.005 s^{-1} to the true strain of 0.1 at room temperature. The EBSD analysis was performed by using Noval 400 NanoSEM scanning electron microscopy to judge the twin types.

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Fig. 1 EBSD patterns of the 0.1 strain AZ31 sample.

3. Results and Discussion

The EBSD patterns for the compressed AZ31 sample are shown in Fig. 1 where the wider twins are the $\{10\overline{1}2\}$ type and the thinner twins are the $\{10\overline{1}1\}$ type. It is shown that most of the twins are the $\{10\overline{1}2\}$ extension twins, while only a few of them are the $\{10\overline{1}1\}$ contraction twins, which indicates that the $\{10\overline{1}1\}$ twinning is much harder to occur than the $\{10\overline{1}2\}$ twinning.

The shear magnitudes are generally regarded as a parameter to measure the difficulty degree of twinning in the HCP materials.²⁵⁾ However some special cases indicated that it is improper to judge the difficulty degree of twinning only by shear magnitudes. As a special case, the shear magnitude of the {1012} twinning is zero when the axis ratio of an HCP material is $\sqrt{3}$, which means the twinning should be the easiest to occur, but the fact is not true.²⁶⁾ To find out the real factor that affects the difficulty degree of twinning, we calculated the displacement vectors of the twinning atoms in the {1011} twinning and based on which established a model to investigate the law of atomic motion in the {1011} twinning.

3.1 Displacement vectors of the twinning atoms

A rectangular coordinate system was constructed in a Mg crystal cell so as to simplify the calculation (Fig. 2). The atomic motion during the {1011} twinning is illustrated in Fig. 3. The {1011} planes were divided into two categories as shown in Fig. 4: the crystal planes through the A-layer atoms of the HCP materials are named main planes (M) and the crystal planes through B-layer atoms of the HCP materials are named sub-planes (S). In addition, the pair of M-plane and S-plane on the {1011} twin boundary is enumerated as "0" and from which to the distant "1,2,...,n" (where *n* is the number of the twinning planes). Thus the *k*-th main plane is expressed as M_k -plane; the rest can be deduced by analogy.

In order to further simplify the calculation, we selected a small piece of typical region as surrounded by the parallelogram "AQSC" (Fig. 4). The positions of the atoms after twinning are determined by the symmetric relation between the twin and the matrix. The atomic displacement vectors are determined by the criterion of the minimum magnitude of displacement;²⁶ i.e. each atom moves to the nearest available



Fig. 2 Three-dimensional Cartesian coordinate system and the corresponding four-axis coordinate system in a crystal cell of Mg.



Fig. 3 Lattice for the atomic motion during the AZ31 {1011} twinning. The colorful spheres represent the atoms before twinning; the white spheres represent the atoms after twinning; and the arrows represent the atomic displacement vectors of the twinning atoms.

twin sites. A part of locations of the twinning atoms are listed in Table 1.

The crystal cell parameters of an AZ31 alloy are as follows: a = 0.321 nm, c = 0.521 nm, $\gamma = c/a = 1.623$, thus the displacement vectors of some atoms in the area of parallelogram "AQSC" can be calculated as follows:

$$v_{\rm F} = v_{\rm S1} = \Delta x_{\rm F} i + \Delta y_{\rm F} j + \Delta z_{\rm F} k$$

$$\approx 0i - 0.194aj - 0.0921ak \qquad (1a)$$

$$\vec{v}_{\rm G} = \vec{v}_{\rm M2} = \Delta x_{\rm G} i + \Delta y_{\rm G} j + \Delta z_{\rm G} k \qquad (1a)$$

$$\vec{v}_{\rm G} = \vec{v}_{\rm M2} = \Delta x_{\rm G} i + \Delta y_{\rm G} j + \Delta z_{\rm G} k \qquad (1b)$$

$$\vec{v}_{\rm J} = \vec{v}_{\rm S2} = \Delta x_{\rm J} i + \Delta y_{\rm J} j + \Delta z_{\rm J} k \qquad (1c)$$

$$\vec{v}_{\rm K} = \vec{v}_{\rm M2} = \Delta x_{\rm K} i + \Delta y_{\rm K} j + \Delta z_{\rm K} k \qquad (1c)$$

$$\vec{v}_{\rm K} = \vec{v}_{\rm M2} = \Delta x_{\rm K} i + \Delta y_{\rm K} j + \Delta z_{\rm K} k \qquad (1d)$$

$$\vec{v}_{\rm N} = \vec{v}_{\rm S3} = \Delta x_{\rm N} i + \Delta y_{\rm N} j + \Delta z_{\rm N} k \qquad (1d)$$

$$\vec{v}_{\rm N} = \vec{v}_{\rm S3} = \Delta x_{\rm N} i + \Delta y_{\rm N} j + \Delta z_{\rm N} k \qquad (1e)$$

$$\vec{v}_{\rm O} = \vec{v}_{\rm M3} = \Delta x_{\rm O} i + \Delta y_{\rm O} j + \Delta z_{\rm O} k \qquad (1e)$$

$$\approx 0\mathbf{i} - 0.230\mathbf{a}\mathbf{j} - 0.154\mathbf{a}\mathbf{k} \tag{1f}$$



Fig. 4 QPAG unit model for the AZ31 {1011} twinning. (a) and (b) are the type-I QPAG units before and after twining respectively; (c) and (d) are the type-II QPAG units before and after twining respectively; (e) and (f) are the arrangement of several QPAG units before and after twinning respectively; and (g) and (h) are the corresponding top views of (e) and (f).

Table 1 A part of the positions of twinning atoms in the $\{10\overline{1}1\}$ twinning.

Twinning planes	M_0	M_1	M_2	M ₃	M_4
Atoms	A, C	E, G, U	I, K, V	M, O, Z	Q, S, Y
Twinning planes	S_0	S_1	S_2	S_3	S_4
Atoms	B, D	F, H	J, L	N, P	R, T

$$\vec{v}_{R} = \vec{v}_{S4} = \Delta x_{R} i + \Delta y_{R} j + \Delta z_{R} k$$
$$\approx 0i - 0.421aj - 0.249ak \qquad (1g)$$

$$\vec{v}_{\rm S} = \vec{v}_{\rm M4} = \Delta x_{\rm S} i + \Delta y_{\rm S} j + \Delta z_{\rm S} k$$

$$\approx 0\mathbf{i} - 0.197\mathbf{a}\mathbf{j} - 0.369\mathbf{a}\mathbf{k} \tag{1h}$$

$$|\vec{v}_{\rm S}| \approx 0.418a \tag{1h'}$$

where \vec{v}_F and \vec{v}_{M1} denote displacement vectors of atom Fand the atoms on the M₁-plane respectively; Δx_F , Δy_F and Δz_F denote the vector components of atom F along the x, y, and z axes respectively (the rest of atoms in the parallelogram can be deduced similarly). Note that \vec{v}_S is the minimum among all the shearing vectors. If the interplanar spacing of the {1011} planes is defined as d_2 , the twinning shear s_2 is obtained:

$$s_2 = \frac{|\vec{v}_S|}{4d_2} = \frac{0.155a}{4\frac{\sqrt{3}\gamma a}{\sqrt{4\gamma^2 + 3}}} \approx \frac{0.155a}{4 \times 0.764a} \approx 0.137 \quad (2)$$

Thus the general formulas for calculating the displacement vectors of the twinning atoms during the $\{10\overline{1}1\}$ twinning are obtained according to the periodicity of the twinning cells:

$$\vec{v}_{\mathrm{M}(4k+i)} = \vec{v}_{\mathrm{M}i} + k\vec{v}_{\mathrm{S}} \tag{3a}$$

$$\vec{v}_{\mathrm{S}(4k+i)} = \vec{v}_{\mathrm{S}i} + k\vec{v}_{\mathrm{S}} \tag{3b}$$

where i = 1, 2, 3, 4; k = 0, 1, 2, ..., n (n is the sum of the twinning planes).

3.2 Establishment of the QPAG model

The moving directions of the shuffling atoms in the $\{10\overline{1}1\}$ twinning seem disordered (Fig. 4). However, it is found that the atomic motions in the {1011} twinning show a good regularity when some twinning atoms in certain area are regarded as an entirety. As shown in Fig. 4(a), atoms W, R, Oand S constitute a "quadrilateral". In fact, each of these atoms represents a row of atoms. Hence, the four rows of atoms represented by W, R, O and S construct a "quadrangular prism", thus it is named as a "quadrangular prism-shaped atomic group" (QPAG) unit. It is noteworthy that the choice of these QPAG units is not arbitrary but follows a principle: the relative positions of the twinning atoms in each unit should keep unchanged. In the {1011} twinning there exists two types of QPAG units classified by their ways of motion: type I QPAG units are represented by the atom group "WROS" (Fig. 4(a),(b)), and these QPAG units rotate simply within the y-o-z plane; type II QPAG units are represented by the atom group "NJGK" (Fig. 4(c),(d)), and these QPAG units not only rotate within y-o-z plane but also shift along xaxis for 0.5 a (Fig. 4(e)–(h)).

Since the atomic motion in the {1011} twinning is ascribed to the rotational motion of the two types of QPAG units, the difficulty degree of the twinning can be measured by calculating the relative displacement magnitudes between the adjacent QPAG units. The relative displacement vectors between atoms of the unit "WROS" and its adjacent QPAG units are calculated as follows:

$$\vec{v}_{\rm N} - \vec{v}_{\rm R} = \pm 0.5 a i + 0.129 a j - 0.027 a k$$
 (4a)

$$\vec{v}_{\rm K} - \vec{v}_{\rm O} = \pm 0.5 a i + 0.129 a j - 0.027 a k$$
 (4b)

$$\vec{v}_{\rm S} - \vec{v}_{\rm P} = \pm 0.5 \mathrm{a} i + 0.096 \mathrm{a} j - 0.092 \mathrm{a} k$$
 (4c)

$$\vec{v}_{\rm O} - \vec{v}_{\rm L} = \pm 0.5 a i + 0.096 a j - 0.092 a k$$
 (4d)

$$|\vec{v}_{\rm N} - \vec{v}_{\rm R}| \approx 0.517a \tag{4a'}$$

$$|\vec{v}_{\rm K} - \vec{v}_{\rm O}| \approx 0.517a \tag{4b'}$$

$$|\vec{v}_{\rm S} - \vec{v}_{\rm P}| \approx 0.517a \qquad (4c')$$

$$|\vec{v}_{\rm O} - \vec{v}_{\rm L}| \approx 0.517a \tag{4d'}$$

The rotational angles of the two types of QPAG units α_I and α_{II} are calculated as follows:

$$\alpha_{I} = \alpha_{WROS} = \arctan \frac{|\Delta z_{\rm R} - \Delta z_{\rm W}|}{WR - |\Delta y_{\rm R} - \Delta y_{\rm W}|}$$

$$\approx \arctan \frac{0.212a}{0.866a - 0.031a} \approx 14.3^{\circ} \qquad (5a)$$

$$\alpha_{II} = \alpha_{NJGK} = \arctan \frac{|\Delta z_{\rm J} - \Delta z_{\rm N}|}{NJ - |\Delta y_{\rm J} - \Delta y_{\rm N}|}$$

$$\approx \arctan \frac{0.212a}{0.866a - 0.031a} \approx 14.3^{\circ} \qquad (5b)$$

According to eq. (4) and eq. (3), it can be concluded that the relative displacement magnitude between the two types of QPAG units is 0.517a (eq. (4a')–(4d')), which is larger than the value of 0.349a in the {1012} twinning.²⁴ According to

eq. (5) and eq. (3), both the two types of QPAG units rotate by an angle of 14.3° , despite the different rotational modes, which is smaller than the value of 15.9° in the $\{10\overline{1}2\}$ twinning.²⁴⁾ Note that it is inappropriate to compare the difficulty degrees of twinning by the rotational angles for the different shapes and rotational directions of the QPAG units between in the $\{10\overline{1}1\}$ twinning and in the $\{10\overline{1}2\}$ twinning. However, it is of physical meaning to measure the difficulty degree of twinning by the relative displacement magnitudes, because the larger value of which means the lager atomic deformation and the larger stress to overcome.

4. Conclusions

The mechanism of the $\{10\overline{1}1\}$ twinning can be well explained through the QPAG model. There exists two types of QPAG units in the $\{10\overline{1}1\}$ twinning: type I QPAG units rotate simply in the plane *y-o-z*; while type II QPAG units not only rotate in plane *y-o-z* but also shift along *x* axis for 0.5 a. These two types of QPAG units are distributed alternately, and both of them rotate by an angle of 14.7° . The relative displacement magnitude between the two types of QPAG units in the $\{10\overline{1}1\}$ twinning is 0.517a, which is larger than in the $\{10\overline{1}2\}$. The reason that the $\{10\overline{1}1\}$ twinning is harder to be activated than the $\{10\overline{1}2\}$ twinning is either for its more complicated movement ways of QPAG units or for its larger value of the relative displacement magnitude.

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