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Triple twins and martensitic transformation in Ti–5Al–2Mo–3Zr alloy

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In Ti–5Al–2Mo–3Zr alloy, TEM observations showed a special feature of "triple twins" in martensite plates after quenching, i.e. three sets of crystals in a martensite plate oriented with the $\{1\bar{1}01\}\langle\bar{1}102\rangle$ twin relationship between any two of them. This is possible because the c/a ratio of the lattice parameters equals 1.588 in this alloy, and thus the triangle consisting of spots 0001, $1\bar{1}01$ and the central spot in a selected-area diffraction pattern has the interior angles of approximately 30, 60 and 90°. The observations also showed that the boundary between twins II and III was the twin plane $\{1\bar{1}01\}$, but the boundary between twins I and II was close to $\{1\bar{1}03\}$, i.e. (1 2 1) of the b.c.c. parent phase. Formation of the triple twins could be explained by the phenomenological theory of crystallography. One pair of twin martensite plates may grow from a pair of twin nuclei which take (1 1 0) and (0 1 1) planes of the parent phase as their respective basal planes. However, the (1 1 0) and (0 1 1) planes are symmetrical with respect to (1 2 1) of the parent phase, which corresponds to a $\{1\bar{1}03\}$ plane of the martensite. The third part of the triple twins forms to meet the need for simple shear according to the phenomenological theory. The formation of triple twins occurs to accommodate the shape change and reduce the elastic energy during the transformation.

1. Introduction

The alloy Ti–5A1–2Mo–3Zr is a promising structural material with high resistance to fatigue crack propagation at room temperature and excellent ductility at − 75 °C [1, 2]. The alloy is an $\alpha + \beta$ type and assumes primary α phase plus h.c.p. martensite α' after quenching from 950 °C. This study investigates the features of twin formation during the martensitic transformation and the relationship between the twins and the transformation mechanism. Some studies [3, 4] have identified the twin elements in titanium alloys as $K_1\{1\bar{1}01\}$, $\eta_1\langle\bar{1}102\rangle$, $K_2\{1\bar{1}03\}$ and $\eta_2\langle\bar{3}302\rangle$. Nishiyama *et al.* [5–7] have investigated the $\{1\bar{1}01\}$ martensitic transformation twins in commercially pure titanium. Hammond and Kelly [8] as well as Knowles and Smith [9] have observed K-type and L-type (M-type) twins in martensites in Ti–Mn alloy. These twins resulted from the invariant plane strain during martensitic transformation according to the phenomenological theory for martensitic transformation crystallography [10–14]. Thus, the twins are related to the transformation mechanism. However, the calculated results based on the phenomenological theory are not consistent with the experimental results of Knowles and Smith [9], which are rather in agreement with expectation from the theory of Bilby *et al.* [15, 16]. Thus, the formation process of the martensitic transformation twin is not yet totally clear. This paper will show some special twin morphologies and try to explain the twin formation in Ti–5A1–2Mo–3Zr alloy.

2. Experimental results and discussion

2.1. Alloy composition and sample preparation

The composition of the alloy studied is shown in Table I and the alloy will be referred to as Ti-523 for brevity. The alloy was melted twice in a consumable-electrode furnace, forged at 1000 °C and rolled at 950 °C. The rolled rods of ϕ 10 mm × 40 mm were quenched from 950 °C after 1 h holding and the microstructure consisted of primary α phase and h.c.p. martensite α'. Some of the quenched samples were tempered at 600 °C for 4 h to observe the precipitation process at the twin boundaries. TEM samples were cut to 0.5 mm thick by a molybdenum wire electrospark machine and ground to less than 0.1 mm thickness with sandpaper. The foils were then electropolished and perforated in an electrolyte containing $HClO_4{:}CH_3OH{:}C_2H_5CH_2CH_2OH = 1{:}6{:}10$ at − 35°C. The transmission electron microscopes used were an H-800 and a Jeol 100 CX.

2.2. Twin morphology in martensite

In the α' phase, three types of twin morphology have been observed: longitudinal twins, transversal twins and "triple twins". Fig. 1a shows the longitudinal twin morphology and Fig. 1b the selected-area diffraction (SAD) pattern and its key diagram, which indicates that this twin is of $\{1\bar{1}01\}$ type. Fig. 2 shows another martensite consisting of transversal twins which are similar to the K-type twins of Hammond and Kelly

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TABLE I Alloy composition

Element	Al	Mo	Zr	Fe	C	Si	N	H	O
Composition (wt %)	4.91–5.00	1.85–2.00	2.65–2.92	0.062–0.063	0.01–0.02	0.01–0.02	0.0090–0.0092	0.0096–0.0098	0.0099–0.0110

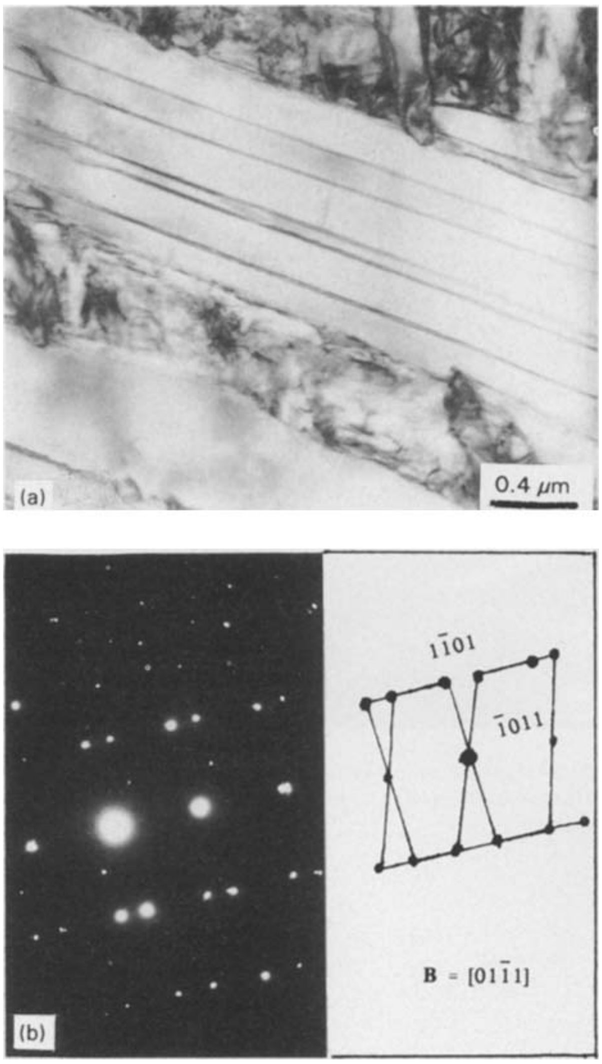

Figure 1 Longitudinal twins in Ti–5Al–2Mo–3Zr alloy: (a) TEM morphology, (b) SAD pattern and its key diagram.

[8] and Knowles and Smith [9]. This twin system is measured also as $\{1\,\bar{1}\,0\,1\}$ type as expected. This type of twin has also been observed in Ti–5Al–1Mo–2Nb–3Zr alloy [17]. Fig. 3 shows a configuration orientation in which the three sets of contacting crystals form a triple twin in which any two of the three sets orient in $\{1\,\bar{1}\,0\,1\}$ twin relationship. Fig. 3a shows the morphology of a triple twin and Fig. 3b the SAD pattern and its key diagram. In order to verify the triple twin relationship, two different dark-field photos (Fig. 3c and d) obtained from two of the fine diffraction spots closest to the centre are shown, and they demonstrate the correspondence between the pattern spots and the twin crystals. By using the technique of Knowles and Smith [9], i.e. tilting the foil until the twin boundary is as thin as possible, it is determined that the twin boundary between twins II and III is close to $(1\,\bar{1}\,0\,1)$ as expected, but the boundary between twins I and II is close to $(1\,\bar{1}\,0\,3)$. This type of twin morphology in titanium martensite, to the authors' knowledge, has not yet been reported. It is noteworthy that within twin II there are twins which can be found by careful observation and called twin IV, in a position making an angle of 60° with twin III, as indicated by arrows in Fig. 3. Twin IV is even clearer after 600 °C tempering and decorating by precipitated β particles, as shown in Fig. 4.

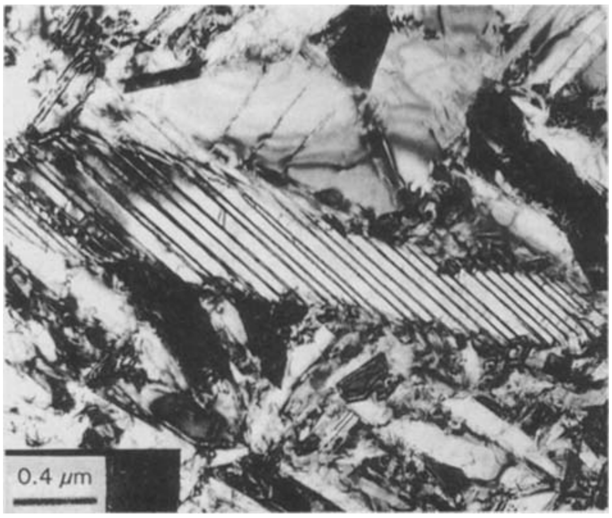

Figure 2 Transversal twins in Ti–5Al–2Mo–3Zr alloy.

2.3. Discussion of triple twins

Comparing Fig. 3b with Fig. 5 in Knowles and Smith [9], it is found that the positions and angles of spots 0002 are similar. The difference between the two patterns is that Fig. 5 in Knowles and Smith is a twin diffraction pattern but Fig. 3b in this paper is a threefold symmetric one, i.e. a pattern of triple twins. The characteristics and elaboration of the triple twins are shown in Fig. 5. The possibility of assuming triple twins comes from the fact that the c/a ratio equals 1.588 in the Ti–523 alloy. This ratio results in a triangle consisting of diffraction spots 0001, $1\,\bar{1}\,0\,1$ and the central spot with interior angles of approximately 30, 60 and 90°. Threefold rotationally symmetric patterns are therefore possible in alloys with a c/a ratio of 1.588. If this is true, it is to be expected that triple twins exist in Ti–5Mn alloy.

Fig. 6 shows the lattice relationship between triple twins and the parent phase. The lattice parameters of the α′ phase in Ti–523 alloy are $a = 0.2949$ nm, $c = 0.4684$ nm and ratio $c/a = 1.588$ [1, 2]. It can then be obtained that the orientation of the three parts of α′, rotated 120° about the $[1\,1\,\bar{2}\,0]$ axis from each

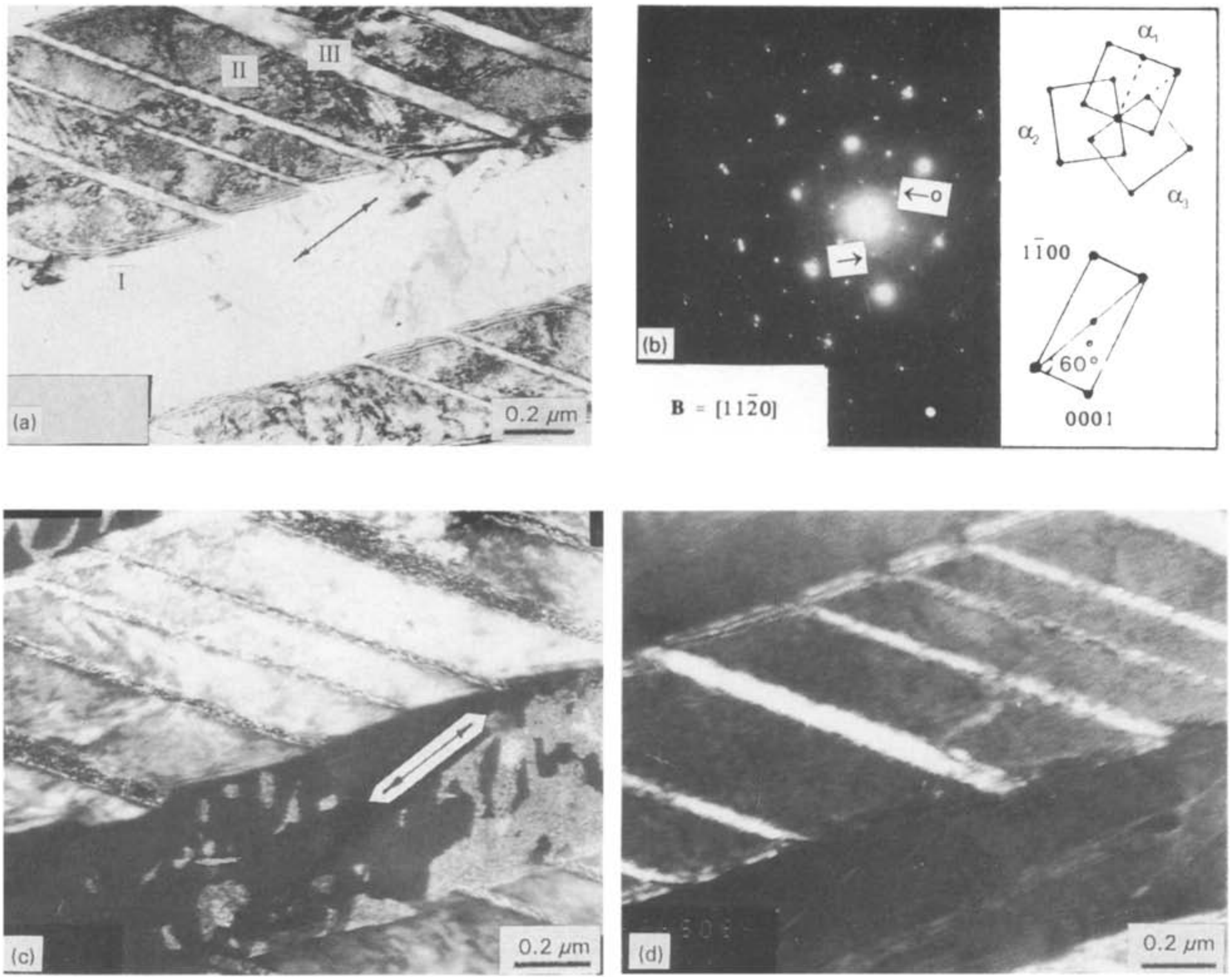

Figure 3 Triple twins in Ti–5Al–2Mo–3Zr alloy: (a) TEM morphology, (b) SAD pattern and its key diagram, (c) dark-field micrograph of twin II (spot 0001 marked ↑ in (b)), (d) dark-field micrograph of twin III (spot 0001 marked $\overset{\uparrow}{\circ}$ in (b)).

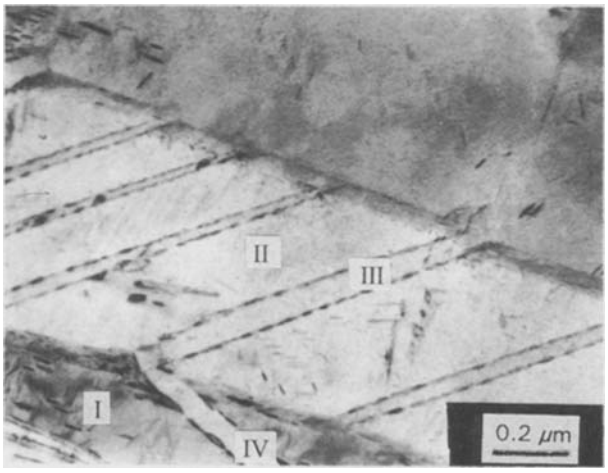

Figure 4 Precipitated β particles at the twin boundaries after tempering for 4 h at 600 °C.

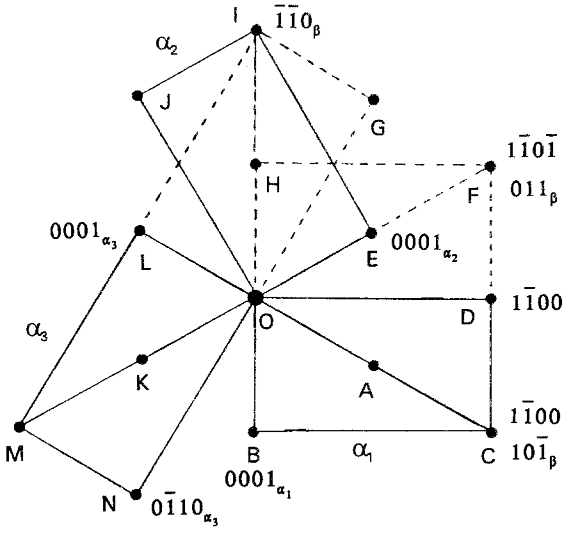

Figure 5 Schematic SAD pattern of the triple twins: $\mathbf{B} = [11\bar{2}0]_\alpha$, $[\bar{1}1\bar{1}]_\beta$. α1 is twin I (BCFH), α2 is twin II (OEIJ) and α3 is twin III (OLMN); α1 (OBCD) and α3 (OGIL) are symmetric with respect to OF ($1\bar{1}0\bar{1}$), while α1 (ODFH) and α3 (OLMN) are symmetric with respect to OJ 1/2 ($\bar{1}10\bar{3}$).

other, shows a $\{1\bar{1}01\}$ twin relationship between any two of the three crystals. Furthermore, each crystal of the triple twins has a Burgers orientation with respect to the parent phase. Because of these geometric features, the $\{1\bar{1}01\}$ triple twins in Ti–523 alloy have $\{1\bar{1}03\}$ symmetry planes perpendicular to the twin planes. In other words, the $\{1\bar{1}01\}$ triple twins are also $\{1\bar{1}03\}$ twins in this alloy, as shown in Figs. 5 and 6. The dark fields of twin II and twin III of the triple twins in Fig. 3c and d confirm the above analysis and demonstrate the existence of the triple twins.

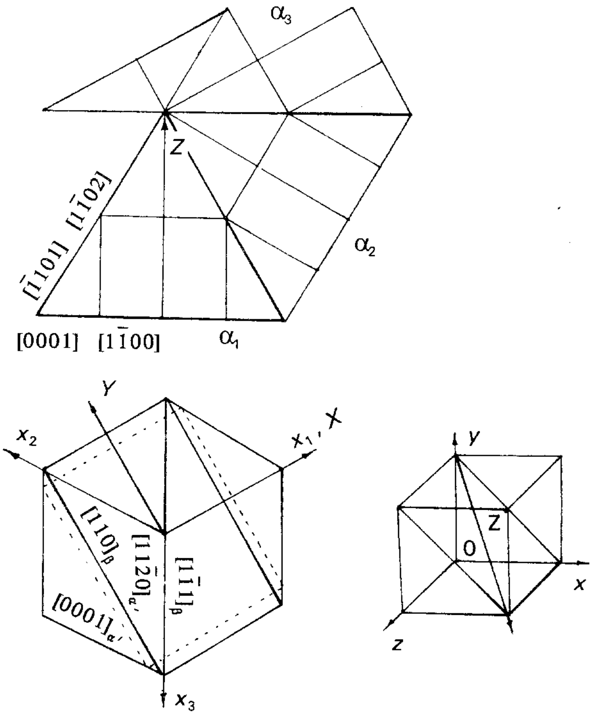

Figure 6 Schematic lattice relationships and twin boundaries of triple twins. Coordinates: (X, Y, Z) for principal axes, (x, y, z) for b.c.c. parent phase, (x_1, x_2, x_3, Z) for h.c.p. martensite. Dotted lines are (1 1 0) before Bain distortion.

3. Formation of triple twins

3.1. Transformation strain

According to Knowles and Smith [9], the K-type and the M-type martensite plates are consistent with the crystallography of the class A ($\alpha -$, $\omega +$) solution. In Fig. 3a the martensite plate consisting of twin II and twin III is identified with the same result, i.e. belonging to class A ($\alpha -$, $\omega +$). The coordinates used in the phenomenological theory calculation are shown in Fig. 6. The invariant plane strain is

$$D = RBS = I + \mathbf{d}\mathbf{p}' \qquad (1)$$

where R, B, S are the matrices of a rotation, Bain strain and a simple shear respectively, and I is an identity matrix and $\mathbf{d}$ and $\mathbf{p}'$ are respectively the displacement vector of, and the normal vector to, the invariant plane. For the alloy studied, the lattice parameters have been measured [1, 2] as $a = 0.3254$ nm for the b.c.c. parent phase and $a = 0.2949$ nm, $c = 0.4684$ nm for h.c.p. martensite. By using the principal axis system (X, Y, Z) shown in Fig. 6, the Bain strain is considered to be

$$B = \begin{bmatrix} 0.906\,27 & 0 & 0 \\ 0 & 1.109\,95 & 0 \\ 0 & 0 & 1.017\,85 \end{bmatrix} \qquad (2)$$

The following data are referred to the b.c.c. co-ordinate in Fig. 6. Assuming that the simple shear (twin) plane is (1 0 $\bar{1}$), it is calculated that the invariant vector and invariant normal of the invariant line strain are respectively

$$\mathbf{x} = \begin{bmatrix} 0.700\,10 \\ -0.140\,36 \\ 0.700\,10 \end{bmatrix} \qquad (3)$$

$$\mathbf{n}' = [0.685\,44 \quad 0.625\,52 \quad -0.372\,68] \qquad (4)$$

The normal to the invariant plane (habit plane) and the displacement vector of the plane are respectively

$$\mathbf{p}' = [0.555\,56 \quad 0.723\,01 \quad -0.410\,62] \qquad (5)$$

$$\mathbf{d} = \begin{bmatrix} -0.105\,13 \\ 0.085\,13 \\ -0.050\,47 \end{bmatrix} \qquad (6)$$

Thus, the invariant line strain tensor and invariant plane strain tensor are respectively

$$L = \begin{bmatrix} 1.016\,65 & 0.047\,34 & -0.003\,33 \\ -0.049\,14 & 0.995\,58 & 0.020\,89 \\ 0.004\,36 & 0.182\,32 & 1.013\,02 \end{bmatrix} \qquad (7)$$

$$D = \begin{bmatrix} 0.941\,59 & -0.076\,01 & 0.043\,17 \\ 0.047\,29 & 1.061\,55 & -0.034\,96 \\ -0.028\,04 & -0.036\,49 & 1.020\,73 \end{bmatrix} \qquad (8)$$

In addition, the reciprocals of the normalization factor for D (shape deformation) and the factor for the simple shear vector (twin amount) are respectively.

$$m_1 = 0.144\,39 \qquad (9)$$

$$m_2 = 0.247\,68 \qquad (10)$$

The results are in agreement with those of Knowles and Smith [9] except for some small calculation errors and different axis directions in b.c.c. (it seemed that their cubic coordinate system [9] was a left-handed one when compared with Fig. 6). The invariant plane (habit plane) is close to a plane of the {3 3 4} family of planes in b.c.c.

3.2. Transformation system

However, the (1 1 0) plane in b.c.c. is a mirror symmetric plane, with respect to which planes (1 0 $\bar{1}$) and (0 1 1) are symmetric with each other. Thus, (0 1 1) can equally act as a simple shear plane just as (1 0 $\bar{1}$) does, and the basal plane of the transformed martensite is parallel to the (1 1 0) plane in both cases. The corresponding calculated results with simple (0 1 1) shear are

$$\mathbf{x} = \begin{bmatrix} 0.140\,36 \\ -0.700\,10 \\ 0.700\,10 \end{bmatrix} \qquad (11)$$

$$\mathbf{n}' = [0.625\,52 \quad 0.685\,44 \quad 0.372\,68] \qquad (12)$$

$$\mathbf{p}' = [0.723\,01 \quad 0.555\,56 \quad 0.410\,62] \qquad (13)$$

$$\mathbf{d} = \begin{bmatrix} 0.085\,13 \\ -0.105\,13 \\ 0.050\,47 \end{bmatrix} \qquad (14)$$

$$L = \begin{bmatrix} 1.016\,65 & -0.047\,34 & 0.003\,33 \\ 0.049\,14 & 0.995\,58 & 0.020\,89 \\ -0.004\,36 & 0.182\,32 & 1.013\,02 \end{bmatrix} \qquad (15)$$

$$D = \begin{bmatrix} 1.061\,55 & 0.047\,29 & 0.034\,96 \\ -0.076\,01 & 0.941\,59 & -0.043\,17 \\ 0.036\,49 & 0.028\,04 & 1.020\,73 \end{bmatrix} \qquad (16)$$

$$m_1 = 0.14439 \quad (17)$$

$$m_2 = 0.24768 \quad (18)$$

These two transformation-invariant plane strains with simple shear planes $(1\,0\,\bar{1})$ and $(0\,1\,1)$, respectively, lead to the $(1\,1\,0)$ plane and $[1\,\bar{1}\,1]$ direction of the parent phase transforming to the $(0\,0\,0\,1)$ plane and $[1\,1\,\bar{2}\,0]$ direction of martensite, as shown in Fig. 6. Thus, the whole system can be called a $(1\,1\,0)$ transformation system. The transformation is expected to result in a Burgers orientation relationship, i.e. $(0\,0\,0\,1)$ and $[1\,1\,\bar{2}\,0]$ of martensite parallel to $(1\,1\,0)$ and $[1\,\bar{1}\,1]$ of the parent phase, respectively. The discrepancies of the transformed orientation from Burgers orientation can be calculated and the results are: $(1\,1\,0)_{\mathrm{b.c.c}} \wedge (0\,0\,0\,1)_{\mathrm{h.c.p}} = 2.78°$ and $[1\,\bar{1}\,1]_{\mathrm{b.c.c}} \wedge [1\,1\,\bar{2}\,0]_{\mathrm{h.c.p}} = 4.07°$. These errors are not negligible and may need some investigation and explanation. However, what is important here is that the symmetrical simple shear planes $(1\,0\,\bar{1})$ and $(0\,1\,1)$ in the $(1\,1\,0)$ system play the same role for the martensite crystallography.

3.3. Transformation twins

During martensite plate growth, $(1\,\bar{1}\,0\,1)$ twins act as a simple shear to meet the needs of the phenomenological theory. This type of twin, i.e. the twins II and III in Fig. 3, could be called growth twins. The growth twins have been discussed thoroughly by Hammond and Kelly [8] and Knowles and Smith [9]. However, planes $(1\,1\,0)$ and $(0\,1\,1)$ are symmetrical with respect to plane $(1\,2\,1)$ in b.c.c. Therefore, $(1\,1\,0)$ and $(0\,1\,1)$ transformation systems should transform martensite plates symmetrically with respect to $(1\,2\,1)$ of b.c.c., which is parallel to $(1\,\bar{1}\,0\,3)$ in h.c.p. martensite. In other words, if two contacting martensite plates are transformed from the $(1\,1\,0)$ system and $(0\,1\,1)$ system, respectively, the plates are $(1\,\bar{1}\,0\,3)$ twins. From the viewpoint of crystallography, a $(1\,\bar{1}\,0\,3)$ twin is also a $(1\,\bar{1}\,0\,1)$ twin in this alloy, as shown in Fig. 5. The difference between these two types of twin lies in the contact interfaces (twin planes). If the inferface is the $(1\,\bar{1}\,0\,1)$ plane, it is the $(1\,\bar{1}\,0\,1)$ twin. If the interface is the $(1\,\bar{1}\,0\,3)$ plane, then it is the $(1\,\bar{1}\,0\,3)$ twin. Thus, the twin relationship between twin I and twin II is $(1\,\bar{1}\,0\,3)$ twin rather than $(1\,\bar{1}\,0\,1)$ twin. Furthermore, this type of twin forms from two transformation systems, i.e. two martensite nuclei or a pair of twin nuclei, but not from the growth of a single martensite plate by the ordinary mechanism; thus they could be called nucleation twins.

It is obvious that, for a certain amount of martensite, the deformation and elastic energy caused by the twin martensites are lower than those caused by a single martensite. This is in favour of the occurrence of twin nuclei. However, the possibility of twin martensite nucleation does depend on the nucleation mechanism. If the mechanism is that suggested by Olson and Cohen [18], the nucleation defects needed are so special that the probability of martensite twin nucleation is extremely low. On the other hand, according to a new nucleation model suggested recently by one of the authors [19], the probability of twin martensite nucleation is high enough to have a practical meaning.

4. Conclusions

1. In the Ti–5Al–2Mo–3Zr alloy, triple twins form during the martensitic transformation. The lattice orientation are rotationally threefold symmetric for the triple twins and mirror-symmetric between any two of the twins, and so are the SAD patterns. However, the morphology is not threefold symmetric, i.e. the interface between twins II and III is the ordinary twin plane $(1\,\bar{1}\,0\,1)$, but the interface between twins I and II is $(1\,\bar{1}\,0\,3)$, i.e. the $(1\,2\,1)$ plane of b.c.c.

2. Two contacting martensite plates containing twins I and II, respectively, might form from a pair of twin nuclei which take $(1\,1\,0)$ and $(0\,1\,1)$ as their basal planes, and thus are symmetric with respect to $(1\,2\,1)$ of b.c.c., i.e. $(1\,\bar{1}\,0\,3)$ of martensite. Naturally, the plane of symmetry becomes the twin boundary. Another type of twin formed during the growth is the ordinary transformation twins of $\{1\,\bar{1}\,0\,1\}$. The configuration of triple twins is favourable in lowering the elastic strain energy.

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