Selection and change in deformation mode to maintain continuity of strains and slip/twinning planes at lamellar boundaries in fatigued TiAl polysynthetically twinned crystals

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Abstract

Change in deformation mode in six types of \(\gamma\) domain \((A_M-C_T)\) and \(\alpha_2\) plates in TiAl polysynthetically twinned (PST) crystals fatigued at a loading axis parallel to lamellar planes with stress amplitude \((\Delta \sigma)\) of 420–450 MPa was examined by the transmission electron microscope focusing on continuity of macroscopic strains and slip/twinning planes at lamellar boundaries. At \(\Delta \sigma = 420\) and 450 MPa, the strain continuity is always maintained at lamellar boundaries by activation of one of the symmetric twinning systems in \(A\)-type domain and selection of the dominant deformation mode between ordinary dislocations and twins in \((B\text{ and }C\text{-type } \gamma\) domain). The \((B\text{ and }C\text{-type } \gamma\) domains of \(B_{54}, B_{53}, C_{52}\) and \(C_{51}\) behave as two sets of \((B_{35}, C_{71})\) and \((B_{75}, C_{51})\), because each set selects either the deformation mode of ordinary dislocations or twins as a dominant system in order to keep macroscopic strain continuity. The set \((B_{54}, C_{52})\) which accounts for a larger volume fraction than the set \((B_{53}, C_{71})\) in TiAl-PST crystals used in this study selected a twinning system at \(\Delta \sigma = 450\) MPa, while ordinary dislocations were selected at \(\Delta \sigma = 420\) MPa. At \(\Delta \sigma = 450\) MPa, twinning deformation prevented the further motion of ordinary dislocations with a Burgers vector parallel to lamellar boundaries, and rapid fatigue hardening occurred accompanied by reduction of the accumulative plastic strain energy. Anomalous change in strain energy during fatigue is influenced by the volume fraction of a set of \((B\text{ and }C\text{-type } \gamma\) domain and the anomalous behavior in fatigued TiAl-PST crystals may disappear when each type of \(\gamma\) domain is equally distributed. © 2002 Elsevier Science Ltd. All rights reserved.

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1. Introduction

A harmonic design of materials by combining different phases with different suitable properties is necessary for development of new functional and/or structural materials. Ni-based super alloys are an example of materials developed successfully on the basis of the harmonic design, and progress has been of sought in Ni-base and other L1\(_2\)-based alloys to improve the registered temperature for practical use [1–4]. A novel combination of intermetallic phases with no disordered phase has recently been focused on the usage of their superior strength at high temperatures. TiAl/Ti\(_3\)Al and MoSi\(_2\)/NbSi\(_2\) containing peculiar lamellae showing good stability at high-temperatures are the most promising candidates because of their excellent oxidation resistance, relatively light weight and superior high-temperature strength. Many excellent reviews and reports on aluminides and silicides have been published [5–13]. Since intermetallics in general show lower crystallographic symmetry than fcc and bcc alloys in disordered state, the operative deformation modes are restricted and deformation transfer at boundaries often affects the macroscopic plastic deformation in duplex intermetallic phases. The transfer mechanisms of deformation in TiAl polysynthetically twinned (PST) crystals with oriented lamellae were investigated as an ideal model for understanding continuity of strains and slip/twinning planes at different types of lamellar boundary such as \(\gamma/\gamma\) domain boundaries and \(\gamma/\alpha_2\) interfaces [14–17]. Detailed transmission electron microscopic studies were also performed in polycrystalline TiAl/Ti\(_3\)Al.
lamellar crystals to determine the reaction and preservation of strain component in two neighboring γ domains and a pair of a γ domain and an α2 plate [18–24]. Zhang et al. for example, showed that the most important factor for slip transfer across γ/α2 interfaces is existence of a common intersection of slip/twinning planes at the interface [22]. The similar transfer was also observed at γ/γ domain boundaries [15,16,22,23].

More recently, lamellar boundaries in TiAl-PST crystals fatigued at φ = 0° where φ is the angle between the loading axis and lamellar plane, at Δσ = 420 MPa were classified into 13 groups composed of three γ/γ true twin, three γ/γ pseudo twin, three γ/γ 120° rotation boundaries and four γ/α2 interfaces on the basis of the Schmid factor for possible slip and twinning systems [17]. They were subdivided into two groups composed of continuous and discontinuous geometry. Detailed analysis of dominant deformation mode by the transmission electron microscope (TEM) showed that macroscopic strain continuity was maintained at all the boundaries. At several boundaries strain continuity was maintained by activation of deformation modes unexpected from Schmid factor consideration. Continuity of macroscopic strains was concluded to be a more effective factor than the continuity of slip/twinning planes and Schmid factors for deformation transfer across the boundary.

In TiAl-PST crystals fatigued at φ = 0° under a constant applied stress amplitude, anomalous behavior in accumulated plastic strain energy appeared with increasing stress amplitude [25]. The energy for each cycle increased with increasing stress amplitude but an anomalous energy drop was observed at around Δσ = 440 MPa. This anomalous behavior was thought to be related to change in the dominant deformation mode from the motion of ordinary dislocations to twinning with increasing stress amplitude in several types of γ domain, but no detailed TEM observation was performed, especially above Δσ = 440 MPa where anomalous accumulation of plastic strain energy appeared in the slip transfer mechanism at lamellar boundaries.

In this article, the continuity of macroscopic strain components at lamellar boundaries was examined geometrically and experimentally in TiAl-PST crystals fatigued at Δσ = 450 MPa in comparison with that at Δσ = 420 MPa reported earlier [17]. The focus was on cause of the anomalous change in plastic strain energy with stress amplitude between 420 and 450 MPa.

2. Experimental procedure

TiAl-PST crystals containing Ti–49.1 at.%Al were prepared and cyclic deformation was performed in a tension/compression mode under a stress amplitude of Δσ = 450 MPa at a frequency of 10 Hz in air at room temperature. The beginning was done in tension. The load was applied at φ = 0° and χ = 0° where χ is the angle between the loading axis and ⟨112⟩ in γ domains. The fatigue test was stopped at 1 × 10⁵ cycles. Experimental details were given in our previous paper [25].

Thin foils were cut parallel to the loading axis and perpendicular to the lamellar planes. As a result, the foil normal was thus selected to be ⟨110⟩ directions in the γ domains and [1210] in the α2 phase. The direction is for example [110] in AM. The foils were thinned to 60 μm thickness and then electrolytically perforated by a twin jet method using a solution of 1:2:7 by volume of perchloric acid/glycerin/methanol at –30 °C. Deformation substructure and continuity of deformation modes in the fatigued samples were examined in a Hitachi H-800 TEM operated at 200 kV.

3. Results

3.1. Geometrical classification of lamellar boundaries

Strain continuity at boundaries is often calculated based on the decomposed reaction of Burgers vector [15–19,21–24]. Lamellar boundaries in TiAl-PST crystals fatigued at Δσ = 420 MPa were classified into 13 types composed of three γ/γ true twin, three γ/γ pseudo twin, three γ/γ 120°-rotation and four γ/α2 interfaces [17]. Since such classification made it possible to understand the roles of slip/twinning transfer at each boundary, the same method was applied to the geometrical classification of boundaries in TiAl-PST crystals fatigued at Δσ = 450 MPa where anomalous accumulation of plastic strain energy appeared.

Since TiAl-PST crystals consist of six types of γ domain, AM, BM, CM, AT, BT and CT, and a single-oriented α2 phase maintaining Blackburn’s orientation relationship, the relationship among γ domains and α2 phase are described on (111) plane in AM, BM and CM, (111) in AT, BT and CT and on the (0001) plane in the α2 phase in Fig. 1. The [X, Y, Z] standard coordinates (S) are also defined in this figure. The loading direction and lamellar plane normal at φ = 0° are parallel to the X and Z axes, respectively. Although the L1₀ structure of γ domain shows a slight tetragonality, the γ phase is regarded as a cubic lattice for simplicity.

Since in TiAl-PST crystals deformed at φ = 0° and χ = 0° slip/twinning occurs on ⟨111⟩ octahedral planes in γ phase and on ⟨110⟩ prism planes in the α2 phase [8,10–12,14,17,25–30], these important crystallographic planes are denoted as 1, 2, 4 and 6 in AM, BM and CM domains, 1, 3, 5 and 7 in AT, BT and CT and 8, 9 and 10 in the α2 phase, respectively, as shown in Fig. 2. They are defined on the basis of the relative orientation relationship to the loading axis and lamellar planes. The same definition was used in our previous paper [17].

The lamellar boundaries can first be classified into three types of γ/γ domain boundary and one γ/α2 interface. The true twin boundary is formed between AM and AT, between BM and CT or between BT and CM; the pseudo twin boundary between AM and BT, between AM and CT, between BM and
Fig. 1. Geometrical orientation relationship among six γ domains, A_M, B_M, C_M, A_T, B_T, and C_T, and the α_2 phase under Blackburn’s orientation relationship on (111) in A_M–C_M, (111) in A_T–C_T, and (0001) in the α_2 phase. The [X, Y, Z] standard coordinate (S) is defined in this figure.

A_T, between B_M and B_T, between C_M and A_T or between A_T and C_T; and the 120° rotation boundary between A_M and B_M, between B_M and C_M, between C_M and A_M, between A_T and B_T, between B_T and C_T or between C_T and A_T. Furthermore, the direction of loading axis should be considered since activated deformation modes roughly depend on the type of γ domain. Schmid factors for possible deformation modes in each γ domain are shown in Table 1. Since the twinning partial moves in one preferential direction, positive and negative values of Schmid factors in compression and tension, respectively, are favorable for twinning. According to Schmid factor consideration, γ domains in

Fig. 2. Schematic illustrations of (111) octahedral slip/twining planes in γ domains and (1100) prism plane in the α_2 phase in TiAl-PST crystals deformed at θ = 0° and χ = 0°. The important crystallographic planes are denoted as (1), (2), (4), and (6) in A_M, B_M and C_M domains, (1), (3), (5) and (7) in A_T, B_T and C_T and (8), (9) and (10) in the α_2 phase.
Table 1
Table 1 shows the Schmid factors for possible slip/twinning systems in TiAl-PST crystals deformed at $\phi = 0^\circ$ and $\chi = 0^\circ$ in γ domains. Twinning in tension and compression is represented by − and +, respectively (twinning in tension: −, twinning in compression: +).

| Slip plane | Type of domain | $A_M$, $A_T$ | $B_M$, $B_T$ | $C_M$, $C_T$ |
|------------|----------------|--------------|--------------|--------------|
| (111)[110] | 0.272          | 0.136        | 0.272        |
| (111)[101] | 0.136          | 0.272        | 0.272        |
| (111)[011] | 0.408          | 0.408        | 0            |
| (111)[112] | +0.314         | −0.395       | −0.157       |
| (111)[110] | 0.272          | 0.272        | 0.136        |
| (111)[011] | 0.408          | 0            | 0.408        |
| (111)[112] | +0.314         | −0.157       | −0.393       |
| (111)[101] | 0              | 0.408        | 0.408        |
| (111)[110] | 0.272          | 0.272        | 0.136        |
| (111)[011] | 0.272          | 0.136        | 0.272        |

TiAl-PST crystals loaded at $\phi = 0^\circ$ and $\chi = 0^\circ$, are classified into two groups of A-type and (B and C)-type, although such a simple classification was finally concluded not to be appreciable in our previous paper [17]; the same conclusion is reached and the simple classification is also not in this article due to the macroscopic strain continuity across the lamellar boundary. For simplicity, however, the Schmid factor is considered in this initial geometrical classification.

Operative deformation modes markedly changed in (B and C)-type γ domain of TiAl-PST crystals fatigued below and above $\Delta \sigma = 440$ MPa [25]. In almost all the (B and C)-type domain, dominant deformation modes seemed to change from the motion of ordinary dislocations with a Burgers vector parallel to lamellar boundaries to twinning across lamellae. Based on Schmid factor and TEM observation in the majority of (B and C)-type domain, dominant deformation modes and their relative incidence in each domain and $\alpha_2$ phase of TiAl-PST crystals fatigued at $\Delta \sigma = 450$ MPa above the critical stress amplitude of 440 MPa are represented by the number of arrows in Fig. 3. The operative deformation modes and their relative incidence are depicted by Burgers vectors projected on the X–Z plane and the number of arrows. The deformation mode with the maximum number of arrows is regarded as the dominant mode in each γ domain or the $\alpha_2$ phase. A similar description was given at $\Delta \sigma = 420$ MPa below 440 MPa in Fig. 2 in our previous paper [17]. The principal difference depending on stress amplitude between 420 and 450 MPa appears in (B and C)-type domain. In $C_M$ domain, for example, (111)[112] twinning in tension and (111)[101] slip in compression are dominant deformation modes at $\Delta \sigma = 450$ MPa, while (111)[110] slip in tension and compression is dominant at $\Delta \sigma = 420$ MPa. Two equivalent deformation modes on symmetrical octahedral [111] planes exist in A-type domain and the $\alpha_2$ phase, while there are no symmetrical planes for the possible operative deformation modes in (B and C)-type domain in tension or compression.

Anyway, Schmid factor consideration leads to classification of three groups composed of ($A_M$, $A_T$), ($B_M$, $B_T$, $C_M$, $C_T$) and the $\alpha_2$ phase independent of the stress amplitude. These three can reconstruct eight types of boundaries similar to the previous classification at $\Delta \sigma = 420$ MPa [17] as shown in Table 2, but the dominant deformation mode at $\Delta \sigma = 450$ MPa is quite different from that at $\Delta \sigma = 420$ MPa as shown in Fig. 3. In this article, hereafter the eight types of boundaries in Table 2 are abbreviated as TT1–In2.

![Fig. 3](image-url)

Fig. 3. The dominant operative deformation modes and their relative intensity in each γ domain and the $\alpha_2$ phase of TiAl-PST crystals fatigued at $\Delta \sigma = 450$ MPa in tension and compression. The relative intensities are qualitatively represented by the number of arrows.
Table 2
Types of boundary formed by adjacent phases in TiAl-PST crystals with oriented lamellae

| Type of boundary | Adjacent phases at boundary |
|------------------|----------------------------|
| True twin-1 (TT1) | $A_T/A_T$ |
| True twin-2 (TT2) | $B_T/B_T$, $B_T/C_T$, $A_T/C_M$ |
| Pseudo twin-1 (PT1) | $A_T/B_R$, $A_T/C_T$, $A_T/B_M$, $A_T/C_M$ |
| Pseudo twin-2 (PT2) | $B_T/B_T$, $B_T/C_T$ |
| Rotation-1 (R1) | $A_T/B_M$, $A_T/B_T$, $A_T/C_M$, $A_T/C_T$ |
| Rotation-2 (R2) | $B_T/C_M$, $B_T/C_T$ |
| Interface-1 (In1) | $\alpha_j/A_M$, $\alpha_j/A_T$ |
| Interface-2 (In2) | $\alpha_j/B_M$, $\alpha_j/B_T$, $\alpha_j/C_M$, $\alpha_j/C_T$ |

3.2. Strain continuity through lamellar boundaries

So far, slip/twinning transfer has been discussed by total strain components represented by Burgers vector before and after the transmission through lamellar boundaries [15,16,21–24]. The same method in our previous paper [17] was applied for the TiAl-PST crystals fatigued at $\Delta\sigma = 450$ MPa.

Macroscopic strain components for each dominant operative deformation mode in TiAl-PST crystals fatigued at $\Delta\sigma = 450$ MPa are given at the true twin boundaries of TT1 and TT2 in Fig. 4, at the pseudo twin boundaries of PT1 and PT2 in Fig. 5, at the $120^\circ$ rotation boundaries of R1 and R2 in Fig. 6 and at the $\gamma/\alpha_2$ interfaces of In1 and In2 in Fig. 7. The depicted dominant deformation modes are based on those in Fig. 3. The components for each mode are regarded as $\langle 110 \rangle$ for two $1/2\langle 110 \rangle$ ordinary dislocations, $\langle 101 \rangle$ for one $\langle 101 \rangle$ superlattice dislocation, $1/2\langle 112 \rangle$ for three $1/6\langle 112 \rangle$ twinning partials and $1/3\langle 1210 \rangle$ for one $1/3\langle 1210 \rangle$ prism dislocation to evaluate the continuity of macroscopic strains at boundaries. The macroscopic components in tension and compression are projected as each vector individually along the X, Y and Z axes on the $X-Z$ plane and $Y-Z$ plane. Conservative and non-conservative components of macroscopic strains through lamellar boundaries are shown by black and white arrows, respectively.

According to our previous study on the continuity of macroscopic strains and slip/twinning planes in TiAl-PST crystals fatigued at $\Delta\sigma = 420$ MPa, the component along the $Y$-axis is the most important to understand the continuity and slip/twinning transfer [17]. The boundaries are distinguished into two groups based on whether the $Y$ component was reserved or not through the boundaries because the direction of this component is useful to determine continuity of the macroscopic strains and slip/twinning planes at boundaries. In $A$-type $\gamma$ domain, choice of the operative mode on the two symmetrical slip/twinning planes determines direction of the $Y$-component, and affects the continuity of the strains and planes. The boundaries neighboring the $A$-type domain are therefore distinguished as $a$-type and $b$-type where the macroscopic strain continuity along the $Y$-axis is or is not maintained, respectively, as seen in TT1, PT1, R1 and In1 boundaries. Although small white arrow at the end of black bar along $Y$-direction can be seen even in $a$-type boundary, macroscopic strain continuity is assumed to be maintained in the present study. A similar classification is possible even at the In2 interface containing no $A$-type domain because the prism slip in the $\alpha_2$ phase can be selected on the symmetrical slip planes. At several boundaries, the strain components are not maintained perfectly

![Fig. 4](image-url)

Continuous and discontinuous components of macroscopic strain projected on the $X-Z$ and $Y-Z$ planes at true twin boundaries (TT1-a, TT1-b and TT2) in TiAl-PST crystals fatigued at $\Delta\sigma = 450$ MPa in tension and compression (labeled T and C, respectively). Continuous and discontinuous components of the macroscopic strain along the X, Y and Z axes are shown by black and white arrows, respectively. The slip/twinning systems assumed in each $\gamma$ domain are described.
along the X and Z axes, but such small discordance may be accommodated by local instigation of the minor deformation mode as observed by several researchers [15,16,18–24]. On the other hand, the continuity of macroscopic strains and slip/twinning planes is essentially maintained at the TT2 boundary and not at PT2 or R2 boundary by the dominant deformation mode expected by Schmid factor consideration.

The continuity for all types of boundary in TiAl-PST crystals fatigued at $\Delta \sigma = 450$ MPa is summarized in Table 3. Although change in strain energy during cyclic deformation is different between $\Delta \sigma = 420$ and 450 MPa, the same classification of boundaries is obtained (see Table 3 in Ref. [17]). However, the dominant deformation mode in (B and C)-type $\gamma$ domain varied depending on the stress amplitude: the motion of ordinary dislocations with a Burgers vector parallel to lamellar boundaries was dominant at $\Delta \sigma = 420$ MPa, while twinning occurred across lamellar

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Fig. 5. Continuous and discontinuous components of macroscopic strain projected on the X–Z and Y–Z planes at pseudotwin boundaries (PT1-a, PT1-b and PT2) in TiAl-PST crystals fatigued at $\Delta \sigma = 450$ MPa in tension and compression (labeled T and C, respectively).

Fig. 6. Continuous and discontinuous components of macroscopic strain projected on the X–Z and Y–Z planes at 120° rotation boundaries (R1-a, R1-b and R2) in TiAl-PST crystals fatigued at $\Delta \sigma = 450$ MPa in tension and compression (labeled T and C, respectively).
boundaries at $\Delta \sigma = 450$ MPa. The $\gamma/\gamma$ domain boundaries and $\gamma/\alpha_2$ interfaces at $\Delta \sigma = 450$ MPa finally can be divided into 13 combinations composed of six continuous and seven discontinuous boundaries similar to those at $\Delta \sigma = 420$ MPa.

3.3. Fatigued microstructure and its analysis in TiAl-PST crystals at $\Delta \sigma = 450$ MPa on the basis of macroscopic strain continuity through lamellar boundaries

Deformation substructures in TiAl-PST crystals fatigued at $\Delta \sigma = 450$ MPa at room temperature to $N = 1 \times 10^5$ cycles were observed by TEM, focusing on slip/twinning transfer through lamellar boundaries on the basis of the 13 classifications in Table 3. The types of $\gamma$ domain, operative dominant deformation modes and boundary types were determined by tilting and g-b analyses in the TEM. Details of the method were described in our previous papers [17,25]. In this crystal, the volume fraction of the ($B_1$, $C_1$) set is relatively larger than that of the ($B_M$, $C_T$) set.

Fig. 8 shows a bright field image and a corresponding schematic illustration in a TiAl-PST crystal fatigued at

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Fig. 7. Continuous and discontinuous components of macroscopic strain projected on the X–Z and Y–Z planes at $\gamma/\alpha_2$ interfaces (In1-a, In1-b, In2-a and In2-b) in TiAl-PST crystals fatigued at $\Delta \sigma = 450$ MPa in tension and compression (labeled T and C, respectively).
Table 3
Classification of the boundaries on the basis of continuity (C, continuous; NC, non-continuous) of macroscopic strains and slip/twinning planes in TiAl-PST crystals fatigued at $\phi = 0^\circ$ and $\chi = 0^\circ$ at $\Delta \sigma = 450$ MPa.

| Type of boundary (wide classification) | Continuity of slip plane (Continuous/Non-continuous) | Type of boundary (narrow classification) |
|---------------------------------------|-----------------------------------------------|----------------------------------------|
| True twin-1 (TT1)                      | C                                             | TT1-a                                  |
| True twin-2 (TT2)                      | NC                                            | TT1-b                                  |
| Pseudo twin-1 (PT1)                    | C                                             | PT1-a                                  |
| Pseudo twin-2 (PT2)                    | NC                                            | PT2                                    |
| Rotation-1 (R1)                        | C                                             | R1-a                                   |
| Rotation-2 (R2)                        | NC                                            | R1-b                                   |
| Interface-1 (In1)                      | C                                             | In1-a                                  |
| Interface-2 (In2)                      | NC                                            | In1-b                                  |

$\Delta \sigma = 450$ MPa. Highly dense deformation twins are observed in all $\gamma$ domains belonging to both A-type and (B and C)-type in this figure, while $B_M$ and $C_T$ domains as the minor constituent do not exist in this area. Since all twinning planes are edged on at the incident beam parallel to [011] in $A_M$, they are determined to be (111) (1:4) in $A_M$, (111) (1:4) in $C_M$, (111) (1:5) in $A_T$ and (111) (1:5) in $B_T$. This beam direction was obtained by the foil rotated 60° about the [111] zone axis. Moreover, the (1100)[1110] prism slip was operative on (111) plane in the $\alpha_2$ phase. Continuity of macroscopic strains and slip/twinning planes is therefore maintained and all boundaries are the continuous type in Table 3. It should be noted that the slip/twinning plane in $A_M$ domain and the prism slip plane in the $\alpha_2$ phase are selected between two symmetrical planes so that macroscopic strain transfer occurs through the boundaries. In addition, (101) superlattice dislocations are also operative on the plane parallel to the deformation twinning planes in $A_M$, $A_T$, $B_T$ and $C_M$ domains. The Burgers vector of (101) dislocations is parallel to the lamellar boundaries as shown in Fig. 3 and often decomposes into 1/2[112] and 1/2[110] dislocations as reported by several researchers [14,31,32].

Fig. 8. A bright-field image and the corresponding schematic illustration in TiAl-PST crystals fatigued at $\Delta \sigma = 450$ MPa to $1 \times 10^5$ cycles. The beam direction is parallel to [011] in $A_M$. 
Of course, minor slip/twinning modes were activated to accommodate local residual strain, and the detailed analysis on the fatigued TiAl-PST crystals was done in our previous paper [25].

Fig. 9 shows the fatigued microstructure containing $B_M$ and $C_T$ domains which are not seen in Fig. 8. In this area, all types of boundary under the wide classification in Table 3 exist: TT1, TT2, PT1, PT2, R1, R2, In1 and In2. Detailed TEM observation and its analysis clarified that the $1/2\langle 110 \rangle$ ordinary dislocations with a Burgers vector parallel to lamellar boundaries were dominantly activated in $B_M$ and $C_T$ domains which account for a relatively smaller volume fraction than $B_T$ and $C_T$ lamellae. The ordinary dislocations by $\langle 110 \rangle$ on $\langle 1\bar{1}1 \rangle$ plane in $B_M$ and $\langle 1\bar{1}0 \rangle$ on $\langle \bar{1}\bar{1}1 \rangle$ plane in $C_T$ were found to operate. Low-dense traces for twins were also observed to maintain the continuity of local strains but dominant strains. If the twins are dominantly activated in spite of the activation of ordinary dislocations on the basis of Schmid factor consideration in $B_M$ and $C_T$ domains, boundaries surrounding the domains would behave as discontinuous boundaries which could not maintain the continuity of macroscopic strains and slip/twinning planes. Such possible discontinuous boundaries of PT1-b, PT2, R1-b and R2 are represented by bold lines in Fig. 9, but change in the dominant deformation mode from twins to ordinary dislocations in the $B_M$ and $C_T$ domains indeed makes it possible to maintain the continuity of macroscopic strains and slip/twinning planes through lamellar boundaries. This result indicates that the continuity of macroscopic strains has priority over Schmid factor consideration as suggested in TiAl-PST crystals fatigued at $\Delta \sigma = 420$ MPa [17]. The operative deformation mode of ordinary dislocations in the minor set of $B_M$ and $C_T$ domains at $\Delta \sigma = 450$ MPa is in good accordance with that in the major set of $B_T$ and $C_M$ domains at $\Delta \sigma = 420$ MPa. Since the dominant deformation mode in the major set of $B_T$ and $C_M$ domains with the larger volume fraction becomes twinning at $\Delta \sigma = 450$ MPa, a favorable applied stress to activate twins as well as ordinary dislocations in (B and C)-type domain must be reached on the viewpoint of Schmid factor consideration, while twins hardly appear in the set of $B_M$ and $C_T$ domains with the smaller volume fraction. This result strongly suggests that the continuity of macroscopic strains and slip/twinning planes is the most important factor in selecting the deformation mode in $\gamma$ domains and the $\alpha_2$ plate.

Fig. 10 shows the fatigued microstructure containing the $\alpha_2$ phase bounded by In1 and In2 boundaries. In the $\alpha_2$ phase, the to-and-fro motion of $1/3[\bar{1}\bar{1}0]$ prism dislocations occurs on the $\langle \bar{1}00 \rangle$ plane (51). As a result, macroscopic continuity is maintained at the interfaces of In1-a and In2-a, and almost all slip traces of the prism dislocations in the $\alpha_2$ phase immediately connect to twinning traces in the neighboring $\gamma$ domains. In TiAl-PST crystals fatigued at $\Delta \sigma = 420$ MPa, the prism slip in the $\alpha_2$ phase was induced by the operation of twins, but by ordinary dislocations in the
neighboring γ domains due to the stress concentration [17].

In the crystal fatigued at Δσ = 450 MPa twinning is a dominant deformation mode in AM, AT, BT and CM, accounting for almost the entire volume fraction in lamellae (as shown later in Fig. 11). Thus, highly dense traces by the prism slip may become marked as shown in Fig. 10. This TEM observation corresponds to the slip trace on prism planes in the α2 phase on the surface of TiAl-PST crystals becoming remarkable and more uniform with increasing stress amplitude over Δσ = 440 MPa, where anomalous strain energy accumulation occurs as shown in the previous paper [17]. According to the high resolution X-ray measurement, the residual strain accumulated in the α2 phase in TiAl-PST crystals fatigued at Δσ = 450 MPa is smaller than that at Δσ = 420 MPa [33]. This suggests that activation of uniform and highly-dense prism dislocations induced by highly dense twins in γ domains accommodates and reduces the residual elastic strain in the α2 phase.

4. Discussion

In TiAl-PST crystals fatigued at Δσ = 450 MPa where plastic strain energy was anomaly accumulated, the continuity of macroscopic strains and slip/twinning planes was maintained through all lamellar boundaries similar to that at Δσ = 420 MPa. The major difference at stress amplitudes of both 450 and 420 MPa appears in dominant deformation modes in (B and C)-type domain: twins at

![Fig. 10. A bright-field image and the corresponding schematic illustration in TiAl-PST crystals fatigued at Δσ = 450 MPa to 1 × 10^5 cycles. The beam direction is parallel to [011] in AM.](image)

![Fig. 11. Schematic illustration showing traces of operative dominant slip/twinning in TiAl-PST crystals below and above Δσ = 440 MPa. Volume fraction of the set of (BT and C2) is assumed to be larger than that of (B24 and C) in this figure. The macroscopic shear direction is changed below and above Δσ = 440 MPa. Continuity of macroscopic strains and slip/twinning planes is maintained.](image)
Δσ = 450 MPa and ordinary dislocations at Δσ = 420 MPa in the set of (Bγ and Cγ) domains with the larger volume fraction than the (B_M and C_T) set.

The γ domains of A_M–C_T are produced during α–γ transformation, avoiding an increase in crystal strain, thus the six types of γ domain are ideally distributed having equal volume fraction for each domain. However, lamellar boundaries in TiAl-PST crystals are not necessarily parallel or perpendicular to the direction of crystal growth and heat transfer. Inui et al. also reported that there is priority in the selection of types of boundary due to their different energies [34]. As a result, distribution of γ domain type A_M–C_T is not necessarily equal as reported by Zghal et al. [35]. This uneven distribution of volume fraction for each γ domain plays as an important role in the anomalous strain energy accumulation and is discussed in this section.

Fig. 11 shows a schematic illustration of traces parallel to the dominantly operative slip/twinning planes in TiAl-PST crystals fatigued below and above Δσ = 440 MPa. Volume fraction of the set of (Bγ and Cγ) is assumed to be larger than that of (B_M and C_T) in accordance with the TEM observation. Since the macroscopic continuity of strains through boundaries is maintained independent of stress amplitude, the similar deformation mode appears in each set of γ domains: below Δσ = 440 MPa, twins in A_M, A_T, B_M and C_T and ordinary dislocations in B_T and C_M and above Δσ = 440 MPa, twins in A_M, A_T, B_T and C_M and ordinary dislocations in B_M and C_T. However, the direction of operative dominant slip/twinning traces and the volume fraction for activation of each mode are, of course, quite different as described in Fig. 11.

Since the dominant deformation mode does not change remarkably in A type domain, a discontinuous change in fatigue behavior with increasing stress amplitude is closely related to the deformation mode in (B and C)-type domain. The dominant deformation mode in each set of (B_M and C_T) or (B_T and C_M) is selected depending on the relative volume fraction of the two sets in the initial stage of fatigue deformation. Twinning observed frequently in the (B and C)-type domain is a possible dominant deformation mode in tension, while that in A-type domain is possible in compression. The twin formation in (B and C)-type domain is known to restrict the following operation of ordinary dislocations on another symmetrical slip plane [17,25].

Although in the initial stage of TiAl-PST crystals fatigued at Δσ = 450 MPa slip by the ordinary dislocations is selected as a dominant deformation mode due to sufficiently high applied stress for activation of the slip, an increase in the number of twin interrupts the to-and-fro motion of the ordinary dislocations in the crystal fatigued above Δσ = 440 MPa and the slip/twinning planes different from those below Δσ = 440 MPa are selected. The restriction of motion of ordinary dislocations by the twins introduced earlier may contribute to rapid fatigue hardening and the following reduction of accumulated plastic strain energy. The uneven distribution of volume fraction for two sets of (B and C)-type domain changes the relative activation of dominant deformation mode between the ordinary dislocations and twins in the two sets, resulting in the anomalous fatigue behavior. This alludes to disappearance of the anomalous change in accumulated plastic strain energy in TiAl-PST crystals when six types of γ domain with equal volume fraction are uniformly distributed in lamellae. Thus, distribution in volume fraction for each (B and C)-type domain, especially between the two sets (B_T and C_M) and (B_M and C_T), is an important factor for controlling the fatigue hardening behavior in TiAl-PST crystals with a loading axis parallel to lamellar boundaries.

Kishida et al. clearly showed that macroscopic shape change during deformation proceeds in an anisotropic manner in TiAl-PST crystals deformed at φ = 0° [14]. The crystals tend to increase the width along the Y-axis but not to change it along the Z-axis. This is explained by negligible value of the normal strain in the direction perpendicular to the lamellar boundaries. Similar anisotropic shape change was observed in TiAl-PST crystals fatigued at φ = 0° at both Δσ = 420 MPa and Δσ = 450 MPa. In the fatigued crystals, dominant operative slip/twinning planes vary with selection of a deformation mode depending on the distribution of (B and C)-type domain; a schematic illustration of anisotropic shape change is predicted in Table 4. In this table, the volume fraction in the set (B_T and C_M) is assumed to be larger than that in the set (B_M and C_T). Since the shear direction changes above and below Δσ = 440 MPa where anomalous plastic strain energy accumulation occurs as shown in Fig. 11, the shape change on lamellar plane of the X–Y plane is symmetrical under both stress conditions. This suggests that the spatial distribution of γ domains in lamellae possibly controls the

| Table 4 | Schematic illustration showing macroscopic shape change on lamellar planes in TiAl-PST crystals fatigued at φ = 0°, χ = 0° below and above Δσ = 440 MPa in tension/compression modes. Volume fraction of the set of (B_T and C_M) is assumed to be larger than that of (B_M and C_T) in this table |
|---------|----------------------------------------------------------------------------------|
| **Below Δσ = 440 Mpa** | ![Diagram](image) |
| **Above Δσ = 440 Mpa** | ![Diagram](image) |
macroscopic deformation, especially fatigue deformation. In particular, twin formation plays an important role in restricting the further operative deformation mode in both tension and compression.

5. Conclusions

For TiAl-PST crystals fatigued at $\phi = 0^\circ$ and $\Delta \sigma = 450$ MPa where anomalous accumulation of plastic strain energy appeared, geometrical classification of lamellar boundaries and detailed TEM observation of dominant deformation mode were carried out focusing on continuity of macroscopic strains and slip/twinning planes. The following conclusions were reached.

1. Lamellar boundaries can be classified into thirteen groups in the TiAl-PST crystal fatigued at $\Delta \sigma = 450$ MPa with $\phi = 0^\circ$ and $\chi = 0^\circ$, and subdivided into two groups of six continuous-types and seven discontinuous-types on the basis of continuity of macroscopic strains and slip/twinning planes.

2. In TiAl-PST crystal fatigued at $\Delta \sigma = 450$ MPa, the dominant deformation mode in the (B_M and C_T) set occupies the relatively smaller volume fraction changes from twins to ordinary dislocations with the Burgers vector parallel to lamellar boundaries to maintain continuity of macroscopic strains and slip/twinning planes. In another set of (B_T and C_M), highly dense twins are activated as the dominant mode. Distribution of (B and C) typ domain is one of the most important controlling factors for rapid accumulation of plastic strain energy because the dominant deformation modes are shifted from the ordinary dislocations to twins and vice versa in each set of (B_M and C_T) and (B_T and C_M), respectively, with increasing stress amplitude through $\Delta \sigma = 440$ MPa. Twinning in the (B and C) type domain in the initial stage of fatigue deformation restricts the subsequent to-and-fro motion of the ordinary dislocations, resulting in the rapid fatigue hardening.

3. Since the shear direction is changed above and below $\Delta \sigma = 440$ MPa where an anomalous peak of accumulated plastic strain energy appears, the shape change on the lamellar plane of $X$–$Y$ plane is symmetrical under both stress conditions. This macroscopic shape change is opposite in tension and compression.

4. A large number of twins promote introduction of homogeneous slip traces on the prism planes in the $\alpha_2$ phase.

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