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Transgranular slip and fracture across an interface in α-β brass two-phase bicrystals

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The passage of slip and the transgranular fracture across the interface of α–β brass two-phase bicrystals were investigated in connection with the orientation relationships of the bicrystals. The passage of slip across the interface was observed in the slip systems with misorientation less than 10 degrees. These results were related to the interface dislocation created when a dislocation propagates across the interface. The twist disclination model proposed by Marcinkowski for the passage of a dislocation across the twist boundary was recognized at the interface of the present two-phase bicrystals. The initiation and the propagation of the transgranular crack was seen at the interface where the passage of slip was investigated. It was noted that this transgranular crack was caused by the high stress field around the deformation ledge created when many dislocations passed through the interface.

1. Introduction

The passage of dislocations across a grain boundary and/or a phase boundary is quite an important problem associated with the deformation of polycrystals and duplex alloys. A series of theoretical studies on the interactions between dislocations and grain boundaries have been reported by Marcinkowski *et al.* [1–6], but there have been very few experimental observations despite current interest in this topic. A few reports have been published about the continuity of slip traces across the boundary, such as those in mono-phase bicrystals [7, 8] and in α-brass [9]. The study of the dislocation (slip) passage phenomenon across the interface in a two-phase bicrystal consisting of two different crystal structures is much more complicated and has not yet been reported.

It was shown by Marcinkowski *et al.* [2, 10] that the passage of dislocations across an interface in general creates grain boundary dislocations (the grain boundary ledges) and the large strain field may cause grain boundary fracture. However, few experimental observations have been made on this phenomenon.

The present authors have been studying the deformation behaviours [11–13] of the α–β brass two-phase bicrystals which consist of a f c c (α) and b c c (β) single crystals. The two-phase bicrystals satisfied an orientation relationship; the close packed planes $\{1\,1\,1\}$ in α crystal and $\{1\,1\,0\}$ in β crystal matched at the interface to within few degrees. Since these matching planes corresponded to the predominant slip planes in both crystals, the passage of the dislocation [11] and the resultant fracture phenomenon [13] were observed.. The precise interpretation of these observations is now possible since the information of the microscopic interface structure has been reported [14]. In the present investigation, the propagation of slip and the transgranular fracture across the interface of the α–β brass two-phase bicrystals are represented and discussed in connection with the pre-existing theories.

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2. Experimental procedure

2.1. Preparation of bicrystals and the tensile test

A detailed procedure for the preparation of the α–β two-phase bicrystals was described elsewhere [11]. The orientation relationship between the two single crystals was determined by the X-ray Laue method. A tensile specimen in which the interface was parallel to the tensile axis was cut from a bicrystal by a spark-cutting machine with the gauge dimensions of length 18 mm, width 3 mm and thickness 2 mm. The specimen was electro-polished in a solution of three parts phosphoric acid, one part water and one part ethyl alcohol. Tensile test was carried out at room temperature with a cross-head speed of 0.05 mm min^{-1} using an Instron type machine. The slip traces were observed by optical microscopy at the desired tensile strain stage. In order to investigate the dynamic fracture behaviour, an *in situ* observation was done using scanning electron microscopy (SEM). The bicrystals unnotched and notched in each crystal, and 0.1 to 0.2 mm in diameter were tensile-tested on a special stage at a cross-head speed of 0.05 mm min^{-1} which permits a reasonable rate of deformation, and initiation and growth of the crack. In conjunction with SEM was a high performance video tape unit prepared for recording the dynamic fracture process.

3. Experimental results and discussion

3.1. Propagation of slip across an interface

In the present α–β brass two-phase bicrystals, the predominant slip plane $\{1\,1\,1\}_\alpha$ in α crystal and $\{1\,1\,0\}_\beta$ in β crystal always plane-matched at the interface within few degrees. Therefore, if the resolved shear stress on these planes is high enough and the slip on one of these planes is activated, the passage of slip across the interface is anticipated. Since the critical resolved shear stress in α crystal [15] is lower than that in β crystal [16–18], the passage of slip from α crystal across the interface may be expected in the early stage of deformation. Figs. 1a and b show the evidence of the passage of slip across the interface at about three per cent plastic strain. In both bicrystals, the matching plane $(1\,1\,1)_\alpha$ in α crystal was activated as the primary slip plane (the highest resolved shear stress). Where the slip bands activated in the matrix of α crystal met the interface, slip is observed to have propagated a short distance along the matching plane of β crystal though the primary slip plane $(\bar{1}\,0\,1)$ in β crystal was activated. The difference between the two slip systems in which the passage of slip was observed is characterized by both the angle difference between the normal directions to slip planes ($\cos^{-1}(n_\alpha \cdot n_\beta)$) and that between the slip directions ($\cos^{-1}(b_\alpha \cdot b_\beta)$). The two parameters in bicrystals observed in Figs. 1a and b were 2° and 4°, and 6° and 7° respectively. The passage behaviour in the former bicrystal was more remarkable than in the latter bicrystal. The passage of slip depends not only on the angle difference between the two slip systems but also on the difference in the magnitudes of the two Burgers vectors. According to the lattice parameters for the chemical compositions in both crystals equilibrated at the interface, i.e. $a_\alpha = 3.692$ Å and $a_\beta = 2.955$ Å [19], the magnitudes of the Burgers vectors of the dislocations in both crystals, i.e. $b_\alpha = 2.611$ Å and $b_\beta = 2.559$ Å are obtained. The difference between them is about 2% which is very small. Thus, a small angle difference between the two slip systems and a small difference of the

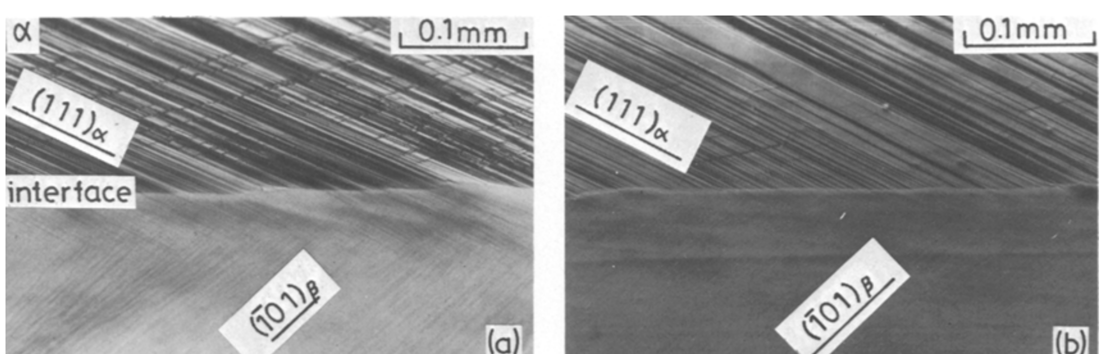

Figure 1 Transgranular slip across an interface of α–β brass two-phase bicrystal. (a) $\cos^{-1}(n_\alpha \cdot n_\beta) = 2^\circ$, $\cos^{-1}(b_\alpha \cdot b_\beta) = 4^\circ$; (b) $\cos^{-1}(n_\alpha \cdot n_\beta) = 6^\circ$, $\cos^{-1}(b_\alpha \cdot b_\beta) = 7^\circ$.

TABLE I Orientation parameters in bicrystals in which the passage of slip was observed

Bicrystal	Orientation parameter (°)			
	$\cos^{-1}(n_\alpha \cdot n_\beta)$	$\cos^{-1}(b_\alpha \cdot b_\beta)$	$\cos^{-1}(n_\alpha \cdot n_I)$	$\cos^{-1}(b_\alpha \cdot n_I)$
1	2	4	30	72
2	2	1	21	86
3	10	10	84	71
4	3	2	24	86
5	8	2	47	86
6	6	7	31	76

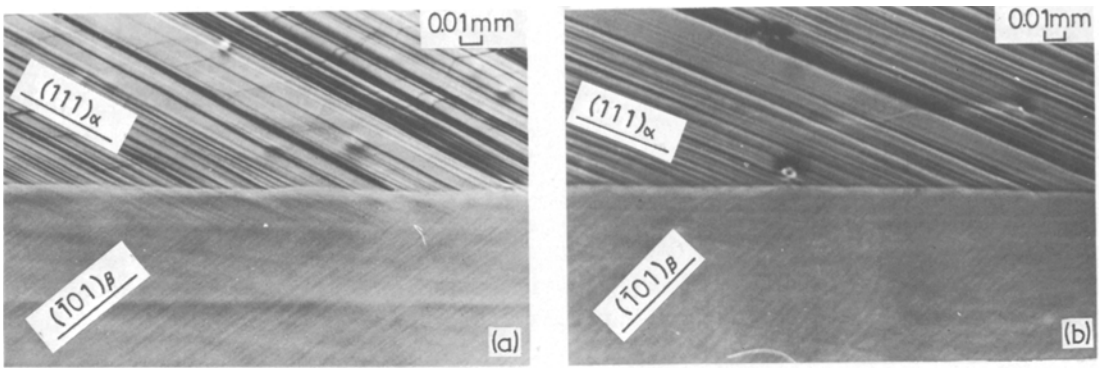

Figure 2 Slip patterns in two bicrystals whose α crystals have the same orientations but whose β crystals have a different orientation. Note that the passage of slip is seen in (a) [$\cos^{-1}(n_\alpha \cdot n_\beta) = 6°$, $\cos^{-1}(b_\alpha \cdot b_\beta) = 8°$], but not in (b) [$\cos^{-1}(n_\alpha \cdot n_\beta) = 13°$, $\cos^{-1}(b_\alpha \cdot b_\beta) = 19°$].

magnitudes between the two Burgers vectors intimate that the interface would be penetrated by the dislocations.

Table I lists the bicrystals in which the passage of slip across the interface occurred. In this table, the second column shows the angle difference between two normal directions to the slip planes, $\cos^{-1}(n_\alpha \cdot n_\beta)$, the third column the angle difference between two slip directions, $\cos^{-1}(b_\alpha \cdot b_\beta)$. The fourth and fifth columns mean the angle difference between the normal to the interface and the normal to the slip plane in α crystal, $\cos^{-1}(n_\alpha \cdot n_I)$, and that between the normal to the interface and the slip direction in α crystal, $\cos^{-1}(b_\alpha \cdot n_I)$. From this table we can see that the passage does not depend on the last two parameters but depends on the first two parameters. Only in the bicrystals in which the angle difference between the two slip systems is less than about 10 degrees was the passage of slip observable. The passage behaviour has never been observed in slip systems with an angle difference greater than 10 degrees.

Figs. 2a and b show the slip patterns in two bicrystals whose α crystals are in the same orientation relationship with respect to the interface plane but β crystals are differently oriented. The passage of slip was seen in (a) but not in (b). The angle differences between the two normals to the slip planes and that between the two slip directions were 6° and 8° in the former bicrystal, while in the latter bicrystal were 13° and 19°, respectively. It is clear from the observation of these two bicrystals that the passage of slip is suppressed with increasing the difference between two slip systems.

Fig. 3 shows the slip pattern in a bicrystal in which double slip occurred in α crystal. While the

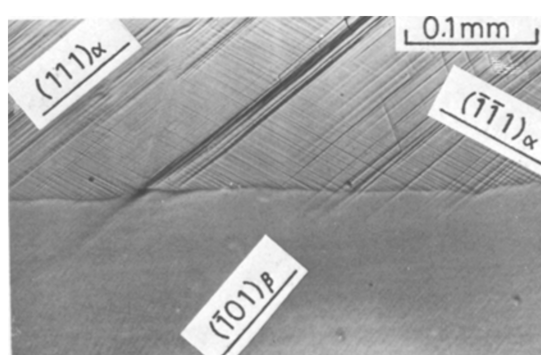

Figure 3 Slip pattern in the bicrystal in which double slip occurred in the α crystal. Note that the slip on $(1\,1\,1)_\alpha$ propagated across the interface, but the slip on $(\bar{1}\,\bar{1}\,1)_\alpha$ did not.

slip bands on one slip plane $(1\,1\,1)_\alpha$ propagated into β crystal, the slip bands on another slip plane $(\bar{1}\,\bar{1}\,1)_\alpha$ did not cross the interface. The passage of slip occurred in the slip systems with the plane-matching relation. It is also found in this observation that one of the factors which controls the passage of slip is the angle difference between two slip systems.

Marcinkowski *et al.* [1–5] reported that the Burgers vector of an interface dislocation b_I which is formed when a dislocation of one crystal passes through the interface and moves on the other crystal, can be represented as

$$b_\mathrm{I} = (b_\alpha - a b_\beta) \quad (1)$$

where b_α and b_β are the Burgers vectors when a dislocation lies on two crystals, respectively, and a is the transformation matrix described. In bicrystals of a given orientation relationship (as in the present bicrystals), the interface dislocation b_I created by the passage of a dislocation across the interface is presented as follows.

$$|b_\mathrm{I}| \simeq 2b_\alpha \sin(\theta/2) \simeq 2b_\beta \sin(\theta/2) \quad (2)$$

It is a mixed sessile dislocation, where θ is the angle difference between the Burgers vectors of two dislocations.

A large misorientation requires an interface dislocation with a larger Burgers vector which is energetically unfavourable. It is energetically more favourable that a dislocation in α crystal penetrates into the slip system in β crystal with smaller misorientation. Thus, the passage of dislocations in slip systems with the plane-matching relation is interpreted primarily by the low strength of the interface dislocation created. Furthermore, Equation 2 suggests that the creation of the interface dislocation (the passage of a dislocation) does not depend on the parameter of the interface normal direction n_I. This prediction is in agreement with the present results as seen in Table I. The critical misorientation (about 10 degrees) for the passage of a dislocation is not deduced from the conservation rule of the Burgers vector and its energy consideration.

The interface structure in the present bicrystal has been observed by transmission electron microscopy [14]. The spacing and direction of the intrinsic interface dislocation depend on the misorientation and spacing between $\{1\,1\,1\}_\alpha$ and $\{1\,1\,0\}_\beta$, as shown in Fig. 4. Since the intrinsic interface dislocations in general incline to the traces of the slip planes in both crystals, they will act as the resistance against the passage of a dislocation. With increase of misorientation, the spacing of the intrinsic dislocation becomes smaller. Therefore, the passage of a dislocation across the interface with larger misorientation becomes restricted.

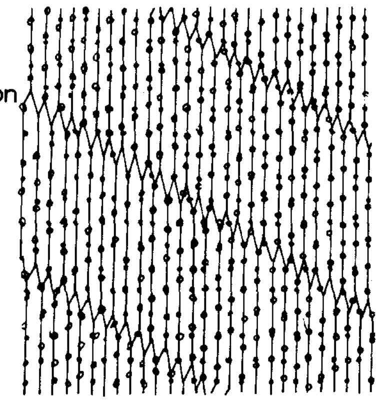

Figure 4 Interface structure observed in the present α–β brass two-phase bicrystal.

Marcinkowski *et al.* [1–4] studied several cases involving the passage of edge, screw and mixed dislocations across symmetric, asymmetric or twist boundaries. They reported that the disturbance b_I left at a twist boundary after the passage of an edge dislocation could not be explained satisfactorily by the interface dislocations, and suggested the "twist disclination loop" model [5] for this passage as shown in Fig. 5. This brings two crystals to crystallographic matching within the disclination loop and allows the edge dislocation to slip from one crystal to another crystal. The orientation relation for plane-matching of the two crystals observed in the present bicrystals has a twist component. An atom relaxation on or near the interface creates the fit region and misfit

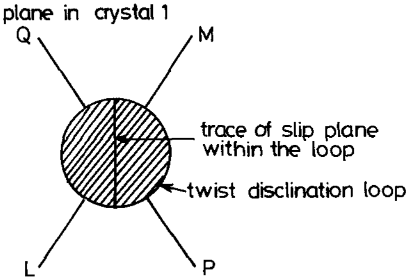

Figure 5 Schematic illustration showing a twist disclination model (after Das [6]).

region. The former region corresponds to the "twist disclination loop" and the latter region corresponds to the intrinsic interface dislocation. Thus, the "twist disclination loop" proposed by Marcinkowski [5] is recognized in the present α–β brass two-phase bicrystals. The edge dislocation can propagate across the interface with the twist component through this fit region (twist disclination loop). It should be noted that the precise and more microscopic interpretation for the passage of a dislocation should be given by the direct observation.

3.2. Transgranular fracture across the interface

Before discussing this subject, the predominant fracture planes in both crystals must be mentioned. It was clarified by the trace analysis of the fracture planes that β crystal fractured on the $\{1\,1\,0\}_\beta$ and α crystal fractured on the $\{1\,1\,1\}_\alpha$ in a ductile fracture mode [13]; each fracture plane coincided with each slip plane.

The clear evidence for the initiation of the transgranular fracture is shown in Fig. 6a which was taken during the direct observation in a SEM. The dynamic observation showed that the crack appeared from notch root in β crystal and propagated as 1 in Fig. 6a on $(\bar{1}\,\bar{1}\,0)_\beta$ then new transgranular crack 2 having a different direction initiated at the interface before the former crack arrived at the interface. This new crack propagated along predominant fracture planes in both phases, i.e. along slip planes $(\bar{1}\,0\,\bar{1})_\beta$ and $(1\,1\,1)_\alpha$ both of which coincided with the matching planes. The appearance of the transgranular crack just at the interface and the resultant alternation of the fracture plane is qualitatively explained by the lack of predominant fracture planes on the extension of the crack 1 propagated from the notch root. The fracture surface after the complete fracturing, as represented in Fig. 6c, revealed such a fracture sequence. The passage of the slip across the interface is seen in the region in which this transgranular crack appeared. Therefore, it seems that the newly appeared transgranular crack was caused by the passage of slip across the interface.

Marcinkowski *et al.* [2, 20] reported a detailed discussion on the grain boundary fracture associated with the "deformation ledge" created by the passage of the dislocations. As the deformation increases and many dislocations pass through the interface, the strength of the "deformation ledge" becomes larger and introduces a high strain field around this as shown in Fig. 7. Since the deformation ledge created in present bicrystal is in general a mixed one as predicted already, a complicated strain field will be created. The strain field

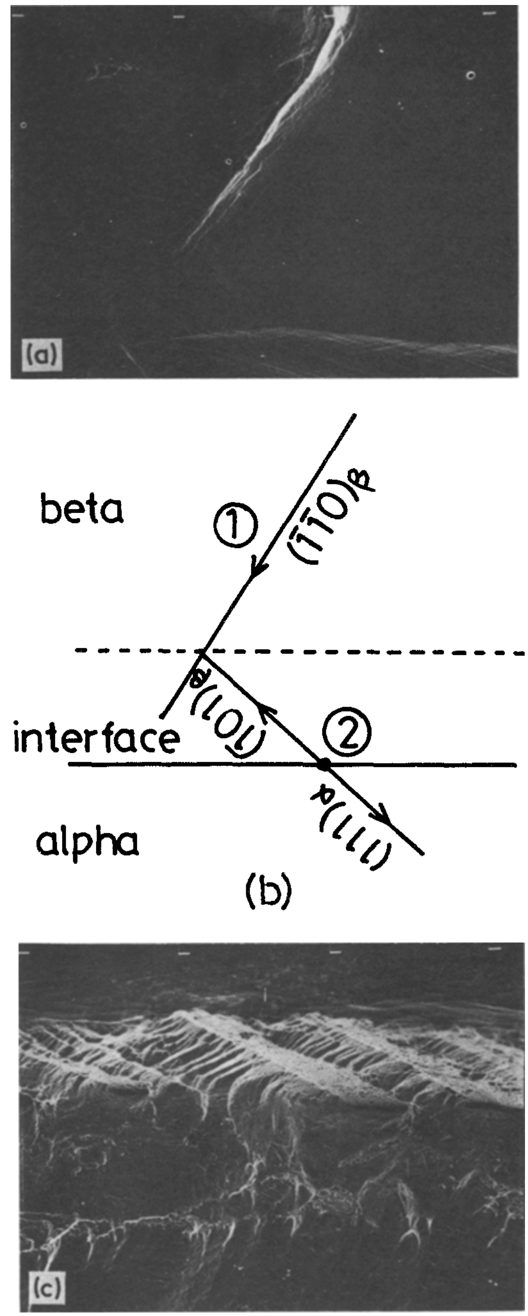

Figure 6 (a) Initiation of the transgranular fracture at the interface. (b) Schematic illustration showing the sequence of the crack propagation. (c) Fracture surface after the complete fracturing.

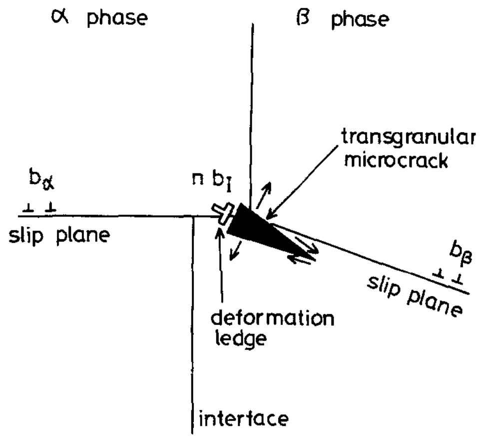

Figure 7 Schematic illustration showing the deformation ledge created by the passage of several dislocations and the transgranular microcrack caused by the high stress.

activates the crystallographic slip (dislocation) up to a given plastic strain. As this crystallographic slip work-hardens and the strength of the deformation ledge increases by the further passages of dislocations, the crack is spontaneously formed depending on the energy of cracked surface and the total applied stress (normal applied stress and incompatible stress induced by the constraint). In general, this crack is a mixed type, i.e. a transgranular microcrack having tensile and shear components. Thus, it is believed that the transgranular microcrack shown in Fig. 6 was caused by a high stress created by the deformation ledge and with the assistance of the total applied stress. The estimation of the exact direction, the size and the beginning strain of the transgranular crack is difficult because they depend not only upon the orientation relation but also upon the work-hardening properties and the surface energies of both crystals.

4. Summary

The transgranular slip and fracture across the interface of α–β brass two-phase bicrystals were investigated by the optical and scanning electron microscopies. The following results are summarized.

(1) The slips activated in α crystal were observed to pass through the interface when the misorientation of slip systems between two crystals were less than about 10 degrees. This behaviour was discussed in relation to the property of the interface dislocation. It was shown that the smaller misorientation at the interface leads to a lower strength of the Burgers vector of the interface dislocation and allows the easy passage of slips. The twist disclination model proposed by Marcinkowski for the passage of an edge dislocation across the twist boundary was recognized at the interface of the present α–β brass two-phase bicrystal.

(2) The initiation and propagation of the transgranular crack were observed at the interface where the passage of slip was severe. This transgranular crack seemed to be caused by the high stress field around the deformation ledge created by many dislocations passing through the interface.

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