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Effect of compositional deviations from stoichiometry on the plastic behaviour of Ti_3Al single crystals

T. Nakano and Y. Umakoshi*
Department of Materials Science and Engineering, Faculty of Engineering, Osaka University, 2-1, Yamada-oka, Suita, Osaka 565 (Japan)

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Abstract

Ti_3Al single crystals containing 24.4, 33.0 and 40.0 at.% Al were grown by a floating zone method and deformed in compression at room temperature. The effect of Al content on the slip geometry, yield stress and ductility was investigated. Prism $\{10\bar{1}0\}\langle 1\bar{2}10\rangle$, basal $(0001)\langle 1\bar{2}10\rangle$ and pyramidal $\{11\bar{2}1\}\langle 11\bar{2}\bar{6}\rangle$ slips were observed depending on the crystal orientation. The prism slip was more common than the other slip systems and the pyramidal slip was limited to orientations near [0001]. The critical resolved shear stress for the prism and pyramidal slip systems increased with increasing Al content, while the basal slip was not strongly affected by the aluminium content. Ti_3Al crystals could easily be deformed by the prism slip up to more than 30% strain without any cracks, while deformation by the pyramidal and/or basal slips was accompanied by poor ductility. Brittleness was increasingly noticeable with higher Al content.

1. Introduction

Extensive study of the deformation behaviour of TiAl alloys has proven TiAl to be a new high temperature structural material with superior strength-to-weight ratio and excellent oxidation resistance. In particular, attractive mechanical properties have been found in two-phase Ti-rich TiAl alloys composed of the γ matrix and a small amount of α_2 (ordered Ti_3Al) phase with lamellar structure [1–3]. Very recently, Umakoshi and coworkers found that the plastic behaviour of TiAl was strongly influenced by the anisotropy of the deformation mode of the α_2 phase in lamellae [4–6]. More information on the plastic behaviour of the α_2 phase and attempts to control it are required to obtain TiAl with a good balance of higher strength and better ductility.

According to recent results using single crystals, Ti_3Al with a near-stoichiometric composition is predominantly deformed by the prism $\{10\bar{1}0\}\langle 1\bar{2}10\rangle$ slip, while the pyramidal $\{11\bar{2}1\}\langle 11\bar{2}\bar{6}\rangle$ slip appears only for an orientation very close to [0001] [7–9]. The critical resolved shear stress (CRSS) for the pyramidal slip is 7.4 times higher than that for the prism slip [9]. In the equilibrium phase diagram of the Ti–Al system the α_2 phase has wide solubility on the Al-rich side of off-stoichiometry [10]. The α_2 phase in equilibrium with the γ matrix in lamellar TiAl has a high Al concentration, deviating from a stoichiometric Ti_3Al alloy. It is well known that the plastic behaviour of intermetallics depends strongly on their composition, particularly deviations from stoichiometry as seen in NiAl, FeAl, Ni_3Al and so on (see the review by Yamaguchi and Umakoshi [11]).

In this study the effect of Al content on the slip systems and mechanical properties of Ti_3Al was examined using single crystals of stoichiometric and Al-rich Ti_3Al to understand the plastic behaviour of the α_2 phase in lamellar TiAl alloys.

2. Experimental procedure

Master ingots of Ti–24.4at.%Al, Ti–33.0at.%Al and Ti–40.0at.%Al alloys were prepared by melting high purity Ti and Al in a plasma arc furnace. Single crystals were grown by a floating zone method using an NEC SC-35HD single-crystal growth apparatus at a growth rate of 5 mm h^{-1}. The rods of the crystals were homogenized at 1000 °C for 72 h, then cooled in a furnace to 500 °C and subsequently annealed at 500 °C for 168 h in order to obtain a fully long-range-ordered DO_{19} structure. Compression specimens approximately 2 mm × 2 mm in cross-section and 5 mm long with four selected orientations were cut by spark machining. They were electrolytically polished in a 6:35:59 (vol.%) perchloric acid–butanol–methanol solution to remove surface damage. Compression tests

*Author to whom correspondence should be addressed.

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were performed on an Instron-type testing machine at room temperature. Slip traces were observed with an optical microscope using Nomarski interference contrast and the slip systems were determined.

3. Results and discussion

Specimens of Ti–33.0at.%Al with four selected compressive axes which have favourable stress components for the pyramidal, basal and prism slips were prepared. The Schmid factors for these slip systems are given in Table 1.

Figure 1 shows the slip traces of Ti–33.0at.%Al single crystals deformed at room temperature. For the specimen with orientation A, pyramidal $\{11\bar{2}1\}\langle 11\bar{2}\bar{6}\rangle$-type slips were activated, but they were observed only at limited orientations close to [0001] because of their high Peierls stress. The basal $(0001)\langle 1\bar{2}10\rangle$ slip appeared at orientation B accompanied by the prism slip as shown in Fig. 1(b). The CRSS for the basal slip is about 2.7 times higher than that for the prism slip. Specimens with orientations C and D were deformed by the prismatic $\{10\bar{1}0\}\langle 1\bar{2}10\rangle$ slip as shown in Figs. 1(c) and 1(d). The CRSS for the $\{10\bar{1}0\}\langle 1\bar{2}10\rangle$ slip at orientations C and D was 91.0 and 90.0 MPa respectively and obeys Schmid's law as well as the previous result for Ti–24.4at.%Al [9]. The orientation dependence of the slip geometry in Ti–24.4at.%Al was similar to that in Ti–33.0at.%Al.

TABLE 1. Schmid factors for possible slip systems of Ti_3Al single crystals

Compressive axis	Slip system		
	$\{10\bar{1}0\}\langle 1\bar{2}10\rangle$	$(0001)\langle 1\bar{2}10\rangle$	$\{11\bar{2}1\}\langle 11\bar{2}\bar{6}\rangle$
A	0	0	0.45
B	0.027	0.22	0.49
C	0.22	0.50	0.28
D	0.50	0	0.42

Addition of manganese or vanadium, which is thought to decrease the stacking fault energy in Ti_3Al, resulted in a significant violation of Schmid's law for the $\{10\bar{1}0\}\langle 1\bar{2}10\rangle$ slip [9, 12]. Namely, the CRSS increased with increase in the relative stress component for the $(0001)\langle 1\bar{2}10\rangle$ slip to the $\{10\bar{1}0\}\langle 1\bar{2}10\rangle$ slip, suggesting that extended faults on the basal plane inside the $\langle 1\bar{2}10\rangle$-type dislocation core act as an obstacle to the motion of the entire dislocation on the prismatic plane. The extended faults may develop as a result of the decrease in stacking fault energy. On the other hand, no information which suggests the existence of extended faults was obtained in the three binary Ti_3Al alloys.

The orientation dependence of the operative slip systems of Ti–40.0at.%Al containing a small amount of γ plates is quite similar to that of the Ti–24.4 and Ti–33.0at.%Al alloys. Since there is no significant difference in the slip geometry and the orientation dependence of the CRSS among the three tested alloys, compositional deviation from stoichiometry is not

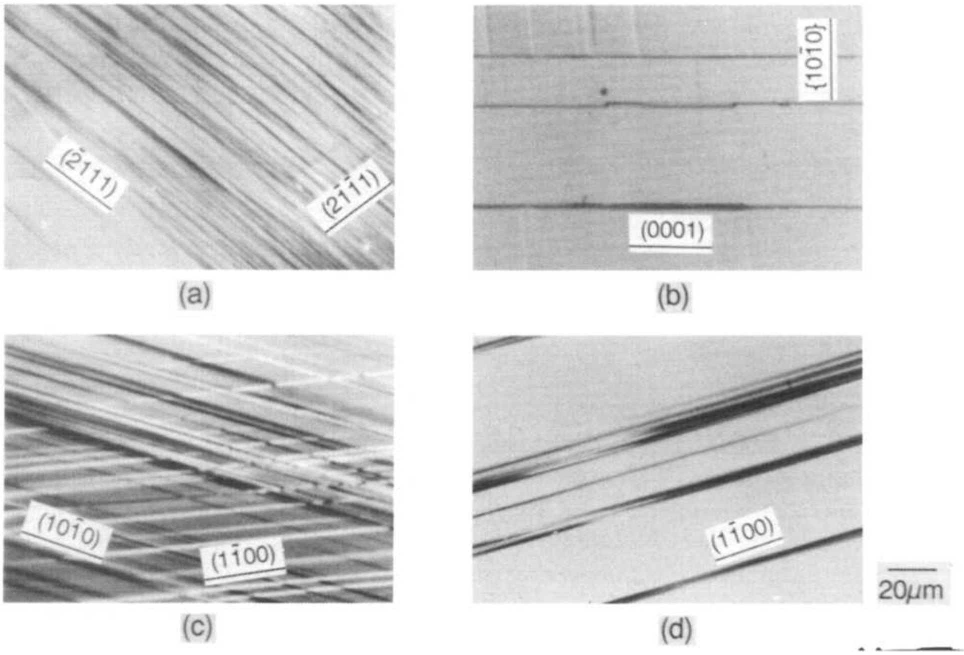

Fig. 1. Slip traces of Ti–33.0at.%Al single crystals deformed at room temperature: (a) orientation A, (b) orientation B, (c) orientation C, (d) orientation D.

thought to affect the glissile core configuration of $\langle 1\bar{2}10\rangle$ superpartials bound with an antiphase boundary (APB) on the prismatic plane.

Figure 2 shows the stress–strain curves of Ti–33.0at.%Al and Ti–24.4at.%Al single crystals deformed at room temperature. The plastic behaviour depends strongly on the orientation of samples in which different slip systems can be activated. When the prismatic slip occurs predominantly at orientation D, the specimen can be deformed in a dented shape by the easy mode of deformation and no cracks can be observed even at plastic strains of more than 30%. At this orientation the samples are deformed too highly to evaluate the difference in deformability among the three alloys. When deformed at orientation C, the specimen was broken at about 8% compressive strain. In this case the $\{10\bar{1}0\}\langle 1\bar{2}10\rangle$ slip occurs as the primary slip and subsequently at further deformation the basal slip is secondarily activated owing to the highly applied stress component for this slip. Slip traces on the basal plane were distributed inhomogeneously and exhibited coarse slip bands. High Peierls stress for the basal slip, which may be due to the non-planar dislocation core, leads to high stress concentration at the coarse slip bands and often results in crack initiation. Therefore at orientation B, where the basal slip is predominantly operative, sufficient plastic flow cannot be obtained after yielding. The effect of Al content on the fracture strain can be clearly found in specimens with orientation A which are deformed by the pyramidal slip. Compositional deviation from stoichiometry to the Al-rich side is harmful for ductility. The reason is not yet clear but this is a general trend similar to that found in NiAl, FeAl and TiAl [11]. Since the α_2 phase in equilibrium with the γ matrix in lamellar TiAl alloys has an off-stoichiometric Al-rich composition, an effective alloying element to move the α_2 solvus to stoichiometry should be sought to improve the ductility of TiAl alloys.

Figure 3 shows the variation in the CRSS for the possible slip systems as a function of Al composition. The CRSS for the prism and pyramidal slip systems increases markedly with increasing Al content but the CRSS for the basal slip does not change much. Such strengthening due to the defect structure on the basis of off-stoichiometry has been found in many intermetallics such as NiAl, AgMg, Ni_3Al and Ni_3Ga (see the review by Yamaguchi and Umakoshi [11]). Activation of the pyramidal slip is required to satisfy the von Mises criterion concerning the number of independent slip systems for general ductility of polycrystals in addition to the basal and prismatic slips. The ratio of the CRSS for the $\{11\bar{2}1\}\langle 11\bar{2}\bar{6}\rangle$ slip to that for the $\{10\bar{1}0\}\langle 1\bar{2}10\rangle$ slip increases from 7.4 to 8.1 with increasing Al content from 24.4 to 33.0 at.%Al. Therefore the increase in Al content suppresses the activation of the pyramidal slip and results in poor ductility.

Ti–40.0at.%Al alloy contains a small amount of γ plates which are unidirectionally aligned in the α_2 matrix in the framework of the orientation relations

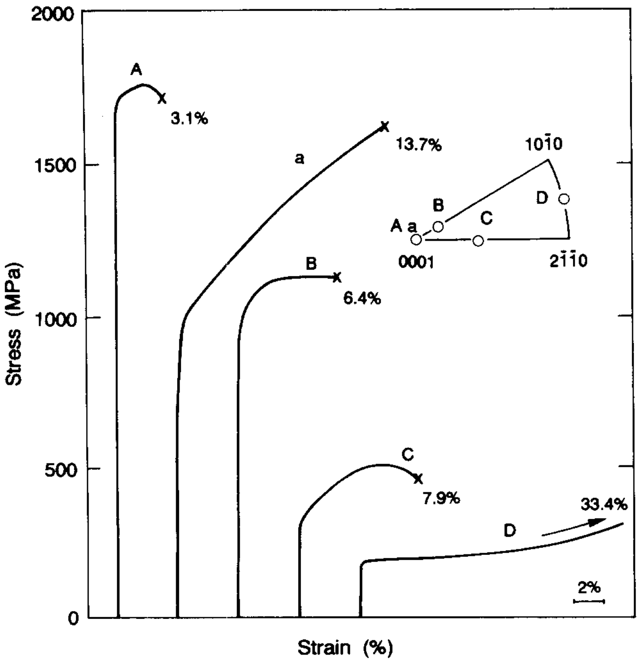

Fig. 2. Stress–strain curves of Ti_3Al single crystals deformed at room temperature: A–D, Ti–33.0at.%Al; a, Ti–24.4at.%Al.

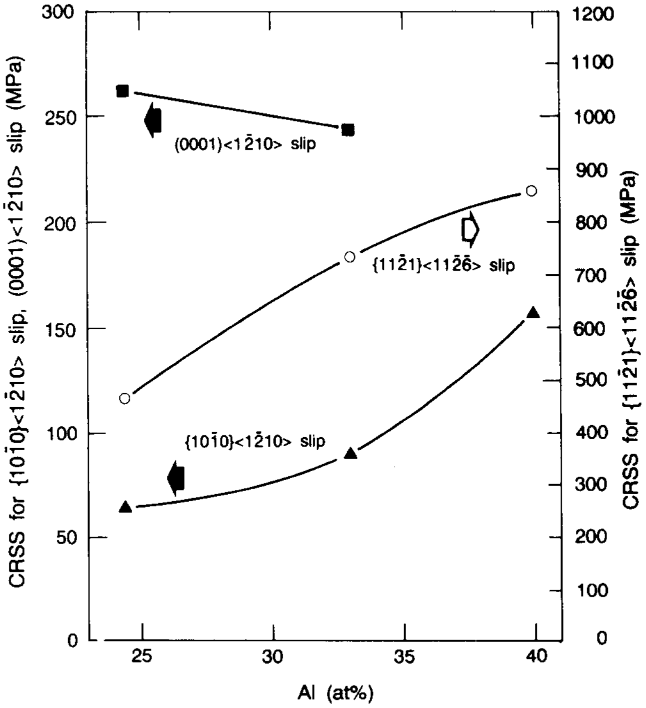

Fig. 3. Variation in CRSS of Ti_3Al single crystals with aluminium content.

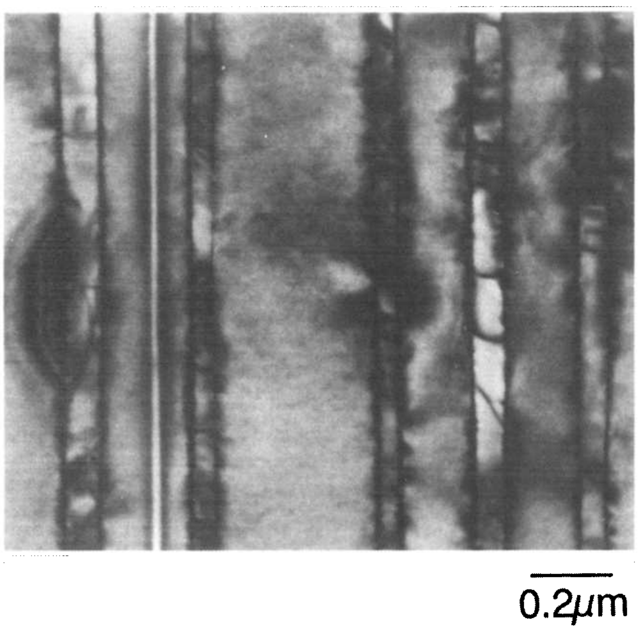

Fig. 4. Electron micrograph of Ti–40.0at.%Al alloy.

$\{111\}_\gamma \| (0001)_{\alpha_2}$ and $\langle 1\bar{1}0\rangle_\gamma \| \langle 1\bar{2}10\rangle_{\alpha_2}$ as shown in Fig. 4. THe α_2–γ interface may act as an effective barrier to prevent the motion of dislocations. However, the slip geometry and orientation dependence of the operative slip systems in Ti–40.0at.%Al alloy are similar to those in the other two alloys. Since the CRSS of Ti–40.0at.%Al lies on the curve extrapolated from the relation between the CRSS and Al content, the effect of the γ plates on the strength must be small.

4. Conclusions

(1) In Ti_3Al single crystals containing 24.4, 33.0 and 40.0 at.%Al the prism $\{10\bar{1}0\}\langle 1\bar{2}10\rangle$, basal $(0001)\langle 1\bar{2}10\rangle$ and pyramidal $\{11\bar{2}1\}\langle 11\bar{2}\bar{6}\rangle$ slips are activated depending on the crystal orientation. The prism slip is more favoured than the other slip systems. The orientation dependence of the operative slip systems is not influenced by compositional deviation from stoichiometry.

(2) The CRSS for the $\{10\bar{1}0\}\langle 1\bar{2}10\rangle$ and $\{11\bar{2}1\}\langle 11\bar{2}\bar{6}\rangle$ slips increases with increasing Al content, while activation of the $(0001)\langle 1\bar{2}10\rangle$ slip does not depend strongly on the aluminium content. The compositional deviation from stoichiometry does not lead to a violation of Schmid's law.

(3) The off-stoichiometric deviation increases the Peierls stress for the motion of $\langle 11\bar{2}\bar{6}\rangle$-type dislocations on the pyramidal plane and suppresses the pyramidal slip. It is conducive to the plastic anisotropy and results in poor ductility of Ti_3Al crystals.

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