Low and high temperature deformation mechanisms in TiAl alloys

A. Couret \(^1\,^2\)

\(^1\) CNRS ; CEMES (Centre d’Elaboration de Matériaux et d’Etudes Structurales) ; BP 94347, 29 rue J. Marvig, F-31055 Toulouse, France
\(^2\) Université de Toulouse ; UPS ; F-31055 Toulouse, France
couret@cemes.fr

Abstract. The deformation mechanisms involving ordinary dislocations are studied at various temperatures, in single-phased and lamellar TiAl alloys. In situ straining and heating experiments are performed in the transmission electron microscope (TEM) as well as post-mortem studies of deformed samples. It is shown that the dislocations can move by glide or climb depending on the temperature range and that some dynamic strain aging occurs at intermediates temperatures. In lamellar alloys, the crossing of interfaces is found to play a determining role.

1. Introduction
During the last two decades, gamma titanium aluminides (\(\gamma\)-TiAl) have attracted considerable interest among industrial and research institutions for structural applications at high temperatures. This is due to a unique combination of properties, i.e. reduced weight, high temperature strength and good oxidation resistance. According to the phase diagram, \(\gamma\)-TiAl alloys can solidify in a single phase state only when Al content exceeds the composition of the peritectic point corresponding to the reaction: \(L + \alpha \rightarrow \gamma\). On the other hand, two phased alloys can be achieved with compositions in the \((\alpha + \gamma)\) two phase region. In particular, slow cooling of \(\alpha\) grains provides lamellar grains, which are formed by an irregular piled-up of \(\gamma\) (L1\(_0\)) and \(\alpha_2\) (D0\(_{19}\)) lamellae. Depending on the respective proportion of \(\gamma\) and lamellar grains, the microstructures were classified in four groups: near-\(\gamma\), duplex, near lamellar and fully lamellar [1]. The plasticity of these \(\gamma\) TiAl alloys is mainly localised in the \(\gamma\) phase. Near-\(\gamma\) microstructures and fully lamellar ones which have generally large grains suffer of a poor ductility at room temperature in such way that the best compromise between ductility, strength and fracture toughness is achieved for duplex and refined lamellar alloys. In this context, to understand the mechanical properties of these various \(\gamma\)-TiAl alloys, it appears necessary to study the elementary deformation mechanisms activated in the \(\gamma\) phase and the deformation spreading in the lamellar microstructure.

The \(\gamma\) phase of TiAl alloys has the L1\(_0\) tetragonal crystal structure which is a derivative of the fcc structure (Fig. 1). The c/a ratio is about 1.02. As per the \(<uvw\>\) mixed brack notation, all permutations amongst \(u\) and \(v\) are allowed while the third index is fixed. Due to the tetragonality of the structure, the \(<110\>\) and \(<101\>\) directions are not equivalent to each other. Two types of perfect dislocations are usually considered in literature: a\(2\times110\) ordinary dislocations similar to the dislocation of the fcc
structure and a<101> superlattice dislocations similar to the dislocations of the L1₂ ordered structure. A few studies have been performed in single crystals on these perfect dislocations [2-5]. They have shown that the corresponding resolved shear stresses are strongly dependent on the aluminium content and exhibit a so-called yield stress anomaly. Twinning due to the glide of a/6<112> Shockley dislocations in (111) plane is also observed [6]. Note that a/6<211> Shockley dislocations are not operative because their glide would produce a complex stacking fault. Except in single crystals, a<101> superlattice dislocations are scarcely observed in comparison with a/2<110> ordinary dislocations and twinning is the second operative mode. This paper is devoted to the study of the deformation mechanisms involving ordinary dislocations at different temperatures. It will also be studied how they are moving in the lamellar microstructure. In situ and post-mortem TEM experiments were performed on Ti₄₈Al₄₈Cr₂Nb₂ and Ti₅₀₈Al₄₇Cr₁Si₀₂ alloys.

![Atomic arrangement and Burgers vector of perfect dislocations in the L1₂ structure](image1)

**Figure 1.** Atomic arrangement and Burgers vector of perfect dislocations in the L1₂ structure

2. Glide at low temperature

Fig. 2 shows ordinary dislocations moving during an in situ experiment performed at room temperature. These dislocations are elongated along their screw direction and they are anchored at many pinning points. The stereographic analysis of the slip traces left by the dislocations has shown that they are moving in their {111} glide plane. Such elongated and anchored configurations have been observed in deformed samples by post mortem TEM studies [7,8]. The dislocations glide by jumps between these elongated positions. Video recordings indicate that the jump times are always smaller than a fiftieth of second and that the duration of the locking varies between 0.02s and 1s.

![Ordinary dislocations and Superlattice dislocations](image2)

**Figure 2.** Two ordinary dislocations 1 and 2 gliding in (111) planes. P1, P2 and P3 are pinning points. (Ti₄₈Al₄₈Cr₂Nb₂ alloy).
As illustrated in Fig. 3, Shockley dislocations involved in twinning are also anchored at small pinning points. In various TiAl alloys, the separating distance between pinning points anchoring moving ordinary and twinning dislocations has been measured to be 0.15 µm. This demonstrates that the pinning is not due to cross-slip, as proposed in Refs. [7,8] since the Shockley dislocations are not able to cross slip because their Burgers vector belong to only one {111} plane. Moreover, Fig. 2 shows that successive dislocations 1 and 2 can anchor at the same location (points P1 and P2). From these observations, it is concluded that these pinning points are due to fixed extrinsic obstacles that are randomly distributed in the crystal. This explanation is consistent with the observation of anchoring points on superlattice dislocations [9] and with the measurement of a decrease of their density during annealing treatments [5]. On the basis of atom probe analysis of TiAl alloys [10], the pinning points have been proposed to have a chemical origin, as a local enrichment in titanium, a segregation of interstitials oxygen atoms and/or the ordering of a small region [11].

**Figure 3.** Three Shockley (1, 2 and 3) dislocations gliding on adjacent twinning planes. Triangles indicate pinning points. (Ti$_{48}$Al$_{48}$Cr$_2$Nb$_2$ alloy)

Fig. 4 displays three successive positions of an ordinary dislocation. In view (a), it is anchored at point (P). Between views (a) and (b), the screw segments (S) jumps. Between views (b) and (c), the macrokink at the pinning point glides quickly, forming a long screw segment which jumps and locks in a straight configuration. This rectilinear shape of the screw dislocations indicates the existence of a strong frictional force acting on the screw segments whereas no evidence of the same kind has been obtained for the non-screw segments. This frictional force has been attributed to the core spreading of screw segments in consistency with atomistic calculations [12,13].

**Figure 4.** Three successive positions of an ordinary dislocation.
S : screw segment,
P : Pinning point,
bp : projection of the Burgers vector.
3. Glide at intermediate temperatures (400°C-600°C)
At intermediate temperatures (T ≥ 400°C), glide ordinary dislocations are still elongated along their screw orientation and anchored at many pinning points (Fig. 5a). However, they are highly concentrated in bands. During in situ experiments (Fig. 5), movements are faster and more heterogeneous than at room temperature. When the strain is applied, the deformation occurs suddenly by bursts of dislocations, namely tens or hundreds of dislocations move instantaneously and quickly, and stop (Fig. 5b). Then, these dislocations will stay immobile and will not move again. Further strain application will generate a new burst.

![Figure 5](image)

**Figure 5. In situ observation of the formation of a band of ordinary dislocations at 400°C.**
F are fixed points in the crystal. (Ti_{48}Al_{48}Cr_{2}Nb_{2} alloy)

4. Mixed climb at high temperature
At high temperatures, ordinary dislocations look very different to those described above. As shown on Fig. 6, these dislocations exhibit no preferential direction and are not anchored at pinning points. The planes of some dislocation loops were determined by tilt experiments associated with a stereographic analysis. Fig. 7 shows one example of such determination. The dislocation is tilted around the dashed line joining the two dislocation extremities, which is thus the trace of the intersection between the loop plane and the surface. From the variation of the apparent width of the loop, its plane is determined with an experimental uncertainty of ± 5° [14]. In more than fifty percents of cases, this plane deviates significantly from the (111) glide planes. However, this deviation was never found to be greater than 20°. This indicates that the movement occurs by a mixed climb mechanism, which involves climb and glide components.
Figure 6. Ordinary dislocations in a sample crept at 750°C under 150 MPa. (Ti_{48}Al_{48}Cr_{2}Nb_{2} alloy).

Figure 7. Tilts experiment performed on an ordinary dislocations, in a thin foil cut in a sample crept at 750°C under 150 MPa. (Ti_{48}Al_{48}Cr_{2}Nb_{2} alloy).

In situ heating experiments were performed at 750°C on a thin foil cut from a sample crept (2% of strain) at the same temperature (Fig. 8). During this sequence, rectilinear non-screw segments are observed to move viscously, at a very low velocity as indicated by the time information. It has been evidenced that this movement in thin foil occurs in pure climb plane [14].
5. Ordinary dislocations in the lamellar microstructure

In consistency with the formation mechanism of γ lamellae during cooling [15-17], the interface planes of the lamellar microstructure are {111}_γ and (0001)_α₂ planes. Due to the tetragonality of the structure, the L1₀ lamellae can take six orientation variants corresponding to six possible orientations. Between these lamellae, three interface relationships can be found: ordered domain, twin and pseudo-twin [16-17]. Statistical analyses of the lamellar microstructure have shown a predominance of twin related interfaces and that the width of α₂ lamellae is smaller than that of γ lamellae [18].

Fig. 9 shows lamellar zones deformed at 600°C [19]. In both cases, the majority of the lamellae were deformed by ordinary dislocations, the Burgers vector of which is either parallel (view a), or inclined (view b) to the interface plane. These dislocations are elongated along their screw orientation and anchored as described previously. Some loops seem to have been emitted at the interfaces. Few lamellae (view b) are deformed by a combination of twins and ordinary dislocations.

Black arrows in view b (Fig. 9) indicate that ordinary dislocations are localized near areas where twins have impacted the γ/α₂ interface. This suggests that the activation of ordinary dislocations was influenced by the accumulation of stress due to the pile-up of twinning dislocations at interfaces. It has been shown elsewhere that the propagation of deformation across α₂ lamellae occurs by an elastically-mediated transfer under the effect of these dislocation piled-up [20].

Figure 8. Heating *in situ* experiments performed on a thin foil cut from a sample crept (2% of strain, 750°C and 150 MPa). (Ti₄₈Al₄₈Cr₂⁺₂ alloy).

Figure 9. Deformation microstructures in two lamellar zones of a Ti₃₀Al₁₅Cr₁Si₀₂ alloy deformed at 600°C.
Fig. 10 shows an example of the transmission of the deformation at interfaces at room temperature. It can be seen that pile-ups of dislocations are formed at the interfaces and that the transmission occurs. Several situations differing by the incident system, the interface relationship and the orientation of the stress were analysed in details [21,22]. In general, part of the incident shearing is transferred under the effect of the internal stress due to dislocation pile-up. The crossing is easier at twin interfaces and when the incident system is formed by a twin. It is promoted by favourable geometric conditions based on orientations of the Burgers vector, of the dislocation lines and of the glide planes.

\[ d_c = \frac{2T}{\tau b} \cos\left(\frac{\theta_c}{2}\right), \]

where $T$ is the line tension, $\theta_c$ the critical angle between the two anchored segments when the obstacle breaks, $\tau$ the resolved shear stress and $b$ the Burgers vector ($b = 0.28$ nm). In fact, the dislocations never stop at pinning points as long as there is at least one rectilinear segment able to move. The sequence of events of Fig. 4 illustrates this point since it shows that the pinning point (P) overcoming results of the reaching of the critical configuration by the moving screw segment (S). For the case of ordinary dislocations of TiAl, it has been found that $d_s$ is twice $d_c$ [24]. As a conclusion, the ordinary dislocation glide is controlled by the frictional force, in consistency with the experimental observations showing rectilinear screw segments free of pinning points (see for instance Fig. 4).

The fast and catastrophic behavior observed at intermediate temperatures is correlated to plastic instabilities measured at the same temperature during tensile tests at constant strain rate [5]. It was observed in several intermetallics. It has been attributed to dynamic strain ageing [9,25] and correlated to yield stress anomalies. For ordinary dislocations, the coupling of an easy cross-slip and of a strong frictional force leads to easy multiplication processes by open loops, as identified for instance in titanium [26]. During the deformation at imposed constant strain rate, this intensive dislocation multiplication is at the origin of the deformation by bursts since it induces a decrease of the dislocation velocity leading to a decrease of the stress and eventually to a strong locking of the dislocations due to the frictional force.

At high temperature, during creep experiments (750°C) these ordinary dislocations are generally moving by a mixed climb mechanism, for which the moving plane is close but distinct from the glide
plane [14]. The corresponding elementary process is the nucleation and lateral propagation of a jog pair, in consistency with the rectilinear shape of non screw segments. On the one hand, this movement allows the dislocations to escape from the frictional force which is operative only when they are lying along their screw direction in (111) planes. On the other hand, in terms of dislocation displacement, it is more efficient than pure climb for one diffusion event, in consistency with activation parameters measurements [14]. As a matter of fact, the moving distance for one elementary jump is proportional the jog height which is the distance between adjacent (111) planes in the inclined moving plane and this distance is higher for mixed plane due to the inclination of the moving plane.

7. Concluding remark
In the present paper, it has been shown that the frictional force acting on ordinary dislocations of TiAl plays a determining role in the entire temperature range. It controls the movement at low temperature, produces the strong locking of the dislocations which induce instabilities at intermediate temperature and is at the origin of the activation of mixed climb. In lamellar areas, it is also operative but the controlling process is the crossing of the interface.

References
[1] Kim YW and Dimiduk DM 1991 JOM 43 40
[2] Kawabata T, Kanai T and Izumi O 1985 Acta Metall. Mater. 38 1381
[3] Inui H, Matsumuro M, Wu DH and Yamaguchi M 1997 Phil. Mag. A 75 395
[4] Nakano T, Hagihara K, Seno T, Sumida N, Yamamoto M and Umakoshi Y 1998 Phil. Mag. Lett. 78 385
[5] Grégori F, 1999 Ph D Thesis Université de Paris VI
[6] Farenc S, Coujou A and Couret A 1993 Phil. Mag. A 67 127
[7] Viguier B, Hemker KJ, Bonneville J, Louchet F and Martin J L 1995 Phil. Mag. A 71 1295
[8] Sriram S, Dimiduk D M, Hazledine P and Vasudevan V K 1997 Phil. Mag. A 76 965
[9] Haussler D, Bartsch M, Aindow, Jones I P and Messerschmidt U 1999 Phil. Mag. A 79 1045
[10] Menand A, Huguet A and Nérac-Partaix A 1996 Acta. Metall. Mater. 44 4729
[11] Zghal S, Menand A and Couret A. 1998 Acta Metall. Mater. 46 5899
[12] Mahapatra R, Girshick, Pope D and Vitek V 1995 Scripta Metall. Mater. 33 1921
[13] Simmons J P., Rao S I and Dimiduk D M. 1997 Phil. Mag. A 75 1299
[14] Malaplate J, Caillard D and Couret A 2004 Phil. Mag. A 84 3671
[15] Denquin A and Naka S 1996 Acta Metall. Mater. 44 343
[16] Inui H, Oh M H, Nakamura A and Yamaguchi M 1992 Phil. Mag. A 66 539
[17] Zghal S, Naka S and Couret A 1997 Acta Metall. Mater. 45 3005
[18] Zghal S, Thomas M, Naka, S, Finel A and Couret A 2005 Acta Mater. 53 2653
[19] Singh JB, Molénat G, Sundararaman M, Banerjee S, Saada G, Veyssière P and Couret A 2006. Phil. Mag. A 86 2429
[20] Singh JB, Molénat G, Sundararaman M, Banerjee S, Saada G, Veyssière P and Couret A 2006. Phil. Mag. Lett. 86 47
[21] Zghal S, Coujou A and Couret A 2001. Phil. Mag. A 81 345
[22] Zghal S and Couret A 2001. Phil. Mag. A 81 365
[23] Caillard D and Couret A 2002 Mater. Sci. Eng. A322 108
[24] Couret A 1999 Phil. Mag. A 79 1977
[25] Molénat G, Couret A and Caillard. 1997 Mater. Sci. Eng. 234 66
[26] Farenc S, Caillard D and Couret A 1993 Acta Metall. Mater. 41 2701