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To cite this version:
M. Biget, G. Saada. Effect of Interstitial Impurities on Twinning of Titanium and Zirconium. Journal de Physique III, EDP Sciences, 1995, 5 (11), pp.1833-1840. <10.1051/jp3:1995219>. <jpa-00249418>

HAL Id: jpa-00249418
https://hal.archives-ouvertes.fr/jpa-00249418
Submitted on 1 Jan 1995

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Effect of Interstitial Impurities on Twinning of Titanium and Zirconium

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(Received 6 February 1995, revised 9 August 1995, accepted 21 August 1995)

Abstract. — It is shown by a simple analysis that twinning in α-Zr polycrystals is strongly influenced by the presence of impurity atoms in low concentration. Motion of impurity atoms appears therefore as an important element to be taken into account when trying to define a criteria for twinning.

1. Introduction

α-Ti and Zr alloys are present as hcp phases at low temperature. Since it is difficult to purify these alloys, in fact, even very “pure” samples may contain more than 100 at ppm of oxygen. In the hexagonal cell (Fig. 1), metals atoms are located either on the basal plane or at the plane displaced by c/2 from the basal plane, where the oxygen atoms occupy octahedral sites at planes c/4, 3c/4 [1-5]. At low oxygen contents the former sites are preferably occupied. At low temperature, these crystals deform both by glide and by deformation twinning. One reason for the occurrence of twinning is that pyramidal slip, which is the only slip system which has a glide component in the c-direction, is not very active at low temperature.

The problem of predicting the twinning system of a given crystal is still poorly understood despite many clever attempts [6]. It is quite clear from available experimental results that both the magnitude of the shear, and local atomic shuffles play an important role, particularly in alloys. Table I shows the two most frequently observed twinning system in α-Zr Recent observations summarized in Table II suggest that the content of oxygen may influence the twinning behaviour of such crystals [7]. One may verify that for a given content in oxygen the {1121}(10̅11) is preferred at low temperatures and that its propensity increases at a given temperature with increasing oxygen content. In this short note, we shall show that the observed results can be understood as a consequence of the motion of oxygen atoms during deformation twinning.

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Fig. 1. — Projection of metal atoms (○) level 0, (●) level c/2 and of oxygen atoms (+) level c/4 and 3c/4 in the (0001) plane.

Table I. — Most frequently observed twinning modes in uniaxial deformation of α-Ti and α-Zr at low temperature. The shear $s$ and the $c/a$ ratio are: $\alpha - Ti c/a = 1.588$, $s_{10\overline{1}2} = 0.174, s_{\overline{1}1\overline{2}1} = 0.629$; $\alpha - Zr c/a = 1.593, s_{10\overline{1}2} = 0.167, s_{\overline{1}1\overline{2}1} = 0.627$.

<table>
<thead>
<tr>
<th>Twinning plane (1st undeformed) $K_1$</th>
<th>Twinning shear direction $\eta_1$</th>
<th>2d undeformed plane $K_2$</th>
<th>plane of shear $\pi$</th>
<th>expression of shear magnitude $s$</th>
<th>magnitude of twinning shear (c/a=1.59)</th>
</tr>
</thead>
<tbody>
<tr>
<td>${10\overline{1}2}$</td>
<td>$\langle 10\overline{1}\overline{1}\rangle$</td>
<td>${10\overline{1}2}$</td>
<td>${1\overline{2}10}$</td>
<td>$c^2 - a^2$</td>
<td>0.171</td>
</tr>
<tr>
<td>${1\overline{1}\overline{2}1}$</td>
<td>$\langle 1\overline{1}\overline{2}6\rangle$</td>
<td>(0002)</td>
<td>${1\overline{1}00}$</td>
<td>$a$</td>
<td>0.628</td>
</tr>
</tbody>
</table>

Figure 2 represents the elements defining a given twinning mode: the invariant $K_1$ and its conjugate $K_2$ planes, the shear direction $\eta_1$ and its conjugate $\eta_2$, the plane of shear $\Pi$. The shear $s$ is:

$$s = 2 \cot \alpha$$  \hspace{1cm} (1)

Let $e_1$ be the unit vector corresponding to $\eta_1$, $n$ the unit vector normal to $K_1$, the displacement $u$ of a point $M$ of the shear plane $\Pi$ is:

$$u = s(r \cdot n)e_1$$  \hspace{1cm} (2)

Here $r$ stands for the vector $OM$, the origin $O$ is taken on the twin boundary.
Table II. — Influence of temperature and plastic strain on the twinning mode. Samples A are the purest sample, samples B, C correspond to the addition of 96 atppm 386 atppm of oxygen respectively. $e$ is the deformation of the specimen in %. The twinning ratio is the percentage of the twinned crystal with respect to the total number of grains.

<table>
<thead>
<tr>
<th>Sample (*)</th>
<th>Temperature Kelvin</th>
<th>Deformation $e$ %</th>
<th>Total twinning ratio M(II)</th>
<th>Twinning mode ratio $M{10\overline{1}2}$</th>
<th>Twinning mode ratio $M{1\overline{1}21}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zr A</td>
<td>295</td>
<td>12</td>
<td>0.27</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td></td>
<td>77</td>
<td>38</td>
<td>0.32</td>
<td>0.32</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4 2</td>
<td>10</td>
<td>0.65</td>
<td># 0.65</td>
<td></td>
</tr>
<tr>
<td>Zr B</td>
<td>295</td>
<td>12</td>
<td>0.18</td>
<td>0.15</td>
<td>0.3</td>
</tr>
<tr>
<td></td>
<td>77</td>
<td>33</td>
<td>0.33</td>
<td>0.21</td>
<td>0.12</td>
</tr>
<tr>
<td></td>
<td>4 2</td>
<td>17 6</td>
<td>0.74</td>
<td>0.03</td>
<td>0.71</td>
</tr>
<tr>
<td>Zr C</td>
<td>295</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>77</td>
<td>15</td>
<td>0.45</td>
<td>0.09</td>
<td>0.36</td>
</tr>
<tr>
<td></td>
<td>4 2</td>
<td>15</td>
<td>0.85</td>
<td>0.10</td>
<td>0.75</td>
</tr>
</tbody>
</table>

Fig. 2. — Twinning elements of twinning.

To describe the twinning transformation, it is convenient to visualize the crystal as a stacking of planes parallel to the shear plane, and to assume that the unit cell can be defined by two vectors $P$ and $Q$ belonging to the II plane (the third vector being perpendicular to the II plane is irrelevant). During twinning $P$ and $Q$ transform into $P'$ and $Q'$, and a point $M$ defined by:

$$r = x_P P + x_Q Q$$

(3)
Fig. 3. — Position of the octahedral sites in the \((c, a')\) cell of the \((2\overline{1}10)\) shear plane. a) A planes, b) B planes.

transform into a point \(M'\) defined by:

\[
r' = x_P P' + x_Q Q'
\]  

(4)

Let \(M'(x_P', x_Q')\) be the point crystallographically equivalent to \(M\) in the cell defined by \(P', Q'\). To restore the initial lattice the point \(M'\) has to be moved by a translation \(t\):

\[
t = (x_P' - x_P)P' + (x_Q' - x_Q)Q'
\]  

(5)

It should be noticed that these situations exist where by interchanging identical atoms one may describe the transformation by a motion smaller than described by formula (5) (see Fig. 4).

2. Twinning of \(\alpha\)-Zr

2.1. \(\{10\overline{1}2\}\{10\overline{1}1\}\) System. — Figure 1 shows that the lattice can be viewed as an ABAB... stacking of prismatic plane parallel to the \(\Pi\) plane. The \(P, Q\) unit cell, as well as the coordinate system are represented Figure 3a,b. In this coordinate system, \(P\) and \(Q\) have coordinates
EFFECT OF INTERSTITIAL IMPURITIES ON TWINNING

Fig. 4. — Position of the previous sites in the \((a', c)\) cell of the \((2\overline{1}10)\) shear planes and suffling. Notice that in this case, the shuffling of the metal atoms is smaller than that calculated in formulae (5, 6). The motion is indicated by the arrow (—→).

\[(0, c)\) and \((a', 0)\), respectively. The shear \(s = (a'^2 - c^2)/a'c\). A straightforward application of formulae (1 - 5) shows that the coordinates \(P'\) and \(Q'\) in the same coordinate system are respectively: \([a'/(a'^2 + c^2)], (a'^2 - c^2), 2a'c\] and \([c/(a'^2 + c^2)], [2a'c(a'^2 - c^2)]\). These vectors are perpendicular and of length respectively \(a'\) and \(c\). Therefore, the motion \(t\) for an atom at the initial coordinates \((x_P, x_Q)\) is:

\[t = (x_P - x_Q)(a' - c)\]  

These results are summarized in Table III and Figure 4. Thus the motion of interstitial atoms is quite important in this twinning system.

2.2. \(\{11\overline{2}1\}\)(11\(\overline{2}6\)) SYSTEM. — Figure 5 shows that in order to describe the stacking planes \(A, B, C, D\) containing metal atoms must be distinguished from planes \(A', B'\) containing interstitial oxygen atoms. \(A\) and \(B\) contain atoms at level \(0\) or \(c\), \(C\) and \(D\) contain atom at level \(c/2\). \(A'\) and \(B'\) contain atoms at level \(c/4\) and \(3c/4\) respectively. The projection of the atoms on the plane \(\Pi\) is shown Figure 6a. The stacking can be describe as \(AB'DCA'BA...\), the shear \(s = a/c\).
Table III. — Coordinates and shuffling of atoms in \{10\bar{1}2\}(10\bar{1}1) twinning system.

<table>
<thead>
<tr>
<th>TWINNING {10\bar{1}2}(10\bar{1}1)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Sites</td>
<td>Coordinates in the unit cell</td>
</tr>
<tr>
<td>Metal atoms</td>
<td>A LAYER</td>
</tr>
<tr>
<td></td>
<td>(0, 0)</td>
</tr>
<tr>
<td></td>
<td>(2/3, 1/2)</td>
</tr>
<tr>
<td>Interstitials</td>
<td>(1/3, 1/4)</td>
</tr>
<tr>
<td></td>
<td>(1/3, 3/4)</td>
</tr>
<tr>
<td>Metal atoms</td>
<td>B LAYER</td>
</tr>
<tr>
<td></td>
<td>(1/2, 0)</td>
</tr>
<tr>
<td></td>
<td>(1/6, 1/2)</td>
</tr>
<tr>
<td>Interstitials</td>
<td>(5/6, 1/4)</td>
</tr>
<tr>
<td></td>
<td>(5/6, 3/4)</td>
</tr>
</tbody>
</table>

Fig. 5. — Description of the hexagonal cell as a stacking of (\bar{1}100) planes.
Fig. 6. — a) Position of atoms and octahedral sites in the \((c - a, a)\) cell of the shear plane \((\overline{1}00)\). b) Motion (possible via a shuffling mechanism) of the metal atoms and oxygen atoms. The motion is indicated by an arrow \((-\rightarrow\)). (●) A plane, (Δ) C plane; metal atoms: (○) B plane, (□) D plane; Octahedral sites: (⊗) A' plane, (⊕) B' plus.

Table IV. — Coordinates and shuffling of atoms in \(\{11\overline{2}1\}\{11\overline{2}6\}\) twinning system.
The \( P, Q \) unit cell is represented Figure 6a, the transformed cell \( P', Q' \) is represented Figure 6b. In the coordinate system of Figure 6a:

\[
P(-a, c) \rightarrow P' \left[ \frac{c}{4c^2 + a^2} \right] [-4ac, 4c^2 - a^2]
\]
\[
Q(a, 0) \rightarrow Q' \left[ \frac{a}{4c^2 + a^2} \right] [4c^2 - a^2, 4ac]
\]

\( P' \) and \( Q' \) are perpendicular and have length \( c \) and \( a \) respectively.

The metal sites belonging to planes A and C are not modified, the metal sites belonging to planes B and D are interchanged. However the interstitial atoms need to be moved, shown in Figure 6b, possibly via a shuffling mechanism. These results are summarized in Table IV.

3. Conclusion

The above analysis strongly suggests that twinning in \( \alpha \)-Zr is influence by the motion of interstitial impurity atoms, even in small concentration. Preliminary observations show that the situation is similar in \( \alpha \)-Ti: \( \{10\overline{1}2\}\{10\overline{1}1\} \) twinning dominates at 300 K while \( \{11\overline{2}1\}\{11\overline{2}6\} \) twinning dominates at 4.2 K.

The effects reported above occur very likely in other alloys. They should be taken into account when trying to define twinning criteria.

References


