STRUCTURAL RELATIONSHIPS BETWEEN THE T AND O PHASES IN Ti-24Al-11Nb

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Introduction

In an earlier study of phase evolution during aging of a rapidly solidified Ti-24Al-11Nb alloy, we discovered the existence of an ordered tetragonal (T) phase[1]. The T phase formed through a B2 -> T ordering transition, and can be regarded as a tetragonally distorted DO3-like phase formed by further ordering of Nb atoms in the B2 superlattice. Later, we reported on the metastability of the T phase; a sequential transition T -> O (ordered orthorhombic) -> α₂ (ordered hexagonal) phase was found to take place during aging[2]. To elucidate the mechanism of the T -> O transition, a study of the structural relationships between the T and O phases has been carried out using transmission electron microscopy (TEM) and electron diffraction methods. The results are presented here.

Experimental

A plasma-sprayed Ti₃Al+Nb alloy with a nominal composition of Ti-24at%Al-11at%Nb was chosen for this study. The sample was produced from powder through an inductively coupled plasma deposition (ICPD) process by GE Aircraft Engines, Lynn, MA[3]. During the ICPD process, titanium aluminide powder was melted by passing through a plasma. The molten droplets were immediately deposited onto a mandrel inside a vacuum chamber where they were rapidly quenched to a solid state. Before aging, specimens were wrapped with tantalum foils and sealed in cleaned and evacuated quartz ampoules. Isothermal aging was subsequently performed for different times at 650°C. The microstructure of the alloy was examined for its aged status using transmission electron microscopy (TEM), selected area diffraction (SAD), microdiffraction (MD) and convergent beam electron diffraction (CBED) methods in a Philips-400T transmission electron microscope.

Results and Discussion

Microstructure

A typical microstructure observed in a sample after aging for 40 min at 650°C is shown in Fig. 1(a). A lath-like O phase was found to coexist with the T phase. The T and O phases were distinguished using the dark-field (DF) imaging method as shown in Figs. 1(b) and 1(c). Figure 1(b) shows the matrix of the T phase. Figure 1(c) shows the lath-like O phase. Notice that two different orientation variants of the O lath can be found in Fig. 1(c). The T/O interface (habit) planes were found to be 44° away from (001)ₜ, i.e. parallel to (223)ₜ and (223)ₜ (Fig. 1(d)). Note that these are different from the {211}bcc habit plane found in an equilibrium bcc/orthorhombic Ti-Al-Nb system by Bendersky et al.[4]. A selected area
diffraction (SAD) pattern generated from the (T + O) two-phase region in Fig. 1(a) is shown in Fig. 2. The orientation relationships between the T and O phases derived from the SAD pattern are the following: (110)$_T$(001)$_O$ and (110)$_T$(010)$_O$ = (001)$_T$(100)$_O$ = 4.5°.

When the aging time was extended, the O phase was found to grow by consumption of the T phase. The morphology of the O phase eventually altered from a plate to an equiaxed grain (after aging for 2h at 650°C) as a result of phase coarsening. This is shown in Fig. 3(a). Microdiffraction and CBED whole patterns generated from the <001> zone of a coarsened O phase are shown in Fig. 3(b). A 2mm symmetry is displayed in the <001>$_O$ zone CBED pattern[5].

**Structural relationships between the T and O phases**

The lattice correspondence between the T and O phases can be derived in the manner shown in Fig. 4(a). Let a lattice vector $[x_1,x_2,x_3]_O$ in the O lattice correspond to a lattice vector $[x_1,x_2,x_3]_T$ in the T lattice. From the relative orientations of the two lattices (001)$_T$ -> (100)$_O$, (110)$_T$ -> (010)$_O$ and (110)$_T$ -> (001)$_O$, the relation between the $[x_1,x_2,x_3]_O$ and $[x_1,x_2,x_3]_T$ can be expressed as follows:

\[
\begin{bmatrix}
  x_1 \\
  x_2 \\
  x_3
\end{bmatrix}_O = \begin{bmatrix}
  0 & 0 & 2 \\
  -1 & 1 & 0 \\
  -1 & -1 & 0
\end{bmatrix} \begin{bmatrix}
  x_1 \\
  x_2 \\
  x_3
\end{bmatrix}_T
\]

(1)

Structural relationships between these two phases can be derived by assuming a shuffling of atoms on alternating (110)$_T$ planes along [110]$_T$, accompanied by homogeneous lattice deformations along the [001]$_T$, [110]$_T$ and [110]$_T$ directions. These are illustrated in Figs. 4(b) & 4(c).

An important aspect of the T -> O transition is the shape deformation $P$ required to convert a tetragonal to an orthorhombic lattice. The shape deformation ($P$) must be consistent with the experimental observation that the habit (invariant strain) plane is essentially undistorted and unrotated. In practice, $P$ is composed of a homogeneous lattice distortion $B$, a lattice-invariant inhomogeneous shear $S$ (corresponding to slip and twinning), and a rigid-body rotation $Q$, i.e. $P = QB[6]$. The lattice dimensions of the O phase can be obtained by contracting the T lattice by 8.8% along [001]$_T$ to create [100]$_O$, expanding [110]$_T$ by 6.6% to create [010]$_O$, and expanding [110]$_T$ by 2% to create [001]$_O$. Referring to the directions [001]$_T$, [110]$_T$ and [110]$_T$ as x-, y-, z- axes, these can be expressed as follows:

\[
\begin{bmatrix}
  e_{11} & 0 & 0 \\
  0 & e_{22} & 0 \\
  0 & 0 & e_{33}
\end{bmatrix} = \begin{bmatrix}
  -0.088 & 0 & 0 \\
  0 & 0.066 & 0 \\
  0 & 0 & 0.02
\end{bmatrix}
\]

(2)

The principal strains, denoted by $\eta_{ij}$ of the homogeneous distortion $B$ for the T -> O transformation are given by:

\[
B = \begin{bmatrix}
  \eta_{11} & 0 & 0 \\
  0 & \eta_{22} & 0 \\
  0 & 0 & \eta_{33}
\end{bmatrix} = \begin{bmatrix}
  1+e_{11} & 0 & 0 \\
  0 & 1+e_{22} & 0 \\
  0 & 0 & 1+e_{33}
\end{bmatrix} = \begin{bmatrix}
  a_0c_T & 0 & 0 \\
  0 & b_0\sqrt{2}a_T & 0 \\
  0 & 0 & 2c_0\sqrt{2}a_T
\end{bmatrix} \begin{bmatrix}
  0.912 & 0 & 0 \\
  0 & 1.066 & 0 \\
  0 & 0 & 1.02
\end{bmatrix}
\]

(3)
plane strain $B'$:

$$B' = B + e = \begin{bmatrix} \eta_{11} & 0 & 0 \\ 0 & \eta_{22} & 0 \\ 0 & 0 & \eta_{33} \end{bmatrix} + \begin{bmatrix} \nu e_{33} & 0 & 0 \\ 0 & \nu e_{33} & 0 \\ 0 & 0 & -e_{33} \end{bmatrix} = \begin{bmatrix} \eta_{11} & 0 & 0 \\ 0 & \eta_{22} & 0 \\ 0 & 0 & 1 \end{bmatrix} + \begin{bmatrix} 0.918 & 0 & 0 \\ 0 & 1.072 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$  \(4\)

where $\nu$ is Poisson ratio (-0.3). Since the magnitude of shear deformation is small, the shape deformation $P$ required for the $T \rightarrow O$ transformation is approximately equal to the invariant plane strain combined with a rigid-body rotation, i.e. $\Omega B'$. The Rotation matrix $\Omega$ is:

$$\Omega = \begin{bmatrix} \cos \theta & \sin \theta & 0 \\ -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$  \(5\)

where $\theta$ is the rotation angle about the [001] direction of the O phase with respect to the T phase.

A theoretical prediction of the habit (invariant strain) plane, rotation angle and orientation relationships between the T and O phases can be made in the manner shown in Fig. 5[6]. The effect of the invariant plane strain $B'$ on a spherical crystal, viewed along the z-axis, is illustrated. The spherical crystal was deformed into an ellipsoid due to the strain $B'$. The planes $OQ'$ and $OP'$ are not distorted by the strain, yet they were rotated from their initial positions $OQ$ and $OP$. To produce an unrotated as well as undistorted habit plane, a rotation about the z-axis has to be added to the invariant plane strain $B'$ to return one of these planes to the initial position ($OQ'$ to $OQ$ for instance). Let $Q$ be the point $(x,y)$. The coordinates of $Q'$ $(x',y')$ can then be given by the matrix multiplication:

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 0.918 & 0 & 0 \\ 0 & 1.072 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ 0 \end{bmatrix}$$  \(6\)

whence, $x' = 0.918x$, $y' = 1.072y$. Since $OQ = OQ'$, or $x^2 + y^2 = (0.918x)^2 + (1.072y)^2$. Thus, $z_{Q'OY} = \tan^{-1}(x/y) = 44.2^\circ$. The habit (T/O interface) plane therefore makes an angle $44.2^\circ$ with $(001)_T$, this is only $0.3^\circ$ away from the $(223)_T$ plane $(223)_T \cap (001)_T = 43.9^\circ$. $z_{Q'OY} = \tan^{-1}(x'/y') = 39.9^\circ$, thus the rotation angle $\theta = 4.3^\circ$. This rotation makes the $(223)_T$ plane nearly parallel to $(340)_O$, $(223)_T \cap (340)_O = 0.4^\circ$. The predicted orientation relationships between the T and O phases are $(110)_T \parallel (001)_O$, and $(110)_T \parallel (010)_O = [001]_T \parallel [100]_O = 4.3^\circ$. These are in agreement with the experimental results shown above. Consequently, we conclude the shape deformation $P$ for the T $\rightarrow$ O transition is:

$$P = \Omega B' = \begin{bmatrix} 0.915 & 0.069 & 0 \\ -0.080 & 1.069 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$  \(7\)

**Summary**

Structural relationships between the T and O phase have been studied, and our results are summarized as follows:

1. The T $\rightarrow$ O transition can be explained by a shape deformation mechanism.
2. The T/O interface (habit) plane is near to $(223)_T$.
3. The orientation relationships between the T and O phases are $(110)_T \parallel (001)_O$, and $(110)_T \parallel (010)_O = [001]_T \parallel [100]_O = 4.3^\circ$. 


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References


Fig. 1. (a) Bright-field (BF) image showing a typical microstructure observed in a sample after aging for 40 min at 650°C, Z (zone axis) = [110]_T[001]_O, (b) dark-field (DF) image showing the matrix of the T phase, (c) dark-field (DF) image showing the lath-like O phase, (d) a [110]_T stereographic projection showing the orientation of the T/O interface.
Fig. 2. A selected area diffraction pattern generated from the (T + O) two-phase region in Fig. 1(a), Z = [110]_T||[001]_O.

Fig. 3. (a) Dark-field (DF) image showing the formation of equiaxed O grains in a sample after aging for 2 h at 650 °C, (b) microdiffraction (MD) and CBED whole patterns of the <001>_O zone generated from a coarsened O phase.
Fig. 4. Schematic illustrations of (a) lattice correspondence between the T and O phases, (b) lattice deformation and (c) atomic shuffling during the T -> O transition. Only part of the T and O lattices were drawn in (c).

Fig. 5. An ellipsoid developed from a sphere of the T crystal by the invariant plane strain $B'$. The diagram is normal to $[110]_T$. 