Precipitation Behavior of $\omega_0$ Phase in Ti-37.5Al-12.5Nb Alloy

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Abstract: Mutual transformation between $\alpha_2$ and $\omega_0$ phases has been an interesting topic in recent years. In this study, martensitic $\alpha_2$ was obtained by air-cooling from 1250 °C in Ti-37.5Al-12.5Nb (at%) alloy while four $\omega_0$ variants formed in the $\beta_o$ phase matrix during the cooling process. Nonetheless, only one $\omega_0$ variant was observed at the periphery of the $\alpha_2$ plates in the $\beta_o$ phase and the orientation relationship between these two phases was $\{0001\} \alpha_2 // \{12\1\0\} \omega_0$; $(11\2\0) \alpha_2 // (0002) \omega_0$. Thin $\gamma$ plates precipitated within the $\alpha_2$ phase and were thought to be related to the appearance of $\omega_0$ phase. The redistribution of the compositions during the phase transformations was studied by energy dispersive X-ray spectroscopy analysis. The corresponding mechanisms of the phase transformations mentioned above are discussed.

Keywords: titanium aluminides; $\omega_0$ phase; TEM; HRTEM

1. Introduction

High Nb-containing TiAl (Nb-TiAl) alloys have been considered as potential materials for high-temperature applications due to their low density, high strength, good oxidation resistance, and creep properties [1–3]. Recently, Stark et al. showed that the amount of $\omega_0$ phase increased with the content of Nb in high Nb-TiAl alloy [4,5]. Meanwhile, Nb is a $\beta$ phase stabilizer that extends the $\beta$ phase field and facilitates the ordered $\omega_0$ ($\omega_o$) phase transitions in the $\beta_o$ phase in high Nb-TiAl alloys [6–9]. Numerous studies have reported the $\omega_o$ phase transformations in high Nb-TiAl alloys, indicating that the $\omega_o$ phase is stable at 700–900 °C [10,11]. However, these studies have mainly focused on the transition process between the $\beta_o$ and $\omega_o$ phases [6–13] or the $\alpha_2$ to $\beta_o$ phase [14–16]. Recently, some reports concentrated on the precipitation of the $\omega_o$ phase in $\alpha_2$ laths during aging and studied the relationship between the $\alpha_2$ and $\omega_o$ phases [10,17–20]. To summarize, there are two different thoughts regarding the precipitation of $\omega_o$ from $\alpha_2$ phase. First, Huang et al. reported the perpendicular decomposition of coarse $\alpha_2$ laths in Ti-44Al-8Nb-B alloy and suggested that the $\alpha_2$ to $\beta_o(\omega)$ transformation occurred after exposing at 700 °C in air for up to 10,000 h, indicating the occurrence of $\alpha_2 \rightarrow \beta_o \rightarrow \omega_o$ transformation [17]. Similar cases of $\alpha \rightarrow \beta \rightarrow \omega$ transformation in titanium alloys had been reported by Vohra et al. [18] and Gupta et al. [19]. Second, Bystrzanowski et al. observed that the applied stress could enhance the $\omega_o$ precipitation and suggested that the $\omega_o$ precipitation was directly transformed from the $\alpha_2$ phase [20]. Furthermore, Song et al. observed the direct $\alpha_2$ to $\omega_o$ phase transformation in Ti-45Al-9Nb alloy after aging at 900 °C [10]. Although
these studies discussed the transformation process and orientation relationships (ORs) between the ω₀ and α₂ phases, few reports focused on the nucleation sites of the ω₀ phase and the preferential ORs between the ω₀ and α₂ phases. Moreover, the nucleation behavior of ω₀ particles associated with α₂ phase in β₀ phase has scarcely been reported. In this work, the precipitation of ω₀ phase in Ti-37.5-12.5Nb alloy was examined. The preferential OR between the ω₀ and α₂ phases was evaluated. The corresponding mechanisms were also discussed.

2. Materials and Methods

An ingot of the Ti-37.5Al-12.5Nb (at%) used in this study was prepared using induction levitation melting. The ingot was flipped and remelted three times to ensure compositional homogeneity. Table 1 lists the chemical compositions measured via wet chemical analysis. Specimens with sizes of 10 × 10 × 10 mm were cut from the center of the ingot by electric-discharge machining. The specimens were heat treated at 1250 °C for 2 h followed by air cooling with a cooling rate of approximately 20 K/s. The microstructures after heat treatments were examined using a Zeiss Supra 55 scanning electron microscope (SEM) in back-scattered electron (BSE) mode. Thin foils used for transmission electron microscopy (TEM) observation were prepared by twin-jet electro-polishing in a solution of 65 vol% methanol, 30 vol% butanol, and 5 vol% perchloric acid at 30 V and −30 °C. TEM analysis was conducted on a Tecnai G² F30 field emission transmission electron microscope operating at 300 kV. The compositions were obtained by energy dispersive X-ray spectroscopy (EDS) on TEM. Each parameter was an average value of more than five results measured at different locations.

| Table 1. Chemical composition of the as-cast material. |
|-----------------|-----|-----|-----|-----|-----|
| Elements        | Ti  | Al (at%) | Nb (at%) | O (wt%) | N (wt%) |
| Composition     | Bal.| 37.0 | 13.0 | 0.018 | 0.0086 |

3. Results

The actual composition of the alloy is Ti-37.0Al-13.0 Nb, as obtained by chemical analyses, which is close to the nominal composition. Figure 1a shows the BSE image of the Ti-37.5Al-12.5Nb alloy after air-cooling. The microstructure is composed of α₂ plates and β₀ matrix which can be identified by TEM as in Figures 1b and 2b. The well-defined dark lines (arrowed in Figure 1a) observed in α₂ plates are believed to be the midribs of the martensite, which is similar to the result for the α₂ phase form from the β phase by iced-brine quenching in Ti-44Al-4Nb-4Hf-0.1Si [21]. It is difficult to distinguish whether the ω₀ phase exists in the β₀ region or not from the SEM image. Thus, the precipitation behavior of the ω₀ phase can be studied by using TEM. Figure 1b shows the bright-field TEM image of the air-cooled sample. Some particles with sizes of tens of nanometers distribute uniformly in the β₀ region. The corresponding selected area diffraction (SAD) pattern of the β₀ region is shown in Figure 1c, indicating that β₀ phase can readily transform to ω₀ phase during air cooling in this alloy.

Commonly, the observed ω₀ phase in high Nb-TiAl alloys can form from the “ω-collapse” in β₀ phase [6], i.e., the [111] β₀ layers “collapse” and the “-A-B-A-B-A-B-A-” stacking sequence in β₀ phase transforms into “-A-B/A-B-A/B-A-”. There are four equivalent [111] β₀ layers so that four possible ω₀ variants can form in one β₀ grain. Considering the ORs between these four ω₀ variants and β₀ phase, the [01T0] ω₀ diffraction spots of two ω₀ variants (denoted as “ω₀₁” and “ω₀₂” in Figure 1c) can be observed at 1/3[112] β₀ under the zone axes: <110> β₀ // <2T0> ω₀₁, ω₀₂. However, the <01T2> zone axes of “ω₀₃” and “ω₀₄” are parallel with <110> β₀ thus the diffraction patterns of these zone axes are overlapped completely. As a result, the intensities of the superposition spots of the ω₀ and β₀ phases are significantly increased in Figure 1c.
were obtained by EDS equipped on TEM in Table 2. The results show that the \( \omega \) phases \[22–24\]. Thus, \( \alpha \) periphery of the \( \omega \) phase. This case can be interpreted in that Nb is a stabilizing element of the \( \omega \) phase rather than of the \( \beta \) and \( \alpha \) 2 phases during the cooling process.

Figure 2a shows the bright-field image of the \( \alpha \) 2 plates. The circled area in Figure 2a demonstrates an almost precipitate-free region except for some particles that precipitate at the boundary of the \( \alpha \) 2 phase. The corresponding SAD pattern of this area is shown in Figure 2b. Only one \{011\} \( \omega \) variant exists at the \( \alpha \) 2 boundary are of one kind of \( \beta \) variant, as circled in the SAD pattern in Figure 2b. It is indicated that the precipitates at the periphery of the \( \beta \) 2 phase are more concentrated in Nb than \( \beta \) 0 and \( \alpha \) 2 phases during the cooling process.

\[ 110 \] \( \beta \) 0, // / [0001] \( \alpha \) 2, // / [11\overline{2}10] \( \omega \) 0; (1\overline{1}0) \( \beta \) 0, // / (1\overline{1}2\overline{2}0) \( \alpha \) 2, // / (0002) \( \omega \) 0.

Figure 2c is the corresponding dark field image taken by using the diffraction spot of the \( \omega \) 0 variant, as circled in the SAD pattern in Figure 2b. It is indicated that the precipitates at the \( \alpha \) 2/\( \beta \) 0 boundary are of one kind of \( \omega \) 0 variants. The compositions of the different phases (denoted in Figure 2a) were obtained by EDS equipped on TEM in Table 2. The results show that the \( \omega \) 0 precipitates at the periphery of the \( \alpha \) 2 phase are more concentrated in Nb than \( \beta \) 0-martix and \( \alpha \) 2 phase. This case can be interpreted in that Nb is a stabilizing element of the \( \omega \) 0 phase rather than of the \( \beta \) 0 and \( \alpha \) 2 phases \[22–24\]. Thus, \( \omega \) 0 precipitations at the \( \alpha \) 2/\( \beta \) 0 boundary are more concentrated in Nb than \( \beta \) 0 and \( \alpha \) 2 phases because of the expulsion of Nb in the \( \beta \) 0 and \( \alpha \) 2 phases during the cooling process.
Figure 2. TEM images of (a) bright-field image of the $\alpha_2/\beta_o$ boundary; (b) the corresponding SAD pattern at the $\alpha_2/\beta_o$ boundary; (c) dark-field image of the same area obtained by taking the spot of the $\omega_o$ phase circled in the SAD pattern in (b).

Table 2. Energy dispersive X-ray spectroscopy (EDS) results of different phases.

<table>
<thead>
<tr>
<th>Regions</th>
<th>Composition (at %)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Ti</td>
</tr>
<tr>
<td>$\beta_o$ matrix</td>
<td>49.9 ± 0.8</td>
</tr>
<tr>
<td>$\omega_o$</td>
<td>49.5 ± 0.7</td>
</tr>
<tr>
<td>$\alpha_2$ plate</td>
<td>51.1 ± 0.8</td>
</tr>
</tbody>
</table>

Figure 3 shows the High-resolution TEM (HRTEM) image of the $\alpha_2/\beta_o$ interface obtained under $[0001]_{\alpha_2}$ direction. The fast Fourier transformation (FFT) images of the $\omega_o$ and $\beta_o$ areas are shown in Figure 3b,c respectively. It is demonstrated that $\omega_o$ phases sized about a few tens of nanometers nucleate at the $\alpha_2$ boundary in Figure 3a. This indicates that the preferential $\omega_o$ phase can nucleate at the boundary of $\alpha_2$ phase and keep a certain OR with $\alpha_2$ phase.

Further studies on the interior of the $\alpha_2$ phase reveal that there are a few stacking faults in it. Figure 4a shows some fine-scale planar defects within the $\alpha_2$ phase, indicating certain phase transformations occur, as also suggested by the distortions at the boundary of the $\alpha_2$ plate. Figure 4b is the HRTEM image of the interface between the $\alpha_2$ and $\beta_o$ phase. The $\beta_o$ region and an $\omega_o$ precipitate nucleated at the $\alpha_2$ boundary are observed (the corresponding FFT images are shown in Figure 4c,d). It is worth pointing out that although the beam direction is $[11\overline{2}0]_{\alpha_2}$ and the $\omega_o$ precipitate is under $[0001]_{\omega_o}$ direction, the OR between these two phases is as same as those obtained in Figures 2 and 3. The magnified image of Figure 4b is shown in Figure 4e, the atomic stacking sequence of the $\alpha_2$ phase changes from “-ABAB-“ to “-ABCABC-“ (FCC-stacking) due to Shockley partial dislocations moving on alternate basal plane (0001) $\alpha_2$ planes. Repeating this mechanism every two basal planes of the hexagonal matrix leads to the crystal structure change, thus, the stacking faults can act as the nucleus of the $\gamma$ phase [25,26]. Moreover, it has also been reported that $\gamma$ phase precipitated in this alloy.
after annealing at 700 °C for 26 days [6]. However, the γ phase observed in [6] consists of γ grains precipitated directly from the matrix and not thin γ laths transformed from the α2 phase. Despite the different morphologies, these facts suggest that the γ phase is an equilibrium phase.

Figure 3. (a) High resolution TEM (HRTEM) image of the α2/βo interface, the corresponding fast Fourier transformation (FFT) images of ωo and βo areas denoted in (a) are shown in (b,c) respectively.

Figure 4. (a) TEM image of the α2 plate; (b) HRTEM image of the α2 boundary; (c,d) the corresponding FFT images transformed from the ωo and βo regions in (b); (e) the magnified image of (b) at the α2/ωo interface.
4. Discussion

4.1. Single $\omega_0$ Variant Nucleated at the $\alpha_2$ Boundary

Transformation matrices are useful for calculating the ORs between the precipitation and matrix phase, which has been widely used in calculating the habit-planes and misorientations [27–30]. As described above, four possible $\omega_0$ variants exist in the $\beta_0$ phase. The ORs between the $\omega_0$ variants and $\beta_0$ phase and between the $\omega_0$ and $\alpha_2$ phases are calculated by using the transformation matrices. The transformation matrices $B$ for $\beta_0$ to $\omega_0$ phases are shown in Table 3 (see Appendix A.2 for details). The hypothesis is that the ORs between the $\alpha_2$ and $\beta_0$ phases: $\{110\} \beta_0//(0001) \alpha_2$; <11T1> $\beta_0//<11\overline{2}0> \alpha_2$, six $\beta_0$ variants can form from the $\alpha_2$ phase and the transformation matrices $C$ for these variants are shown in Table 4 (see Appendix A.2 for details). The hypothesis is that the ORs between the $\alpha_2$ and $\omega_0$ phases can be transferred by the relationships between $\alpha_2$ to $\omega_0$. The OR between the $\alpha_2$ and $\omega_0$ phases (matrices $T$) can be readily obtained by

$$ T_{\alpha_2 \rightarrow \omega_0} = B \times C $$

$\omega_0$ is shown in Table 4 (see Appendix A.2 for details). The hypothesis is that the ORs between the $\alpha_2$ and $\omega_0$ phases can be transferred by the relationships between $\alpha_2$ to $\beta_0$ and $\beta_0$ to $\omega_0$. The OR between the $\alpha_2$ and $\omega_0$ phases (matrices $T$) can be readily obtained by

$$ T_{\alpha_2 \rightarrow \omega_0} = B \times C $$

Table 3. The transformation matrices $B$ for four $\omega_0$ variants from the $\beta_0$ phase.

<table>
<thead>
<tr>
<th>Variants</th>
<th>Orientation Relationship</th>
<th>Transformation Matrices $B$ for $\beta_0$ to $\omega_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>B1</td>
<td>(111) $\beta_0//(0001)$ $\omega_0$; [1T1] $\beta_0//[2\overline{2}0]$ $\omega_0$</td>
<td>$\sqrt{3}/2$ $-\sqrt{3}/2$ 0 $\sqrt{3}/3$ $\sqrt{3}/3$ $\sqrt{3}/3$</td>
</tr>
<tr>
<td>B2</td>
<td>(1T1) $\beta_0//(0001)$ $\omega_0$; [110] $\beta_0//[2\overline{2}0]$ $\omega_0$</td>
<td>$\sqrt{3}/2$ $\sqrt{3}/2$ 0 $\sqrt{3}/3$ $\sqrt{3}/3$ $\sqrt{3}/3$</td>
</tr>
<tr>
<td>B3</td>
<td>(1T1) $\beta_0//(0001)$ $\omega_0$; [110] $\beta_0//[2\overline{2}0]$ $\omega_0$</td>
<td>$\sqrt{3}/2$ $\sqrt{3}/2$ 0 $\sqrt{3}/3$ $\sqrt{3}/3$ $\sqrt{3}/3$</td>
</tr>
<tr>
<td>B4</td>
<td>(1T1) $\beta_0//(0001)$ $\omega_0$; [1T1] $\beta_0//[2\overline{2}0]$ $\omega_0$</td>
<td>$\sqrt{3}/2$ $\sqrt{3}/2$ 0 $\sqrt{3}/3$ $\sqrt{3}/3$ $\sqrt{3}/3$</td>
</tr>
</tbody>
</table>

Table 4. The transformation matrices $C$ for six $\beta_0$ variants from the $\alpha_2$ phase.

<table>
<thead>
<tr>
<th>Variants</th>
<th>Orientation Relationship</th>
<th>Transformation Matrices $C$ for $\alpha_2$ to $\beta_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>(110) $\beta_0//(0001)$ $\alpha_2$; [1T1] $\beta_0//[2\overline{2}0]$ $\alpha_2$</td>
<td>$\sqrt{3}/3$ $\sqrt{3}/3$ $\sqrt{3}/3$</td>
</tr>
<tr>
<td>C2</td>
<td>(110) $\beta_0//(0001)$ $\alpha_2$; [1T1] $\beta_0//[2\overline{2}0]$ $\alpha_2$</td>
<td>$\sqrt{3}/3$ $\sqrt{3}/3$ $\sqrt{3}/3$</td>
</tr>
<tr>
<td>C3</td>
<td>(110) $\beta_0//(0001)$ $\alpha_2$; [1T1] $\beta_0//[2\overline{2}0]$ $\alpha_2$</td>
<td>$\sqrt{3}/3$ $\sqrt{3}/3$ $\sqrt{3}/3$</td>
</tr>
<tr>
<td>C4</td>
<td>(110) $\beta_0//(0001)$ $\alpha_2$; [1T1] $\beta_0//[2\overline{2}0]$ $\alpha_2$</td>
<td>$\sqrt{3}/3$ $\sqrt{3}/3$ $\sqrt{3}/3$</td>
</tr>
<tr>
<td>C5</td>
<td>(110) $\beta_0//(0001)$ $\alpha_2$; [1T1] $\beta_0//[2\overline{2}0]$ $\alpha_2$</td>
<td>$\sqrt{3}/3$ $\sqrt{3}/3$ $\sqrt{3}/3$</td>
</tr>
<tr>
<td>C6</td>
<td>(110) $\beta_0//(0001)$ $\alpha_2$; [1T1] $\beta_0//[2\overline{2}0]$ $\alpha_2$</td>
<td>$\sqrt{3}/3$ $\sqrt{3}/3$ $\sqrt{3}/3$</td>
</tr>
</tbody>
</table>
**L** is the transformation matrix from the crystallographic coordinate system to the orthogonal coordinate system (see Appendix A). By using Equation (1), the matrices **T** for \( \alpha_2 \) to \( \omega_0 \) phases are obtained, deriving the arbitrary parallel crystallographic directions between the \( \alpha_2 \) and \( \omega_0 \) phases. According to these results, only four \( \omega_0 \) variants have good lattice matching and two ORs between the \( \alpha_2 \) and \( \omega_0 \) phases are obtained (see Appendix A.2 for details):

\[
<2\overline{1}00> \alpha_2//<0001> \omega_0; \quad \{0002\} \alpha_2//(2\overline{1}00) \omega_0, \text{ORI}
\]

\[
<2\overline{1}00> \alpha_2//<2\overline{2}01> \omega_0; \quad \{0002\} \alpha_2//(01\overline{2}2) \omega_0, \text{ORII}
\]

ORII can be also expressed as \(<\overline{1}0\overline{1}0>\alpha_2/<2\overline{2}32>\omega_0; \quad \{0002\} \alpha_2//(01\overline{2}2) \omega_0\) by using a superimposed stereographic projection. Thus, both ORs calculated from the transformation matrices are the same as the results obtained by edge-to-edge matching calculation in Ti-45Al-9Nb alloy [10]. According to the results, the selection of OR between the \( \alpha_2 \) and \( \omega_0 \) phases is essentially based on which \( \omega_0 \) variant has good lattice matching with \( \alpha_2 \) phase. It was reported that the misfit between the \( \alpha_2 \) and \( \omega_0 \) phases had a minimum value if ORI was formed [10]. Thus, it is believed that only one \( \omega_0 \) variant nucleated at the \( \alpha_2 \) boundary.

Moreover, according to the EDS results in Table 2, the composition of the \( \omega_0 \) particle nucleated at the boundary of the \( \alpha_2 \) phase is more concentrated in Nb than the \( \beta_2 \) matrix. It is suggested that the \( \omega_0 \) phase primarily nucleates at the boundary of the \( \alpha_2 \) phase and enriches in Nb during growth. Thus, the untransformed area of the periphery of the \( \alpha_2 \) phase is depleted in Nb so that the precipitate-free regions are observed.

### 4.2. Thin \( \gamma \) Plates Precipitated within the \( \alpha_2 \) Phase

Because of the misfit matching between the \( \alpha_2 \) and \( \omega_0 \) phases, distortions at the interface are expected. The interplanar spacings of the (0002) \( \alpha_2 \) and (11\overline{2}0) \( \omega_0 \) planes measured by HRTEM and SAD software are 0.233 nm and 0.229 nm, respectively. That is a 1.7% mismatch in the interplanar spacing when ORI is formed between the \( \alpha_2 \) and \( \omega_0 \) phases. It means that \( \alpha_2 \) phase may have an extra (0002) \( \alpha_2 \) plane after successive stacking of 59 pairs of (11\overline{2}0) \( \omega_0 \) and (0002) \( \alpha_2 \) planes. The interplanar spacing of (111) \( \gamma \) is 0.232 nm is smaller than that of the (0002) \( \alpha_2 \) but larger than (11\overline{2}0) \( \omega_0 \). Thus, the fine \( \gamma \) plates may relieve the distortion at the interface of the \( \omega_0 \) and \( \alpha_2 \) phases (Figure 4e). It has been reported that the precipitation of \( \gamma \) in \( \alpha_2 \) is simply a HCP → FCC structure change which can be brought about if \( a/6 <10\overline{1}0> \) type Shockley partials move on alternate basal plane (0001) \( \alpha_2 \) planes [31,32]. As mentioned above, an extra (0002) \( \alpha_2 \) plane exists after successive stacking of 59 pairs of (11\overline{2}0) \( \omega_0 \) and (0002) \( \alpha_2 \) planes. This case may cause the distorted-region separated along the \( \alpha_2 \) and \( \omega_0 \) interface. As a consequence, the sliding of the partial dislocations in the distorted-region can produce separated fine \( \gamma \) plates at certain intervals. Moreover, the interplanar spacing of 59 (0002) \( \alpha_2 \) planes is approximate 13.7 nm, which is consistent with the average spacing of the \( \gamma \) laths, which is approximate 12 nm as obtained from Figure 4a.

### 5. Conclusions

In this work, the precipitation of \( \omega_0 \) phase in Ti-37.5Al-12.5Nb alloy was examined mainly by TEM. The ORs between different phases were calculated. The main results are summarized as follows:

1. Only one \( \omega_0 \) variant preferentially nucleates at the \( \alpha_2 \) boundaries. This is because the minimum misfit exists at the \( \alpha_2/\omega_0 \) interface if the OR between these two phases is: \(<2\overline{1}00>\alpha_2//<0001>\omega_0; \quad \{0002\} \alpha_2//(2\overline{1}00) \omega_0\).

2. Precipitate-free regions are observed at the \( \alpha_2 \) boundaries. EDS results indicate that the \( \omega_0 \) precipitates are more concentrated in Nb than \( \beta_2 \)-matrix. The preferred nucleation of the \( \omega_0 \) variant causes solute depletion surrounding the \( \alpha_2 \) plates, which inhibits the nucleation and growth of new \( \omega_0 \) precipitates in the un-precipitated regions.
3. Thin γ plates precipitate within the α2 phase. These fine γ plates can relieve the distortion caused by the mismatch at the α2/ωo interface.

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**Author Contributions:** Lin Song and Junpin Lin conceived and designed the experiments; Teng Ye, Maohua Quan and Jianping He performed the experiments; Teng Ye analyzed the data and wrote the paper.

**Conflicts of Interest:** The authors declare no conflict of interest.

**Appendix A**

Because ωo and α2 phases have a hexagonal structure, we can define an orthogonal coordinate system with ‘x’ axis is [2110] direction, ‘y’ axis is [0110] direction and ‘z’ axis is [0001] direction. Then, the transformation matrix from the crystallographic coordinate system to the orthogonal coordinate system can be written as:

\[
L = \begin{bmatrix}
  a & -a/2 & 0 \\
  0 & \sqrt{3}a/2 & 0 \\
  0 & 0 & c
\end{bmatrix}
\]

here ‘a’ and ‘c’ are lattice parameters.

In order to calculate the ORs between these phases, the indices of the crystallographic direction [uvtw] and the crystallographic face (hkil) in the four-index vector must transform into a three-index vector \([u'v'w']\) and \([h'k'l']\) in the hexagonal coordinate system, e.g.,

\[
u^h = 2u + v; v^h = u + 2v; w^h = w \tag{A1}
\]

and

\[
h^h = h; k^h = k; l^h = l \tag{A2}
\]

Considering a hexagonal structure, the indices of the normal of the crystallographic face \([h'k'l']\) in the hexagonal coordinate system are: \([2h + k \cdot h + 2k \cdot 3l (a/c)^2]/2\). Thus, the index vector \([u'v'w']\) and \([h'k'l']\) in the orthogonal coordinate system can be obtained by \(L \times [u^h v^h w^h]^T\) and \(L \times [h^h k^h l^h]^T\), the relationship between the \([u'v'w']\) and \([uvtw]\) is:

\[
u' = 3u/2; v' = (u + 2v)\sqrt{3}/2; w' = wc/a \tag{A3}
\]

and

\[
U = 2u'/3; v = \left(\sqrt{3}v' - u'\right)/3; t = -(u + v); w = aw'/c \tag{A4}
\]

Similarly, the relationship between the \([h'k'l']\) and \([hkil]\) is:

\[
h' = \sqrt{3}h; k' = h + 2k; l' = \sqrt{3}a/c \tag{A5}
\]

and

\[
H = h' \sqrt{3}/3; k = (k' - h' \sqrt{3}/3)/2; l = cl' \sqrt{3}/3a \tag{A6}
\]

**Appendix A.1. Transformation Matrices B from βo to ωo**

The observed ωo phase in high Nb-TiAl alloys can be formed from ‘ω-collapse’ in the (111) βo plane. The OR between ωo and βo phase can be described as:

\[
<110> \beta_o / <1210> \omega_o; \{1T1\} \beta_o / \{0001\} \omega_o \tag{A7}
\]
There are four different crystallographic equivalent \(<111>\) \(\beta_0\) directions in \(\beta_0\) lattice. Thus, four possible \(\omega_0\) variants exist in the \(\beta_0\) phase with specific ORs between \(\omega_0\) and \(\beta_0\) phases. It is convenient to describe the ORs by using \('(hkl) [uvw]'\) matrix, which is written as:

\[
\begin{align*}
\mathbf{u} & = rh \\
\mathbf{v} & = sk \\
\mathbf{w} & = tl
\end{align*}
\]

All the vectors have been normalized and the orientation matrix \(\mathbf{A}\) of the \(\beta_0\) phase can be written as in Table A1.

### Table A1. The orientation matrix \(\mathbf{A}\) of the \(\beta_0\) phase.

<table>
<thead>
<tr>
<th>Variants</th>
<th>Orientation Relationship</th>
<th>Orientation Matrix (\mathbf{A}) of the (\beta_0) Phase</th>
</tr>
</thead>
</table>
| A1       | \((111)\beta_0//\langle0001\rangle\omega_0;\) \([1\bar{1}0]\) \(\beta_0//[2\bar{1}0\bar{0}]\) \(\omega_0\) | \[
\begin{pmatrix}
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
-\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\
0 & -2/\sqrt{6} & 1/\sqrt{3}
\end{pmatrix}
\]
| A2       | \((1\bar{1}0)\beta_0//\langle0001\rangle\omega_0;\) \([1\bar{1}0]\) \(\beta_0//[2\bar{1}0\bar{0}]\) \(\omega_0\) | \[
\begin{pmatrix}
\frac{1}{\sqrt{2}} & -1/\sqrt{6} & -1/\sqrt{2} \\
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & 1/\sqrt{3} \\
0 & -2/\sqrt{6} & 1/\sqrt{3}
\end{pmatrix}
\]
| A3       | \((1\bar{1}0)\beta_0//\langle0001\rangle\omega_0;\) \([1\bar{1}0]\) \(\beta_0//[2\bar{1}0\bar{0}]\) \(\omega_0\) | \[
\begin{pmatrix}
\frac{1}{\sqrt{2}} & -1/\sqrt{6} & 1/\sqrt{3} \\
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & -1/\sqrt{3} \\
0 & 2/\sqrt{6} & 1/\sqrt{3}
\end{pmatrix}
\]
| A4       | \((1\bar{1}0)\beta_0//\langle0001\rangle\omega_0;\) \([1\bar{1}0]\) \(\beta_0//[2\bar{1}0\bar{0}]\) \(\omega_0\) | \[
\begin{pmatrix}
\frac{1}{\sqrt{2}} & -1/\sqrt{6} & 1/\sqrt{3} \\
-\frac{1}{\sqrt{2}} & -1/\sqrt{6} & 1/\sqrt{3} \\
0 & -2/\sqrt{6} & -1/\sqrt{3}
\end{pmatrix}
\]

Thus, the transformation matrices \(\mathbf{B}\) from \(\beta_0\) to \(\omega_0\) can be obtained by inverse matrices of \(\mathbf{A}\): \(\mathbf{B} = \mathbf{A}^{-1}\), (see Table 3 in the article).

Having noted that the calculated crystal directions of the \(\omega_0\) phase are described in the orthogonal coordinate, thus, they can be transformed from orthogonal coordinate to crystal coordinate by using the Equation (A4).

### Appendix A.2. Transformation Matrices \(\mathbf{C}\) from \(\alpha_2\) to \(\beta_0\)

According to the so-called Burgers OR between the \(\alpha_2\) and \(\beta_0\) phases: \((\langle110\rangle) \beta_0//\langle0001\rangle \alpha_2;\) \(\langle1\bar{1}0\rangle\) \(\beta_0//\langle1\bar{1}0\rangle\) \(\alpha_2\), six \(\beta_0\) variants can form from the \(\alpha_2\) phase (see Table A2). As described above, we can obtain the transformation matrices \(\mathbf{C}\) from \(\alpha_2\) to \(\beta_0\). However, variants 3 and 4 indicate that the direction of \([\bar{2}10\bar{0}]\) \(\alpha_2\) parallels the ‘\(\chi\)’ axis in the reference coordinate system (which means the crystal coordinate rotates 120° counterclockwise around the \([0001]\) \(\alpha_2\)). Thus, the transformation matrices should be multiplied by the three-fold rotation matrix under the \([0001]\) axis:

\[
\mathbf{R} = 
\begin{pmatrix}
-1 & 1 & 0 \\
-1 & 0 & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

Moreover, variant 5 and 6 must be multiplied by the three-fold rotation matrix twice because the crystal coordinate rotates 240° counterclockwise around the \([0001]\) \(\alpha_2\). Thus, the transformation matrices \(\mathbf{C}\) from \(\alpha_2\) to \(\beta_0\) can be obtained by \(\mathbf{L}\) and \(\mathbf{R}\). (see Table 4 in the article).

Then, we can calculate the transformation matrices \(\mathbf{T}\) from \(\alpha_2\) to \(\omega_0\), \(\mathbf{T} = \mathbf{B} \times \mathbf{C}\). As described above, the calculated crystal directions of the \(\omega_0\) phase should be transformed from orthogonal coordinate to crystal coordinate by using the Equation (A2).

For instance, when the view direction is \([\bar{2}110]\) \(\alpha_2\) and \([000\bar{1}]\) \(\alpha_2\), the paralleled crystallographic directions of \(\alpha_o\) are shown in Tables A2 and A3 (Moreover, the parallel crystallographic plane can be obtained from the normal of the crystal face by using Equation (A3)).
Table A2. The paralleled crystallographic directions of different $\omega_0$ variants under $[2110] \alpha_2$ direction.

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Table A3. The paralleled crystallographic directions of different $\omega_0$ variants under $[0001] \alpha_2$ direction.

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