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LATTICE CORRESPONDENCE AND CRYSTALLOGRAPHY OF MARTENSITES IN TITANIUM ALLOYS

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Abstract.—Lattice correspondence, crystallography and internal structure of various martensites in titanium alloys are discussed in a unified manner. Strain energy minimization criterion is applied to discuss the orientation of habit planes and lattice invariant strains. A comparison of the present analysis with experimental observations has been carried out.

Introduction.—Quenching from the high-temperature β (b.c.c.) phase of titanium alloys results in the formation of various kinds of martensites such as α' (h.c.p.), α" (orthorhombic), f.c.c. (face-centered orthorhombic) and f.c.c. (face-centered cubic) martensites. Except for the f.c.c. martensite, which is considered to occur only in thin films [1], the other three martensites have been found in bulk titanium alloys. Although there are many studies available for the crystallography of these martensites, it seems that no unified understanding of the martensitic transformations in titanium alloys has been developed.

In this study, the lattice correspondence and the crystallography of the α', α" and f.c.c. martensites will be investigated systematically by using experimental observations available in the literature. It will also be shown that the strain energy minimization criterion can be applied to discuss the crystallography and internal structure (lattice invariant shear, habit plane, etc.) of these martensites.

Lattice Correspondence and Crystal Structure Change.—Figure 1 shows the four unit cells of the b.c.c. β-phase and its face-centered tetragonal equivalent. It has been demonstrated [2 - 4] that all of the martensites (α', α" and f.c.c.) can be generated from this tetragonal lattice. By using lattice parameter values of the parent β-phase and the martensites, the lattice variant strain (Bain strain) can be calculated. Table 1 shows the lattice parameters of the parent and martensite phases [1, 3, 4] used in the present study. From these values, the Bain strains based on the x-y'-z' coordinate system (t-system) in the tetragonal cell in Fig. 1 can be calculated and these are also shown in Table 1. For the case of the α' martensite, the Bain strain is brought about by the well-known Burgers mechanism where the operation of the (112)<111> shear systems followed by a small volume increase results in the (0001)α' plane from the (011)β plane. In addition to the above Bain strain, a small shuffling on every other (011)β plane.
Table 1.- Lattice parameters and the calculated Bain strains in titanium alloys analyzed in the present study.

<table>
<thead>
<tr>
<th>Martensite</th>
<th>(a')</th>
<th>(a'')</th>
<th>f.c.c.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alloy</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ti-5Mn [1]</td>
<td>3.259</td>
<td>3.22</td>
<td>3.263</td>
</tr>
<tr>
<td>Ti-10V-2Fe-3Al [3]</td>
<td>3.259</td>
<td>3.22</td>
<td></td>
</tr>
<tr>
<td>Ti-12.6V [4]</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Lattice parameter of B-phase (Å)</th>
<th>(a)</th>
<th>(c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>2.950</td>
<td>4.585</td>
</tr>
<tr>
<td>(c)</td>
<td>4.62</td>
<td>4.667</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Bain strain</th>
<th>(\epsilon_1)</th>
<th>(\epsilon_2)</th>
<th>(\epsilon_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\epsilon_1)</td>
<td>-0.0748</td>
<td>0.1086</td>
<td>0.0165</td>
</tr>
<tr>
<td>(\epsilon_2)</td>
<td>-0.0652</td>
<td>0.0607</td>
<td>-0.0495</td>
</tr>
<tr>
<td>(\epsilon_3)</td>
<td>-0.0913</td>
<td>0.0145</td>
<td>-0.0370</td>
</tr>
</tbody>
</table>

The formation of the \(a''\) martensite can be explained in essentially the same manner. The difference lies in the fact that after the operation of the \([112]<111>\) shear, the \((011)_{B}\) plane does not completely change into the hexagonal close-packed plane but stops midway between the \((011)_{B}\) and the \((0001)_{a'}\) leaving the angles \(\theta_1\) and \(\theta_2\) in Fig. 2(b) slightly different from 120 degrees. Thus, the \(a''\) martensite can be considered as a "distorted" \(a'\) martensite. It has been reported [2, 3, 5] that a transition from the \(a'\) to \(a''\) martensite occurs with an increasing \(B\)-stabilizing solute content. This issue will be further discussed.

The f.c.c. martensite, on the other hand, is a rather unique one found only in a bulk Ti-12.6% V alloy [4]. In this case, no shuffling is necessary and the lattice correspondence is very similar to that in the Au-Cd martensite [6]. It should be noted, from Table 1, that the components of the Bain strain for the f.c.c. martensite have the opposite signs to those for the \(a'\) and \(a''\) martensites. Thus, the f.c.c. martensite cannot be considered to be a "distorted" \(a'\) martensite.

Phenomenological Analysis Based on the Strain Energy Minimization Criterion.- Mura et al. [7] and Kato et al. [8] have shown that there is a one-to-one correspondence between the phenomenological crystallographic theory of martensitic transformations [9, 10] and the strain energy minimization approach based on the small deformation theory [7, 8]. According to their analysis, if the transformation strain \(\epsilon_{14}\) (Bain strain plus lattice invariant strain) in an \(x_1-x_2-x_3\) cartesian coordinate system

![Fig. 2.- Crystal structure change from b.c.c. to (a) h.c.p. (\(a'\)) and (b) orthorhombic (\(a''\)).](image-url)
satisfies the condition of
\[ \varepsilon_{11}^T = \varepsilon_{22}^T = \varepsilon_{12}^T = 0, \]  
(1)
the strain energy becomes minimum (zero) and the condition in equation (1), with the \( x_3 \)-axis as an invariant plane (habit plane) normal, is equivalent to the invariant plane condition in the phenomenological theory. The advantage of using the small-deformation theory is that the calculation becomes much simpler and even if the three principal components of the Bain strain are different, such as the case in the present martensites, the final solutions can be obtained in simple analytical forms.

Let us now apply this strain energy minimization criterion to simultaneously analyse the crystallography of the \( \alpha' \), \( \alpha'' \) and the f.c.c. martensites. As shown in Table 1, the Bain strain in the t-system for the all three martensites can be written in a form of
\[ \varepsilon^1_{ij} = \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_2 & 0 \\ 0 & 0 & \varepsilon_3 \end{pmatrix}. \]  
(2)
As can be seen in Table 1, \( \varepsilon_1 < 0 \) (contraction) and \( \varepsilon_2, \varepsilon_3 > 0 \) (expansion) for the \( \alpha' \) and \( \alpha'' \) martensites whereas \( \varepsilon_1 > 0 \) and \( \varepsilon_2, \varepsilon_3 < 0 \) for the f.c.c. martensite. If equation (2) is viewed based on the \( x-y-z \) system in the parent \( \beta \)-phase (\( \beta \)-system), we have
\[ \varepsilon^1_{ij} = \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & (\varepsilon_2 + \varepsilon_3)/2 & (\varepsilon_3 - \varepsilon_2)/2 \\ 0 & (\varepsilon_3 - \varepsilon_2)/2 & (\varepsilon_2 + \varepsilon_3)/2 \end{pmatrix}, \]  
(variant 1).
\[ \varepsilon^2_{ij} = \begin{pmatrix} (\varepsilon_2 + \varepsilon_3)/2 & 0 & (\varepsilon_3 - \varepsilon_2)/2 \\ 0 & \varepsilon_1 & 0 \\ (\varepsilon_2 - \varepsilon_3)/2 & 0 & (\varepsilon_2 + \varepsilon_3)/2 \end{pmatrix}, \]  
(variant 2).

It has been reported that the lattice invariant shear for each martensite occurs dominantly by twinning and the twinning planes are \{10\bar{1}\} \( \alpha' \), \{11\bar{1}\} \( \alpha'' \) [5] and \{11\bar{1}\} f.c.c. [4]. Interestingly, all of these twinning planes correspond to the \{110\} plane of the parent \( \beta \)-phase in Fig. 1. Thus, by using the \( \beta \)-system, the twinned variant should have the Bain strain of
\[ \varepsilon^T_{ij} = \varepsilon^1_{ij} + (1 - f)\varepsilon^2_{ij}, \]  
(0 < f < 1),
where \( f \) is the volume fraction of the variant 1 which is to be determined. The habit plane and \( f \) can be obtained in the following manner.

Let the unit vector \( \vec{h} \), normal to the habit plane, be written in the \( \beta \)-system as
\[ \vec{h} = [\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta]_\beta. \]  
(6)
By rotating the coordinate system, we can find a new \( x_1-x_2-x_3 \) system in which the total transformation strain (5) satisfies the invariant plane condition of equation (1). In this new system, \( \vec{h} \) becomes parallel to the \( x_3 \)-axis. It should be noted that equation (1) actually gives three simultaneous equations with \( f, \theta \) and \( \phi \) as the...
three unknown parameters. These can be solved easily and the results become;

$$
\tan^2 \phi = \frac{2(1 - f)\epsilon_1 + f(\epsilon_2 + \epsilon_3)}{2\epsilon_1 + (1 - f)(\epsilon_2 + \epsilon_3)},
$$

(7)

$$
\tan \theta = \frac{\sin \phi (2(2f - 1)\epsilon_1 + (1 - 2f)(\epsilon_2 + \epsilon_3))}{(\epsilon_2 - \epsilon_3)((1 - f)\tan \phi + f)},
$$

(8)

where

$$
f = \frac{1}{2} \pm \frac{\sqrt{A^2 - 4AB}}{2A},
$$

(9)

It can easily be shown that solutions corresponding to the positive and negative signs in equation (9) are crystallographically equivalent. Moreover, it should be noted that there are two independent (crystallographically different) solutions for the orientation of the habit plane, depending on the positive and negative values of $\tan \phi$ in equation (7).

By using the data for the Bain strain in Table 1, the habit plane normal and the volume fraction of the variant 1 were calculated from equations (7) through (9) for each of the three martensites and the results are shown in Table 2. The habit plane normals are also plotted in Fig. 3 where the stereographic projection is based on the indices of the parent B-phase.

**Discussion.** To investigate the accuracy of the present small deformation analysis, the results of the numerical calculation of the habit plane normal for the a' martensite in a Ti-Mn alloy by Knowles and Smith [11], based on the phenomenological theory, are also shown in Fig. 3. Since the same input data are adopted in the present analysis, it is not surprising to see from Fig. 3 that both the present analysis and the phenomenological theory predict essentially the same orientation of the habit plane normals; one of the solutions belonging to the Class A (a-u^+), and the other to the Class A (a^+ w^-) in the Mackenzie-Bowles notation [1, 11, 12]. From this, we can say that the small-deformation strain energy minimization criterion can be used in lieu of the phenomenological theory to discuss the crystallography of the titanium alloy martensites. One main advantage in the small deformation theory is that no numerical calculation is involved and a systematic investigation is possible to find the change in solutions due to the change in input parameters.

It has been found in Ti-Mn alloys [1, 11] that there are two different types of a' martensites, one with the {334}B and the other with the {344}B habit planes. As can be seen from Fig. 3, none of the two solutions for the a' martensite accurately explains the above habit plane indices. Hammond and Kelly [1] were thus forced to use an adjustable "dilatation" parameter, $\delta$, in the phenomenological theory to bring the irrational habit plane normals to the observed indices.

Knowles and Smith [11] took a different approach. They analyzed the zig-zag

<table>
<thead>
<tr>
<th>Table 2. Calculated solutions for titanium alloy martensites.</th>
</tr>
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<tbody>
<tr>
<td><strong>martensite</strong></td>
</tr>
<tr>
<td>----------------</td>
</tr>
<tr>
<td>volume fraction of variant 1, $f$</td>
</tr>
<tr>
<td>habit plane, $h_0$</td>
</tr>
<tr>
<td></td>
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</tbody>
</table>
Fig. 3.- Calculated habit plane normals for titanium alloy martensites.

The reason why the calculated orientations of the habit plane in Fig. 3 do not coincide with the observed (334) or (344) plane might simply be understood if we make the following analysis. Hammond and Kelly [1] as well as Knowles and Smith [11] used the lattice parameter of the 6-phase of the Ti-5% Mn alloy ($a = 3.259 \text{ Å}$ as shown in Table 1) measured at room temperature. Since the $\beta \rightarrow \alpha'$ martensitic transformation takes place at a higher temperature, the lattice parameter should be compensated by taking into account the thermal dilatation. Davis et al. [5], on the other hand, have systematically obtained the lattice parameters of the $\beta$-phase and the $\alpha'$ and $\alpha''$ martensites in Ti-Mo alloys taking into account the thermal dilatation as well as the change in the lattice parameter of the $\beta$-phase due to the change in the molybdenum content. According to their observation, the $\alpha'$ martensite is formed in the alloy with as much as 4% Mo and the $\alpha''$ martensite is observed in Ti-6% Mo and Ti-8% Mo alloys. Similar tendency from h.c.p. to orthorhombic structure change associated with increasing $\beta$-stabilizing elements is also observed in other titanium alloys [2, 4].

Table 3 shows the systematic change in the Bain strain due to the change in the molybdenum content obtained by Davis et al. [5]. By using these data, trial calculation based on the strain energy minimization criterion was made to see the systematic change in the orientation of the habit plane with increasing molybdenum content.

<table>
<thead>
<tr>
<th>Table 3.- Bain strains for Ti-Mo martensites [5].</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_1$</td>
</tr>
<tr>
<td>-------</td>
</tr>
<tr>
<td>Ti</td>
</tr>
<tr>
<td>Ti-2I Mo</td>
</tr>
<tr>
<td>Ti-4I Mo</td>
</tr>
<tr>
<td>Ti-6I Mo</td>
</tr>
<tr>
<td>Ti-8I Mo</td>
</tr>
</tbody>
</table>
Figure 4 summarizes the results of the calculation. As can be seen, the habit plane normals lie close to the $[434]_g$ and $[433]_b$ poles. As recently pointed out by several investigators [2, 5], there is a continuous change in crystal structure of martensite from $a'$ to $a''$ with increasing $b$-stabilizing elements. This fact results in the continuous change in the orientation of the habit plane as shown in Fig. 4.

The f.c.c. martensite, on the other hand, is considered to have a totally different crystal structure and the transformation resembles that in a Au-Cd [6] or Cu-Al-Ni [13] system. It is interesting to know that all of these martensites are reported to have (133) habit planes [4, 6, 13]. As shown in Fig. 3, both of the solutions of the habit plane normals for the f.c.c. martensite lie reasonably close to the $<133>_g$-type poles. Thus, further investigation is necessary to know which solution is the better description of this transformation.

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References.