THE CRYSTALLOGRAPHY OF THE BCC TO HCP (ORTHOHEXAGONAL) MARTENSITIC TRANSFORMATION IN DILUTE Zr-Nb ALLOYS:

Part I: Lattice Strain and Lattice Invariant Shear

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ABSTRACT

The Bain strain (homogenous strain or lattice strain), the inhomogeneous shear (LIS) and the rigid body rotation in relation with the martensitic transformation in Zr-2.5%Nb alloy has been calculated. The homogenous lattice strain has been uniquely determined by invoking Lomer’s criterion and the minimum distortion criterion. Both the minimum strain energy and the minimum distortion considerations lead to the same type of Bain strain and lattice correspondence. A systematic study has been carried out to identify the possible lattice invariant shears (LIS) which meet the IPS condition for both slip type and twin type shears. Mathematical and graphical methods have been employed to determine the slip and the twin systems which qualify as the LIS from amongst the possible deformation systems of the hcp structure. In this manner, the most frequently observed \{\(1\overline{1}0\overline{1}\)\}_H <2\(\overline{1}\overline{1}3\)>_H; \{\(2\overline{1}2\)\}_H <2\(\overline{1}\overline{1}3\)>_H; \{\(\overline{1}\overline{1}2\)\}_H <2\(\overline{1}\overline{1}3\)>_H slip systems and the \{\(1\overline{1}0\overline{1}\)\}_H <4\(1\overline{5}\)3>_H; \{0\(1\overline{1}2\)\}_H <0\(1\overline{1}\)1>_H twin systems have been found to qualify as the LIS.

1. INTRODUCTION

Bcc to hcp martensitic transformation is observed to occur in Ti, Zr, Li, Hf and their alloys. This group of metals and alloys when rapidly quenched from temperatures at which the \(\beta\) (bcc) phase is stable transforms to the \(\alpha'\) (hcp) phase. The crystal structure of the \(\alpha'\) phase is the same as that of the \(\alpha\) phase, which forms on slow cooling. The crystallographic and microstructural features associated with bcc-hcp martensitic transformation have been reviewed by Christian 1, Nishiyama 2. In 1934 Burger 3 recognized that the polymorphic phase change in zirconium could be brought about by a shear mechanism. In this context he proposed, the first single shear mechanism for a martensitic change. The transformation temperatures, the lattice parameters, and the measured crystallographic parameters are very similar for elemental titanium and zirconium and for dilute alloys based on these metals. A detailed crystallographic analysis of the bcc-orthorhombic (equivalent to bcc-hcp transformation) martensitic transformation in Ti alloys was carried out by Lieberman et al 4, Bowles and Mackenzie 5 and other workers 6-8. However, in the literature such systematic studies on the crystallography of the martensitic transformation in Zr and Zr-base alloys are not available. Substructural and morphological studies of several binary Zr-X 9-17 (X = Nb, Cr, Ti, Cu and Mo) and Ti-X 6,18-31 (X = Cu, Fe Ta, Mn, Cr, Mo and V) alloys have been studied extensively.
In the present work, the phenomenological theory of martensitic crystallography (PTMC) has been applied to the bcc-hcp martensitic transformation, using the lattice parameters of Zr-2.5\% Nb alloy. The results of the martensitic crystallography have been presented in the two-part paper. Part I of the present work deals with the determination of the Bain strain (homogenous strain or lattice strain) and the selection of possible inhomogeneous shear or lattice invariant shear, LIS, (both slip as well as twin type). A simple model has been proposed for determining the factors, which influences the selection of the preferred LIS mode. In Part II of the paper, the Bain strain, the inhomogeneous shear and the rigid body rotation determined in the Part I has been used to calculate the shape strain and related crystallographic parameters, such as, shape strain, orientation relationship and habit plane etc. for each possible LIS mode for the martensitic transformation of Zr-2.5\% Nb alloys. This treatment of PTMC for Zr-2.5Nb is very general in nature and the results obtained here would be applicable for all the dilute Zr-Nb alloys.

2. THE CRYSTALLOGRAPHY OF MARTENSITIC TRANSFORMATION

The basic concept inherent in the current phenomenological theories of the martensitic crystallography (PTMC) is that the interface between the parent and the product phases is an invariant strain plane (one that is undistorted and unrotated during the transformation) \(^{1-2}\). Such a plane will give rise to the minimum transformation strain energy\(^{1-2}\).

A characteristic of the martensitic transformation is that it proceeds through cooperative movement of atoms, in which atomic neighbours are maintained before and after the transformation. The numbers and type of atoms is also conserved in this transformation. A homogenous distortion was suggested as one of the possible mechanisms, although the amount of deformation would be large compared with ordinary elastic deformation. Bain \(^{32}\) proposed such a model for steels in which a bct lattice can be generated from an fcc (\(\gamma\)) lattice by compression along one axis, say \(<001>_{\text{fcc}}\) and uniform expansion along the other two axes perpendicular to it. There can be several possible lattice deformation alternatives to generate the daughter (bct) lattice from the parent (fcc) lattice. Bain deformation is most reasonable among these because it involves the smallest relative atomic displacement and thus the smallest strain energy. Jawson and Wheeler \(^{33}\) have also given a mathematical treatment to deduce a simple correspondence for the fcc-bct transformation by finding the one which causes the minimum atom movements. It is possible to confirm the validity of Bain deformation in steels since the interstitial atom tetragonality of a specific orientation with respect to the austenite lattice is known \(^{34}\). However, the validity of the Bain distortion can be proved more clearly for ordered alloys which give rise to diffraction patterns containing super lattice spots \(^{35}\). In the Zr-2.5\% Nb alloy, which is disordered in nature it is not possible to validate the correspondence. Such a homogenous distortion, which transforms one lattice to another, is termed a lattice distortion (Bain distortion). In some transformations, a lattice distortion alone may not be able to move the majority of the atoms to the correct positions. In such cases, a shuffle is required to bring the atoms to the proper positions \(^{1-2}\).

It is in general, difficult to obtain a coherent undistorted planar interface under the operation of lattice (Bain) distortion only. The necessary and sufficient condition of PTMC can be ensured by incorporating an additional shear, which does not affect the lattice structure but nevertheless, produces a macroscopic change in shape \(^{1-2}\). Such an additional distortion can be a slip shear or a twinning shear over a fraction of the crystal \(^{1-2}\). This shear is termed as “inhomogeneous” or “lattice invariant” shear. In PTMC the critical amount of lattice invariant shear (LIS) is determined in such a way that the combined operation of the lattice distortion and the LIS ensures the existence of a plane of zero distortion (IPS condition) \(^{1}\). A microscopic IPS is obtained by averaging over the two lattice deformations of a finely twinned product or by forming an interface containing an array of “misfit”, “interface” or “anti coherency” dislocations, each of which has a Burgers vector equal to a lattice vector. Electron microscope studies have confirmed the presence of internal twins as well as dislocation substructure in the martensitic
microstructure. In this context, the work of Bywater and Christian may be cited in which a suitable alloy composition, Ti-22%Ta, was chosen for making one of the principal strain values equal to zero \( \eta_1 = 0 \). The IPS condition was thus fulfilled even without the operation of any LIS. The absence of twins and dislocations substructure in the martensitic microstructure of the Ti-22%Ta alloy experimentally validated the absence of any LIS.

The pure lattice strain transforms the parent lattice into the product lattice and the combination of LIS will, in general, leave one plane undistorted but rotated to a new position; a rigid body rotation is applied to bring back the undistorted plane into the original position. Thus the total shape deformation involved in the martensitic deformation is obtained by combining three operations consisting of a pure lattice distortion, B (the “Bain distortion”), the lattice invariant shear, P, and a rigid body rotation, R. The two most widely cited phenomenological theories have been developed by Wechsler, Lieberman and Read (W-L-R theory) and by Bowles and Mackenzie (B-M theory). The Bain strain, the inhomogeneous shear and the rigid body rotation pertinent to calculating the shape strain and related crystallographic parameters for Zr-2.5% Nb alloys are described in the following sections.

2.1 Bain Strain and Lattice Correspondence:

2.1.1 Lattice Correspondence and Orientation Relationship in Zr-2.5% Nb Alloy

Assuming the Bain distortion, a lattice correspondence between lattice points in the initial and final lattices can be determined uniquely which defines a one to one relationship between selected vectors, planes and cells of the two lattices. It is generally possible to determine the Bain correspondence uniquely on the basis of minimum atomic movements. However, in certain cases, e.g., in \( \beta-\alpha \) transformation of uranium, the situation can be very complex. Since \( \beta \) uranium structure involves 30 atoms per unit cell, there can be very large number of possible lattice correspondences. Bain distortion is concerned with the initial and the final lattices, and does not give the actual crystal orientation relationship between them. However, the lattice correspondence, in general, is found to be very close to the orientation relationship.

The cubic (bcc) to close packed hexagonal (hcp) transformation in Zr and Ti alloys was originally described by Burger. The Burgers correspondence was later confirmed in most of the Zr and Ti alloys. Burgers orientation relationship is given by:

\[
\begin{align*}
[110]_C &\parallel [0001]_H; \quad [\overline{1}2\overline{1}]_C &\parallel [10\overline{1}0]_H; \\
[\overline{1}11]_C &\parallel [\overline{1}2\overline{1}0]_H
\end{align*}
\]

As per the Burgers scheme a distorted hexagonal cell can be delineated from the bcc unit cell as shown in Fig. 1. In this a \( \{011\}_C \) plane transforms to the basal plane \( \{0001\}_H \) while the close packed \( [\overline{1}1\overline{1}]_C \) and \( [\overline{1}11]_C \) directions lying on that plane transforms to close packed \( <11\overline{2}0>_H \) directions. The other two \( <11\overline{2}0>_H \) directions are derived from the \( [100]_C \) and \( [\overline{1}00]_C \) directions.

In the literature two additional types of bcc-hcp orientation relationship have been reported. Pitsch and Schrader observed experimentally the following orientation relationship in the formation of \( \epsilon \) carbide.

\[
\begin{align*}
[110]_C &\parallel [0001]_H; \quad [#1\#]_C &\parallel [10\#0]_H; \\
[001]_C &\parallel [\#110]_H
\end{align*}
\]

Fig. 1: The distorted close packed hexagonal cell (hcp) delineated from the parent bcc phase.
Potter has experimentally observed the other orientation relationship for the bcc-hcp transformation associated with V$_2$N formation and is known as Potter orientation relationship. This is given by:

\[
[110]_C || [0001]_H ; [\#10]_C || [01\#0]_H ; \\
[001]_C || [\$110]_H 
\]  

These three orientation relationships are closely connected by small fixed rotations. The atomic arrangement of the two superimposed close packed planes i.e., (011)$_C$ and (0001)$_H$ is shown in Fig. 2(a). The symmetries of these two dimensional arrangements are two fold and six fold rotation.

Two orthogonal strains along \(<100>_C\) and \(<01\#>_C\) bcc directions produce one lattice from the other in the position of the highest composite symmetry (Fig. 2(a)). This choice of strain irrespective of lattice parameters results in a misalignment of the close packed directions in the two lattices by 5.26° (Fig. 2(a)). Therefore a rotation of one of the lattices through this angle of 5.26° will be required. The two arrangements of atom shown in (Fig. 2(b)) describe all the three above mentioned orientation relationships (OR). These three OR’s are illustrated in [110] stereographic projections in Fig. 2(c) and Fig. 2(d) respectively. The Burgers OR can then be

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Fig. 2: Superposition of close packed planes of bcc (open circles) and hcp (full circles) lattices. The lattices are related in (a) by the strain along axes x and y and in (b) by aligning the close packed directions through a relative rotation of 5.26°. The stereograms illustrating the relationship between the three possible orientation relationships in bcc-hcp transformation, that of Pitsch Schraeder in (c) and that of Burgers and Potter in (d).
obtained from the Pitsch-Schreder OR by effecting an anticlockwise rotation through 5.26° about [011]_C [0001]_H. The rotation matrix R_1 in the cubic basis for the same can be written as:

\[
R_{1,C} = \begin{bmatrix}
0.99789 & 0.00211 & 0.006482 \\
0.00211 & 0.99789 & -0.006482 \\
-0.006482 & 0.006482 & 0.99579
\end{bmatrix}
\]

This rotation R_1 is independent of the lattice parameters of the bcc and the hcp phases. A second rotation around [111]_C || [110]_H pole (Fig. 2(d)) produces Potter’s O.R. from Burgers O.R. Unlike the previous rotation, this rotation does depend on the lattice parameters, i.e. the c/a ratio. For Zr and its alloys (c/a \leq 1.59) a rotation of 5° is required to bring the (101)_C and (100)_H poles into coincidence. The rotation matrix R_{2,C} in the cubic basis in this case is given by:

\[
R_{2,C} = \begin{bmatrix}
0.99777 & -0.01523 & 0.01500 \\
0.01500 & 0.99777 & 0.01523 \\
-0.01523 & 0.01500 & 0.99977
\end{bmatrix}
\]

In most of the experimental studies of bcc-hcp transformation in Zr and Ti base alloys either Burgers OR \(^9\)\(^{31}\) or Potter’s OR \(^39\) has been reported. Burgers OR is more frequently reported than Potters OR. Furthermore, it is very difficult to make a distinction between these two orientation relationships by experimental techniques due to the very small angular difference.

In the present work, the Burgers correspondence has been assumed for the bcc-hcp martensitic transformation. It is convenient to use an orthorhombic unit cell rather than a hexagonal cell for the matrix algebra treatment. A orthorhombic unit cell of dimensions a_1, a_1 + 2a_2, and c can be defined where a_1, a_2, and c are vectors defined in the conventional hcp cell. In the hexagonal case, the edge lengths of the orthorhombic cell are a_1, \(\sqrt{3}a_1\) and a_1 \(\gamma a_1\) where \(\gamma\) is the axial ratio, c/a. The relationship between the parent cubic (bcc), the orthorhombic and the hexagonal cells is shown in Fig. 3.

Pertinent to the lattice correspondence, assuming Burgers relationship, the six possible correspondence variants of the parent cubic (C) phase and the orthorhombic (O) cell are listed in Table 1. The lattice correspondence matrices \((O^{R_{12}})\) relating the planes and directions of the hexagonal cell and the orthorhombic cell have been worked out and the results are presented in Table 2. The indices of the planes and the directions in different basis (e.g. conversion from cubic to orthorhombic basis) are obtained by using the following expressions respectively:

\[
P_O = P_C R_C^O
\]

\[
V_O = c R_D^O V_C
\]

Where \(P_O\), \(P_C\), \(V_O\) and \(V_C\) are the indices of the planes and vectors in orthorhombic and cubic unit cells respectively. The correspondence matrices for relating planes and directions in the hexagonal cell to those in the cubic cell is obtained from the relationship.
Table 1
CORRESPONDENCE BETWEEN ORTHOHEXAGONAL AND CUBIC CELL (ORH)

<table>
<thead>
<tr>
<th>Variant</th>
<th>$[100]_c$</th>
<th>$[010]_c$</th>
<th>$[001]_c$</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>$[100]_k$</td>
<td>$[010]_k$</td>
<td>$[001]_k$</td>
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<tr>
<td>2</td>
<td>$[001]_k$</td>
<td>$[110]_k$</td>
<td>$[101]_k$</td>
</tr>
<tr>
<td>3</td>
<td>$[001]_k$</td>
<td>$[110]_k$</td>
<td>$[101]_k$</td>
</tr>
<tr>
<td>4</td>
<td>$[010]_k$</td>
<td>$[101]_k$</td>
<td>$[101]_k$</td>
</tr>
<tr>
<td>5</td>
<td>$[010]_k$</td>
<td>$[101]_k$</td>
<td>$[101]_k$</td>
</tr>
<tr>
<td>6</td>
<td>$[100]_k$</td>
<td>$[011]_k$</td>
<td>$[011]_k$</td>
</tr>
</tbody>
</table>

Table 2
CORRESPONDENCE MATRICES RELATING ORTHOHEXAGONAL CELL AND HEXAGONAL CELL

<table>
<thead>
<tr>
<th>Variant</th>
<th>$\alpha_{RH}$</th>
<th>$\beta_{RO}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>For Direction</td>
<td>$\begin{bmatrix} 2 &amp; 0 &amp; 0 \ 1 &amp; 3 &amp; 0 \ 0 &amp; 0 &amp; 3 \end{bmatrix}$</td>
<td>$\begin{bmatrix} 3 &amp; 0 &amp; 0 \ 1 &amp; 2 &amp; 0 \ 0 &amp; 0 &amp; 2 \end{bmatrix}$</td>
</tr>
<tr>
<td>For Planes</td>
<td>$\begin{bmatrix} 1 &amp; 1 &amp; 0 \ 0 &amp; 2 &amp; 0 \ 0 &amp; 0 &amp; 1 \end{bmatrix}$</td>
<td>$\begin{bmatrix} 2 &amp; 1 &amp; 0 \ 0 &amp; 1 &amp; 0 \ 0 &amp; 0 &amp; 2 \end{bmatrix}$</td>
</tr>
</tbody>
</table>

$\beta_{RH} = \alpha_{RO} \cdot \beta_{RO}$  \hspace{1cm} (8)

$\alpha_{RC} = \beta_{RO} \cdot \beta_{RO}$  \hspace{1cm} (9)

The correspondence matrices for conversion from the cubic to the hexagonal cell, $\beta_{RH}$, have been calculated using expression (Eqn.9) and the results are given in Table 3. The correspondence matrices relating hexagonal cell vectors to orthorhombic cell vectors and cubic cell vectors to hexagonal cell vectors would be different from the matrices pertaining to the conversion of the planes. The six possible correspondence matrices for converting vectors (and directions) in the cubic cell to those in the hexagonal cell ($\beta_{RH}$) have been worked out and are listed in Table 4. The six possible Burgers correspondences pertaining to the bcc-hcp transformation in Zr and Ti base alloys are shown in Table 5.

2.1.2 Determination of Bain Strain in Zr-2.5 Nb Alloy

The principal distortions $\eta_1$, $\eta_2$, $\eta_3$ along the three principal axes are determined and the corresponding Bain strain or distortion matrix is written as

$$B = \begin{bmatrix} \eta_1 & 0 & 0 \\ 0 & \eta_2 & 0 \\ 0 & 0 & \eta_3 \end{bmatrix}$$  \hspace{1cm} (10)
The lattice parameters of the parent β phase (bcc) and the martensitic α’ phase (hcp) in the Zr-2.5 Nb alloy were determined by X-ray diffraction method by Banerjee et al. to be $a_\beta = 0.3577$ nm for β and $a_H = 0.3211$ nm, $c_H = 0.5115$ nm, and $c/a = 1.593$ for the α’ phases. Using these values and referring to Fig. 4(a), $\eta$, have been calculated on the basis of the Burgers correspondence. The Bain strain matrix ($B_p$) in the principal axis system assumes the form and given by

$$B_p = \begin{bmatrix}
\frac{\sqrt{3}}{2} a_\alpha & 0 & 0 \\
0 & \frac{1}{2} c_\alpha & 0 \\
0 & 0 & \frac{a_\alpha}{a_\beta}
\end{bmatrix}$$

so that for the Zr-2.5 Nb alloy one has

$$B_O = \begin{bmatrix}
0.89768 & 0.0 & 0.0 \\
0.0 & 1.09942 & 0.0 \\
0.0 & 0.0 & 1.01213
\end{bmatrix}$$

In a schematic diagram (Fig.4(b)) the Bain strain is shown for the correspondence variant indicated in Fig. 4(a). The principal strains and the corresponding Bain strain matrix have also been determined by following the minimum strain energy criterion as suggested by Lomer for the β→α transformation in the U-1.4at% Cr alloy and by minimum distortion criterion of Madangopal for the cubic to monoclinic transformation in Ni-Ti alloy, as indicated below.;

A. Lomer’s Approach

For the β→α transformation in uranium, an alternative approach was suggested by Lomer, which considers only the relations between the fundamental lattice vectors of the two structures and does not take into account the atomic positions. In this method it is assumed that each β cell is transformed in the same way as every other β cell. This implies that each of the β cell vectors transforms into some integral multiple of the corresponding a lattice vector. Lomer derived a correspondence matrix by finding a set of three vectors in the a lattice of uranium which are nearly orthogonal and nearly equal in length to the fundamental β vectors. Furthermore, the parallelepiped defined by these three a lattice vectors must contain the same number of atoms as the β unit cell from which it is derived.

The total strain $S$ required for the change in the lattice structure is calculated from the knowledge of the correspondence and the lattice dimensions of the parent β and product α’ phase, which may require a rigid body rotation in addition to the change of

![Fig. 4:](image)

(A) The lattice correspondence between the hexagonal and the bcc is shown along (110)$_c$ || (0001)$_h$ plane. Closed and open circles represent lattice points corresponding to bcc and hcp structures respectively. (b) Unit sphere and the ellipsoid produced by the application of lattice strain are shown. Vector OA’ andOX’ which are rotated into vectors OA and OX respectively remains undistorted. If the strain along [110]$_c$ is neglected, vertical plane passing through vectors OA and OX will be the undistorted planes.

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Table 4
CORRESPONDENCE MATRICES FOR CORRELATING VECTORS AND DIRECTIONS OF THE HEXAGONAL AND CUBIC CELL FOR ALL THE SIX VARIANT OF BURGERS CORRESPONDENCE

<table>
<thead>
<tr>
<th>Variant</th>
<th>Correspondence matrix $\mathbf{C}_{RH}^{(Dir)}$</th>
<th>Correspondence matrix $\mathbf{C}_{RC}^{(Dir)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\begin{bmatrix} 4 &amp; 0 &amp; 0 \ 2 &amp; 3 &amp; \frac{3}{2} \ 0 &amp; 3 &amp; 3 \end{bmatrix}$</td>
<td>$\begin{bmatrix} 3 &amp; 0 &amp; 0 \ 1 &amp; 2 &amp; 2 \ 1 &amp; 2 &amp; 2 \end{bmatrix}$</td>
</tr>
<tr>
<td>2</td>
<td>$\begin{bmatrix} 0 &amp; 0 &amp; 4 \ 3 &amp; 3 &amp; 2 \ 3 &amp; \frac{3}{2} &amp; 0 \end{bmatrix}$</td>
<td>$\begin{bmatrix} 1 &amp; 2 &amp; 2 \ 1 &amp; 2 &amp; 2 \ 3 &amp; 0 &amp; 0 \end{bmatrix}$</td>
</tr>
<tr>
<td>3</td>
<td>$\begin{bmatrix} 0 &amp; 4 &amp; 0 \ 3 &amp; 2 &amp; 3 \ 3 &amp; 0 &amp; 3 \end{bmatrix}$</td>
<td>$\begin{bmatrix} 1 &amp; 2 &amp; 2 \ 1 &amp; 2 &amp; 2 \ 3 &amp; 0 &amp; 0 \end{bmatrix}$</td>
</tr>
<tr>
<td>4</td>
<td>$\begin{bmatrix} 0 &amp; 4 &amp; 0 \ 3 &amp; \frac{3}{2} &amp; 3 \ 3 &amp; 0 &amp; 3 \end{bmatrix}$</td>
<td>$\begin{bmatrix} 1 &amp; 2 &amp; 2 \ 1 &amp; 2 &amp; 2 \ 3 &amp; 0 &amp; 0 \end{bmatrix}$</td>
</tr>
<tr>
<td>5</td>
<td>$\begin{bmatrix} 4 &amp; 0 &amp; 0 \ 2 &amp; 3 &amp; \frac{3}{2} \ 0 &amp; 3 &amp; 3 \end{bmatrix}$</td>
<td>$\begin{bmatrix} 3 &amp; 0 &amp; 0 \ 1 &amp; 2 &amp; 2 \ 1 &amp; 2 &amp; 2 \end{bmatrix}$</td>
</tr>
<tr>
<td>6</td>
<td>$\begin{bmatrix} 0 &amp; 4 &amp; 0 \ 3 &amp; 2 &amp; 3 \ 3 &amp; 0 &amp; 3 \end{bmatrix}$</td>
<td>$\begin{bmatrix} 1 &amp; 2 &amp; 2 \ 1 &amp; 2 &amp; 2 \ 3 &amp; 0 &amp; 0 \end{bmatrix}$</td>
</tr>
</tbody>
</table>

The matrix $\mathbf{M}$ and the correspondence matrix $\mathbf{C}_{RO}^{(Dir)}$ correlating the orthohexagonal and the cubic cells are given by:

$$\mathbf{M} = \begin{bmatrix} a_H & 0 & 0 \\ 0 & c_H & 0 \\ 0 & 0 & \gamma a_H \end{bmatrix}$$

(15)

For variant 1,

$$\mathbf{C}_{RO}^{(Dir)} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

(16)

Here $\mathbf{M}^*$ and $\mathbf{I}$ are the transpose of $\mathbf{M}$ and the unit matrix respectively, and $a$, $c$ and $a_0$ are the lattice parameters of the hcp and bcc cells. Using the lattice parameters for the Zr-2.5 alloy and the lattice correspondence matrix for variant 1, the Strain matrix (Bain matrix), $\mathbf{S}$, in the orthohexagonal basis is given by:

$$\mathbf{S}_{0,1} = \begin{bmatrix} -0.10180 & 0.0 & 0.0 \\ 0.0 & 0.09893 & 0.0 \\ 0.0 & 0.0 & 0.01117 \end{bmatrix}$$

(17)

From the strain matrix $\mathbf{S}_{0,1}$, the magnitude of the principal distortions in the three principal directions are given by $d_1 = -0.101798$ ($\approx -10.18\%$), $d_2 = 0.098925$ ($\approx 9.89\%$) and $d_3 = 0.011165$ ($\approx 1.12\%$) respectively. Therefore, keeping in view the relation $\eta_i = 1 - d_i$, the corresponding Bain strain matrix is given by:

$$\mathbf{B}_{0,1} = \begin{bmatrix} 0.89820 & 0.0 & 0.0 \\ 0.0 & 1.09893 & 0.0 \\ 0.0 & 0.0 & 1.01117 \end{bmatrix}$$

(18)

B. The Minimum Distortion Approach

As pointed out earlier, the preferred lattice correspondence is that which generates the product phase lattice from the parent phase lattice with the minimum distortion. The following illustrates the approach followed to determine the lattice correspondence associated with the minimum distortion for the cubic to hexagonal (orthohexagonal) transformation in the Zr-2.5Nb alloy. This approach

shape. A symmetrical homogenous strain matrix $S$, referred to the original cubic lattice, for the change of the lattice, in which any arbitrary relative rotation of the lattices is eliminated, is given by:

$$(\mathbf{I} + \mathbf{S})^2 = \mathbf{M}^* \mathbf{M}$$

(13)

$$S = \frac{1}{2} \left( \mathbf{M}^* \mathbf{M} - \mathbf{I} \right) \left( \mathbf{I} - \frac{1}{4} \left( \mathbf{M}^* \mathbf{M} - \mathbf{I} \right) \right)$$

(14)
is based on the method that followed by Madangopal \textsuperscript{35} for the cubic to monoclinic transformation in Ni-Ti alloys.

Taking the value for the lattice parameter of the cubic (bcc) parent phase to be, $a_C = 0.3577\, \text{nm}$ the magnitude of a few low index crystal directions are determined to be:

- $<1\,0\,0>_C = 0.3577\, \text{nm}$
- $<1\,1\,0>_C = 0.5059\, \text{nm}$
- $<1\,1\,1>_C = 0.6196\, \text{nm}$
- $<1\,2\,0>_C = 0.7998\, \text{nm}$
- $<1\,1\,2>_C = 0.8762\, \text{nm}$
- $<1\,2\,2>_C = 1.0731\, \text{nm}$

Comparing the above values with the lattice parameters of the orthohexagonal martensite in the Zr-2.5\% Nb alloy: $a_O = a_H = 0.3211\, \text{nm}$, $b_O = \sqrt{3}a_H = 0.5562\, \text{nm}$ and $c_O = c_H = 0.5115\, \text{nm}$, the two possible lattice correspondences deduced by the minimum distortion criterion are:

<table>
<thead>
<tr>
<th>Variant</th>
<th>Correspondence A</th>
<th>Correspondence B</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$(1,1,0)_C$</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>$(1,0,0)_C$</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>$(1,0,1)_C$</td>
<td></td>
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<tr>
<td>4</td>
<td>$(1,0,0)_C$</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>$(0,0,1)_C$</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>$(0,1,0)_C$</td>
<td></td>
</tr>
</tbody>
</table>

Comparing the values of the Bain strain derived by above two approaches, it can be seen that both of them result in almost the same distortion values.

The principal distortions corresponding to the three principal axes referred to the orthohexagonal basis, calculated as per correspondence A are:

- $d_1 = (a_{\alpha} - a_{\beta})/a_{\alpha} = -0.1023203 \approx -10.23\%$
- $d_2 = (\sqrt{3}a_{\alpha} - \sqrt{3}a_{\beta})/\sqrt{3}a_{\alpha} = 0.0994267 \approx 9.94\%$
- $d_3 = (c_{\alpha} - \sqrt{2}a_{\beta})/\sqrt{2}a_{\beta} = 0.0110693 \approx 1.11\%$

Using the relation $\eta_i = 1 - d_i$ the relevant Bain matrix can be written as

$$B_{CI} = \begin{bmatrix} 0.89768 & 0.0 & 0.0 \\ 0.0 & 1.09943 & 0.0 \\ 0.0 & 0.0 & 1.01107 \end{bmatrix} \tag{20}$$

Comparing the values of the Bain strain derived by above two approaches, it can be seen that both of them result in almost the same distortion values. These two analyses, which are based on minimum strain energy/ minimum distortion considerations, lead to the same type of Bain strain and lattice correspondence. The lattice correspondences derived from these methods are also equivalent to the Burger’s correspondence. However, it is not possible to verify the Bain strain because of absence of any superlattice reflections in the diffraction patterns obtained from the Zr-2.5\% Nb alloy specimens which have undergone the bcc-hcp transformation. If the martensitic transformation does not involve shuffle then the chosen correspondence should predict the correct habit plane and orientation relationship as determined experimentally.
The Bain matrix, referred to the cubic basis, can be obtained by employing the similarity transformation as suggested by Wayman. For variant 1,

\[
B_{C,1} = \rho R^C B_{O,1} (\rho R^C)^{-1}
\]

For variant 1,

\[
\begin{bmatrix}
2 \eta_1 & 0 & 0 \\
0 & \eta_3 + \eta_2 & \eta_3 - \eta_2 \\
0 & \eta_3 - \eta_2 & \eta_3 + \eta_2
\end{bmatrix}
\]

\[
= \begin{bmatrix}
0.89768 & 0.0 & 0.0 \\
0.0 & 1.05578 & -0.04365 \\
0.0 & -0.04365 & 1.05578
\end{bmatrix}
\]

For determining the shape strain and other crystallographic parameters for all variants of the Zr-2.5Nb martensite, it is necessary to determine the Bain deformation matrices for all the six correspondence variants. Using the Bain deformation matrix in the orthohexagonal basis and the correspondence matrices for all the six variants the Bain matrices in the cubic (parent) basis have been computed by employing the similarity transformation method. The results of the computation are presented in Table 6.

Table 6
BAIN STRAIN MATRICES (\(B_{C,1}\)) OF BCC TO HCP TRANSFORMATION IN Zr-2.5 Nb ALLOY IN THE CUBIC BASIS FOR THE SIX POSSIBLE CORRESPONDENCE VARIANTS OF THE MARTENSITIC PHASE

<table>
<thead>
<tr>
<th>Variant</th>
<th>Bain Stress</th>
<th>Variant</th>
<th>Bain Stress</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>([\alpha \ 0 \ 0])</td>
<td>4</td>
<td>([\beta \ 0 \ \gamma])</td>
</tr>
<tr>
<td>0 (\beta \ \gamma)</td>
<td>0 (\alpha \ 0)</td>
<td>(\gamma \ 0 \ \beta)</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>([\beta \ \gamma \ 0])</td>
<td>5</td>
<td>([\beta \ 0 \ \gamma -\gamma \ 0 \ \beta])</td>
</tr>
<tr>
<td>(\gamma \ 0 \ \alpha)</td>
<td>0 (\alpha \ 0)</td>
<td>(\gamma \ 0 \ \beta)</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>([\beta \ 0 \ \gamma])</td>
<td>6</td>
<td>([\alpha \ 0 \ 0])</td>
</tr>
<tr>
<td>(\gamma \ 0 \ \alpha)</td>
<td>0 (\beta \ \gamma)</td>
<td>(0 \gamma \ \beta)</td>
<td></td>
</tr>
</tbody>
</table>

The eigen values for the Bain strain in the above analysis for the correspondence variant 1 are given by: \(\eta_1 = 0.898 (< 1.0)\), \(\eta_2 = 1.099 (> 1.0)\) and \(\eta_3 = 1.011 (>1.0)\). It is thus observed that the Bain strain for the bcc to hcp martensitic transformation in the Zr-2.5 Nb alloy cannot form an IPS because i.e. the condition as deduced in the phenomenological theory of martensitic transformation that in order to meet the IPS condition, one of the \(\eta_i\) should be 1 and the other two \(\eta_i\) should be greater than 1 and less than 1 respectively. The magnitude of distortion along one of the principal axes is very small 1.011 (close to zero) and the eigen value \(\eta_3 = 1.011\) is approximately equal to 1. Thus, the Bain strain, by itself, nearly satisfies the IPS condition. It can also be inferred that the magnitude of the LIS required in the martensitic transformation in the Zr-2.5 Nb alloy needs to be very small to meet the IPS condition. The possible LIS for the bcc-hcp martensitic transformation in this alloy have been dealt with in what follows.

2.2 Lattice Invariant Strain

In bcc-hcp (\(\beta - \alpha'\)) martensitic transformation in zirconium base alloys the principal strain along one of the principal directions is very close to zero (2%) while the strains along the other two principal directions are of opposite sign. Therefore, the IPS condition is approximately satisfied in these alloys without any LIS. However, the experimental observation of dislocation substructure and internal twins suggests the presence of LIS in the form of twinning and slip.

In phenomenological theories of martensitic transformation, the dislocation and twin models were shown to be equivalent if shear plane (\(K_1\)) corresponds to mirror plane of the parent phase, and shear direction (\(\eta_3\)) is parallel to the Burgers vector, and the magnitude of the shear produced by the array of anti coherency dislocations is a positive fraction of the twinning shear. The phenomenological theories give, in the most general case, four independent solutions for the orientation relations, habit planes and shape deformation, but, certain symmetry dictated conditions reduce the solutions to crystallographically equivalent variants of either two solutions or of a unique solution for each set of input data. The choice of \(K_1\) plane and
the \( \eta_1 \) direction is restricted if the two lattice correspondences of a twinned product are equivalent variants. Either the parent plane \( (K_1) \) must be a mirror plane or the \( \eta_1 \) direction must be derived from a two fold axis of the parent phase. When \( K_1 \) or \( \eta_1 \) is chosen for a given shear system, the other crystallographic parameters get fixed. The input data for the PTMC are the crystal structures and the lattice parameters of the two phases and the plane and the direction of twinning or slip (LIS). The precise value of the LIS should always satisfy the IPS condition and the predicted values of the habit plane and the orientation relation should be validated.

Systematic studies on the determination of the possible shear systems in martensitic transformations occurring in zirconium base alloys are not available in literature. However, in the case of titanium base alloys several experimental observations \(^{24-31}\) and theoretical analysis \(^{5,6,42}\) are reported. Otte \(^{43}\) has reviewed all the theoretically possible and experimentally observed shear systems for titanium base alloys. Bowles and Mackenzie \(^{5}\) have carried out a detailed treatment of the bcc to hcp transformation in two special cases; class A involving the \{01\}\( _H \) bcc shear plane and an irrational shear direction in this plane; and the other class B involving the \(<1010>_C \{001\}_C \) bcc shear system.

In the present work an attempt has been made to determine the possible shear systems and twinning modes that qualify as LIS in martensitic transformation in zirconium base alloys. The usual slip and twinning modes associated with mechanical deformation of zirconium base alloys have been used as the starting data. The reported slip modes and twin modes in the hcp phase \( (Cv) \) phase are listed in Table 7 \(^{44-45}\).

### Table 7

<table>
<thead>
<tr>
<th>Slip Systems</th>
<th>Twin systems</th>
</tr>
</thead>
<tbody>
<tr>
<td>(&lt;110&gt;_H {0110}_H )</td>
<td>(&lt;#011&gt;_H {105}_H )</td>
</tr>
<tr>
<td>(&lt;110&gt;_H {0001}_H )</td>
<td>(&lt;#26&gt;_H {11\bar{1}2}_H )</td>
</tr>
<tr>
<td>(&lt;110&gt;_H {0113}_H )</td>
<td>(&lt;#23&gt;_H {11\bar{1}2}_H )</td>
</tr>
<tr>
<td>(&lt;113&gt;_H {10#1}_H )</td>
<td>(&lt;#012&gt;_H {10#1}_H )</td>
</tr>
<tr>
<td>(&lt;113&gt;_H {11\bar{1}3}_H )</td>
<td></td>
</tr>
</tbody>
</table>

2.2.1 Possible Twinning Systems

One of the characteristics of the martensitic transformation in the case of internally twinned martensites is that the twinning plane \( (K_1) \) should be derived from a mirror plane of the parent phase for Type I twinning and twinning direction \( (\eta_1) \) should be derived from a diad in the parent phase for Type II twinning. The possible mirror planes and diads in the parent bcc structure are given in Table 8(a) and 8(b) respectively. These mirror planes and diads, with the exception of, those which transform to a mirror or a diad of the hcp product phase, transform to the \( K_1 \) plane and \( \eta_2 \) direction of the Type I twinning mode or the \( K_2 \) plane and \( \eta_1 \) direction of the conjugate Type II twinning mode. The symmetry of the parent phase results in the conjugate mode of a Type I twinning derived from a mirror plane, to be a twinning axes derived from the diad normal to the mirror plane. The possible \( K_1 \) planes and \( \eta_2 \) directions in the product hcp structure, are also listed in the Table 8(a) and 8(b) respectively. It can be seen that one of the \{100\}_C mirror planes remains a mirror plane after the bcc-hcp transformation, and hence cannot be a twinning plane in the product phase. The other two \{100\}_C planes are transformed into crystallographically equivalent planes of type \{10\#2\}_H in the product martensitic phase. Two of the parent bcc \{110\}_C planes also remain mirror planes after the transformation, whilst the other four become equivalent possible twinning planes of type \{10\#1\}_H in the product phase. Similarly, it can be seen from Table 8 that one of the \(<100>_C \) and two of the \(<110>_C \) diads in the parent phase remain diads in the product phase after the transformation, whilst two \(<100>_C \) and four \(<110>_H \) diads transform to crystallographically equivalent directions of the types \(<01\#1>_H \) and \(<41\#3>_C \) respectively. There are thus two possible types of transformation that can occur, utilizing different product twinning planes, in pure Zr and dilute Zr base alloys. Bowles and Mackenzie referred to these two possibilities as class A and class B transformation for correspondence variant 1 in the manner indicated below:

\[
\begin{align*}
\{110\}_C (\overline{1}101)_H \cdot \{110\}_C [41\overline{5}3]_H \\
(010)_C (01\overline{1}2)_H \cdot [010]_C [01\overline{1}]_H
\end{align*}
\]
The correspondence variants of the martensite structure related by these possible twinning planes have been computed as follows.

The rotation matrix, $R_{\text{Twin}}$, for twinning operation can be written as [42]

$$R_{\text{Twin}} = \begin{bmatrix}
2p_1^2 - 1 & 2p_1p_2 & 2p_1p_3 \\
2p_1p_2 & 2p_2^2 - 1 & 2p_2p_3 \\
2p_1p_3 & 2p_2p_3 & 2p_3^2 - 1
\end{bmatrix} \tag{24}$$

where $P = [p_1, p_2, p_3]$ is the rotation axis.

From the knowledge of one twin variant (e.g. the major twin fraction) the other twin variant (minor twin fraction) related by a given twinning plane can be obtained by matrix algebra operations. For example, for the twinning plane $(010)_C \parallel (0\bar{1}\bar{2})_H$ and with the major twin fraction as correspondence variant 1, the minor twin fraction is obtained by

$$c_{x} R^O = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix} \cdot \begin{bmatrix}
0 & 1 & 1 \\
0 & 1 & 1 \\
1 & 0 & 0
\end{bmatrix} = \begin{bmatrix}
0 & 1 & 1 \\
0 & 1 & 1 \\
1 & 0 & 0
\end{bmatrix} \tag{25}$$

It can be seen from Table 8(a) that the above matrix corresponds to the correspondence matrix of variant 6. Therefore, the correspondence variant 1 is twin related to the variant 6 for the twinning plane $(010)_C \parallel (0\bar{1}\bar{2})_H$. Similarly, other correspondence variants related by all the possible twinning planes mentioned in Table 8 have been worked out and the results are presented in Table 9.

### Table 8(a)

**POSSIBLE TWIN PLANES IN THE HEXAGONAL PRODUCT PHASE DERIVED FROM PLANES OF THE PARENT BCC PHASE.**

<table>
<thead>
<tr>
<th>Plane (H)</th>
<th>Mirror</th>
<th>Variant 1</th>
<th>Variant 2</th>
<th>Variant 3</th>
<th>Variant 4</th>
<th>Variant 5</th>
<th>Variant 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>(100)</td>
<td></td>
<td>(2#0)</td>
<td>(0#12)</td>
<td>(0#12)</td>
<td>(0#12)</td>
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<td>(2#0)</td>
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<tr>
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<td>(0#2)</td>
<td>(2#0)</td>
<td>(2#0)</td>
<td>(2#0)</td>
<td>(0#2)</td>
</tr>
<tr>
<td>(001)</td>
<td></td>
<td>(0#2)</td>
<td>($110$)</td>
<td>($110$)</td>
<td>(0#2)</td>
<td>(0#2)</td>
<td>(0#2)</td>
</tr>
<tr>
<td>(110)</td>
<td></td>
<td>(1#0)</td>
<td>(0#00)</td>
<td>(0#1)</td>
<td>(1#0)</td>
<td>(1#0)</td>
<td>(1#0)</td>
</tr>
<tr>
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<td></td>
<td>(1#0)</td>
<td>(0#10)</td>
<td>(0#11)</td>
<td>(1#10)</td>
<td>(1#01)</td>
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</tr>
<tr>
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<td></td>
<td>(1#01)</td>
<td>(#11)</td>
<td>(#101)</td>
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<td>(0#01)</td>
<td>(1#01)</td>
</tr>
<tr>
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<td>(1#0)</td>
<td>(1#0)</td>
<td>(0#10)</td>
<td>(0#10)</td>
<td>(0#10)</td>
<td>(1#01)</td>
</tr>
<tr>
<td>(10#)</td>
<td></td>
<td>(1#0)</td>
<td>(1#0)</td>
<td>(0#10)</td>
<td>(0#10)</td>
<td>(0#10)</td>
<td>(1#01)</td>
</tr>
<tr>
<td>(011)</td>
<td>Mirror</td>
<td>(0001)</td>
<td>(#101)</td>
<td>(#101)</td>
<td>(10#)</td>
<td>(10#)</td>
<td>(0#01)</td>
</tr>
<tr>
<td>(0#1)</td>
<td>Mirror</td>
<td>(0#10)</td>
<td>(#11)</td>
<td>(#101)</td>
<td>(#101)</td>
<td>(#101)</td>
<td>(0#01)</td>
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<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 8(b)

POSSIBLE POSSIBLE TWIN SHEAR DIRECTIONS ($\eta_j$) IN THE HEXAGONAL PRODUCT PHASE DERIVED FROM DIADS OF THE PARENT BCC PHASE AND LIST OF TWIN VARIANTs RELATED BY DERIVED DIADS IN THE PRODUCT PHASE.

<table>
<thead>
<tr>
<th>Diads in bcc</th>
<th>Variant 1</th>
<th>Variant 2</th>
<th>Variant 3</th>
<th>Variant 4</th>
<th>Variant 5</th>
<th>Variant 6</th>
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</thead>
<tbody>
<tr>
<td>[100]</td>
<td>[2#0]</td>
<td>[0#11]</td>
<td>[0#11]</td>
<td>[0#11]</td>
<td>[01#1]</td>
<td>[2#0]</td>
</tr>
<tr>
<td></td>
<td>Diad</td>
<td>Diad</td>
<td>Diad</td>
<td>Diad</td>
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<tr>
<td>[010]</td>
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<td>[01#1]</td>
<td>[01#1]</td>
<td>[0#11]</td>
<td>[2#0]</td>
<td>[01#1]</td>
</tr>
<tr>
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<td>Diad</td>
<td>Diad</td>
<td>Diad</td>
<td>Diad</td>
<td>Diad</td>
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<tr>
<td>[001]</td>
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<td>[0#11]</td>
<td>[0#11]</td>
<td>[01#1]</td>
<td>[01#1]</td>
<td>[01#1]</td>
</tr>
<tr>
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<td>Diad</td>
<td>Diad</td>
<td>Diad</td>
<td>Diad</td>
<td>Diad</td>
<td>Diad</td>
</tr>
<tr>
<td>[110]</td>
<td>[41*3]</td>
<td>[0001]</td>
<td>[010]</td>
<td>[41*3]</td>
<td>[41*3]</td>
<td>[41*3]</td>
</tr>
<tr>
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<td>Diad</td>
<td>Diad</td>
<td>Diad</td>
<td>Diad</td>
<td>Diad</td>
<td>Diad</td>
</tr>
<tr>
<td>[1#0]</td>
<td>[4*13]</td>
<td>[0#10]</td>
<td>[0001]</td>
<td>[01#53]</td>
<td>[05#3]</td>
<td>[01*3]</td>
</tr>
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<td>Diad</td>
<td>Diad</td>
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<tr>
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<td>[05#3]</td>
<td>[05#3]</td>
<td>[010]</td>
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<td>Diad</td>
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<td>Diad</td>
<td>Diad</td>
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<tr>
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<td>[41*3]</td>
<td>[4*13]</td>
<td>[41*3]</td>
<td>[0001]</td>
<td>[01#0]</td>
<td>[41*3]</td>
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</tbody>
</table>

Table 9

THE COMBINATION OF MAJOR AND MINOR TWIN CORRESPONDENCE VARIANTS RELATED BY THE POSSIBLE TWINNING PLANES IN THE HCP Zr-2.5Nb ALLOY.

<table>
<thead>
<tr>
<th>Twinning Plane</th>
<th>Major-Minor Twin Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>(01#2)$_H$</td>
<td>1-6 2-3 3-2 4-5 5-4 6-1</td>
</tr>
<tr>
<td>(#101)$_H$</td>
<td>1-4 2-5 3-1 4-2 5-6 6-3</td>
</tr>
<tr>
<td>(1#01)$_H$</td>
<td>1-3 2-1 3-4 4-6 5-3 6-5</td>
</tr>
<tr>
<td>(#011)$_H$</td>
<td>1-2 2-6 3-5 4-1 5-2 6-4</td>
</tr>
<tr>
<td>(10#1)$_H$</td>
<td>1-5 2-4 3-6 4-3 5-1 6-2</td>
</tr>
</tbody>
</table>

The twinning elements $K_2$ and $\eta_1$ of the two twinning modes have been computed from the knowledge of $K_1$ and $\eta_2$ and by employing the crystallographic relationship for the twinning elements derived by Jawson and Dove:

\[
k = k' - N \frac{[010].[pqr]}{[pqr] J^2} \tag{26b}
\]
\[
l = l' - N \frac{[001].[pqr]}{[pqr] J^2} \tag{26c}
\]
\[
h = h' - N \frac{[100].[pqr]}{[pqr] J^2} \tag{26a}
\]

where, $K_1 = (h' k' l')$, $K_2 = (h k l)$, $\eta_2 = [p q r]$ and $N = h' p + k' q + l' r$.
The results of this computation for all the possible twinning modes have been presented in Table 10. It can be seen from Table 10 that both the twinning modes are of Type I.

2.2.2 Possible Lattice Invariant Shears

Experimental observations made on morphology and substructure of martensitic microstructure do not confirm the presence of all the slip and twin modes mentioned in Table 7 as LIS. The primary requirement for any shear system to be a LIS is that it should meet the IPS condition and it should yield the habit plane solution. Based on this requirement, Wechsler and Otte 48-49 have proposed generalized theory of the martensitic transformation for cubic to orthorhombic 48 and cubic to tetragonal transformation 49 in which they have worked out restrictions that have to be imposed on the starting data (possible LIS) for the existence of the habit plane solution. Crocker and Bilby 50-52 have considered these restrictions for the most general case of the martensitic transformation, using the Bullough and Bilby phenomenological theory 47.

The additional strain due to LIS is assumed to be a simple shear on a plane m in a direction l. The m and l is referred to the principal axis system (since principal directions remain unrotated by pure strain). In the Bilby and Crocker’s “m” and “l” restrictions, it is possible to determine whether a given twinning mode or slip mode qualifies as a LIS. This method has been applied as a first step to select the possible shear system from those listed in Table 7. From the knowledge of the principal strains ($\eta_i$) two inequality conditions referred to as “m” and “l” restrictions 52 are expressed as:

“m” restriction:

$$m_i^3(1-\eta_i^2)(1-\eta_i^2) + m_{i+1}^3(1-\eta_i^2)(1-\eta_i^2) + m_{i+2}^3(1-\eta_i^2)(1-\eta_i^2) \leq 0$$

(27)

“l” restriction:

$$l_i^2\eta_i^2(1-\eta_i^2)(1-\eta_i^2) + l_{i+1}^2\eta_i^2(1-\eta_i^2)(1-\eta_i^2) + l_{i+2}^2\eta_i^2(1-\eta_i^2)(1-\eta_i^2) \leq 0$$

(28)

The geometrical interpretation of the above restrictions in martensitic crystallography indicates that (1) the shear plane must intersect the cone of directions left undistorted by the pure (Bain) strain and (2) planes normal to the shear direction must intersect the cone of plane normals (i.e., of reciprocal lattice directions) left undistorted by this strain. The inequality conditions in the equation imply the restriction that all the $(1-\eta_i^2)$ should not be of the same sign for the existence of the habit plane solution.

In order to determine the possible LIS modes the “m” and “l” restrictions were employed to the LIS modes listed in Table 7 in the following manner; For correspondence variant 1 and the shear system $(\overline{T}01)c[111]_c ||(\overline{T}011)_H[2\overline{T}3]_H$, the principal axes system (eigen value system) and cubic axes system can be related by the following matrix

$$p^R = c^R P = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \sqrt{2} & \sqrt{2} & \sqrt{2} \end{bmatrix}$$

(29)

Therefore $m = (1, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ and $l = (1, \frac{\sqrt{2}}{2}, 0)$

Putting the values of $m$, $l$ and $\eta_i$ for the Zr-2.5Nb alloy in the expressions 27 and 28 we obtain

for “m” restriction = -0.03781 i.e., < 0

and for “l” restriction = -0.00735 i.e., < 0

From the above computational results it can be seen that for the above mentioned shear system, both restrictions of the Bilby and Crocker are fulfilled. Therefore, the shear system $[111]_c ||(\overline{T}011)_H[2\overline{T}3]_H$ qualifies to be LIS for correspondence variant 1. In a similar manner, the computations were carried out for all the possible slip modes listed in the Table 7 and the twinning mode listed in the Table 8. The results of the computation are presented in Table 11 for twin modes and in Table 12 for the slip systems. It can be seen from Table 12 that in the case of slip pertaining to Zr-2.5Nb alloy, several shear systems...
Table 10
ELEMENTS OF TWINNING MODES IN HCP STRUCTURE (AS LIS) FOR BCC-HCP MARTENSITIC TRANSFORMATIONS

<table>
<thead>
<tr>
<th>Twinning mode</th>
<th>$K_1$</th>
<th>$K_2$</th>
<th>$\eta_1$</th>
<th>$\eta_2$</th>
<th>shear</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(10#1) [41*3]$</td>
<td>$(10#1)$</td>
<td>$(2.509, 3.263)$</td>
<td>$[2.019, 3.445]$</td>
<td>$[41*3]$</td>
<td>$-0.168$</td>
</tr>
<tr>
<td>$(01#2) [01#1]$</td>
<td>$(01#2)$</td>
<td>$(0#12)$</td>
<td>$[0#12]$</td>
<td>$[01#1]$</td>
<td>$0.562$</td>
</tr>
</tbody>
</table>

Table 11
THE RESULT OF BILBY AND CROCKER CRITERION (l AND m CRITERION) FOR ALL POSSIBLE TWINNING MODES IN THE PRODUCT HCP MARTENSITIC PHASE FOR CORRESPONDENCE VARIANT 1.

<table>
<thead>
<tr>
<th>S.No.</th>
<th>bcc</th>
<th>hcp</th>
<th>'l'</th>
<th>'m'</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Direction Plane</td>
<td>Direction Plane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>[010] (010)</td>
<td>[01#1] (01#2)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>2</td>
<td>[001] (001)</td>
<td>[0#11] (0#12)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>3</td>
<td>[110] (110)</td>
<td>[41*%] (10#1)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>4</td>
<td>[1#0] (1#0)</td>
<td>[4*1%] (1#0#)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>5</td>
<td>[101] (101)</td>
<td>[4*13] (1#01)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>6</td>
<td>[10#] (10#)</td>
<td>[41*3] (10#3)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
</tbody>
</table>

It is possible to express Bilby and Crocker restrictions \(^2\) approximately by a graphical method which is more illustrative. The loci corresponding to the equality sign in the two restrictions (equations 27 and 28) in the expressions can be represented on a stereogram as “m” and “l” curves. As per the restrictions if either the shear plane normal or the shear direction lies inside the regions whose limits are shown by the elliptical section of the cone, then no solution for the habit plane will be obtained. The shear plane normals (m) and shear directions (l) of the possible slip modes listed in Table 12 for correspondence variant 1 are plotted in the [100]C projection on a stereogram along with the “m” and “l” curves for Zr-2.5 Nb alloy in the Fig. 5. Similarly the twinning plane normals ($K_2$) and the twinning shear directions ($\eta_1$) of the possible twinning modes for this alloy are plotted in the [100]C stereographic projection in Fig. 6. The shear plane normal and shear direction which lie within the “l” and “m” curve do not yield any habit plane solution are underlined in the Table 11 and Table 12. It can be seen that the results obtained by the stereographic method are similar to those obtained analytically.

Using an alternative graphical method Christian \(^1\) has given the necessary conditions for the existence of the habit plane solution. In this method the invariant plane of the shear ($K_1$) and the plane normal to the shear direction ($K_2$) must intersect the initial and the final Bain cones respectively; i.e. the shear plane m ($K_1$) should intersect the initial Bain cone and the plane containing the shear direction l($\eta_1$) must intersect the final Bain cone. The initial and the final Bain cones of unextended vectors are given by

$$x_1^2\left(\frac{1}{\eta_1^2} - 1\right) + x_2^2\left(\frac{1}{\eta_2^2} - 1\right) + x_3^2\left(\frac{1}{\eta_3^2} - 1\right) = 0$$

(30)

respectively.
<table>
<thead>
<tr>
<th>S.No.</th>
<th>Direction bcc</th>
<th>Plane bcc</th>
<th>Direction hcp</th>
<th>Plane hcp</th>
<th>'l'</th>
<th>'m'</th>
</tr>
</thead>
<tbody>
<tr>
<td>1(a)</td>
<td>[111]</td>
<td>(10#)</td>
<td>[2#3#]</td>
<td>(#101)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>1(b)</td>
<td>[111]</td>
<td>(01#)</td>
<td>[2#3#]</td>
<td>(01#0)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>1(c)</td>
<td>[111]</td>
<td>(10#)</td>
<td>[2#3#]</td>
<td>(10#0)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>1(d)</td>
<td>[111]</td>
<td>(11#)</td>
<td>[2#3#]</td>
<td>(11#0)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>1(e)</td>
<td>[111]</td>
<td>(11L)</td>
<td>[2#3#]</td>
<td>(11L#)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>1(f)</td>
<td>[111]</td>
<td>(01L)</td>
<td>[2#3#]</td>
<td>(01L#)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>2(a)</td>
<td>[11#]</td>
<td>(011)</td>
<td>[1S10]</td>
<td>(0001)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>2(b)</td>
<td>[11#]</td>
<td>(10#)</td>
<td>[1S10]</td>
<td>(10#0)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>2(c)</td>
<td>[11#]</td>
<td>(110)</td>
<td>[1S10]</td>
<td>(10#1)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>2(d)</td>
<td>[11#]</td>
<td>(121)</td>
<td>[1S10]</td>
<td>(10#3)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>2(e)</td>
<td>[11#]</td>
<td>(#12)</td>
<td>[1S10]</td>
<td>(#013)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>2(f)</td>
<td>[111]</td>
<td>(011)</td>
<td>[1S10]</td>
<td>(10#0)</td>
<td>&gt; 0.0</td>
<td>&gt; 0.0</td>
</tr>
<tr>
<td>3(a)</td>
<td>[01#]</td>
<td>(011)</td>
<td>[01#0]</td>
<td>(0001)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>3(b)</td>
<td>[01#]</td>
<td>(111)</td>
<td>[01#0]</td>
<td>(2#4#)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>3(c)</td>
<td>[01#]</td>
<td>(211)</td>
<td>[01#0]</td>
<td>(2#2#)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>3(d)</td>
<td>[01#]</td>
<td>(311)</td>
<td>[01#0]</td>
<td>(30#4)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>4(a)</td>
<td>[010]</td>
<td>(010)</td>
<td>[01#1]</td>
<td>(1#10)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>4(b)</td>
<td>[010]</td>
<td>(001)</td>
<td>[01#1]</td>
<td>(0#12)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>4(c)</td>
<td>[010]</td>
<td>(100)</td>
<td>[01#1]</td>
<td>(2#0#)</td>
<td>&gt; 0.0</td>
<td>&gt; 0.0</td>
</tr>
<tr>
<td>4(d)</td>
<td>[010]</td>
<td>(102)</td>
<td>[01#1]</td>
<td>(2#14#)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>5(a)</td>
<td>[100]</td>
<td>(011)</td>
<td>[2#0#]</td>
<td>(0001)</td>
<td>&gt; 0.0</td>
<td>&gt; 0.0</td>
</tr>
<tr>
<td>5(b)</td>
<td>[100]</td>
<td>(010)</td>
<td>[2#0#]</td>
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<td>&gt; 0.0</td>
<td>&gt; 0.0</td>
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<tr>
<td>5(c)</td>
<td>[100]</td>
<td>(001)</td>
<td>[2#0#]</td>
<td>(0112)</td>
<td>&gt; 0.0</td>
<td>&gt; 0.0</td>
</tr>
<tr>
<td>5(d)</td>
<td>[100]</td>
<td>(012)</td>
<td>[2#0#]</td>
<td>(0114)</td>
<td>&gt; 0.0</td>
<td>&gt; 0.0</td>
</tr>
<tr>
<td>6(a)</td>
<td>[113]</td>
<td>(0#0)</td>
<td>[1S13]</td>
<td>(1#0#)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>6(b)</td>
<td>[113]</td>
<td>(02#)</td>
<td>[1S13]</td>
<td>(11#0)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>6(c)</td>
<td>[113]</td>
<td>(21#)</td>
<td>[1S13]</td>
<td>(10#0)</td>
<td>&gt; 0.0</td>
<td>&gt; 0.0</td>
</tr>
<tr>
<td>7(a)</td>
<td>[#13]</td>
<td>(110)</td>
<td>[#223]</td>
<td>(10#1)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>7(b)</td>
<td>[#13]</td>
<td>(2#1)</td>
<td>[#223]</td>
<td>(1#00)</td>
<td>&gt; 0.0</td>
<td>&gt; 0.0</td>
</tr>
<tr>
<td>7(c)</td>
<td>[#13]</td>
<td>(151)</td>
<td>[#223]</td>
<td>(151#)</td>
<td>&lt; 0.0</td>
<td>&lt; 0.0</td>
</tr>
<tr>
<td>8(a)</td>
<td>[3#1]</td>
<td>(011)</td>
<td>[1#00]</td>
<td>(0001)</td>
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<td>&gt; 0.0</td>
</tr>
<tr>
<td>8(b)</td>
<td>[3#1]</td>
<td>(115)</td>
<td>[1#00]</td>
<td>(112#)</td>
<td>&gt; 0.0</td>
<td>&gt; 0.0</td>
</tr>
<tr>
<td>8(c)</td>
<td>[3#1]</td>
<td>(12#)</td>
<td>[1#00]</td>
<td>(11#1)</td>
<td>&gt; 0.0</td>
<td>&gt; 0.0</td>
</tr>
</tbody>
</table>
Fig. 5: The shear plane normals (m) and the shear directions (l) of the possible shear systems listed in Table 12 are plotted in the [100]c stereographic projection along with m and l restriction curves of the Bilby and Crocker 52. The shear plane normals and the shear directions lying inside the elliptical cone region do not yield any habit plane solution.

Fig. 6: The twinning plane normals (K) and the twinning shear directions (JJJJJ) of the possible twinning modes for Zr-2.5Nb alloy are plotted in the [100]c stereographic projection along with m and l restriction curves of the Crocker and Bilby 52. The twinning plane normals and the twinning directions lying inside the elliptical cone region do not yield any habit plane solution.

Fig. 7: Traces of the shear planes (K) of the possible shear systems are superimposed on [100]c stereographic projection of the initial Bain cone for the Zr-2.5 Nb alloy.

Fig. 8: Traces of the shear planes (K) of the possible shear systems are superimposed on [100]c stereographic projection of the initial Bain cone for the Zr-2.5 Nb alloy.

Using the above expressions the locus of all vectors that are unchanged in magnitude in the initial and final Bain cones can be plotted on a stereogram. Fig. 7 gives the (100)c pole stereographic projection.

\[ X_1^2(\eta_1^2 - l) + X_2^2(\eta_2^2 - l) + X_3^2(\eta_3^2 - l) = 0 \]  

(31)
of the initial Bain cone for the Zr-2.5 Nb alloy on which the traces of the shear planes of the possible slip modes are superimposed. Likewise, the (100)_C projection of the final Bain cone along with the traces of K_2 planes are superimposed in Fig. 8. The results arrived at in this manner are equivalent to those obtained by the Bilby and Crocker methods. From the above analysis of Bilby and Crocker method and graphical method it can be concluded that the twinning modes and the shear systems shown in Table 11 and Table 12 can qualify as LIS.

3. SUMMARY

In the present work the Bain strain (homogenous strain or lattice strain), the inhomogeneous shear (LIS) and the rigid body rotation in relation with the martensitic transformation in Zr-2.5%Nb alloy has been calculated. The possible inhomogeneous shear or lattice invariant shear, LIS, (both slip as well as twin type) has been identified. A simple model has been proposed for determining the factors, which influences the selection of the preferred LIS mode.

(i) The Bain strain matrix for Zr-2.5 Nb alloys has been shown to be

\[
B_0 = \begin{bmatrix}
0.89768 & 0.0 & 0.0 \\
0.0 & 1.09942 & 0.0 \\
0.0 & 0.0 & 1.01213 \\
\end{bmatrix}
\]

Both the minimum strain energy and the minimum distortion considerations, lead to the same type of Bain strain and lattice correspondence.

(ii) The possible shear systems and twinning modes that qualify as LIS in martensitic transformation in Zr-2.5Nb alloy on the basis of generalized theory of the martensitic transformation have been identified. In the case of slip pertaining to Zr-2.5Nb alloy, several shear systems do not qualify to be LIS, whereas both \{\overline{1}10\}_H <4\overline{1}3>_H and \{01\overline{1}2\}_H <01\overline{1}_1>_H twinning modes do qualify as LIS from the “m” and “l” criteria of Bilby and Crocker and graphical analysis method.

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