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Theoretical Analysis of the Crystallography for $DO_3 \rightarrow$ M18R Martensitic Transformation

Seyfettin AKMAK, Ekrem ARTUN
Department of Physics
Faculty of Arts and Sciences
Sleyman Demirel University
32260 Isparta - TURKEY

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Abstract

A mathematical approach of the phenomenological theory has been applied to the martensitic transformation of $DO_3 \rightarrow$ M18R close-packed structure. The crystallography of $DO_3 \rightarrow$ M18R martensitic transformation in Fe-25.8 wt%Mn-7.4wt%Al-0.11wt%C alloy was studied using single crystals. Martensitic crystallographic parameters such as habit plane, magnitude of lattice invariant shear, shape deformation direction and orientation relationships are calculated with new mathematical approach. Phenomenological theoretical calculations were compared with predictions of the phenomenological crystallographic CRAB theory and with experimental observations.

1. Introduction

On the basis of the experimentally observed parent-martensite orientation relationship, and other features such as stacking faults on the martensite basal plane, it is now well accepted that the basal plane of 18R martensites originates from one of the {110} planes of the parent DO_3 phase and that the inhomogeneous shear of the crystallography theory during transformation occurs on the basal plane. There are six {110} planes in the DO_3 structure and two possible shear directions for each {110} plane. Thus, there are 12 possible combinations of stacking planes and shear directions, each combination of which leads to two possible crystallographically equivalent unrotated and undistorted habit planes. Thus, 24 martensite variants can result from a single crystal parent.

The 18R martensite phase was observed in the bcc matrix of an Fe-25.8wt%Mn-7.4wt%Al-0.11wt%C [1] alloy, after cooling from high temperature. When FeMnAlC

alloy was water-quenched from 1300°C to room temperature, $\gamma + \alpha$ duplex structures was found. The γ phase is a fcc structure and the α phase is bcc. There is a needle-like martensite phase in the α grains. The bcc phase is the stable phase at high temperature. The crystal structure of the needle-like martensite phase can be determined from the selected-area diffraction technique [2, 3]. In the FeMnAlC alloy system, a high stacking fault density is found within the 18R martensite phase. Basically, the martensite phase in this system is similar to the 9R martensite in CuZn [4, 5] or the 18R martensite in CuZnAl [6, 7, 8].

It is well known that the so-called phenomenological theory of martensitic transformation is based on the assumptions that the parent-martensite interface (i.e., at the habit plane) should remain unrotated during the transformation. From this basic condition crystallographic features such as habit plane, magnitude of lattice invariant shear, shape deformation direction and orientation relationships can be calculated. Almost all of such calculations so for done followed the mathematical approach originally developed by Wechsler et.al. [9], Bowles and Mackenzie [10] or Crocker et.al. [11]. This approach consists of rather lengthy and complicated matrix algebra. On the other hand, Suzuki [12] developed in 1954 a much simpler method of calculating those crystallografic features of martensitic transformation, assuming the almost same strain condition at the habit plane. Although his approach is quite easily applicable to any system of martensitic transformations and is very convenient for actual numerical calculations.

In this work the Suzuki's mathematical approach is applied to the transformation of $DO_3 \rightarrow$ M18R close-packed structure, and analytical equations for the magnitude of the lattice invariant shear and habit plane indices are derived. The numerical calculations of various crystallographic features are performed for FeMnAlC [1] alloy. The predicted crystallographic features will be compared with the calculations of CRAB martensitic crystallography. Martensitic crystallographic parameters such as habit plane, magnitude of lattice invariant shear, shape deformation direction and orientation relationships were analysed with a program written in FORTRAN 77.

2. Derivation of Analytical Equations

2.1. Magnitude of the Lattice Invariant Shear and Habit Plane Indices

It is well known that the theory of martensitic transformation crystallography is based on the assumption that there should be no average distortion at the parent/product interface (i.e. at the habit plane). From this basic condition, crystallographic features such as habit plane, orientation relationships, direction and magnitude of the shape deformation and magnitude of the lattice invariant shear can be calculated. We accomplish this by inserting the lattice parameters introduced earlier for the bcc parent and 9R martensite into the formula derived by Kajiwara [4], which incorporated the Suzuki martensite crystallographic theory [12]. First we discuss the structural change from DO_3 to M18R

structure, referring to Fig. 1 [13]. The DO_3 superlattice and the 18R structure in the monoclinic representation are drawn schematically in Fig. 1(b).

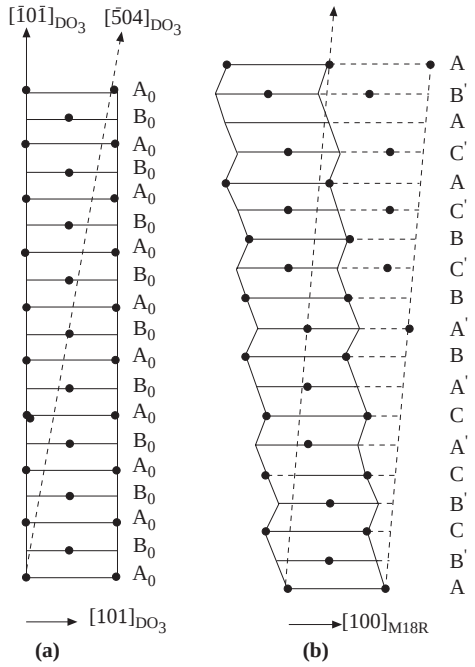

Figure 1. Structural change from DO_3 parent to M18R martensite for C.V.3ı. a) DO_3 structure viewed from $[0\ \overline{1}\ 0]_{DO_3}$ direction. b) 18R structure viewed from $[0\ 1\ 0]_{18R}$ direction [13].

Similar to what has been shown by Kajiwara [4], it can be seen that the axes in the 18R structure are related to those in the DO_3 superlattice as follows [13]:

$$\begin{aligned} a[1\ 0\ 0]_{18R} &\rightarrow \frac{a_{DO_3}}{2}[\overline{1}\ 0\ \overline{1}] \\ b[0\ 1\ 0]_{18R} &\rightarrow a_{DO_3}[0\ \overline{1}\ 0] \\ c[0\ 0\ 1]_{18R} &\rightarrow a_{DO_3}[\overline{5}\ 0\ 4]. \end{aligned}$$

From the relations above, the matrix C relating any vector $\vec{V}$ of the DO_3 structure to a vector $\vec{V}'$ of the 18R structure can be deduced as

$$\vec{V} = C\vec{V}'. \tag{1}$$

Here, the matrix C is correspondence matrix and is given by:

$$C = \frac{1}{2}\begin{pmatrix} -1 & 0 & -10 \\ 0 & -2 & 0 \\ -1 & 0 & 8 \end{pmatrix}.$$

The inverse of this relation

$$\vec{V}' = C^{-1}\vec{V} \tag{2}$$

with

$$C^{-1} = \frac{1}{9}\begin{pmatrix} -8 & 0 & -10 \\ 0 & -9 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

is also valid and can be used for calculating the vector $\vec{V}'$ in martensite into which a given vector $\vec{V}$ in the parent phase is transformed. Accordingly, plane normals $\vec{n}$ in the parent phase and $\vec{n}'$ in martensite are related by

$$\vec{n} = \vec{n}'C^{-1} \tag{3}$$

$$\vec{n}' = \vec{n}C. \tag{4}$$

By means of Eqs. (1) to (4) the vectors originally present in martensite or in the parent phase can be redefined in terms of other structure.

Since there are six $\{\bar{1}01\}_{DO_3}$ planes and two choices in the direction of the shear, there are 12 lattice correspondence variants (C.V.). These are listed in Table 1, where the C.V. with and without primes for the same numbers refer to C.V.'s with opposite shear directions. Obviously, the C.V. described above corresponds to C.V.3′ in Table 1.

Table 1. Lattice correspondence between DO_3 parent and 18R martensite

C.V.	$[100]_{18R}$	$[010]_{18R}$	$[001]_{18R}$	$(001)_{18R}$
1	$\frac{1}{2}[011]_{DO_3}$	$[100]_{DO_3}$	$[05\bar{4}]_{DO_3}$	$(0\bar{1}1)_{DO_3}$
1′	$\frac{1}{2}[0\bar{1}\bar{1}]_{DO_3}$	$[\bar{1}00]_{DO_3}$	$[04\bar{5}]_{DO_3}$	$(0\bar{1}1)_{DO_3}$
2	$\frac{1}{2}[0\bar{1}1]_{DO_3}$	$[100]_{DO_3}$	$[054]_{DO_3}$	$(011)_{DO_3}$
2′	$\frac{1}{2}[01\bar{1}]_{DO_3}$	$[\bar{1}00]_{DO_3}$	$[045]_{DO_3}$	$(011)_{DO_3}$
3	$\frac{1}{2}[101]_{DO_3}$	$[010]_{DO_3}$	$[\bar{4}05]_{DO_3}$	$(\bar{1}01)_{DO_3}$
3′	$\frac{1}{2}[\bar{1}0\bar{1}]_{DO_3}$	$[0\bar{1}0]_{DO_3}$	$[\bar{5}04]_{DO_3}$	$(\bar{1}01)_{DO_3}$
4	$\frac{1}{2}[10\bar{1}]_{DO_3}$	$[010]_{DO_3}$	$[405]_{DO_3}$	$(101)_{DO_3}$
4′	$\frac{1}{2}[\bar{1}01]_{DO_3}$	$[0\bar{1}0]_{DO_3}$	$[504]_{DO_3}$	$(101)_{DO_3}$
5	$\frac{1}{2}[110]_{DO_3}$	$[001]_{DO_3}$	$[4\bar{5}0]_{DO_3}$	$(\bar{1}10)_{DO_3}$
5′	$\frac{1}{2}[\bar{1}\bar{1}0]_{DO_3}$	$[00\bar{1}]_{DO_3}$	$[5\bar{4}0]_{DO_3}$	$(\bar{1}10)_{DO_3}$
6	$\frac{1}{2}[\bar{1}10]_{DO_3}$	$[001]_{DO_3}$	$[540]_{DO_3}$	$(110)_{DO_3}$
6′	$\frac{1}{2}[1\bar{1}0]_{DO_3}$	$[00\bar{1}]_{DO_3}$	$[450]_{DO_3}$	$(110)_{DO_3}$

Based on the stacking of close packed planes, we assume the lattice invariant shear direction in the 18R structure martensite is $[100]_{18R}$ and the plane of lattice invariant deformation is $(001)_{18R}$. By this shear the lattice vector $\vec{V}'$ and the plane $\vec{n}'$ are transformed into $\vec{V}''$ and $\vec{n}''$, respectively, through the following equations:

$$\vec{V}'' = G \cdot \vec{V}' \tag{5}$$

$$\vec{n}'' = \vec{n}' \cdot G^{-1} \tag{6}$$

where

$$G = \begin{pmatrix} 1 & 0 & g \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and g is the magnitude of lattice invariant shear. The matrix G^{-1} is the inverse of the matrix G. A combined effect of the lattice deformation and the lattice invariant deformation is seen by the substitution of Eqs. (3) and (4) into Eqs. (5) and (6), which leads to

$$\vec{V}'' = G \cdot C^{-1} \cdot \vec{V} \tag{7}$$

$$\vec{n}'' = \vec{n} \cdot C \cdot G^{-1}. \tag{8}$$

The matrix G^{-1} is calculated as follows:

$$G^{-1} = \begin{pmatrix} 1 & 0 & -g \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

It is concluded that, as a result of lattice deformation and the lattice invariant deformation, the vector and the plane in the DO_3 crystal are transformed by the above equations into the vector and the plane in the 18R crystal, respectively.

Now denote a habit plane as $(1 \;\; Y \;\; Z)_{DO_3}$ and an arbitrary vector lying in this habit plane as $[1 \;\; y \;\; z]_{DO_3}$, then the following equation holds:

$$1 + yY + zZ = 0. \tag{9}$$

In the DO_3 to 18R transformation the vector $[1 \;\; y \;\; z]_{DO_3}$ is transformed into the vector $[\frac{1}{9}\{-8 - g + (g - 10)z\}, \; -y, \frac{1}{9}(z - 1)]_{18R}$by Eq. (7). The latter vector must, of course, lie in the habit plane. Since the habit plane is undistorted, the lengths of the above two vectors must be the same. Therefore

$$\begin{aligned} \frac{a^2}{81}\{(-8 - g) \;\; &+ \;\; (g - 10)z\}^2 + b^2y^2 + \frac{c^2}{81}(z - 1)^2 \\ &+ \;\; \frac{2ca}{81}\cos\beta_0\{(-8 - g) + (g - 10)z\}(z - 1) = a_{DO_3}^2(1 + y^2 + z^2). \end{aligned} \tag{10}$$

Eliminating y from Eqs. (9) and (10), we obtain

$$A(Y,Z,g)z^2 + B(Y,Z,g)z + C(Y,g) = 0, \tag{11}$$

where

$$\begin{aligned}
A(Y,Z,g) &= \frac{a^2}{81}(10-g)^2 + b^2\frac{Z^2}{Y^2} + \frac{c^2}{81} - \frac{2}{81}ac(10-g)\cos\beta_0 - a_{DO_3}^2(1+\frac{Y^2}{Z^2}) \\
B(Y,Z,g) &= \frac{2a^2}{81}(8+g)(10-g) + \frac{2b^2}{81}\frac{Z}{Y^2} - \frac{2c^2}{81} + \frac{4}{81}ac(1-g)\cos\beta_0 - 2a_{DO_3}^2\frac{Z}{Y^2} \\
C(Y,g) &= \frac{a^2}{81}(8+g)^2 + b^2\frac{1}{Y^2} + \frac{c^2}{81} + \frac{2}{81}ac(8+g)\cos\beta_0 - a_{DO_3}^2(1+\frac{1}{Y^2}).
\end{aligned}$$

Since $[1 \quad y \quad z]_{DO_3}$ represent an arbitrary direction lying in the habit plane, Eq. (11) should hold for any value of z, hence each coefficient of z in the equation must be zero. That is,

$$A(Y,Z,g) = 0, \quad B(Y,Z,g) = 0, \quad C(Y,g) = 0. \tag{12}$$

From Eq. (12) g, Y and Z are obtained as follows:

$$g = 1 - \frac{c}{a}\cos\beta_0 \pm \frac{9a_{DO_3}}{\sqrt{2}a}\sqrt{\left(\frac{2a^2}{a_{DO_3}^2} - 1\right)\left(\frac{2c^2\sin^2\beta_0}{81a_{DO_3}^2} - 1\right)} \tag{13}$$

$$Y = \pm\sqrt{\frac{81a_{DO_3}^2 - b^2}{a^2(8+g)^2 + 2ac(8+g)\cos\beta_0 + c^2 - 81a_{DO_3}^2}} \tag{14}$$

$$Z = \sqrt{\frac{a^2(10-g)^2 + 2ac(10-g)\cos\beta_0 + c^2 - 81a_{DO_3}^2}{a^2(8+g)^2 + 2ac(8+g)\cos\beta_0 + c^2 - 81a_{DO_3}^2}}. \tag{15}$$

By using the relation $g' = ga/c\sin\beta_0$, the magnitude of the lattice invariant shear g' is then

$$g' = \frac{a}{c\sin\beta_0} - ctg\beta_0 \pm \frac{9a_{DO_3}}{\sqrt{2}c\sin\beta_0}\sqrt{\left(\frac{2a^2}{a_{DO_3}^2} - 1\right)\left(\frac{2ca^2\sin^2\beta_0}{81a_{DO_3}^2} - 1\right)}. \tag{16}$$

As seen in the above equation g' is a function of only lattice constants, a, b, c, β_0, and a_{DO_3}, and accordingly Y and Z are also dependent only on the lattice constants of both phases.

2.2. Orientation Relationships

The derivation of the orientation relationships was performed on the martensite variant of which the habit plane indices have positive sign. It is seen by Eq. (8) with g that the habit plane $(1YZ)_{DO_3}$ is transformed into $(HKL)_{18R}$. Since the habit plane is invariant during the transformation, $(1YZ)_{DO_3}$ must be parallel to $(HKL)_{18R}$. Any given vector lying on the habit plane must also be invariant during the transformation. For example, the intersection of $(100)_{DO_3}$ plane with the habit plane $(1YZ)_{DO_3}$ is $[u_1 \quad u_2 \quad u_3]_{DO_3}$ and this direction is transformed into $[u'_1 \quad u'_2 \quad u'_3]_{18R}$ by Eq. (7). Since the direction $[u_1 \ u_2 \ u_3]_{DO_3}$ lies on the habit plane, it must be invariant and hence parallel to the direction $[u'_1 \ u'_2 \ u'_3]_{18R}$. Therefore the following orientation relationship is obtained:

$$(1YZ)_{DO_3}//(HKL)_{18R}$$

$$[u_1 \ u_2 \ u_3]_{DO_3}//[u'_1 \ u'_2 \ u'_3]_{18R}.$$

A relationship between some prominent planes and directions is derived from the above relation by the following procedures. First, set up a new orthogonal coordinate with its origin on the habit plane, of which x_0- and y_0-axes are taken to be parallel to $[u_1 \ u_2 \ u_3]_{DO_3}$ and the habit plane normal $[1YZ]_{DO_3}$, respectively. The unit length in the DO_3 lattice coordinate is taken as the unit length in this new orthogonal coordinate. That is, the unit vector along x_0-axis in the above orthogonal coordinate is taken equal to normalized direction of $[u_1 \ u_2 \ u_3]_{DO_3}$, i.e.

$$\frac{1}{\sqrt{u_1^2+u_2^2+u_3^2}}[u_1 \ u_2 \ u_3]_{DO_3}$$

and the unit vector y_0-axis equal to the normalized direction of $[1YZ]_{DO_3}$, i.e.,

$$\frac{1}{\sqrt{1+Y^2+Z^2}}[1YZ]_{DO_3} \quad \text{or} \quad \frac{1}{\sqrt{v_1^2+v_2^2+v_3^2}}[v_1 \ v_2 \ v_3]_{DO_3}.$$

A direction perpendicular to the above two directions is parallel to z_0-axis and its normalized direction is

$$\frac{1}{\sqrt{w_1^2+w_2^2+w_3^2}}[w_1 \ w_2 \ w_3]_{DO_3}.$$

Therefore the following relation holds between the direction $[u \quad v \quad w]_{DO_3}$ in DO_3 coordinate and the direction $[u \ v \ w]_{DO_3}$ in DO_3 coordinate and the direction $[u \ v \ w]_0$ in the $x_0y_0z_0$-coordinate:

$$\begin{bmatrix} u \\ v \\ w \end{bmatrix}_{DO_3} = \begin{pmatrix} u_1 & v_1 & w_1 \\ u_2 & v_2 & w_2 \\ u_3 & v_3 & w_3 \end{pmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix}_0. \tag{17}$$

The next step is to obtain a similar relation between the direction $[u\ \ v\ \ w]_{18R}$ in monoclinic coordinate of 18R martensite and direction $[u\ \ v\ \ w]_0$. The vectors

$$\frac{1}{\sqrt{u_1^2+u_2^2+u_3^2}}[u_1\ \ u_2\ \ u_3]_{DO_3} \quad \text{and} \quad \frac{1}{\sqrt{w_1^2+w_2^2+w_3^2}}[w_1\ \ w_2\ \ w_3]_{DO_3}$$

which are the unit vectors along x_0- and z_0-axes are transformed by Eq. (7) into $[u_1\ \ u_2\ \ u_3]_{18R}$ and $[w_1\ \ w_2\ \ w_3]_{18R}$, respectively. Since x_0- and z_0-axes lie on the habit plane, the above two vectors are invariant during the transformation. Therefore, the transformed vectors, $[u_1'\ \ u_2'\ \ u_3']_{18R}$ and $[w_1'\ \ w_2'\ \ w_3']_{18R}$, in monoclinic coordinate of the 18R martensite correspond to the unit vectors along x_0- and z_0-axes in the $x_0y_0z_0$-coordinate. A vector corresponding to the unit vector along y_0-axis is calculated to be $[v_1'\ \ v_2'\ \ v_3']_{18R}$ from these two vectors. Thus the following relationship is obtained:

$$\begin{bmatrix} u \\ v \\ w \end{bmatrix}_{18R} = \begin{pmatrix} u_1' & v_1' & w_1' \\ u_2' & v_2' & w_2' \\ u_3' & v_3' & w_3' \end{pmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix}_0 . \tag{18}$$

Now a relation between $[u\ \ v\ \ w]_{DO_3}$ and $[u\ \ v\ \ w]_{18R}$ is obtained from Eqs. (17) and (18).

$$\begin{bmatrix} u \\ v \\ w \end{bmatrix}_{DO_3} = \begin{pmatrix} u_1 & v_1 & w_1 \\ u_2 & v_2 & w_2 \\ u_3 & v_3 & w_3 \end{pmatrix} \begin{pmatrix} u_1' & v_1' & w_1' \\ u_2' & v_2' & w_2' \\ u_3' & v_3' & w_3' \end{pmatrix}^{-1} \begin{bmatrix} u \\ v \\ w \end{bmatrix}_{18R} . \tag{19}$$

A relation between the planes $(hkl)_{DO_3}$ and $(hkl)_{18R}$ is obtained from the above equation by calculating the inverse of the multiplication of these two matrices.

$$(h\ \ k\ \ l)_{DO_3} = (h\ \ k\ \ l)_{18R} \left(\begin{pmatrix} u_1 & v_1 & w_1 \\ u_2 & v_2 & w_2 \\ u_3 & v_3 & w_3 \end{pmatrix} \begin{pmatrix} u_1' & v_1' & w_1' \\ u_2' & v_2' & w_2' \\ u_3' & v_3' & w_3' \end{pmatrix}^{-1} \right)^{-1} . \tag{20}$$

From Eqs. (19) and (20) the relations between some prominent planes and directions are obtained.

2.3. Shape Deformation

It is well known that the total shape change which produces the surface relief effect in the martensitic transformation is an invariant plane strain. The total shape change (deformation) is considered to be an invariant plane strain, which corresponds to a simple shear on the habit plane plus an extension or contraction perpendicular to the habit plane to account for the change in volume upon transformation. The invariant plane is, of course, the habit plane $(1YZ)_{DO_3}$. This total shape change is simply called the shape deformation. The direction and the magnitude of the shape deformation are

defined by the direction and the amount of the displacement of the unit vector normal to the habit plane.

The unit vector,

$$\frac{1}{\sqrt{v_1^2+v_2^2+v_3^2}}[v_1 \;\; v_2 \;\; v_3]_{DO_3}$$

of the habit plane normal is transformed into $[v'_{1n} \;\; v'_{2n} \;\; v'_{3n}]_{18R}$ by Eq. (7). This vector is equivalent to $[v'_{1n} \;\; v'_{2n} \;\; v'_{3n}]_{DO_3}$ according to Eq. (19). The vector difference between the above vector and unit normal of the habit plane is $\vec{S}''$. That is, the shape deformation is

$$\vec{S}'' = [s''_1 \;\; s''_2 \;\; s''_3]_{DO_3} = [v'_{1n} \;\; v'_{2n} \;\; v'_{3n}]_{DO_3} - \frac{1}{\sqrt{v_1^2+v_2^2+v_3^2}}[v_1 \;\; v_2 \;\; v_3]_{DO_3}. \tag{21}$$

The magnitude of the shape deformation is $\sqrt{(s''_1)^2+(s''_2)^2+(s''_3)^2}$. The normalized direction of the shape deformation $\vec{s}''$ is

$$\vec{s}'' = \frac{1}{\sqrt{(s''_1)^2+(s''_2)^2+(s''_3)^2}}[s''_1 \;\; s''_2 \;\; s''_3]_{DO_3}. \tag{22}$$

3. Numerical Calculations of the Lattice Invariant Shear, Habit Plane, Orientation Relationship and Shape Deformation

In order to obtain reliable results single crystals were used, and were studied by X-ray diffraction technique. The lattice parameter a_{DO_3} of the DO_3 matrix is determined to be 0.582 nm from X-ray diffractometry. The lattice parameter of the monoclinic 18R unit cell is determined to be $a = 0.448$ nm, $b = 0.518$ nm, and $c = 3.865$ nm [1]. The a and b lie in the basal plane, the c direction corresponds to 18 close packed layers, making an angle β_0 different from 90° between a and c axes. The distortion of the close-packed hexagonal in the close-packed plane leads to a deviation from the ideal (b/a) and (c/a) ratios. The ratios between the lattice parameters in the case of an ideally close-packed 18R structure are $a/b/c = 1/1.155/8.485$ [14]. In the ideally close-packed structure, the angle β_0 is 90 deg. The lattice parameters of 18R phase for FeMnAlC alloy [1] are very close to the ideal ratios. That is, the ratios for FeMnAlC [1] alloy are $a/b/c = 1/1.156/8.627$.

It is well known that the theory of martensitic transformation crystallography is based on the assumption that there should be no average distortion at the habit plane. From this basic condition, crystallographic features such as habit plane, orientation relationships, direction and magnitude of the shape deformation and magnitude of the lattice invariant shear can be calculated. Kajiwara applied the Suzuki theory to calculate the martensitic crystallography of bcc to 9R structure in Cu-Zn or Cu-El alloys [4]. Lee et.al. [1] applied the CRAB [11] theory to calculate the martensitic crystallography for a FeMnAlC [1] alloy and the calculated crystallography fits very well with experimental observation by TEM. In this paper, the Suzuki mathematical approach is applied to the

transformation of the DO_3 to 18R close-packed structure, and the numerical calculations of various crystallographic features are performed for FeMnAlC [1] alloy. The calculated results and the calculations of CRAB theory are given in Table 2.

Table 2. Theoretical crystallographic comparison between in the present work and CRAB theory for a FeMnAlC [1] alloy. The experimental habit plane is nearly $(1\ 6\ 8)_{bcc}$

	in the present	CRAB
Habit plane	(1 6.108 7.151)	(1 6.303 7.712)
Direction of shape deformation	[0.096 -0.723 0.684]	[0.089 -0.721 0.688]
Magnitude of shape deformation	0.2355	0.2522
Magnitude of lattice invariant shear	0.0606	0.0968

The orientation relationships were calculated by using for the lattice parameters of the FeMnAlC alloy [1]. From equations (20) and (21), the relationships between some planes and directions can be obtained and are given in Table 3. From Table 3, it can be seen that $[\bar{1}11]_{DO_3}$ is approximately parallel to $[1\bar{1}0]_{18R}$ and $(011)_{DO_3}$ approximately parallel to $(\bar{1}\bar{1}8)_{18R}$. This orientation relationship is also similar to those in FeMnAlC alloy [1].

From the crystallographic calculation for FeMnAlC [1] alloy, the magnitude of lattice invariant shear g is 0.0606. The solution of habit plane from the calculation of martensitic crystallography is $(1, 6.303, 7.7119)_{DO_3}$, which is very close to that determined from experiment.

Table 3. Theoretical comparison between planes or directions in FeMnAlC [1] alloy during martensitic transformation

18R	in present	calc. angle	CRAB	calc. angle
$(\bar{1}\ \bar{1}\ 8)$	$(012)_{DO_3}$	1.23°	$(011)_{bcc}$	0.35°
$(\bar{1}\ \bar{1}\ \bar{1}0)$	$(210)_{DO_3}$	3.03°	$(110)_{bcc}$	5.42°
$(\bar{2}\ 0\ 2)$	$(101)_{DO_3}$	6.08°	$(101)_{bcc}$	6.24°
$(0\ 0\ 18)$	$(\bar{1}01)_{DO_3}$	5.13°	$(\bar{1}01)_{bcc}$	5.53°
$(1\ \bar{1}\ 10)$	$(\bar{2}01)_{DO_3}$	5.18°	$(\bar{1}10)_{bcc}$	7.04°
$(\bar{1}\ 1\ 8)$	$(0\bar{1}2)_{DO_3}$	12.26°	$(0\bar{1}1)_{bcc}$	13.9°
$[\bar{1}\ \bar{1}\ 0]$	$[111]_{DO_3}$	10.08°	$[111]_{bcc}$	12.23°

4. Conclusions

The martensite crystallographic parameters such as orientation relationships, habit plane, shape deformation direction and magnitude of lattice invariant shear have been calculated using new mathematical approach in the present work. The predicted orientation relationship of $DO_3 \rightarrow 18R$ martensitic transformation is near $(011)_{DO_3}//(\bar{1}\ \bar{1}\ 8)_{18R}$ and $[\bar{1}1\bar{1}]_{DO_3}//[1\bar{1}0]_{18R}$. The habit plane is $(1\ \ 6.108\ \ 7.151)_{DO_3}$ and shape deformation direction is $[0.096\ \ -0.723\ \ 0.684]_{DO_3}$ with the magnitude of 0.2355.

The theoretical analysis in this present paper confirms the crystallography of $DO_3 \rightarrow 18R$ martensitic transformation in the Fe-25.8 wt % Mn-7.4 wt % Al-0.11 wt % C alloy. Phenomenological crystallographic CRAB theory, in good agreement with experimental observations. Overall, the calculated crystallographic features fit very well with CRAB theory.

As shown in this work, the Suzuki method is especially powerful when a complicated lattice deformation is involved, and mathematical equations for the magnitude of the lattice invariant shear and the habit plane indices can be quite easily obtained by this mathematical approach.

References

[1] W.B. Lee, Fu-Rong Chen, S.K. Chen, G.B. Olson and C.M. Wan, *Acta metall. mater.*, **43** (1995) 21.

[2] C.H. Chao and N.J. Ho, *Scripta metall.*, **26** (1992) 1863.

[3] C.H. Chao and N.J. Ho, *Scripta metall.*, **27** (1992), 499.

[4] S. Kajiwara, *Trans. Japan Inst. Metals*, **17** (1976) 436.

[5] I. Cornelis and C.M. Wayman, *Acta metall.*, **22** (1974) 291.

[6] S. Chakravorty and C.M. Wayman, *Acta metall.*, **25** (1977) 989.

[7] S. akmak, Doctoral Thesis, Graduate School of Natural and Applied Sciences, Frat Univ. (1992) (in Turkish).

[8] S. akmak, N. Kayal, E. Artun and O. Adgzel, *Turkish Jr. of Physics*, **22** (1994) 331.

[9] M.S. Wechsler, D.S. Lieberman and T.A. Read, *Trans. AIME*, **197** (1953) 1503.

[10] J.S. Bowles and J.K. Mackenzie, *Acta metall.*, **2** (1954) 129, 138, 224.

[11] A.F. Acton, M. Bevis, A.G. Crocker and N.D.H. Ross, *Proc. Roy. Soc.* (Lond.), **A320** (1970) 101.

[12] H. Suzuki, *Sci. Rep. Res. Inst. Tohoku Univ.*, **A6** (1954) 30.

[13] M. Andrade and L. Delaey, *Transactions of the Japan Institute of Metals*, **25** (1984) 778.

[14] W.R. Dong, Eon-Sik Lee and G.K. Young, *Metallurgical Transactions A*, **23A** (1992) 2753.