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Rigorous version of infinitesimal deformation approach to the crystallography of fcc → bcc martensitic phase transformation observed in Fe-31 wt % Ni and zirconia alloys

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Following the mathematical approach of Kelly (2003), rigorous version of infinitesimal deformation approach (ID) was applied to analyze fcc → bcc martensitic phase transformation observed in Fe-31wt% Ni alloys considering the twinning shear system as the lattice invariant system (LIS). The expressions for crystallographical parameters associated with the martensitic phase transformation such as habit plane orientation, rotation matrix, total shape deformation matrix, orientation relationships between austenite and martensite phases, etc., have been obtained by using the rigorous version of infinitesimal deformation approach, taking into account only the information about the lattice parameters of the austenite and martensite phases. The habit plane orientation obtained from the infinitesimal deformation approach (ID), for example, for the value of volume fraction 0.39876 in Fe-31wt% Ni alloy, is found as (0, 0.58033, 0.81438) while the habit plane obtained from rigorous version of (ID) approach associated with the martensite transformation is (0.185064, 0.594242, 0.782705) which is an agreement with that calculated from the Wechsler-Lieberman-Read (W-L-R) theory. The difference between the two habit plane orientations is 10.8° . Moreover, the calculations carried out for zirconia, in which there are small values of the principal distortions, in the present study certainly indicate that infinitesimal deformation approach (ID) gives almost the same results as (W-L-R) theory. For the other crystallographical parameters, such as magnitude of total shape deformation, volume fraction, orientation relationship, the rigorous version of (ID) approach gives essentially the same crystallographical solutions as those calculated (W-L-R) theory. So, it is concluded that the rigorous version of (ID) approach in the habit plane orientation is better than the infinitesimal deformation approach (ID) for the alloys in question.

Key words: Martensitic transformation, solid-solid phase transitions, crystallography of martensite phase transformations.

INTRODUCTION

Phenomenological crystallographic theories of martensite transformation were introduced in 1950's and are based on the concept that the interface plane between the martensite and parent phase is essentially macroscopically invariant – that is, undistorted and rotated. The

equivalence of the various formulations by Wechsler-Lieberman-Read (W-L-R) (Wechsler et al., 1953) and Bowles-Mackenzie (B-M) (Bowles and Mackenzie, 1954) has been demonstrated many time (Christians, 1955). These theories have gained general acceptance because of the agreement between theory and experiment in a number of cases. However, one must conclude that only a few specific martensite transformations are adequately accounted for, when these theories are applied to various martensitic transformation in iron alloys and steels

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(Wechsler et al, 1953; Bowles and Mackenzie, 1954; Bullough and Bilby, 1956; Dunne and Wayman, 1971; Christians, 1955; Nishiyama, 1978; Wayman, 1964). In recent years, some researchers (Kato and Shibata-Yanagisawa, 1990; Shibata-Yanagisawa and Kato, 1990) adopted a theory based on the infinitesimal deformation approach (ID) taking into consideration both symmetric strain components and the antisymmetric rotation components of deformation in which this theory is an approximation of the finite deformation-based phenomenological crystallographic theory (FD) or (PT). In the infinitesimal deformation approach, there is superposition of the solutions since this approach neglects the second- and higher- order terms of the magnitude of the lattice distortions.

However, the advantage of ID-based phenomenological theory is that all solutions can be expressed in simple and analytical forms while the disadvantage of it is that the miller indices can be expressed in the form as $\{hk0\}$ instead of $\{hkl\}$ observed experimentally. The difference in habit plane indices between ID and FD becomes larger as the lattice distortion components involved in a transformation become larger. However, it is of course true that the ID analysis is the approximation of the FD analysis. Therefore, in a recent paper by Kelly (2003), a modification was carried out on this approach. It is very convenient for the actual numerical calculations since this approach, which is called rigorous version of infinitesimal deformation approach, is quite easily applicable to some of the systems associated with martensitic transformations.

In the present study, taking the $(101)_\gamma$ $[\bar{1}01]_\gamma$ twinning system as the lattice invariant shear (LIS) deformation observed in Fe-31 wt% Ni alloys, the reformulation of rigorous version of the infinitesimal deformation approach is given briefly and the results calculated from the crystallographic parameters are applied for the fcc to bcc martensite transformation in the above alloy. However, the results obtained in the (W-L-R) or (B-M) theories are suitable for a comparison with the results of the rigorous version of ID approach treated in the present study, ID approach and experimental values.

DETERMINATION OF CRYSTALLOGRAPHIC PARAMETERS ASSOCIATED WITH MARTENSITE TRANSFORMATION

In the phenomenological theory of the martensitic transformation, the total shape deformation can be written in matrix form as follows:

$$T = R.B.P \quad (1)$$

where R is the rigid body rotation matrix which describes the orientation relationship and the invariant plane distortion, B is Bain strain and P is the simple shear. Whereas, it is assumed that this expression in the ID approach is taken as in the form $T = R + B + P$, because

this approach neglects the second- and higher- order terms of the magnitude of the lattice distortions. However, the following form is more convenient to treat the case twinning as the LIS deformation:

$$\mathbf{F} = R + (1-f)\mathbf{B}_2 + f(\Phi + \mathbf{B}_1)$$

\mathbf{B}_1 and \mathbf{B}_2 are the lattice deformation matrices for variant 1 and 2, respectively, and Φ denotes a rotation which is geometrically necessary to make variant 1 twin related to variant 2. Here, f is the volume fraction of variant 1 of the product phase which is twin-related to variant 2. In order for T to describe invariant plane deformation (IPS), the elements of the matrix T^n must be satisfied as: $T_{11}^n, T_{12}^n, T_{21}^n, T_{22}^n, T_{31}^n$ and $T_{32}^n = 0$ (Kato and Shibata-Yanagisawa, 1990; Shibata-Yanagisawa and Kato, 1990). These constitute the necessary (but not sufficient) condition for the IPS deformation. The n indicates that the matrix is described on $x_1^n - x_2^n - x_3^n$ orthonormal coordinate system (n system) with the x_3^n plane parallel to the invariant plane that is the habit plane. It is well known that the matrix T^γ expressed on the austenite coordinate system (γ) can be converted into T^n expressed on the n coordinate system, which is defined by the usual tensor conversion given in Equation (9). In order for the habit plane to be invariant (undistorted and unrotated), the rotation matrix, R, must become an antisymmetric form. The elements of this matrix must satisfy $R_{11}^\gamma = 0, R_{22}^\gamma = 0, R_{33}^\gamma = 0, R_{12}^\gamma = -w_3, R_{13}^\gamma = w_2, R_{21}^\gamma = w_3, R_{23}^\gamma = -w_1, R_{31}^\gamma = -w_2$ and $R_{32}^\gamma = w_1$. Here, w_1, w_2 and w_3 are unknown angles of rotation. These angles, f, the direction cosine angles θ and ϕ (these angles determines the habit plane direction) can be found from the condition $T^n = 0$. Then, the orientation relationship between parent and product phase can be determined from the R^γ matrix.

In the present study dealing with rigorous version of the ID approach, T matrix in Equation (1) can be defined as follows (Kelly, 2003; Ledbetter and Dunn, 1999; Ledbetter and Dunn, 2000):

$$T = \frac{1}{2} [F^T F - I] \quad (2)$$

where F^T is the transpose of the $F = B P$ matrix, which leaves the habit plane undistorted, and so that F matrix is taken in the form:

$$\mathbf{F} = (1-f)\mathbf{B}_1 + f\Phi\mathbf{B}_2 \quad (3)$$

Here, f is the relative amount of twins. For the selected $(101)_\gamma$ $[\bar{1}01]_\gamma$ twinning shear system as LIS, the Bain strain matrices in Equation (3) can be taken in the following forms:

$$\mathbf{B}_1 = \begin{bmatrix} \eta_1 & 0 & 0 \\ 0 & \eta_2 & 0 \\ 0 & 0 & \eta_3 \end{bmatrix} \quad (4)$$

and

$$\mathbf{B}_2 = \begin{bmatrix} \eta_3 & 0 & 0 \\ 0 & \eta_2 & 0 \\ 0 & 0 & \eta_1 \end{bmatrix} \quad (5)$$

In order for the martensitic phase to be internal twinned, the α phase crystal subjected to a lattice deformation \mathbf{B}_1 called crystal 1 must be rotated relative to the α phase crystal subjected to the lattice deformation \mathbf{B}_2 called crystal 2 by an angle ϕ . The expression of relative rotation matrix Φ is calculated as

$$\Phi = \begin{pmatrix} \cos \varphi & 0 & -\sin \varphi \\ 0 & 1 & 0 \\ \sin \varphi & 0 & \cos \varphi \end{pmatrix} = \begin{bmatrix} \frac{2\eta_1\eta_3}{\eta_1^2 + \eta_3^2} & 0 & -\left(\frac{\eta_1^2 - \eta_3^2}{\eta_1^2 + \eta_3^2}\right) \\ 0 & 1 & 0 \\ \left(\frac{\eta_1^2 - \eta_3^2}{\eta_1^2 + \eta_3^2}\right) & 0 & \frac{2\eta_1\eta_3}{\eta_1^2 + \eta_3^2} \end{bmatrix} \quad (6)$$

Furthermore, F matrix in the obtained total shape deformation T via Lagrangean-strain formulation (Wayman, 1964) is obtained as using Equations (3) to (6):

$$F = \begin{bmatrix} \eta_1(1 - \xi f) & 0 & -\eta_1 \xi f \\ 0 & \eta_2 & 0 \\ \eta_3 \xi f & 0 & \eta_3(1 + \xi f) \end{bmatrix} \quad (7)$$

Here, ξ is defined as $\xi = (\eta_1^2 - \eta_3^2) / (\eta_1^2 + \eta_3^2)$. Taking into consideration of $\det \frac{1}{2}(\mathbf{F}^T \mathbf{F} - \mathbf{I}) = 0$ in Equation (2), the two values of volume fractions f are derived as:

$$f_{\pm} = \frac{1}{2} \left\{ 1 \mp \sqrt{1 + \frac{2(\eta_1^2 + \eta_3^2)(\eta_1^2 - 1)(\eta_3^2 - 1)}{(\eta_1^2 - \eta_3^2)^2}} \right\} \quad (8)$$

The total shape deformation matrix \mathbf{T}_{ij}^n expressed on particular orthonormal x_1^n, x_2^n, x_3^n coordinate system can be derived from \mathbf{T}^γ matrix expressed on the γ -coordinate system by an usual tensor transformation

$$\mathbf{T}_{ij}^n = \sum_{k=1}^3 \sum_{l=1}^3 \mathbf{A}_{ki} \mathbf{A}_{lj} \mathbf{T}_{kl}^\gamma \quad (9)$$

where the a_{ij} are direction cosines between x_1^n, x_2^n, x_3^n and $x_1^\gamma, x_2^\gamma, x_3^\gamma$ axes. It can be given that the

elements of direction cosines A_{ij} as: $A_{11} = \cos \theta \cos \phi$, $A_{12} = -\sin \phi$, $A_{13} = \sin \theta \cos \phi$, $A_{21} = \cos \theta \sin \phi$, $A_{22} = \cos \phi$, $A_{23} = \sin \theta \sin \phi$, $A_{31} = -\sin \theta$, $A_{32} = 0$ and $A_{33} = \cos \theta$.

In order for T to describe the invariant plane deformation, the following elements of the matrix \mathbf{T}^γ have the form:

$$\mathbf{T}_{11}^n = \mathbf{T}_{12}^n = \mathbf{T}_{22}^n = 0 \quad (10)$$

θ and ϕ angles determining the habit plane direction (That is, $n = [\cos \theta, \sin \theta \sin \phi, \sin \theta \cos \phi]$ in the spherical coordinate system) can be calculated from Equation (10), as:

$$\tan \phi = \mp \sqrt{-\frac{T_{22}^\gamma}{T_{11}^\gamma}} \quad (11)$$

and

$$\tan \theta = \frac{T_{11}^\gamma - T_{22}^\gamma}{T_{13}^\gamma} \cos \phi \quad (12)$$

On the other hand, the orientation relationship between γ and α phase can be obtained when the rotation matrix R is determined. Details of these calculations are not presented here, since they are found easily in some advanced books (Nishiyama, 1978; Wayman, 1964).

RESULTS AND DISCUSSION

Lattice parameter of the γ phase (austenite) associated with the alloy Fe-31 wt% Ni is $a_\gamma = 3.591 \pm 0.001 \text{ \AA}$ and the lattice parameters of α phase (martensite) are $a_\alpha = 2.875 \pm 0.001 \text{ \AA}$ (Nishiyama, 1978). Using these values, the principal distortions are determined as:

$$\eta_1 = \eta_2 = \sqrt{2} \frac{a_\alpha}{a_\gamma} = 1.132237 \quad \text{and}$$

$$\eta_3 = \frac{a_\alpha}{a_\gamma} = 0.800613 \quad (13)$$

In order for a suitable comparison, if these values of η_1 and η_2 for the alloy Fe-31 wt% Ni are substituted into the expressions for the solution in Equations (8) to (12), some numerical values for various crystallographic parameters can be listed in Table 1. Using these values, Navruz and Durlu (1999) gave a reformulated infinitesimal deformation approach to martensite crystallography for the only slip system $(101)_\gamma [-1 \ 0 \ 1]_\gamma$. From Table 1, it can be seen that the obtained habit plane in the ID approach for $f^- = 0.39876$ is given as (0,

Table 1. A comparison of the numerical solutions of rigorous version of ID and WLR theory, ID Approach with experimental results for fcc to bcc martensitic transformation observed in an Fe-31 wt% Ni alloy. For the detailed experimental analysis and applications of WLR theory, it can be referred to the references (Nishiyama, 1978; Wayman, 1964).

Parameter	ID Approach	Rigorous version of ID Approach		WLR Theory	Experimental
Habit plane, n	$\begin{bmatrix} 0 \\ 0.58033 \\ 0.814380 \end{bmatrix}$	$\begin{bmatrix} 0.594242 \\ 0.782705 \\ 0.185064 \end{bmatrix}$	$\begin{bmatrix} 0.185064 \\ 0.782705 \\ 0.594242 \end{bmatrix}$	$\begin{bmatrix} 0.1848 \\ 0.7823 \\ 0.5948 \end{bmatrix}$	$\begin{bmatrix} 0.1656 \\ 0.7998 \\ 0.5770 \end{bmatrix}$
Volume fraction, f	0.398760	0.225753	0.225756	0.360576	-
Magnitude of total shape deformation (m_T)	0.1994	0.225753	0.225756	0.22580	-
Orientation relationship					
$[100]_\gamma - [100]_\alpha$	6.66°	2.36°	6.23°	7.61°	-
$[010]_\gamma - [010]_\alpha$	4.76°	6.31°	6.31°	6.32°	-
$[001]_\gamma - [001]_\alpha$	11.47°	6.23°	2.36°	9.68°	-
$\begin{bmatrix} \bar{1}01 \end{bmatrix}_\gamma - \begin{bmatrix} \bar{1}\bar{1}1 \end{bmatrix}_\alpha$	4.41°	3.61°	3.61°	3.62°	2.4°
$(111)_\gamma - (011)_\alpha$	9.12°	0.53°	0.53°	0.54°	0.3°

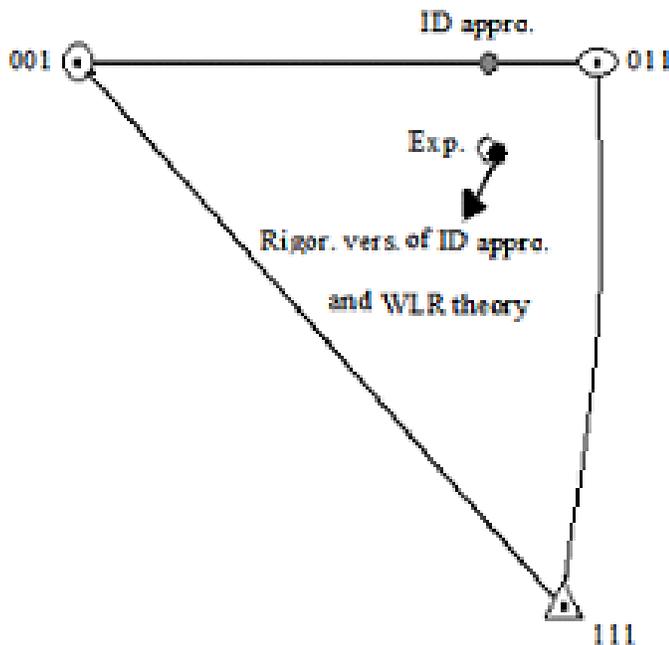


Figure 1. In unit stereographic triangle, theoretical and experimental habit plane determinations for Fe-31wt.% Ni alloy.

0.58033, 0.81438) (Dogan and Havvatoglu, 2003) while the habit plane obtained from Rigorous version of (ID)

approach associated with the martensite transformation is (0.185064, 0.594242, 0.782705) = (3 10 14)_γ. It is easily seen from the investigation of the results mentioned above that the difference between habit plane calculated in the ID approach and that obtained from the rigorous version of (ID) approach is about 0.18 radians or approximately 10.8° which is expected from the ID approach, because the habit plane derived from the ID approach and that from the phenomenological crystallographic theory at small principal transformation distortions are identical to each other (Kelly, 2006; Zhang and Kelly, 2009). It is also seen that the habit plane direction obtained from the rigorous version of (ID) departs from the normal for the observed habit plane (3 14 10)_γ (Dunne and Wayman, 1971; Nishiyama, 1978) only by 1.78°. In order to observe these differences among the reported habit planes more clearly for the transformation observed in Fe-31 wt% Ni alloy, we drew them together in a unit stereographic triangle, as shown in Figure 1.

In order for a suitable comparison of the orientation relationship, it is of interest to focus attention on the closed packed planes and directions in the two lattices which are nearly parallel that is, $\begin{bmatrix} \bar{1}01 \end{bmatrix}_\gamma \wedge \begin{bmatrix} \bar{1}\bar{1}1 \end{bmatrix}_\alpha$ and $(111)_\gamma \wedge (011)_\alpha$. For example, the orientation relationship for $(111)_\gamma$ and $(011)_\alpha$ planes between the result in

Table 2. A comparison of the numerical solutions of Rigorous version of ID approach and WLR theory, ID Approach with experimental results for fcc to bcc martensitic transformation observed in a zirconia alloy. For the ID approach and WLR Theory it can be referred to the references (Kato and Shibata-Yanagisawa, 1990) and (Nishiyama, 1978; Wayman, 1964), respectively.

Parameter	ID Approach	Rigorous version of ID Approach	ID Approach	WLR Theory
Habit plane, n	$\begin{bmatrix} 0.8247 \\ 0.5556 \\ 0 \end{bmatrix}$	$\begin{bmatrix} -0.82674 \\ -0.56264 \\ 0.011909 \end{bmatrix}$	$\begin{bmatrix} -0.826745064 \\ -0.01191 \\ 0.562465 \end{bmatrix}$	$\begin{bmatrix} 0.8267 \\ 0.5625 \\ -0.0118 \end{bmatrix}$
Volume fraction, f	0.4048	0.593178	0.406822	0.4068
Magnitude of total shape deformation, m_T	0.009752	0.009666	0.009716	0.009688
Orientation relationship				
$[100]_\gamma - [100]_\alpha$	0.261°	0.26°	0.26°	0.258°
$[010]_\gamma - [010]_\alpha$	0.617°	0.26°	0°	0.613°
$[001]_\gamma - [001]_\alpha$	0.599°	0.01°	0.26°	0.556°

the present study and that of the experimental result differs only by 0.24°. We thus found that the orientation relationship for $(111)_\gamma$ and $(011)_\alpha$ planes calculated from the rigorous version of ID approach well fits the results of WLR theory and experiment for the alloy Fe-31 wt% Ni. It is seen from Table 1 that this difference is about 9° when a calculation of orientation relationship associated with $(111)_\gamma$ and $(011)_\alpha$ planes is carried out for the work treated in the present study and the ID approach. On the other hand, as can be seen in Table 1, an excellent agreement for magnitude of total shape deformation, m_T , among the rigorous version of ID, WLR theory, ID approach and experiment is found.

Moreover, the crystallographic parameters in Tables 1 and 2 for zirconia were recalculated in order for a comparison between the two results from the point of view that the habit planes of the alloy Fe-31 wt% Ni and zirconia alloy have the small strains.

Before examining the features of the crystallographic analysis associated with the cubic (c) to tetragonal (t) transformation in zirconia alloys using the aforementioned theories, it is appropriate to give a brief information on this transformation. One of the zirconia alloys is ZrO₂-3 mol Y₂O₃ and occurring at high cooling rates in this arc-melted sample, the c-to-t transformation produces a marked surface relief at a free surface, consistent with the simple shear displacements (Srinivasan, 1989). Combined with the absence of detectable composition fluctuations in the transformed volume, this relief has been taken to indicate that the transition is displacive and diffusionless. The cubic-tetragonal displacive transformation in zirconia is a ferroelastic transition and the representative species is given by $m3mF4/mmm$. Their morphology contains

closely spaced twin platelets of certain crystallographic orientations. In most cases, more than one twin orientation, including sometimes the so-called herringbone structure, are present within a single grain. Some variants apparently intersect each other. The twins could come either from the c-to-t transformation itself, as incorporated in the so-called LIS operation during the transformation, or from the mechanical accommodation of the product t phase subsequent to the transformation. Indeed, from a phenomenological, crystallographic viewpoint, it can be readily predicted that the cubic-to-tetragonal transfor-

mation will most likely entail $\{011\}(0\bar{1}1)$ twinning systems in the microstructure to minimize the distortional energy (Kato and Shibata-Yanagisawa, 1990). Such an analysis has been performed by Kato and co-workers for zirconia systems, which explains the experimental observations very well.

Zirconia alloy have the following lattice parameters (Kato and Shibata-Yanagisawa, 1990): The lattice parameter of the cubic phase is $a_\gamma = 5.127 \text{ \AA}$ and the lattice parameter of the tetragonal phase are $a_\alpha = b_\alpha = 5.093 \text{ \AA}$ and $c_\alpha = 5.177 \text{ \AA}$. These give

$$\eta_1 = \eta_2 = \frac{a_\alpha}{a_\gamma} = 0.993368 \quad \text{and} \quad \eta_3 = \frac{c_\alpha}{a_\gamma} = 1.009752 \quad (14)$$

It is clearly seen from Table 2 that the differences associated with the crystallographic parameters, for example the habit plane direction, for the work treated in the present study and the ID approach are negligible. We find from the rigorous version of (ID) approach that the habit plane normal $(-0.82674, 0.562465, -0.01191)$ is in agreement with the habit plane normal $(-0.8247, 0.5656, 0) = (-3\ 2\ 0)$ which is calculated from the ID approach

(Kato and Shibata-Yanagisawa, 1990). This plane is of the form $\{hk0\}$. It can be inferred that the habit plane calculated in the alloy Fe-31 wt% Ni (Navruz and Durlu, 1999) shifts from $(14\ 10\ 3)_\gamma$ to $(230)_\gamma$ calculated in zirconia alloy. The angle between the planes $(14\ 10\ 3)_\gamma$ and $(230)_\gamma$ is about 11° and this is the remarkable difference in the martensite phase transformations in the alloy having large principal distortions such as Fe-31 wt% Ni alloy.

In summary, in the present study, taking into consideration some alloys having values of small and large principal distortions in Bain deformation matrix, the purpose of the present study is to provide simple solutions for some parameters associated with crystallography of martensite phase transformation observed in Fe-31 wt% Ni and zirconia alloys by using the rigorous version of (ID) approach, which depends on the Kell's mathematical approach. In addition, a realistic comparison between the rigorous version of (ID) approach, ID approach and experimental observations to the crystallography of martensite phase transformation from the point of view principal distortions is presented. Although the ID approach offers simple picture of the calculation model associated with crystallography of the martensite phase transformation, its predictions do not agree with the WLR theory in a number areas, especially such as habit plane, because it assumes the principal strains are infinitely small. Thus, for infinitely thin martensite plate it is obviously seen from the investigation treated in the present study that the ID approach can produce no more information than the prediction of WLR theory. Moreover, the results obtained from the Rigorous version of (ID) approach are in good accordance with those calculated from WLR theory as well as experimental observations.

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