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Infinitesimal deformation approach of the phenomenological crystallographic theory of martensitic transformations

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The infinitesimal-deformation approach has been used to reformulate the phenomenological crystallographic theory of martensitic transformations. Simple analytical solutions for the habit plane orientation, the direction and magnitude of the lattice invariant shear, the orientation relationship between parent and product phases, etc. were derived for the cubic to tetragonal transformation. The derived results were numerically compared with those obtained from the original phenomenological theory by taking the cubic to tetragonal transformation in a zirconia alloy as an example. The expected magnitude of the differences in solutions between the present and phenomenological crystallographic analyses was also discussed.

1. Introduction

The so-called phenomenological crystallographic theory of martensitic transformations, originally developed by Wechsler *et al.* [1] and by Bowles and Mackenzie [2], has been applied successfully to the discussion of the crystallography and morphology of various martensites and precipitates embedded in a parent phase. This theory is based on the invariant plane strain (IPS) criterion at the planar interface between parent and product phases. From a knowledge of the lattice deformation and lattice invariant deformation systems which operate during a transformation, such solutions as the habit plane orientation, the total shape deformation of the product phase and the orientation relationship between the parent and product phases can be obtained so as to satisfy the IPS condition.

Since the phenomenological theory employs the finite-deformation (FD) approach, however, numerical calculation on a computer is practically unavoidable to obtain solutions. Although such solutions as habit plane orientation and the amount of lattice invariant deformation can be written analytically when the phenomenological theory is applied to simple transformation systems, the solution for orientation relationship, for example, is very difficult to express analytically. The lack of analytical solutions often prevents us from finding and predicting the systematic dependence of solutions on input parameters.

Several researches [3–7] have shown, using the infinitesimal deformation (ID) approach, that when a product phase embedded in a parent phase has a planar interface between the two phases (called the "habit plane") and when the total transformation strain components in the plane of the interface are zero, the elastic strain energy associated with the transformation completely vanishes. Neglecting the interfacial energy, this condition is of course most favourable for the coexistence of the two phases. With the above physical background in mind, the previous investigators have derived the habit plane orientation and the magnitude of the lattice invariant deformation to satisfy the condition of the vanishing elastic strain energy.

Such a theory based on the ID approach is an approximation of the FD-based phenomenological crystallographic theory. The advantage of the ID-based theory is that all solutions can be expressed in simple and analytical forms. Therefore, numerical calculation on a computer is not needed. However, it must be admitted that the ID-based crystallographic theory so far formulated is still incomplete. For example, the theory lacks the solution for the orientation relationship between parent and product phases. This is probably because of the fact that the ID analysis usually employs symmetric strain tensors and discards the irrelevant rotation components of a deformation. However, the rotation component are in fact essential in describing the orientation relationships.

Therefore, in the present study, asymmetric distortion tensors, instead of symmetric strain tensors, will be employed in the ID analysis to completely formulate the phenomenological theory based on the ID theory. Moreover, the present analysis will also be applied to the cubic to tetragonal transformation in a zirconia alloy to discuss its implication and practical applicability.

2. Fundamental procedure for the analysis

Given a lattice correspondence between a parent phase (hereafter referred to as α phase) and a product phase (β phase) and the lattice parameters of the two

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phases, the distortion matrix to describe the lattice deformation $\boldsymbol{B}$ can be obtained. Appendix 1 shows the definition of the distortion components and matrices in the present study. With a proper orthonormal coordinate system, x_1^α–x_2^α–x_3^α, fixed to the α phase (the α system), $\boldsymbol{B}$ is most generally expressed as

$$\boldsymbol{B}^\alpha = \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix}_\alpha \quad (1)$$

The index α denotes the α coordinate system. Khachaturyan and Shatalov [3] and Mura *et al.* [4] have shown that if the components of a symmetric transformation strain tensor, say $\boldsymbol{F}(S)$, satisfy

$$F_{11}^n(S) = F_{22}^n(S) = F_{12}^n(S) = 0 \quad (2)$$

on a particular orthonormal x_1^n–x_2^n–x_3^n coordinate system (the n system, see Appendix 2), then the elastic strain energy associated with the formation of the plate-shaped β phase (embedded in the α phase) becomes zero when the x_3^n axis becomes perpendicular to the habit plane. In fact, Equation 2 constitutes the necessary condition for the IPS deformation, as will be discussed later.

In general, however, the symmetric strain components of $\boldsymbol{B}$ in Equation 1, $\boldsymbol{B}(S)$, do not satisfy the condition (Equation 2) for any choice of the n system. Therefore, an additional deformation (the lattice invariant deformation) must be introduced in the β phase. For the lattice invariant deformation system, a simple shear, either by slip or by twinning, on a particular plane along a particular direction is taken so as to meet the experimental observation.

Let the distortion tensor as a result of the combination of the lattice deformation and the lattice invariant shear (LIS) deformation be described as $\boldsymbol{F}$. Then, in order for the elastic strain energy to vanish, Equation 2 must be satisfied on a new n coordinate system. It should be noted that we have three unknown parameters to be solved; two angles to describe the direction of the habit plane normal, x_3^n, on the α coordinate system, and the amount of the LIS deformation. Since Equation 2 gives three simultaneous equations, the three unknown parameters and, thus, all the components of $\boldsymbol{F}$ can be obtained in principle.

Although the above derivation procedure assures that the habit plane is undistorted, it does not necessarily mean that the habit plane is unrotated. In other words, Equation 2 is only the necessary (but not sufficient) condition for the IPS deformation. This is because only the symmetric strain components of $\boldsymbol{F}$, $\boldsymbol{F}(S)$, has been dealt with in Equation 2. In order to make the habit plane invariant (undistorted and unrotated), let us introduce an antisymmetric rotation matrix $\boldsymbol{R}$ on the α system. According to Appendix 1, $\boldsymbol{R}$ can be written as

$$\boldsymbol{R}^\alpha = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix}_\alpha \quad (3)$$

where $\omega_i (i = 1, 2, 3)$ are unknown angles of rotation.

The total shape distortion $\boldsymbol{T}^\alpha$ on the α system is written as

$$\boldsymbol{T}^\alpha = \boldsymbol{F}^\alpha + \boldsymbol{R}^\alpha \quad (4)$$

In order for the habit plane to be invariant, any two non-parallel vectors, say $\boldsymbol{v}$(I) and $\boldsymbol{v}$(II), on the habit plane should remain unchanged before and after the transformation. In the present ID analysis, this condition can be written as

$$\boldsymbol{T}^\alpha \boldsymbol{v}^\alpha(i) = 0, \quad i = \text{I and II} \quad (5a)$$

or

$$\begin{pmatrix} T_{11} & T_{12} & T_{13} \\ T_{21} & T_{22} & T_{23} \\ T_{31} & T_{32} & T_{33} \end{pmatrix} \begin{bmatrix} v_1(i) \\ v_2(i) \\ v_3(i) \end{bmatrix}_\alpha = 0, \quad i = \text{I and II} \quad (5b)$$

Since $\boldsymbol{F}^\alpha$ is already known, the above equation determines all the components of $\boldsymbol{R}^\alpha$. Then, the orientation relationship is determined from the matrix $\boldsymbol{R}$. In the following, the above general analysis will be applied to the cubic to tetragonal transformation.

3. Cubic to tetragonal transformation

Many systems belong to this type of transformation such as fcc to bcc (bct) and fcc to fct martensitic transformations in metals and alloys, cubic to tetragonal transformation in zirconia, etc. The original phenomenological theories [1, 2] have been developed to discuss the crystallography of this type of transformation in iron alloys. As an example of the present analysis, we will hereafter focus on this cubic to tetragonal transformation.

Assuming the Bain correspondence or its equivalent between the parent (α) and product (β) crystal lattices, one of the three crystallographically equivalent lattice deformations corresponding to Equation 1 is expressed as

$$\boldsymbol{B}^\alpha = \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_1 & 0 \\ 0 & 0 & \varepsilon_2 \end{pmatrix}_\alpha \quad (6)$$

where ε_1 and ε_2, the principal lattice distortions, can be calculated from the lattice parameter values of the α and β phases and the α coordinate system is chosen as $x_1^\alpha \parallel [1\,0\,0]_\alpha$, $x_2^\alpha \parallel [0\,1\,0]_\alpha$ and $x_3^\alpha \parallel [0\,0\,1]_\alpha$. By following the original phenomenological theories [1, 2], the $(0\,1\,1)_\alpha\,[0\,\bar{1}\,1]_\alpha$ shear system will be chosen as the LIS system. This shear can occur either by slip or by twinning. These two cases will be considered separately.

3.1. Slip as LIS

With an orthonormal x_1^s ($\parallel [0\,1\,1]_\alpha$) – x_2^s ($\parallel [0\,\bar{1}\,1]_\alpha$) – x_3^s ($\parallel [1\,0\,0]_\alpha$) coordinate system (the s system), the $(0\,1\,1)_\alpha\,[0\,\bar{1}\,1]_\alpha$ slip deformation in the ID theory can be expressed as a simple shear of the form

$$\boldsymbol{P}^s = \begin{pmatrix} 0 & 0 & 0 \\ m & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}_s \quad (7)$$

where m is the unknown amount of the shear distortion. When $\boldsymbol{P}$ is viewed on the α coordinate system, the following equation can be obtained as a result of the transformation of the coordinate system

$$\boldsymbol{P}^{\alpha} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -m/2 & -m/2 \\ 0 & m/2 & m/2 \end{pmatrix}_{\alpha} \tag{8}$$

Therefore, the matrix $\boldsymbol{F}$ in the previous section becomes

$$\boldsymbol{F}^{\alpha} = \boldsymbol{B}^{\alpha} + \boldsymbol{P}^{\alpha} = \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_1 - m/2 & -m/2 \\ 0 & m/2 & \varepsilon_2 + m/2 \end{pmatrix}_{\alpha} \tag{9}$$

Using the direction cosines defined in Table AI in Appendix 2, the components of $\boldsymbol{F}^{n}$ viewed on the n coordinate system become from Equation A5

$$F_{ij}^{n} = \sum_{k=1}^{3} \sum_{l=1}^{3} a_{ki} a_{lj} F_{kl}^{\alpha} \tag{10}$$

Therefore, the explicit forms of Equation 2 can be obtained from Equations 9 and 10 and by taking the symmetric strain components of F_{ij}^{n}, i.e., $F_{ij}^{n}(S)$ as

$$\begin{aligned} F_{11}^{n}(S) &= \varepsilon_1 \cos^2\theta \cos^2\phi \\ &\quad + (\varepsilon_1 - m/2) \cos^2\theta \sin^2\phi \\ &\quad + (\varepsilon_2 + m/2) \sin^2\theta = 0 \\ F_{22}^{n}(S) &= \varepsilon_1 \sin^2\phi + (\varepsilon_1 - m/2) \cos^2\phi = 0 \\ F_{12}^{n}(S) &= -m \cos\theta \sin\phi \cos\phi/2 = 0 \end{aligned} \tag{11}$$

As mentioned in the previous section, Equations 11 constitute three simultaneous equations with three unknown parameters θ, ϕ and m. The orientation of the habit plane and the amount of LIS can thus be obtained. Solving Equations 11, we find that there are four sets of solutions, in agreement with the results of the phenomemological theory. However, because of the crystal symmetry, only two solutions (say, solutions I-1 and I-2) are crystallographically independent. They are listed in Table I. It can be seen that solutions I-1 and I-2 give the same combination of the habit plane indices. However, the amounts of LIS are different.

One may think that since the predicted habit plane orientations in Table I are of the form $\{h\,k\,0\}_{\alpha}$, there exists a degeneracy of two different variants, $\{h\,k\,l\}_{\alpha}$ and $\{h\,k\,\bar{l}\}_{\alpha}$, in the FD based analysis. However, this is not the case. The obtained four solutions (two independent ones are shown in Table I) in the ID analysis are actually of the forms $(h\,k\,0)_{\alpha}$, $(h\,0\,k)_{\alpha}$, $(\bar{h}\,k\,0)_{\alpha}$ and $(\bar{h}\,0\,k)_{\alpha}$ and they exactly correspond to the four FD solutions, $(h\,k\,l)_{\alpha}$, $(h\,l\,k)_{\alpha}$, $(\bar{h}\,k\,l)_{\alpha}$ and $(\bar{h}\,l\,k)_{\alpha}$, respectively.

To obtain the orientation relationship, let us consider solution I-1 as an example. Since $m = -2\varepsilon_2$, Equation 9 becomes

$$\boldsymbol{F}^{\alpha} = \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_1 + \varepsilon_2 & \varepsilon_2 \\ 0 & -\varepsilon_2 & 0 \end{pmatrix}_{\alpha} \tag{12}$$

Substituting Equations 3 and 12 into Equation 4, we have

$$\boldsymbol{T}^{\alpha} = \begin{pmatrix} \varepsilon_1 & -\omega_3 & \omega_2 \\ \omega_3 & \varepsilon_1 + \varepsilon_2 & \varepsilon_2 - \omega_1 \\ -\omega_2 & -\varepsilon_2 + \omega_1 & 0 \end{pmatrix}_{\alpha} \tag{13}$$

TABLE I Analytical solutions for various crystallographic parameters resulted from the application of the present ID approach to the cubic to tetragonal transformation with the $(0\,0\,1)_{\alpha}[0\,\bar{1}\,1]_{\alpha}$ slip system as the LIS system

Solution	I-1	I-2
Habit plane	$((-\varepsilon_1/\varepsilon_2)^{1/2}, [(\varepsilon_1 + \varepsilon_2)/\varepsilon_2]^{1/2}, 0)_{\alpha}$	$((-\varepsilon_1/\varepsilon_2)^{1/2}, 0, [(\varepsilon_1 + \varepsilon_2)/\varepsilon_2]^{1/2})_{\alpha}$
Amount of LIS, m	$-2\varepsilon_2$	$2\varepsilon_1$
Total shape deformation		
$\boldsymbol{T}^{n}$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -2\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} \\ 0 & 0 & 2\varepsilon_1 + \varepsilon_2 \end{pmatrix}_{n}$	$\begin{pmatrix} 0 & 0 & 2\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} \\ 0 & 0 & 0 \\ 0 & 0 & 2\varepsilon_1 + \varepsilon_2 \end{pmatrix}_{n}$
Direction	$[-(-\varepsilon_1/\varepsilon_2)^{1/2}, [-\varepsilon_1 + \varepsilon_2)/\varepsilon_2]^{1/2}, 0]_{\alpha}$	$[-(-\varepsilon_1/\varepsilon_2)^{1/2}, 0, [(\varepsilon_1 + \varepsilon_2)/\varepsilon_2]^{1/2}]_{\alpha}$
Magnitude	$\lvert\varepsilon_2\rvert$	$\lvert\varepsilon_2\rvert$
Orientation relationship		
$\boldsymbol{R}^{\alpha}$	$\begin{pmatrix} 0 & \varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & 0 \\ -\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & 0 & -\varepsilon_2 \\ 0 & \varepsilon_2 & 0 \end{pmatrix}_{\alpha}$	$\begin{pmatrix} 0 & 0 & \varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} \\ 0 & 0 & \varepsilon_1 \\ -\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & -\varepsilon_1 & 0 \end{pmatrix}_{\alpha}$
Tilt angles $[1\,0\,0]_{\alpha}$	$[-\varepsilon_1(\varepsilon_1 + \varepsilon_2)]^{1/2}$	$[-\varepsilon_1(\varepsilon_1 + \varepsilon_2)]^{1/2}$
$[0\,1\,0]_{\alpha}$	$[-\varepsilon_1(\varepsilon_1 + \varepsilon_2) + \varepsilon_2^2]^{1/2}$	$\lvert\varepsilon_1\rvert$
$[0\,0\,1]_{\alpha}$	$\lvert\varepsilon_2\rvert$	$(-\varepsilon_1\varepsilon_2)^{1/2}$

From the solution of the habit plane orientation for solution I-1, two non-parallel vectors on the habit plane can be chosen as

$$\begin{aligned} \boldsymbol{v}^{\alpha}(\mathrm{I}) &= [0, 0, 1]_{\alpha} \\ \boldsymbol{v}^{\alpha}(\mathrm{II}) &= [-[(\varepsilon_1 + \varepsilon_2)/\varepsilon_2]^{1/2}, (-\varepsilon_1/\varepsilon_2)^{1/2}, 0]_{\alpha} \end{aligned} \tag{14}$$

From Equations 13, 14 and 5, the components of $\boldsymbol{R}^{\alpha}$ can be obtained in terms of ε_1 and ε_2 as

$$\boldsymbol{R}^{\alpha} = \begin{pmatrix} 0 & \varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & 0 \\ -\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & 0 & -\varepsilon_2 \\ 0 & \varepsilon_2 & 0 \end{pmatrix}_{\alpha} \tag{15}$$

This rotation matrix describes the orientation relationship between the α and β phases and is listed in Table I. It is found from Appendix 1 that the β phase is rotated with respect to the α phase by an angle $\omega_3 = -\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2}$ about the x_3^{α} ($[0\,0\,1]_{\alpha}$) axis and by $\omega_1 = \varepsilon_2$ about the x_1^{α} ($[1\,0\,0]_{\alpha}$) axis. In Table I, the magnitudes of the tilt angles of the principal axes of the α phase as a result of the above rotation are also indicated.

Substituting Equation 15 into Equation 13, the complete information of the total shape deformation $\boldsymbol{T}$ is obtained. When $\boldsymbol{T}$ is viewed on the n coordinate system, from Equation A5 and from the already known direction cosines a_{ij} listed in Table A1, we have

$$\boldsymbol{T}^{n} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -2\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} \\ 0 & 0 & 2\varepsilon_1 + \varepsilon_2 \end{pmatrix}_{n} \tag{16}$$

as shown in Table I. Therefore, the total shape deformation consists of the shear component $T_{23}^{n} = -2\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2}$ on the habit plane along the x_2^{n} ($[-[(\varepsilon_1 + \varepsilon_2)/\varepsilon_2]^{1/2}, (-\varepsilon_1/\varepsilon_2)^{1/2}, 0]_{\alpha}$) direction and the dilational component $T_{33}^{n} = 2\varepsilon_1 + \varepsilon_2$ normal to the habit plane. The magnitude of the total shape deformation is found to be $|\varepsilon_2|$ from $[(T_{23}^{n})^2 + (T_{33}^{n})^2]^{1/2}$ and its direction can be obtained on the α system by the transformation of the coordinate system as shown in Table I. Exactly the same procedure can be repeated to obtain a set of solutions I-2.

3.2. Twinning as LIS

Here, we consider the $(0\,1\,1)_{\alpha}[0\,\bar{1}\,1]_{\alpha}$ twinning shear as the LIS system. As shown in Fig. 1, this twinning can be incorporated in the theory by considering two different (though crystallographically equivalent) lattice deformations, i.e.,

$$\boldsymbol{B}_1^{\alpha} = \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_1 & 0 \\ 0 & 0 & \varepsilon_2 \end{pmatrix}_{\alpha} \quad \boldsymbol{B}_2^{\alpha} = \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_2 & 0 \\ 0 & 0 & \varepsilon_1 \end{pmatrix}_{\alpha} \tag{17}$$

As shown in Fig. 1c, in order for the β-phase to be internally twinned, the β-phase crystal subjected to the lattice deformation $\boldsymbol{B}_1$ (say, crystal 1) must be rotated relative to the β-phase crystal subjected to the lattice deformation $\boldsymbol{B}_2$ (crystal 2) by the angle Φ shown in the figure. From simple geometry, the rotation matrix $\boldsymbol{\Phi}$ of crystal 1 can be found and it is expressed within the framework of the ID theory as

$$\boldsymbol{\Phi}^{\alpha} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\varepsilon_2 + \varepsilon_1 \\ 0 & \varepsilon_2 - \varepsilon_1 & 0 \end{pmatrix}_{\alpha} \tag{18}$$

When the volume fraction of crystal 1 in the twinned β-phase is denoted as f, the total shape deformation $\boldsymbol{T}$ can now be written as

$$\boldsymbol{T} = \boldsymbol{R} + f(\boldsymbol{\Phi} + \boldsymbol{B}_1) + (1 - f)\boldsymbol{B}_2 \tag{19}$$

where $\boldsymbol{R}$ is a rotation matrix to be determined. Similar to the previous case, we define $\boldsymbol{F}$ as

$$\boldsymbol{F} = f(\boldsymbol{\Phi} + \boldsymbol{B}_1) + (1 - f)\boldsymbol{B}_2 \tag{20}$$

From Equations 17 and 18, $\boldsymbol{F}$ is expressed on the α

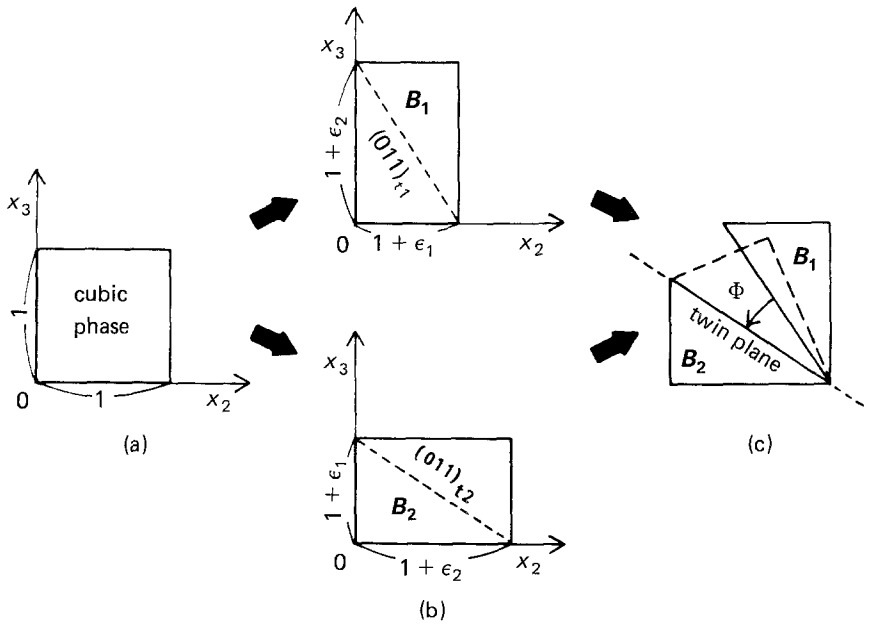

Figure 1 Schematic illustration showing how the $(0\,1\,1)_t[0\,\bar{1}\,1]_t$ (derived from $(0\,1\,1)_c[0\,\bar{1}\,1]_c$) twinning deformation in the product t phase can be incorporated in the present analysis as a result of the combination of two t crystals subjected to different lattice deformations $\boldsymbol{B}_1$ and $\boldsymbol{B}_2$. Note that the rotation of crystal 1 (with $\boldsymbol{B}_1$) by an angle Φ makes this crystal twin related to crystal 2 (with $\boldsymbol{B}_2$).

coordinate system;

$$\boldsymbol{F}^{\alpha} = \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_2 - f(\varepsilon_2 - \varepsilon_1) & -f(\varepsilon_2 - \varepsilon_1) \\ 0 & f(\varepsilon_2 - \varepsilon_1) & \varepsilon_1 + f(\varepsilon_2 - \varepsilon_1) \end{pmatrix}_{\alpha} \tag{21}$$

This matrix with the unknown parameter f for the twinned β-phase corresponds to the matrix (Equation 9) with the unknown parameter m for the slipped β-phase.

We can repeat almost the same procedure as in Section 3.1 to derive f and the habit plane orientation and the results are shown in Table II for the obtained two independent solutions (solutions II-1 and II-2). It is encouraging to find from Tables I and II that the resultant habit plane orientations are exactly the same as those for the slipped β-phase (solutions I-1 and I-2), in agreement with the results in the phenomenological theories [1, 2].

The orientation relationships between the α and β phases can also be derived in a similar manner as in Section 3.1. For the case of solution II-1, for example, $\boldsymbol{R}$ in Equation 19 becomes

$$\boldsymbol{R}^{\alpha} = \begin{pmatrix} 0 & \varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & 0 \\ -\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & 0 & -\varepsilon_1 \\ 0 & \varepsilon_1 & 0 \end{pmatrix}_{\alpha} \tag{22}$$

For the cubic to tetragonal transformation, neither $\boldsymbol{B}_1$ nor $\boldsymbol{B}_2$ rotates the crystal. Therefore, the above $\boldsymbol{R}^{\alpha}$ describes the rotation of crystal 2. On the other hand, in addition to $\boldsymbol{R}^{\alpha}$, the rotation $\boldsymbol{\Phi}^{\alpha}$ in Equation 18 must also be taken into account for the rotation of crystal 1

$$\boldsymbol{R}^{\alpha} + \boldsymbol{\Phi}^{\alpha} = \begin{pmatrix} 0 & \varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & 0 \\ -\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & 0 & -\varepsilon_2 \\ 0 & \varepsilon_2 & 0 \end{pmatrix}_{\alpha} \tag{23}$$

This rotation of crystal 1 is again found to be exactly the same as that for solution I-1 in the previous section. The above orientation relationships are shown in

TABLE II Analytical solutions for various crystallographic parameters resulted from the application of the present ID approach to the cubic to tetragonal transformation with the $(0\,1\,1)_{\alpha}[0\,\bar{1}\,1]_{\alpha}$ twinning system as the LIS system

Solution	II-1	II-2
Habit plane	$((-\varepsilon_1/\varepsilon_2)^{1/2}, [(\varepsilon_1 + \varepsilon_2)/\varepsilon_2]^{1/2}, 0)_{\alpha}$	$((-\varepsilon_1/\varepsilon_2)^{1/2}, 0, [(\varepsilon_1 + \varepsilon_2)/\varepsilon_2]^{1/2})_{\alpha}$
Volume fraction of crystal 1, f	$\varepsilon_1/(\varepsilon_1 - \varepsilon_2)$	$\varepsilon_2/(\varepsilon_2 - \varepsilon_1)$
Total shape deformation		
$\boldsymbol{T}^{n}$	$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -2\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} \\ 0 & 0 & 2\varepsilon_1 + \varepsilon_2 \end{pmatrix}_{n}$	$\begin{pmatrix} 0 & 0 & 2\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} \\ 0 & 0 & 0 \\ 0 & 0 & 2\varepsilon_1 + \varepsilon_2 \end{pmatrix}_{n}$
Direction	$[-(-\varepsilon_1/\varepsilon_2)^{1/2}, [(\varepsilon_1 + \varepsilon_2)/\varepsilon_2]^{1/2}, 0]_{\alpha}$	$[-(-\varepsilon_1/\varepsilon_2)^{1/2}, 0, [(\varepsilon_1 + \varepsilon_2)/\varepsilon_2]^{1/2}]_{\alpha}$
Magnitude	$\lvert\varepsilon_2\rvert$	$\lvert\varepsilon_2\rvert$
Orientation relationship		
Crystal 1		
$\boldsymbol{R}^{\alpha} + \boldsymbol{\Phi}^{\alpha}$	$\begin{pmatrix} 0 & \varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & 0 \\ -\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & 0 & -\varepsilon_2 \\ 0 & \varepsilon_2 & 0 \end{pmatrix}_{\alpha}$	$\begin{pmatrix} 0 & 0 & \varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} \\ 0 & 0 & \varepsilon_1 \\ -\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & -\varepsilon_1 & 0 \end{pmatrix}_{\alpha}$
Tilt angles $[1\,0\,0]_{\alpha}$	$[-\varepsilon_1(\varepsilon_1 + \varepsilon_2)]^{1/2}$	$[-\varepsilon_1(\varepsilon_1 + \varepsilon_2)]^{1/2}$
$[0\,1\,0]_{\alpha}$	$[-\varepsilon_1(\varepsilon_1 + \varepsilon_2) + \varepsilon_2^2]^{1/2}$	$\lvert\varepsilon_1\rvert$
$[0\,0\,1]_{\alpha}$	$\lvert\varepsilon_2\rvert$	$(-\varepsilon_1\varepsilon_2)^{1/2}$
Crystal 2		
$\boldsymbol{R}^{\alpha}$	$\begin{pmatrix} 0 & \varepsilon_1[-\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & 0 \\ -\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & 0 & -\varepsilon_1 \\ 0 & \varepsilon_1 & 0 \end{pmatrix}_{\alpha}$	$\begin{pmatrix} 0 & 0 & \varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} \\ 0 & 0 & \varepsilon_2 \\ -\varepsilon_1[-(\varepsilon_1 + \varepsilon_2)/\varepsilon_1]^{1/2} & -\varepsilon_2 & 0 \end{pmatrix}_{\alpha}$
Tilt angles $[1\,0\,0]_{\alpha}$	$[-\varepsilon_1(\varepsilon_1 + \varepsilon_2)]^{1/2}$	$[-\varepsilon_1(\varepsilon_1 + \varepsilon_2)]^{1/2}$
$[0\,1\,0]_{\alpha}$	$(-\varepsilon_1\varepsilon_2)^{1/2}$	$\lvert\varepsilon_2\rvert$
$[0\,0\,1]_{\alpha}$	$\lvert\varepsilon_1\rvert$	$[-\varepsilon_1(\varepsilon_1 + \varepsilon_2) + \varepsilon_2^2]^{1/2}$

Table II together with the tilt angles of the principal axes.

4. Application of the analysis

The present authors and their colleagues have analysed the crystallography associated with the cubic (c) to tetragonal (t) transformation in zirconia alloys using the Wechsler–Lieberman–Read phenomenological crystallographic theory based on the FD analysis [8]. The results obtained in their study are very suitable for comparison with the results of the present ID analysis. Since the internally twinned t phase on the $(0\,1\,1)_t$ twinning plane derived from the $(0\,1\,1)_c$ plane was considered in the previous study [8], the direct comparison with the present analysis, Section 3.2, is possible.

As an example, let us use Data I shown in Table I of the previous study [8]. The lattice parameter of the c phase is $a_c = 0.5127\,\text{nm}$ and the lattice parameters of the t phase are $a_t = b_t = 0.5093\,\text{nm}$ and $c_t = 0.5177\,\text{nm}$. These give

$$\varepsilon_1 = (a_t/a_c) - 1 = -0.006\,632$$

and

$$\varepsilon_2 = (c_t/a_c) - 1 = 0.009\,752 \qquad (24)$$

Simply substituting these ε_1 and ε_2 values into the expressions for solutions in Table II, we obtain numerical values for various crystallographic parameters. Using solution II-1 as an example, the results are shown in Table III under the column "ID". The solutions from the previous more involved FD analysis, some of which were obtained by a computer, are also listed under the column "FD". The comparison between the two corresponding results readily indicates that the differences are very small. Such differences are immaterial when the calculated results are compared with experimentally observed ones. To help readers find the present results visually, Fig. 2 is also provided. This figure should be compared with Fig. 1 of reference [8] to see the excellent agreement.

5. Discussion

As we have seen, the present ID theory results in very simple analytical solutions for the crystallography and morphology of a transformation product phase. This is a great advantage of the ID analysis since the dependence of the solutions on input data can be found analytically without conducting computer calculations. Moreover, since the ID theory assumes that absolute magnitude of each distortion component is much smaller than unity, the successive occurrence of deformations can be expressed just by the superposition or addition of distortion matrices with no need to pay attention to the order of occurrence of the deformations. This is another advantage of the ID analysis. In the FD analysis, on the other hand, the combination of deformations is expressed by the multiplication of deformation matrices. Since the multiplication of matrices is in general not commutable, the combination of deformations is affected by the order of the occurrence of the deformations.

It is of course true that the ID analysis is the approximation of the more rigorous FD analysis. Then, how large are the differences in the results from the two analyses? Let use define Δ ($\Delta > 0$) as the order of magnitude of the lattice distortion components (such as ε_1 and ε_2) in the ID theory. The superposition of deformations is possible in the ID theory since this theory neglects the second- and higher-order terms of Δ. Therefore, the relative differences in solutions between the ID and FD analyses should be in the order of Δ. Referring to the analytical results in Tables I and II, we find that the components of the habit plane indices (such as $(-\varepsilon_1/\varepsilon_2)^{1/2}$ and $[(\varepsilon_1 + \varepsilon_2)/\varepsilon_2]^{1/2}$ are described by the zeroth order of Δ. Therefore, the absolute differences are in the order of Δ. In other words, the habit plane orientation calculated from the ID theory may differ from the corresponding result of the FD theory by about Δ radian or $180\Delta/\pi$ degrees. For the case of the c → t transformation in zirconia alloys, Δ is in the order of 10^{-2}. Therefore, the difference should be less than 1°, which compares favourably

TABLE III Comparison of the numerical solutions between the present (ID) approach and the usual (FD) approach based on the phenomenological crystallographic theory. As an example, the cubic (c) to tetragonal (t) transformation in a zirconia alloy was used with $\varepsilon_1 = -0.006\,632$ and $\varepsilon_2 = 0.009\,752$. Refer to reference [8] for the FD analysis

	ID	FD
Habit plane	$(0.8247, 0.5656, 0)_c$	$(0.8267, 0.5625, -0.0118)_c$
f	0.4048	0.4068
Total shape deformation		
direction	$[-0.8247, 0.5656, 0]_c$	$[-0.8293, 0.5587, -0.0119]_c$
magnitude	0.009 752	0.009 688
Orientation relationship		
Crystal 1 (t1)		
$[1\,0\,0]_c \Lambda [1\,0\,0]_{t1}$	0.261°	0.258°
$[0\,1\,0]_c \Lambda [0\,1\,0]_{t1}$	0.617°	0.613°
$[0\,0\,1]_c \Lambda [0\,0\,1]_{t1}$	0.559°	0.556°
Crystal 2 (t2)		
$[1\,0\,0]_c \Lambda [0\,1\,0]_{t2}$	0.261°	0.258°
$[0\,1\,0]_c \Lambda [0\,0\,1]_{t2}$	0.461°	0.460°
$[0\,0\,1]_c \Lambda [1\,0\,0]_{t2}$	0.380°	0.381°

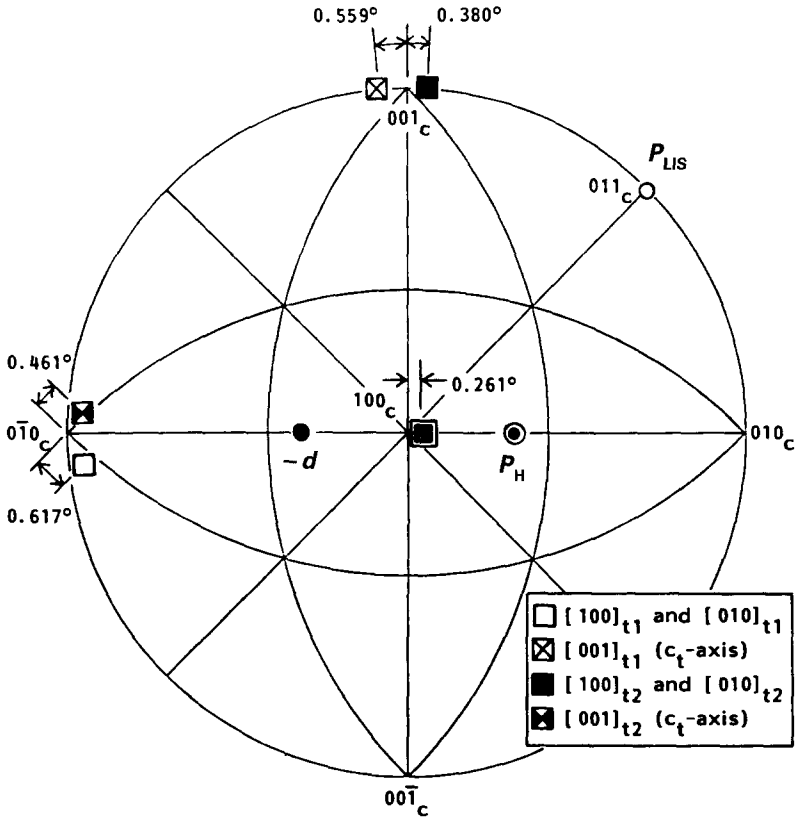

Figure 2 $(1\,0\,0)_c$ stereographic projection showing the calculated habit plane normal ($\boldsymbol{P}_H$), the direction of the total shape deformation ($\boldsymbol{d}$) and the orientation relationships between the c phase and the two twin-related t phase(t_1 and t_2) of a zirconia alloy with $\varepsilon_1 = -0.006\,632$ and $\varepsilon_2 = 0.009\,752$. $\boldsymbol{P}_{LIS}$ indicates the twin plane normal.

with the results in Table II showing the difference of 0.7°.

Similarly, we find that the absolute difference in f is also in the order of Δ since f is expressed in the zeroth order of Δ. However m, the amount of slip, and the rotation angles to describe orientation relationships are expressed in the first order of Δ, as shown in Tables I and II. Therefore, the absolute differences in the numerical values for these parameters are expected to be in the order of Δ^2. The results in Table III correctly indicate that this is the case.

As shown above, the small $\Delta(\sim 10^{-2})$ for the c → t transformation in zirconia alloys naturally resulted in the close agreement in solutions between the ID and FD analyses. For the case of the fcc to bcc (bct) transformation in steels, on the other hand, Δ is in the order of 10^{-1}. In such a case, the above discussion indicates that the ID-based solution for habit plane orientation may differ as much as 10^{-1} radian or about 10° from the corresponding exact FD-based solution. Therefore, the ID solutions may lose their applicability when they are compared with experimental observation.

Nevertheless, compared with 4π steradian of the three-dimensional space, the difference of Δ radian is still small. Moreover, the ID-based analysis certainly gives a handy tool to understand the origin and the meaning of calculated solutions in the FD-based phenomenological theory. For example, it is known from Table I that the magnitude of the total shape deformation is $|\varepsilon_2|$. This means that it should not be very sensitively dependent on the value of ε_1 even when the FD-based analysis is conducted. Such an example can be found in many other crystallographic parameters, as listed in Tables I and II.

The cubic to tetragonal transformation analysed in the present study is one of the simplest transformations to be treated mathematically because of its high crystal symmetry. When a transformation involves phases with lower crystal symmetry, such as the tetragonal to monoclinic transformation in zirconia alloys, the actual calculation to obtain analytical solutions may become rather complicated. In such a case, it is often more convenient to use the condition $|\boldsymbol{F}^{\alpha}(s)| = 0$, as discussed in Appendix 3. From this condition, the amount of slip, m, or the volume fraction of one of the two twin-related crystals, f, can be obtained directly, Then, using two of the three simultaneous Equations 2, θ and ϕ can be obtained easily. The application of the present theory to such cases is currently under progress.

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Appendix 1

Consider a right-handed x_1–x_2–x_3 orthonormal coordinate system fixed to the physical space. When a point in a body whose position vector is originally $\boldsymbol{x} = [x_1, x_2, x_3]$ is displaced by $\boldsymbol{u} = [u_1, u_2, u_3]$ by a deformation, the displacement $\boldsymbol{u} + d\boldsymbol{u} = [u_1 + du_1, u_2 + du_2, u_3 + du_3]$ of an adjacent point $\boldsymbol{x} + d\boldsymbol{x} = [x_1 + dx_1, x_2 + dx_2, x_3 + dx_3]$ is written as

$$du_i = \sum_{k=1}^{3} \frac{\partial u_i}{\partial x_k} dx_k \qquad \text{(A1)}$$

or in a matrix form

$$d\boldsymbol{u} = \boldsymbol{D} \cdot d\boldsymbol{x}$$

TABLE AI The direction cosines a_{ij} relating the α system (fixed to the principal axes of the parent α phase) to the n system (with the x_3^n axis being perpendicular to the habit plane)

α	n		
	x_1^n	x_2^n	x_3^n
$x_1 \parallel [1\,0\,0]_\alpha$	$\cos\theta\cos\phi$ (a_{11})	$-\sin\phi$ (a_{12})	$\sin\theta\cos\phi$ (a_{13})
$x_2 \parallel [0\,1\,0]_\alpha$	$\cos\theta\sin\phi$ (a_{21})	$\cos\phi$ (a_{22})	$\sin\theta\sin\phi$ (a_{23})
$x_3 \parallel [0\,0\,1]_\alpha$	$-\sin\theta$ (a_{31})	0 (a_{32})	$\cos\theta$ (a_{33})

i.e.

$$\begin{bmatrix} du_1 \\ du_2 \\ du_3 \end{bmatrix} = \begin{pmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{pmatrix} \begin{bmatrix} dx_1 \\ dx_2 \\ dx_3 \end{bmatrix} \quad \text{(A2)}$$

where $D_{ij} = \partial u_i/\partial x_j$ are the components of the *distortion tensor* in the ID analysis. If $d\boldsymbol{u} = 0$ regardless of the choice of $d\boldsymbol{x}$, then the part of the body around $\boldsymbol{x}$ exhibits no deformation, i.e., all the components of $\boldsymbol{D}$ are zero.

The distortion tensor $\boldsymbol{D}$ can always be decomposed into symmetric $[\boldsymbol{D}(S)]$ and antisymmetric $[\boldsymbol{D}(A)]$ parts

$$\boldsymbol{D} = \boldsymbol{D}(S) + \boldsymbol{D}(A) \quad \text{(A3)}$$

In the present ID analysis, $D_{ij}(S) = D_{ji}(S) = (\partial u_i/\partial x_j + \partial u_j/\partial x_i)/2$ are called the symmetric *strain* components and $D_{ij}(A) = -D_{ji}(A) = (\partial u_i/\partial x_j - \partial u_j/\partial x_i)/2$ are called the antisymmetric *rotation* components. By defining $\omega_i = -(1/2)\sum_{i=1}^{3}\sum_{k=1}^{3}\varepsilon_{ijk}D_{jk}$ where ε_{ijk} is the permutation tensor ($\varepsilon_{123} = \varepsilon_{231} = \varepsilon_{312} = 1$, $\varepsilon_{132} = \varepsilon_{321} = \varepsilon_{213} = -1$ and other ε_{ijk} are zero), the general form of $\boldsymbol{D}(A)$ is written as

$$\boldsymbol{D}(A) = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix} \quad \text{(A4)}$$

It can be easily seen that the positive values of ω_1, ω_2 and ω_3 express the angles of rotation of the right-handed screw advancing along the positive x_1, x_2 and x_3 directions, respectively. In the ID analysis, the absolute values of all the components D_{ij} are treated as if they are infinitesimally small compared with unity.

Appendix 2

The α coordinate system fixed to the parent α phase and the n coordinate system whose x_3^n axis is perpendicular to the habit plane can be related to each other by the direction cosines a_{ij} defined in Table AI with two angles θ and ϕ. (The mutally perpendicular x_1^n and x_2^n axes can be chosen arbitrarily so that both of them are perpendicular to the x_3^n axis.) Let an arbitrary distortion matrix $\boldsymbol{A}$ be $\boldsymbol{A}^\alpha$ on the α coordinate system and $\boldsymbol{A}^n$ on the n coordinate system. Then, $\boldsymbol{A}^\alpha$ and $\boldsymbol{A}^n$ are related to each other by the following well known transformation of tensor components

$$A_{ij}^n = \sum_{k=1}^{3}\sum_{l=1}^{3} a_{ki}a_{lj}A_{kl}^\alpha \quad \text{(A5)}$$

or conversely,

$$A_{ij}^\alpha = \sum_{k=1}^{3}\sum_{l=1}^{3} a_{ik}a_{jl}A_{kl}^n \quad \text{(A6)}$$

Appendix 3

When the components of a 3 × 3 symmetric strain matrix $\boldsymbol{F}(S)$ satisfy Equation 2 on the n coordinate system, this matrix can be expressed as

$$\boldsymbol{F}^n(S) = \begin{pmatrix} 0 & 0 & c \\ 0 & 0 & b \\ c & b & a \end{pmatrix}_n \quad \text{(A7)}$$

where a, b and c are not necessarily zero. It is clear from the above expression that the determinant of $\boldsymbol{F}^n(S)$, $|\boldsymbol{F}^n(S)|$, is zero. However, since a determinant is an invariant quantity, in order for Equation 2 to be satisfied, $|\boldsymbol{F}(S)| = 0$ must always be satisfied regardless of the choice of the coordinate system. Therefore, choosing the α coordinate system, m or f in the text can be calculated from $|\boldsymbol{F}^\alpha(S)| = 0$. In other words, $|\boldsymbol{F}(S)| = 0$ constitutes one of the necessary conditions for the IPS deformation. Since $|\boldsymbol{F}(S)| = 0$ is the natural result derived from Equation 2, this condition and the three simultaneous Equations 2 are not independent of each other.

To clarify further the implication of Equation A7, let us calculate the principal distortions of $\boldsymbol{F}(S)$. Solving the secular Equation A7, i.e.,

$$\begin{vmatrix} -\lambda & 0 & c \\ 0 & -\lambda & b \\ c & b & a-\lambda \end{vmatrix} = 0 \quad \text{(A8)}$$

we obtain three principal strains as the solutions for λ

$$\lambda = 0, \quad \frac{a \pm [a^2 + 4(b^2 + c^2)]^{1/2}}{2} \quad \text{(A9)}$$

The case for $b = c = 0$ is not of interest to us since only dilatational strain, a, occurs along one direction and a plane perpendicular to it is an invariant plane. Other than the above case, we note that

$$\left(\frac{a + [a^2 + 4(b^2 + c^2)]^{1/2}}{2}\right)\left(\frac{a - [a^2 + 4(b^2 + c^2)]^{1/2}}{2}\right) < 0$$

This, together with Equation A9, indicates that the necessary condition for the realization of the IPS deformation in the ID theory is equivalent to the condition that one of the three principal strains for the symmetric strain matrix $\boldsymbol{F}(S)$ is zero and the signs of the other two principal strains are different. In the present example of the cubic to tetragonal transformation, it can be seen from Equation 12 that the three principal strains are 0, ε_1 and $\varepsilon_1 + \varepsilon_2$. Therefore, in order for the IPS condition to be realized, $\varepsilon_1(\varepsilon_1 + \varepsilon_2)$ must be negative. In this way, it is very easy to examine whether a given lattice distortion matrix $\boldsymbol{B}$ can result in the IPS deformation.

In the FD theory, it has been shown [1, 9] that the necessary condition for the invariant plane deformation is that one of the three principal distortions must be

unity and the other two be, respectively, greater and less than unity. Therefore, the exact correspondence between the ID and FD theories can also be found in the condition for the invariant-plane deformation.

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