Crystallographic Analysis of Cubic (Tetragonal) to Monoclinic Martensitic Transformations based on the Infinitesimal Deformation Approach

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The infinitesimal-deformation approach was applied to analyze the crystallography involved in cubic (tetragonal) to monoclinic martensitic transformations. Using the same basic concepts as in the finite-deformation-based phenomenological crystallographic theories of martensitic transformations, crystallographic solutions for habit plane orientation, orientation relationships between parent and martensite phases, etc. were obtained in a simple and analytical manner. The derived solutions were numerically compared with those obtained from the phenomenological analysis and excellent agreement between the two solutions was found.

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I. Introduction

The interpretation of the phenomenological crystallographic theories of martensitic transformations⁽¹⁾⁽²⁾ in terms of the infinitesimal-deformation (ID) theory of elasticity has been performed by Khachaturyan and Shatalov⁽³⁾ and by Mura *et al.*⁽⁴⁾ It has been pointed out that when a transformed product phase is embedded in a parent phase, the condition of invariant-plane deformation in the phenomenological theories is equivalent to the condition of vanishing elastic strain energy associated with the transformation. Such solutions in the phenomenological theories as habit plane orientation and the amount of lattice-invariant shear deformation have also been obtained by applying the ID approach to cubic to tetragonal transformations⁽³⁾⁻⁽⁷⁾.

The above studies based on the ID approach considered only the symmetric strain components of deformation matrices. This is because antisymmetric rotation components do not contribute to the creation of elastic strain fields. However, in order to obtain solutions such as orientation relationships between parent and product phases and the direction of the total shape deformation, the rotation components cannot be discarded. Recently, the present authors adopted the ID approach taking into account both the symmetric strain components and the antisymmetric rotation components of deformation⁽⁸⁾. Thereby, complete sets of analytical solutions, which correspond exactly to the solutions of the phenomenological theories, have been successfully derived for cubic to tetragonal phase transformations.

The solutions obtained from the ID approach are of course the approximated ones of the phenomenological

theories which are based on the finite-deformation (FD) approach. However, the ID-based analytical solutions are not only much simpler than the FD-based solutions but also often accurate enough for tenable comparison with experimental observations⁽⁸⁾⁽⁹⁾.

As an extension of the previous study⁽⁸⁾, the present study based on the ID approach will analyze more complex crystallography involved in cubic (tetragonal) to monoclinic transformations. Some phase transformations belonging to this category have already been crystallographically analyzed using the FD-based phenomenological theories⁽¹⁰⁾⁻⁽¹⁴⁾. In these studies, solutions were numerically obtained by a computer. On the other hand, computer calculation is not involved in the present analysis and yet, as will be shown later, the derived analytical solutions are very close to those numerically calculated.

II. Formulation of the ID Analysis

On an $x_1-x_2-x_3$ orthonormal coordinate system, a matrix D to describe a three-dimensional deformation in the ID approach is written in a general form as

$$D = \begin{pmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{pmatrix}, \quad (1)$$

where D_{ij} is a distortion component on a plane perpendicular to the x_j axis (the x_j plane) along the x_i direction. The ID approach tacitly assumes that all D_{ij} 's are much smaller compared to one so that the sequential occurrence of multiple deformations can be superimposed as the *summation* of deformation matrices. On the other hand, in the FD approach, the matrix D^L to describe the same deformation as D becomes

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$$\mathbf{D}^L = \begin{pmatrix} 1+D_{11} & D_{12} & D_{13} \\ D_{21} & 1+D_{22} & D_{23} \\ D_{31} & D_{32} & 1+D_{33} \end{pmatrix} = \mathbf{I} + \mathbf{D}, \quad (2)$$

where $\mathbf{I}$ denotes the 3×3 unit matrix. Different from the ID approach, the FD approach expresses the occurrence of multiple deformations as the *multiplication* of deformation matrices. It is clear, therefore, that the ID analysis corresponds to the approximation of the FD analysis, neglecting second- and higher-order terms of distortion components.

In the FD-based phenomenological theories, the total shape deformation of a transformed product phase, $\mathbf{T}^L$, is factorized into rigid body rotation $\mathbf{R}^L$, lattice deformation $\mathbf{B}^L$, and lattice invariant shear deformation $\mathbf{P}^L$ as

$$\mathbf{T}^L = \mathbf{R}^L \mathbf{B}^L \mathbf{P}^L. \quad (3)$$

The corresponding expression in the ID analysis becomes

$$\mathbf{T} = \mathbf{R} + \mathbf{B} + \mathbf{P}. \quad (4)$$

This equation is useful in analyzing the case of slip as the lattice invariant shear deformation. However, the following form is more convenient to treat the case of twinning as the lattice invariant shear deformation:

$$\mathbf{T} = \mathbf{R} + f(\mathbf{B}_1 + \mathbf{\Phi}) + (1-f)\mathbf{B}_2, \quad (5)$$

where f is the volume fraction of variant 1 of the product phase which is twin-related to variant 2, $\mathbf{B}_1$ and $\mathbf{B}_2$ are the lattice deformation matrices for variants 1 and 2, respectively, and $\mathbf{\Phi}$ denotes a rotation which is geometrically necessary to make variant 1 twin-related to variant 2.

In order for $\mathbf{T}$ to describe the invariant plane deformation, the following form must be satisfied:

$$\mathbf{T}^n = \begin{pmatrix} 0 & 0 & T_{13}^n \\ 0 & 0 & T_{23}^n \\ 0 & 0 & T_{33}^n \end{pmatrix}_n, \quad (6)$$

where “ n ” indicates that the matrix is described on the $x_1^n - x_2^n - x_3^n$ orthonormal coordinate system (the n system) with the x_3^n plane parallel to the invariant plane (the habit plane). The physical meaning of eq. (6) is that no distortion exists on the x_1^n and x_2^n planes.

In the ID approach, any deformation matrix can be expressed by the summation of a symmetric strain matrix and an antisymmetric rotation matrix. For example, by defining

$$E_{ij} = (T_{ij} + T_{ji})/2 \quad (\text{strain}), \quad (7a)$$

$$\Omega_{ij} = (T_{ij} - T_{ji})/2 \quad (\text{rotation}), \quad (7b)$$

the matrix $\mathbf{T}$ is decomposed as

$$\mathbf{T} = \mathbf{E} + \mathbf{\Omega}. \quad (8)$$

From eqs. (6) and (7), $\mathbf{E}$ and $\mathbf{\Omega}$ on the n system can be written as

$$\mathbf{E}^n = \begin{pmatrix} 0 & 0 & T_{13}^n/2 \\ 0 & 0 & T_{23}^n/2 \\ T_{13}^n/2 & T_{23}^n/2 & T_{33}^n \end{pmatrix}_n, \quad (9a)$$

Table 1 The definition of direction cosines A_{ij} between the x_i^p axis and the x_j^n axis. Refer to the text for the meaning of the p and n coordinate systems.

$p \backslash n$	x_1^n	x_2^n	x_3^n
$x_1^p // [100]_p$	$\cos \theta \cos \phi$ (A_{11})	$-\sin \phi$ (A_{12})	$\sin \theta \cos \phi$ (A_{13})
$x_2^p // [010]_p$	$\cos \theta \sin \phi$ (A_{21})	$\cos \phi$ (A_{22})	$\sin \theta \sin \phi$ (A_{23})
$x_3^p // [001]_p$	$-\sin \theta$ (A_{31})	0 (A_{32})	$\cos \theta$ (A_{33})

$$\mathbf{\Omega}^n = \begin{pmatrix} 0 & 0 & T_{13}^n/2 \\ 0 & 0 & T_{23}^n/2 \\ -T_{13}^n/2 & -T_{23}^n/2 & 0 \end{pmatrix}_n. \quad (9b)$$

Khachaturyan and Shatalov⁽³⁾ and Mura *et al.*⁽⁴⁾ have conducted elasticity calculations to prove that the elastic strain energy is minimized to be zero when a plate-shaped transformation product phase embedded in a parent phase has transformation strains of the form of eq. (9a) with the x_3^n plane parallel to the plate. In retrospect, eq. (9a) only means that the x_3^n plane is unstrained. In other words, eq. (9a) constitutes necessary but not sufficient condition for the invariant plane deformation. In order for the x_3^n plane to be invariant, it must also be unrotated. Equation (6) satisfies both unstrained and unrotated conditions so that the x_3^n plane is in fact invariant. It is, therefore, clear that not only strain components of deformation but also rotation components (such as $\mathbf{\Omega}$) must be taken into account.

In eqs. (4) and (5), the lattice deformation $\mathbf{B}$ (or $\mathbf{B}_1$, $\mathbf{B}_2$ and $\mathbf{\Phi}$) is known from a proper assignment of a lattice correspondence between parent and product phases together with their lattice parameter values. Therefore, our task is to find appropriate $\mathbf{R}$ and $\mathbf{P}$ (eq. (4)) or $\mathbf{R}$ and f (eq. (5)) so that $\mathbf{T}$ can have a form of eq. (6).

For the following analyses, we will introduce another orthonormal coordinate system $x_1^p - x_2^p - x_3^p$ (the p system) fixed to the parent phase crystal. The component A_{ij} of a matrix $\mathbf{A}$ shown in Table 1 defines the direction cosines between the x_i^p axis and the x_j^n axis. With this definition, the habit plane normal $\mathbf{P}_h$ (parallel to the x_3^n axis) on the p system is written as

$$\mathbf{P}_h = [\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta]_p, \quad (\text{normalized}), \quad (10a)$$

or when $\cos \theta$ is not zero

$$\mathbf{P}_h = [\tan \theta \cos \phi, \tan \theta \sin \phi, 1]_p, \quad (\text{unnormalized}). \quad (10b)$$

Although the procedure to find solutions can be discussed in general forms, we believe that it is more clearly demonstrated by solving example problems.

III. Tetragonal to Monoclinic Transformation with Slip as a Lattice Invariant Shear Deformation

Several investigators applied the FD-based phenomenological theories to analyze the crystallography in-

Fig. 1 The unit cells of the tetragonal (*t*) and monoclinic (*m*) phases in zirconia showing the lattice correspondence *C* described in the text.

involved in the tetragonal (*t*) to monoclinic (*m*) martensitic transformation in zirconia (ZrO_2) alloys^{(10)–(12)}. Figure 1 shows the unit cells of the *t* and *m* phases[†] and Table 2 shows the lattice parameters of these phases used in the analysis by Kriven *et al.*⁽¹¹⁾ As an example, the so-called lattice correspondence *C*⁽¹¹⁾, where a_m , b_m and c_m axes correspond respectively to b_t , a_t and c_t axes, will be chosen. Then, the lattice deformation matrix *B* on the *p* coordinate system ($x_1^p \parallel [100]_t$, $x_2^p \parallel [010]_t$, $x_3^p \parallel [001]_t$) can be written as

$$\mathbf{B}^p = \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_2 & \gamma \\ 0 & 0 & \varepsilon_3 \end{pmatrix}_p, \quad (11)$$

where $\varepsilon_1 = b_m/a_t - 1 = 0.01276$, $\varepsilon_2 = a_m/a_t - 1 = 0.00769$ and $\varepsilon_3 = c_m/c_t - 1 = 0.02169$ and $\gamma = \pi/2 - \beta = 0.15324$ and “*p*” expresses the *p* system.

For the case of the $(110)_t$ – $[\bar{1}\bar{1}0]_t$ slip system as the lattice invariant shear system⁽¹¹⁾, the matrix *P* in eq. (4) becomes

$$\mathbf{P}^p = \begin{pmatrix} -m/2 & -m/2 & 0 \\ m/2 & m/2 & 0 \\ 0 & 0 & 0 \end{pmatrix}_p, \quad (12)$$

where *m* is the unknown amount of the slip deformation to be determined later. The general form of the matrix *R* in eq. (4) can be expressed as an antisymmetric matrix as

$$\mathbf{R}^p = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix}_p. \quad (13)$$

Table 2 The lattice parameters of the *t* and *m* phases in zirconia.

Tetragonal phase	
a_t	= 0.51485 nm
c_t	= 0.52692 nm
Monoclinic phase	
a_m	= 0.51881 nm
b_m	= 0.52142 nm
c_m	= 0.53835 nm
β	= 1.4176 rad
	(= 81.22 deg)

[†] In the present study, the *t*-phase is indexed using the conventional face-centered tetragonal crystal derived from the high-temperature fluorite cubic structure.

Therefore, from eqs. (11) to (13), the total shape deformation *T* in eq. (4) can be expressed in the *p*-coordinate system as

$$\mathbf{T}^p = \begin{pmatrix} \varepsilon_1 - m/2 & -(\omega_3 + m/2) & \omega_2 \\ \omega_3 + m/2 & \varepsilon_2 + m/2 & \gamma - \omega_1 \\ -\omega_2 & \omega_1 & \varepsilon_3 \end{pmatrix}_p. \quad (14)$$

This matrix *T^p* expressed on the *p* coordinate system can be converted into *Tⁿ* expressed on the *n* coordinate system by the usual tensor conversion:

$$T_{ij}^n = \sum_{k=1}^3 \sum_{l=1}^3 A_{ki} A_{lj} T_{kl}^p, \quad (15)$$

where A_{ij} are the direction cosines defined in Table 1.

The resultant matrix *Tⁿ* now has six unknown parameters, i.e., *m*, ω_1 , ω_2 , ω_3 , θ and ϕ . These six parameters can be solved using the condition of the invariant plane deformation in eq. (6). In other words, we have six simultaneous equations to solve the six unknowns; $T_{11}^n = T_{12}^n = T_{21}^n = T_{22}^n = T_{31}^n = T_{32}^n = 0$.

Instead of solving the above six equations, however, it is often more convenient to consider first the symmetric strain components of *T*, i.e., *E* defined in eq. (7a). From eqs. (7a) and (14), we have

$$\mathbf{E}^p = \begin{pmatrix} \varepsilon_1 - m/2 & 0 & 0 \\ 0 & \varepsilon_2 + m/2 & \gamma/2 \\ 0 & \gamma/2 & \varepsilon_3 \end{pmatrix}_p. \quad (16)$$

On the *n* coordinate system, *Eⁿ* must have a form of eq. (9a) and, thus, the determinant of *Eⁿ*, $|E^n|$, should be zero. However, since determinant is an invariant quantity which is independent of the choice of a coordinate system, the determinant of *E^p* in eq. (16) must also be zero. This leads to two independent solutions for *m*:

$$m = 2\varepsilon_1 \text{ and } \gamma^2/(2\varepsilon_3) - 2\varepsilon_2. \quad (17)$$

As done by Kriven *et al.*⁽¹¹⁾, only the former solution (numerically, $m = 0.0255$) will be considered hereafter since this amount of slip is much smaller and, thus, much more reasonable than the latter ($m = -0.5567$). Then, eq. (16) becomes

$$\mathbf{E}^p = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \varepsilon_1 + \varepsilon_2 & \gamma/2 \\ 0 & \gamma/2 & \varepsilon_3 \end{pmatrix}_p. \quad (18)$$

θ and ϕ can be obtained easily using eqs. (18) and (A2) to (A4) in Appendix 1 as^{††}

$$\cos \phi = 0, \sin \phi = 1,$$

and

$$\tan \theta = \frac{1}{2\varepsilon_3} [\gamma \pm \{\gamma^2 - 4\varepsilon_3(\varepsilon_1 + \varepsilon_2)\}^{1/2}]. \quad (19)$$

Therefore, from eq. (10b), two independent solutions for the unnormalized habit plane normal become

^{††} Actually, we have another set of solutions for θ and ϕ . They are $\cos \phi = 0$, $\sin \phi = -1$ and $\tan \theta = (1/2\varepsilon_3)[- \gamma \pm \{\gamma^2 - 4\varepsilon_3(\varepsilon_1 + \varepsilon_2)\}^{1/2}]$. However, this is crystallographically equivalent to the solutions (19).

$$\mathbf{P}_h = \left[0, \frac{1}{2\varepsilon_3} [\gamma \pm \{\gamma^2 - 4\varepsilon_3(\varepsilon_1 + \varepsilon_2)\}^{1/2}], 1 \right]_p. \quad (20)$$

Using the numerical values for ε_1 , ε_2 , ε_3 and γ shown previously, the normalized habit plane indices then become

$$(0, 0.9897, 0.1428)_p \text{ and } (0, 0.1351, 0.9908)_p$$

on the p coordinate system. If these were indexed on the basis of the tetragonal (t) crystal, they become

$$(0, 0.9897, 0.1461)_t \text{ and } (0, 0.1351, 1.0140)_t,$$

(ID approach)

taking into consideration of the c_t/a_t tetragonality. On the other hand, the FD-based phenomenological crystallographic analysis by Kriven *et al.*⁽¹¹⁾ gives the habit plane orientations respectively as (Table IV in ref. (11))

$$(0.013, 0.990, 0.142)_t \text{ and } (0, 0.132, 1.015)_t,$$

(FD approach)

It is clear that the ID and FD approaches give essentially the same habit plane orientation. They differ only within 2° compared with 4π steradian of the three-dimensional space.

In the above simple example, we have intended to show that the three unknown parameters m , θ and ϕ can be obtained by considering only the symmetric strain components of $\mathbf{T}$. We have not yet obtained the solutions for the remaining three unknown parameters ω_1 , ω_2 and ω_3 . Unless we find these rotation components, it is impossible to discuss the orientation relationship between the parent and product phases. In the next example, we will duly consider these rotation components and the full spectrum of the ID-based crystallographic theory will be developed.

IV. Cubic to Monoclinic Transformation with Twinning as a Lattice Invariant Shear Deformation

Knowles and Smith⁽¹³⁾ and Matsumoto *et al.*⁽¹⁴⁾ analyzed the crystallography involved in the ordered B2-type cubic (c) to internally-twinned monoclinic (m) martensitic transformation in Ti-Ni shape memory alloys on the basis of an FD-based phenomenological theory⁽¹⁵⁾. Figure 2 shows the lattice correspondence between the c and m phases and Table 3 lists the lattice parameter values of the two phases adopted previously⁽¹³⁾⁽¹⁴⁾.

As for the lattice invariant twinning system, both Type I $(11\bar{1})_m$ twinning and Type II $[011]_m$ twinning were analyzed by Knowles and Smith⁽¹³⁾ and the latter was also discussed in detail in the light of experimental observation by Matsumoto *et al.*⁽¹⁴⁾ For the purpose of demonstration of the present method of analysis, we will choose Type II $[011]_m$ twinning. The case for Type I $(11\bar{1})_m$ twinning can be analyzed in a similar manner.

The twinning elements for Type II $[011]_m$ twinning are

Fig. 2 The unit cells of the cubic (c) parent phase and the monoclinic (m) martensite phase in a Ti-Ni alloy showing the lattice correspondence of variant 1 adopted in the present study.

Table 3 The lattice parameters of the c and m phases in a Ti-Ni alloy.

Cubic phase
$a_c = 0.3015$ nm
Monoclinic phase
$a_m = 0.2889$ nm
$b_m = 0.4120$ nm
$c_m = 0.4622$ nm
$\beta = 1.690$ rad
($=96.8$ deg)

$$\eta_1 = [011]_m,$$

$$K_1 = (0.72054, 1, \bar{1})_m,$$

$$\eta_2 = [1, 0.63583, -0.63583]_m,$$

$$s = 0.28040,$$

(21)

using the notations adopted by Knowles and Smith⁽¹³⁾. For the lattice correspondence shown in Fig. 2, the lattice deformation matrix $\mathbf{B}_1$ in eq. (5) for variant 1 can be expressed in the p coordinate system fixed to the parent c phase as

$$\mathbf{B}_1^p = \begin{pmatrix} \varepsilon_1 & \zeta & 0 \\ \zeta & \varepsilon_1 & 0 \\ \delta & \delta & \varepsilon_2 \end{pmatrix}_p, \quad (22)$$

where

$$\varepsilon_1 = \sqrt{2}(b_m + c_m)/(4a_c) - 1,$$

$$\varepsilon_2 = a_m/a_c - 1,$$

$$\zeta = \sqrt{2}(-b_m + c_m)/(4a_c),$$

$$\delta = -\sqrt{2}(\beta - \pi/2)/2. \quad (23)$$

Since $\eta_1 = [011]_m$ is the twinning shear direction and since $[011]_m$ corresponds to $[200]_c$ from the lattice correspondence shown in Fig. 2, the lattice deformation matrix $\mathbf{B}_2$ in eq. (5) for variant 2 can be obtained by rotating the matrix $\mathbf{B}_1$ by π around $[200]_c$ ($//x_1^p$ -axis) as

$$\begin{aligned} \mathbf{B}_2^p &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} \varepsilon_1 & \zeta & 0 \\ \zeta & \varepsilon_1 & 0 \\ \delta & \delta & \varepsilon_2 \end{pmatrix}_p \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \\ &= \begin{pmatrix} \varepsilon_1 & -\zeta & 0 \\ -\zeta & \varepsilon_1 & 0 \\ -\delta & \delta & \varepsilon_2 \end{pmatrix}_p. \end{aligned} \quad (24)$$

The rotation matrix Φ in eq. (5) can be written as shown in Appendix 2 as

$$\Phi^p = \begin{pmatrix} 0 & 2\zeta & 2\delta \\ -2\zeta & 0 & 0 \\ -2\delta & 0 & 0 \end{pmatrix}_p. \quad (25)$$

Therefore, by writing

$$R^p = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix}_p, \quad (26)$$

the matrix T in eq. (5) and its symmetric strain components E become

$$T^p = \begin{pmatrix} \varepsilon_1 & (4f-1)\zeta - \omega_3 & 2f\delta + \omega_2 \\ -\zeta + \omega_3 & \varepsilon_1 & -\omega_1 \\ -\delta - \omega_2 & \delta + \omega_1 & \varepsilon_2 \end{pmatrix}_p, \quad (27)$$

$$E^p = \begin{pmatrix} \varepsilon_1 & 2(f-1/2)\zeta & (f-1/2)\delta \\ 2(f-1/2)\zeta & \varepsilon_1 & \delta/2 \\ (f-1/2)\delta & \delta/2 & \varepsilon_2 \end{pmatrix}_p, \quad (28)$$

where f , ω_1 , ω_2 and ω_3 are unknown parameters to be solved. Out of these, f can be calculated easily from $|E^p|=0$, as discussed in the previous section, to have two solutions

$$f = (1 \pm \sqrt{1 - 4B/A})/2, \quad (29)$$

where

$$A = 2\zeta\delta^2 - 4\zeta^2\varepsilon_2 - \delta^2\varepsilon_1,$$

$$B = (\zeta\delta^2 - 2\zeta^2\varepsilon_2 - \delta^2\varepsilon_1 + 2\varepsilon_1^2\varepsilon_2)/2.$$

Then, since all the components E_{ij}^p in eq. (28) have been found, the angles θ and ϕ in eq. (10a) or (10b) can be obtained by substituting these E_{ij}^p components into simultaneous eqs. (A2) to (A4) in Appendix 1 as

$$\tan \phi = \frac{1}{E_{11}^p} [E_{12}^p \pm \{(E_{12}^p)^2 - E_{11}^p E_{22}^p\}^{1/2}],$$

and

$$\tan \theta = \frac{1}{E_{13}^p \sin \phi - E_{23}^p \cos \phi} \{ (E_{11}^p - E_{22}^p) \cos \phi \sin \phi + E_{12}^p (\sin^2 \phi - \cos^2 \phi) \}. \quad (30)$$

Although the remaining unknowns, ω_1 , ω_2 and ω_3 , can be obtained by describing T on the n coordinate system and using the condition of the invariant-plane deformation, eq. (6), it is easier to proceed as follows. Let the two non-parallel vectors, $v(I)$ and $v(II)$, on the habit plane (perpendicular to P_h in eq. (10a)) be described as

$$v^p(I) = [-\sin \theta \sin \phi, \sin \theta \cos \phi, 0]_p,$$

and

$$v^p(II) = [-\cos \theta, 0, \sin \theta \sin \phi]_p. \quad (31)$$

The condition of the habit plane being an invariant plane requires that $v^p(I)$ and $v^p(II)$ on the habit plane be unchanged before and after the transformation. That is

$$T^p \cdot v^p(I) = 0, \text{ or } \sum_{j=1}^3 T_{ij}^p v_j^p(I) = 0,$$

and

$$T^p \cdot v^p(II) = 0, \text{ or } \sum_{j=1}^3 T_{ij}^p v_j^p(II) = 0. \quad (32)$$

With eqs. (31) and (32), we obtain

$$\begin{aligned} \omega_1 &= \varepsilon_2 \tan \theta \sin \phi - \delta, \\ \omega_2 &= -\varepsilon_2 \tan \theta \cos \phi - \delta, \\ \omega_3 &= (\varepsilon_1 / \tan \phi) + \zeta. \end{aligned} \quad (33)$$

Now that all unknown parameters have been solved, the direction of the total shape deformation d_T and its magnitude m_T can be obtained as

$$d_T^n = [T_{13}^n, T_{23}^n, T_{33}^n]_n, \text{ (n system)} \quad (34a)$$

or

$$d_T^p = A \cdot d_T^n, \text{ (p system)} \quad (34b)$$

and

$$m_T = \sqrt{(T_{13}^n)^2 + (T_{23}^n)^2 + (T_{33}^n)^2}, \quad (35)$$

where A is defined in Table 1. The orientation relationship between the c and m phases can be obtained as follows. Rewriting eq. (5), we have

$$T = fS_1 + (1-f)S_2 \quad (36)$$

where

$$S_1 = R + B_1 + \Phi, \text{ (variant 1)} \quad (37a)$$

$$S_2 = R + B_2. \text{ (variant 2)} \quad (37b)$$

A direction vector x^p drawn from the origin before transformation becomes a vector y^p after transformation in accord with the following transformations

$$(I + S_1^p) \cdot x^p = y^p, \text{ (variant 1)} \quad (38a)$$

$$(I + S_2^p) \cdot x^p = y^p, \text{ (variant 2)} \quad (38b)$$

Owing to the low symmetry of the product m phase, two crystallographically different sets of solutions are obtained even when the smaller value of f ($0 < f < 1/2$) is chosen in eq. (29). This is in contrast to the case of the cubic to tetragonal transformation where the two sets of solutions degenerate to be crystallographically equivalent⁽⁸⁾. Following the notations adopted by Knowles and Smith⁽¹³⁾, let us call the two different sets as solutions (X1, N1) and (X2, N2). Since the latter solutions were found to be in good agreement with experimental observations⁽¹⁴⁾, we will compare the (X2, N2) solutions derived in the present study with those derived previously using the FD-based phenomenological theory⁽¹³⁾⁽¹⁴⁾.

Using the lattice parameter values in Table 3 together with eqs. (23), numerical values were obtained for the solutions (X2, N2) in the present study and they are listed in Table 4 under the column ID. The corresponding FD-based solutions are also listed under the column FD. It can be easily recognized that the two sets of solutions are

Table 4 Comparison of numerical solutions for (X2, N2) obtained from the present ID and previous FD approaches⁽¹³⁾ for the c to m transformation in a Ti-Ni alloy with Type II $[011]_m$ twinning as the lattice invariant shear (LIS) deformation. The matrix S_1^p and S_2^p described on the p coordinate system are defined in eqs. (37a) and (37b), respectively.

	ID	FD
Habit plane normal, P_h	$[0.38502, -0.23606, 0.89221]_p$	$[0.40443, -0.21524, 0.88888]_p$
Volume fraction, f	0.26051	0.27102
Total shape deformation		
Direction, d_T^p	$[0.48939, -0.79821, -0.35122]_p$	$[0.48736, -0.75743, -0.43449]_p$
Magnitude, m_T	0.13336	0.13079
S_1^p	$\begin{pmatrix} 0.02513 & 0.15872 & -0.06589 \\ -0.04099 & 0.02513 & -0.09498 \\ -0.01803 & 0.01106 & -0.04179 \end{pmatrix}_p$	$\begin{pmatrix} 0.02578 & 0.15748 & -0.06670 \\ -0.04006 & 0.01464 & -0.08324 \\ -0.02298 & 0.00840 & -0.04775 \end{pmatrix}_p$
S_2^p	$\begin{pmatrix} 0.02513 & -0.07675 & 0.10196 \\ -0.04099 & 0.02513 & -0.09498 \\ -0.01803 & 0.01106 & -0.04179 \end{pmatrix}_p$	$\begin{pmatrix} 0.02578 & -0.07737 & 0.10252 \\ -0.04006 & 0.02381 & -0.08985 \\ -0.02298 & 0.01366 & -0.05154 \end{pmatrix}_p$
Orientation relationship for variant 2	$[100]_m \Delta [00\bar{1}]_c$ 8.27° $[010]_m \Delta [110]_c$ 1.10° $[001]_m \Delta [1\bar{1}0]_c$ 1.44° $(100)_m \Delta (00\bar{1})_c$ 1.16° $(010)_m \Delta (110)_c$ 1.03° $(001)_m \Delta (1\bar{1}0)_c$ 8.71°	$[100]_m \Delta [00\bar{1}]_c$ 8.18° $[010]_m \Delta [110]_c$ 1.12° $[001]_m \Delta [1\bar{1}0]_c$ 1.72° $(100)_m \Delta (00\bar{1})_c$ 1.42° $(010)_m \Delta (110)_c$ 1.12° $(001)_m \Delta (1\bar{1}0)_c$ 8.23°

in excellent agreement. For example, the habit plane orientations differ only by 1.6°, the volume fraction of variant 1 is also very close to each other (26% vs 27%) and the difference in the orientation relationship is at most within 0.5°. Therefore, we conclude that the present ID-based approach can give essentially the same crystallographic solutions as those given by the FD-based phenomenological theories.

It goes without saying that when the calculated solutions are used for comparison with experimental observations, the differences between ID and FD solutions are immaterial. As discussed in detail in the previous study⁽⁸⁾, the differences become larger as distortion components involved in a transformation become larger. However, the fact that crystallographic solutions can be obtained in an analytical manner even for rather complex cases of cubic (tetragonal) to monoclinic transformations will make the present ID-based analysis useful and advantageous in discussing how the invariant plane condition is realized in a given system.

V. Summary and Conclusion

(1) Phenomenological crystallographic analysis for cubic (tetragonal) to monoclinic martensitic transformations was performed on the basis of the infinitesimal-deformation (ID) approach.

(2) The previously known criterion for the minimization of elastic strain energy associated with a transformation was found to constitute the necessary condition for a habit plane to be an invariant plane.

(3) Not only symmetric strain components but also antisymmetric rotation components of a distortion

matrix must be taken into account to make a habit plane invariant (unstrained and unrotated) in the present ID analysis.

(4) Taking advantage of the ID approach, crystallographic solutions for habit plane orientation, total shape deformation, orientation relationships between parent and martensite crystals, etc. were derived in a simple and analytical manner.

(5) The derived solutions were in excellent agreement with those obtained numerically using the phenomenological crystallographic theory.

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Appendix 1

The components of the matrix E in eq. (7a), E_{ij}^n on the n -coordinate system and E_{ij}^p on the p -coordinate system, are related to each other by the usual tensor transformation as

$$E_{ij}^n = \sum_{k=1}^3 \sum_{l=1}^3 A_{ki} A_{lj} E_{kl}^p, \quad (A1)$$

where A_{ij} are defined in Table 1. For the x_3^n plane to be unstrained, eq. (9a) must be satisfied. Therefore, using explicit forms of eq. (A1) with A_{ij} in Table 1, we have

$$\begin{aligned} E_{11}^n &= E_{11}^p \cos^2 \theta \cos^2 \phi + 2E_{12}^p \cos^2 \theta \sin \phi \cos \phi \\ &\quad - 2E_{13}^p \sin \theta \cos \theta \cos \phi + E_{22}^p \cos^2 \theta \sin^2 \phi \\ &\quad - 2E_{23}^p \sin \theta \cos \theta \sin \phi + E_{33}^p \sin^2 \theta = 0, \end{aligned} \quad (A2)$$

$$\begin{aligned} E_{22}^n &= E_{11}^p \sin^2 \phi - 2E_{12}^p \sin \phi \cos \phi \\ &\quad + E_{22}^p \cos^2 \phi = 0, \end{aligned} \quad (A3)$$

and

$$\begin{aligned} E_{12}^n &= -E_{11}^p \cos \theta \sin \phi \cos \phi + E_{12}^p \cos \theta (\cos^2 \phi \\ &\quad - \sin^2 \phi) + E_{22}^p \cos \theta \sin \phi \cos \phi \\ &\quad + E_{31}^p \sin \theta \sin \phi - E_{32}^p \sin \theta \cos \phi = 0. \end{aligned} \quad (A4)$$

From the above three simultaneous equations, the angles θ and ϕ can be obtained in terms of E_{ij}^p .

Appendix 2

For Type II $[011]_m$ twinning, the lattice correspondence shown in Fig. 2 implies that the twinning direction η_1 and the twinning plane K_1 in eqs. (21) correspond respectively to the following direction and plane on the p coordinate system

$$\eta_1 = [011]_m \leftrightarrow [200]_p,$$

$$K_1 = (r1\bar{1})_m \leftrightarrow (0\bar{1}r)_p,$$

where $r=0.72054$. In order for variants 1 and 2 to be twin related to each other, they must possess K_1 and η_1 in common.

Let us describe the antisymmetric rotation matrix Φ in eq. (5) on the p coordinate system as

$$\Phi^p = \begin{pmatrix} 0 & -\theta_3 & \theta_2 \\ \theta_3 & 0 & -\theta_1 \\ -\theta_2 & \theta_1 & 0 \end{pmatrix}_p. \quad (A5)$$

When D is a distortion matrix such as that in eq. (1), the reciprocal matrix of $I+D$, $(I+D)^{-1}$ in the FD approach, is known to be written in the ID approach as $I-D$. Keeping this in mind, it is found that the direction $[200]_p$ and the plane $(0\bar{1}r)_p$ are converted into the following direction and plane after the operation of $B_1 + \Phi$ in eq. (5) for variant 1:

$$(I+B_1^p + \Phi^p) \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}_p = \begin{bmatrix} 2+2\varepsilon_1 \\ 2\zeta+2\theta_3 \\ 2\delta-2\theta_2 \end{bmatrix}_p, \quad (A6)$$

and

$$\begin{aligned} (0\bar{1}r)_p (I-B_1^p - \Phi^p)_p \\ = (\zeta+\theta_3-r\delta+r\theta_2, -1+\varepsilon_1-r\delta-\delta\theta_1, -\theta_1+r-r\varepsilon_2)_p. \end{aligned} \quad (A7)$$

Here, eqs. (22) and (A5) were used. Similarly, for variant 2 in eq. (5), we have

$$(I+B_2^p) \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}_p = \begin{bmatrix} 2+2\varepsilon_1 \\ -2\zeta \\ -2\delta \end{bmatrix}_p, \quad (A8)$$

and

$$(0\bar{1}r)_p (I-B_2^p) = (-\zeta+r\delta, -1+\varepsilon_1-r\delta, r-r\varepsilon_2)_p. \quad (A9)$$

Equating eq. (A6) with (A8) and eq. (A7) with (A9), we obtain

$$\theta_1=0, \theta_2=2\delta, \theta_3=-2\zeta. \quad (A10)$$

Insertion of eqs. (A10) into eq. (A5) gives eq. (25) in the text.