Crystallographic analysis of $fcc \rightarrow bcc$ martensitic phase transformation observed in Fe-31 wt % Ni alloy using infinitesimal deformation approach

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The solutions for crystallographical parameters such as habit plane orientation, rotation matrix, total shape deformation matrix, orientation relationship between austenite and martensite crystal axis, etc. have been obtained by using infinitesimal deformation approach, taking into account the basic concepts of finite deformation phenomenological crystallographic theories associated with martensitic transformations. Numerical values obtained have been compared with the predictions of the crystallographic theories and experimental results.

Keywords: Martensitic transformation, Crystallographic analysis, Infinitesimal deformation approach

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1 Introduction

Diffusionless phase transformation in metals and alloys has been a widely studied subject of both practical and theoretical interest since seventy years ago. The crystallographic martensite transformation has been investigated in the field of physics and materials science. A quite complete theoretical system which includes the transformation crystallographic theory has been established\(^{1-5}\). Their phenomenological crystallographic theories (PCT) are based on the invariant plane strain (IPS) criterion at the planar interface between parent and product phase. When phenomenological crystallographic theory is applied to some simple transformation system, the solutions for the orientation relationship according to these theories are very difficult to express analytically. The lack of analytical solutions often prevents researcher from finding and predicting the systematic dependence of solutions on input parameters associated with transformation observed in metals and alloys. Although a few crystallographic theories which determine the crystallographic parameters concerning austenite and martensite in some metals and alloys give good results, there is no theory explaining simply all the features of the martensitic phase transformation yet.

In the recent years, some researchers\(^ {7,8}\) adopted a theory based on the infinitesimal approach (ID) taking into consideration both symmetric strain components and the antisymmetric rotation components of deformation. These theories are an approximation of the PCT-based phenomenological crystallographic theory. However, the advantage of ID-based phenomenological theory is that all solutions can be expressed in simple and analytical forms.

The purpose of this study, considering twinning case as the lattice invariant shear (LIS) system, an ID-based phenomenological theory is to formulate for martensic phase transformation from $fcc$ ($\gamma$) to $bcc$ ($\alpha$) observed in the alloy Fe-31 wt % Ni. The obtained solutions for the crystallographic parameters such as habit plane orientation relationship, total shape deformation and orientation relationships between phase $\gamma$ and phase $\alpha$, etc. will be compared numerically with those found from the original PCT analysis and experimental results.

2 Theory

The lattice deformation $B_1^\gamma$ associated with $fcc$ to $bcc$ martensitic transformation is expressed as:

$$B_1^\gamma = \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_1 & 0 \\ 0 & 0 & \varepsilon_2 \end{pmatrix}$$

...(1)

where $\varepsilon_1$ and $\varepsilon_2$ represent the principle strains on the $\gamma$ coordinate system ($x_1^\gamma$//[100], $x_2^\gamma$//[010] and...
According to the application of the phenomenological theory, the \((101)_{\gamma}\|\{10\overline{1}\}\) are chosen as lattice invariant shear system (LIS). This shear can occur either slip or twinning. In the present study, twinning case is considered in order to analyze the crystallography by using ID approach. This twinning can be incorporated in the theory by considering two different deformations. Both of them are actually crystallographically equivalent Bain strain and its expression has:

\[
B_2^\gamma = \begin{pmatrix} \varepsilon_2 & 0 & 0 \\ 0 & \varepsilon_1 & 0 \\ 0 & 0 & \varepsilon_1 \end{pmatrix} \quad \text{(2)}
\]

As shown in Fig. 1(c), in order for the cubic phase to be internally twinned, the cubic crystal subjected to the lattice deformation \(B_1^\gamma\), say crystal 1, must be rotated relative to the cubic phase crystal subject to the lattice deformation \(B_2^\gamma\), i.e. crystal 2 by an angle \(\Phi\).

The rotation matrix \(\Phi\) of the crystal 1 can be obtained within the framework of the ID theory as in the following form:

\[
\Phi_{\gamma} = \begin{pmatrix} 0 & 0 & \varepsilon_1 - \varepsilon_2 \\ 0 & 0 & 0 \\ \varepsilon_2 - \varepsilon_1 & 0 & 0 \end{pmatrix}_\gamma \quad \text{(3)}
\]

According to the ID theory, total shape deformation matrix \(T\) has:

\[
T^\gamma = R^\gamma + f(\Phi_{\gamma} + B_1^\gamma) + (1 - f)B_2^\gamma \quad \text{(4)}
\]

where the coefficient \(f\) denotes the volume fraction of crystal 1 in the twinned cubic phase and \(R^\gamma\) in Eq. (4) represents the rotation matrix. Similar to the previous case, a matrix \(F^\gamma\) can be defined as

\[
F^\gamma = f(\Phi_{\gamma} + B_1^\gamma) + (1 - f)B_2^\gamma \quad \text{(5)}
\]

and together with Eqs (1-3), this expression then becomes:

\[
F^\gamma = \begin{pmatrix} \varepsilon_2 + f(\varepsilon_1 - \varepsilon_2) & 0 & f(\varepsilon_1 - \varepsilon_2) \\ 0 & \varepsilon_1 & 0 \\ -f(\varepsilon_1 - \varepsilon_2) & 0 & \varepsilon_1 - f(\varepsilon_1 - \varepsilon_2) \end{pmatrix}_\gamma \quad \text{(6)}
\]

On the other hand, in order for the habit plane to make invariant, in other words undistorted and

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Fig. 1—Schematic illustration showing how the \((101)_{\alpha}\|\{10\overline{1}\}\) twinning deformation in the product \(\alpha\) phase can be incorporated in the present analysis as a result of the combination of \(\alpha_1\) and \(\alpha_2\) crystals subjected to different deformations \(B_1\) and \(B_2\). An angle \(\Phi\) is produced between crystal 1 and crystal 2, which is twin related to each other.
unrotated, the general form of the antisymmetric rotation matrix, \( \mathbf{R}^\gamma \) is expressed as:

\[
\mathbf{R}^\gamma = \begin{pmatrix}
0 & -w_3 & w_2 \\
w_3 & 0 & -w_1 \\
-w_2 & w_1 & 0
\end{pmatrix}
\]

where \( w_1, w_2 \) and \( w_3 \) represent the angles of rotation to be determined later. Thus, from Eqs (4), (5) and (7), an expression for the total shape deformation, \( \mathbf{T}^\gamma \), in the coordinate system \( \gamma \) as:

\[
\mathbf{T}^\gamma = \mathbf{T}_1^\gamma + \mathbf{T}_2^\gamma - \mathbf{T}_3^\gamma
\]

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

\[
\mathbf{E}^\gamma_{ij} = \left( \mathbf{T}^\gamma_{ij} + \mathbf{T}^\gamma_{ji} \right)/2
\]

Since determinant is an invariant quantity which is independent of the choice of a coordinate system, the determinant of \( \mathbf{E}^\gamma \) in Eq. (9) must also be zero. Thus, this leads to two independent solutions for \( f \):

\[
f_1 = \varepsilon_1/(\varepsilon_1 - \varepsilon_2) \quad \text{and} \quad f_2 = \varepsilon_2/(\varepsilon_2 - \varepsilon_1)
\]

The matrix in Eq. (8) can be converted into the matrix \( \mathbf{T}^n \) expressed on the particular orthonormal coordinate system, say \( n \), by usual tensor conversion:

\[
\mathbf{T}^n_{ij} = \sum_{k=1}^{3} \sum_{l=1}^{3} A_{ik} A_{lj} \mathbf{T}^\gamma_{kl}
\]

where \( A_{ij} \) are direction cosines defined in Table 1. In order for this matrix to describe the invariant plane deformation, the matrix \( \mathbf{T}^n_{ij} \) in Eq. (11) must satisfy the following form:

\[
\mathbf{T}^n = \begin{pmatrix}
0 & 0 & \mathbf{T}^n_{13} \\
0 & 0 & \mathbf{T}^n_{23} \\
0 & 0 & \mathbf{T}^n_{33}
\end{pmatrix}
\]

The physical meaning of this matrix is that no distortion exists on \( x_1^n \) and \( x_2^n \) planes.

For \( f_1 = \varepsilon_1/(\varepsilon_1 - \varepsilon_2) \) in Eq. (10), there are five unknown parameters such as \( w_1, w_2, w_3, \theta \) and \( \phi \) in Eq. (12). In order to determine these parameters, using Eqs (11) and (12) together with Table 1 the following expressions for the elements of the matrix \( \mathbf{T}^n_{ij} \) are obtained as:

\[
\begin{align*}
\mathbf{T}^n_{11} &= (\varepsilon_1 + \varepsilon_2 \cos^2 \phi) \cos^2 \theta = 0 \\
\mathbf{T}^n_{12} &= - (\varepsilon_1 \sin \theta + \varepsilon_2 \cos \theta \cos \phi) \sin \phi \\
& \quad - (w_1 \cos \phi + w_2 \sin \phi) \sin \theta - w_3 \cos \theta = 0 \\
\mathbf{T}^n_{21} &= (\varepsilon_1 \sin \theta - \varepsilon_2 \cos \theta \cos \phi) \sin \phi \\
& \quad + (w_1 \cos \phi + w_2 \sin \phi) \sin \theta + w_3 \cos \theta = 0 \\
\mathbf{T}^n_{22} &= \varepsilon_1 + \varepsilon_2 \sin^2 \phi = 0 \\
\mathbf{T}^n_{31} &= (\varepsilon_1 + \varepsilon_2 \cos^2 \phi) \sin \theta \cos \theta \\
& \quad - \varepsilon_1 \cos \phi + w_1 \sin \phi - w_2 \cos \phi = 0 \\
\mathbf{T}^n_{32} &= (\varepsilon_1 \cos \theta - \varepsilon_2 \sin \theta \cos \phi) \sin \phi \\
& \quad + (w_1 \cos \phi + w_2 \sin \phi) \cos \theta - w_3 \sin \theta = 0 \\
\mathbf{T}^n_{13} &= (\varepsilon_1 + \varepsilon_2 \cos^2 \phi) \sin \theta \cos \theta \\
& \quad + \varepsilon_1 \cos \phi - w_1 \sin \phi + w_2 \cos \phi = 0 \\
\mathbf{T}^n_{23} &= - (\varepsilon_1 \cos \theta + \varepsilon_2 \sin \theta \cos \phi) \sin \phi \\
& \quad - (w_1 \cos \phi + w_2 \sin \phi) \cos \theta + w_3 \sin \theta = 0
\end{align*}
\]

<table>
<thead>
<tr>
<th>( \gamma )</th>
<th>( n )</th>
<th>( x_1^n )</th>
<th>( x_2^n )</th>
<th>( x_3^n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x_1^\gamma ) //([100])</td>
<td>( \cos \theta \cos \phi )</td>
<td>(- \sin \phi )</td>
<td>( \sin \theta \cos \phi )</td>
<td></td>
</tr>
<tr>
<td>( x_2^\gamma ) //([010])</td>
<td>( \cos \theta \sin \phi )</td>
<td>( \cos \phi )</td>
<td>( \sin \theta \sin \phi )</td>
<td></td>
</tr>
<tr>
<td>( x_3^\gamma ) //([001])</td>
<td>(- \sin \theta )</td>
<td>( 0 )</td>
<td>( \cos \theta )</td>
<td></td>
</tr>
</tbody>
</table>
\[ T_{33}^n = (e_1 + e_2 \cos^2 \phi) \sin^2 \theta \]  
\[ n = (1) \]  

From Eqs (14) and (15), it is obviously seen \( \cos \theta = 0 \) or \( \sin \theta = 1 \). In this case, an expression for the angle \( \phi \) can be obtained from Eq. (16) as:

\[ \tan^2 \phi = -e_1 / (e_1 + e_2) \]  
\[ n = (22) \]

Similarly, for \( f_2 = e_2 / (e_2 - e_1) \) in Eq. (10), the new equations corresponding to Eqs (13)-(21) will become as in the following form:

\[ T_{11}^n = e_1 \cos \theta \sin^2 \phi + (e_1 + e_2) \sin^2 \theta = 0 \]  
\[ n = (23) \]

\[ T_{12}^n = (e_1 \cos \theta \cos \phi + e_2 \sin \theta) \]
\[- (w_1 \cos \phi + w_2 \sin \phi) \sin \theta - w_3 \cos \theta = 0 \]  
\[ n = (24) \]

\[ T_{21}^n = (e_1 \cos \theta \cos \phi - e_2 \sin \theta) \]
\[ + (w_1 \cos \phi + w_2 \sin \phi) \sin \theta + w_3 \cos \theta = 0 \]  
\[ n = (25) \]

\[ T_{22}^n = e_1 \cos^2 \phi = 0 \]  
\[ n = (26) \]

\[ T_{31}^n = -(e_1 \cos^2 \phi + e_2) \sin \theta \cos \theta \]
\[ + e_2 \cos \phi + w_1 \sin \phi - w_2 \cos \phi = 0 \]  
\[ n = (27) \]

\[ T_{32}^n = (e_1 \sin \theta \cos \phi - e_2 \cos \theta) \sin \phi \]
\[ + (w_1 \cos \phi + w_2 \sin \phi) \cos \theta - w_3 \sin \theta = 0 \]  
\[ n = (28) \]

\[ T_{13}^n = -(e_1 \cos^2 \phi + e_2) \sin \theta \cos \theta \]
\[ - e_2 \cos \phi - w_1 \sin \phi + w_2 \cos \phi \]  
\[ n = (29) \]

\[ T_{23}^n = (e_1 \sin \theta \cos \phi + e_2 \cos \theta) \sin \phi \]
\[ - (w_1 \cos \phi + w_2 \sin \phi) \cos \theta + w_3 \sin \theta \]  
\[ n = (30) \]

\[ T_{33}^n = e_1 \sin^2 \phi \sin^2 \phi + (e_1 + e_2) \cos^2 \theta \]  
\[ n = (31) \]

In this case, it is clear that \( \cos \phi = 0 \) or \( \sin \phi = 1 \) and

\[ \tan^2 \theta = -e_1 / (e_1 + e_2) \]  
\[ n = (32) \]

Using Eqs (22) and (32) for two values of \( f \), normalized habit planes \( P_h \) can be obtained as:

\[ P_h = [\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta] \]  
\[ n = (33) \]

\[ P_{h1} = \sqrt{(e_1 + e_2)} / (e_2, \sqrt{-e_1 / e_2}, 0) \]  
\[ n = (34) \]

and

\[ P_{h2} = [0, \sqrt{-e_1 / e_2}, \sqrt{(e_1 + e_2) / e_2}] \]  
\[ n = (35) \]

Considering \( \cos \theta = 0 \) for \( f_1 \) and \( \cos \phi = 0 \) for \( f_2 \), the angles \( w_1, w_2 \) and \( w_3 \) can be obtained by solving Eqs (15), (17) and (18) for \( f_1 \) and Eqs (25), (27) and (28) for \( f_2 \). They are listed in Table 2. Two solutions according to the values of \( f_1 \) and \( f_2 \) give the same combinations of the habit planes (Table 2).

The orientation relationship between \( \gamma \) and \( \alpha \) phases can be obtained as follows. A direction vector \( x^\gamma \) drawn from the origin before transformation becomes a vector \( y^\alpha \) after transformation in accordance with the following transformations:

\[ (I + S_1) x^\gamma = y^\alpha \]  
\[ n = (36) \]

and

\[ (I + S_2) x^\gamma = y^\alpha \]  
\[ n = (37) \]

so that \( I \) is unit matrix. \( S_1 \) and \( S_2 \) in Eqs (36) and (37) are \( S_1 = R^\gamma + B_1^\gamma + \Phi_\gamma \), \( S_2 = R^\gamma + B_2^\gamma \) respectively.

3 Results and Discussion

Lattice parameter of the \( \gamma \) phase is \( a_\gamma = 3.591 \pm 0.001 \) Å and the lattice parameters of \( \alpha \) phase are \( a_\alpha = 2.875 \pm 0.001 \) Å. These give:

\[ e_1 = \sqrt{2} \frac{a_\alpha}{a_\gamma} - 1 = 0.132136 \]  
\[ n = (38) \]

and

\[ e_2 = \frac{a_\alpha}{a_\gamma} - 1 = -0.199459 \]  
\[ n = (39) \]

If these values of \( e_1 \) and \( e_2 \) for the alloy Fe-31 wt % Ni are substituted into the expressions for the solution in Table 2 in order for a suitable comparison,
numerical values for various crystallographic parameters can be obtained. These results are listed in Tables 3 and 4. Because the ID approach neglects the second and higher order terms of the lattice distortion, \( \varepsilon \), the relative differences in solutions of the habit planes between the ID and PCT analyses should be also in the order of this distortion. On the other hand, the components of the habit plane indices are also described by the zero order of the lattice distortions. So, the absolute differences are in the same orders of the value of \( \varepsilon \). According to the case, the habit plane orientation calculated from the ID approach may differ from the corresponding results of the experimental observations by amount of 180 \( \varepsilon / \pi \) degrees. For example, concerning the angle between the determination of the habit plane indices, the following angles can be calculated: the angle between
Table 3 — Numerical solutions for the ID approach

<table>
<thead>
<tr>
<th>Solution</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Habit plane</td>
<td>[0.580972, 0.813924, 0]</td>
<td>[0, 0.813924, 0.580972]</td>
</tr>
<tr>
<td>Volume fraction of crystal 1, f</td>
<td>0.398486</td>
<td>0.601514</td>
</tr>
</tbody>
</table>
| Total shape deformation T'' | \[
\begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & -0.188635 \\
0 & 0 & 0.064813
\end{pmatrix}
\] | \[
\begin{pmatrix}
0 & 0 & -0.188635 \\
0 & 0 & 0 \\
0 & 0 & 0.064813
\end{pmatrix}
\] |
| Magnitude of total shape deformation, m_T | 0.199459               | 0.199459               |

Orientation relationship

Crystal 1

\[
R' \Phi' = \begin{pmatrix}
0 & 0.0943175 & 0.199459 \\
-0.0943175 & 0 & 0 \\
-0.199459 & 0 & 0
\end{pmatrix}
\]

Tilt angles

| [100]_γ | 0.2206347 | 0.132136 |
| [010]_γ | 0.0943175 | 0.0943175 |
| [001]_γ | 0.199459 | 0.1623444 |

Crystal 2

\[
R' = \begin{pmatrix}
0 & 0.0943175 & -0.132136 \\
-0.0943175 & 0 & 0 \\
0.132136 & 0 & 0
\end{pmatrix}
\]

Tilt angles

| [100]_γ | 0.1623444 | 0.199459 |
| [010]_γ | 0.0943175 | 0.0943175 |
| [001]_γ | 0.132136 | 0.2206347 |

Table 4 — Comparison of the numerical solution among infinitesimal approach, phenomenological theory and some experimental results\(^{13}\) for fcc to bcc martensitic phase transformation observed in the alloy Fe-31 wt % Ni

<table>
<thead>
<tr>
<th>Habit plane</th>
<th>ID</th>
<th>PT</th>
<th>Experimental</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0, 0.813924, 0.580972]</td>
<td>[0.184765, 0.782337, 0.594820]</td>
<td>[0.1656, 0.7998, 0.5770]</td>
<td></td>
</tr>
<tr>
<td>Amount of LIS, m</td>
<td>0.26447</td>
<td>0.25679</td>
<td>-</td>
</tr>
<tr>
<td>Magnitude of the total shape deformation, m_T</td>
<td>0.19940</td>
<td>0.22560</td>
<td>-</td>
</tr>
</tbody>
</table>

Orientation Relationship for variant 2

| [100]_γ \Lambda [100]_α | 11.46° | 7.61° | - |
| [010]_γ \Lambda [010]_α | 4.76° | 6.32° | - |
| [001]_γ \Lambda [001]_α | 6.66° | 9.68° | - |
| [101]_γ \Lambda [101]_α | 4.42° | 3.62° | 2.4° |
| [1 \bar{1} 2]_γ \Lambda [0 \bar{1} 1]_α | 2.03° | 1.67° | 2.2° |
ID and experimental observation 0.17 radians and the angle between ID and PCT 0.19 radians. It can be inferred that the ID approach is adapted with an error of about 0.18 radians or approximately 10° which is expected from the ID approach. A comparison between the two results from the point of view of the amount of LIS and the magnitude of the total lattice deformation, obviously indicates that the differences are negligible. The difference gradually decreases in calculation for the alloy In-Tl and an ordered fcc-based iron nitride with the stoichiometric composition, Fe₄N, having rather the small principal distortions. For example, the lattice distortion is nearly in the order of 0.01 in an In – 20.75 at. % Tl alloy. We find that the habit plane normal (0, 0.7746, 0.6324) is in agreement with the (0 1 1) habit plane normal observed experimentally. The difference is only 2.61° or 0.046 radian. In the present study, the values of the habit plane indices are in moderate, but not in entire agreement with the experimental values. By contrast, the orientation relationships between the results in the present study and those of the experimental results differ only by 0.875°. An inspection of the orientation relationship shows that there is an agreement with the ID approach and the experimental results. Applications of the present theory to the other transformation systems are currently under progress.

In summary, in the present study, we have formulated the ID approach in order to analyze the martensitic transformation from fcc to bcc observed in an Fe-31 wt % Ni alloy. From the results obtained in this study, the following main conclusions can be drawn:

1. The ID approach considered in the present study offers very simple and clear analytical equations to be solved for the crystallography of martensite from fcc to bcc observed in alloy Fe-31 wt % Ni without requiring much complex numerical computations;
2. Although two amounts of the volume fractions of crystal 1 having the product phase which is twin-related to crystal 2 in question have different values, the two solutions give rise to same combination of the habit plane indices.

References