A DISLOCATION REACTION MODEL FOR VARIANTS SELECTION DURING THE AUSTENITE-TO-MARTENSITE TRANSFORMATION

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Variant selection rules are described that predict the austenite-to-martensite transformation textures of an Fe–30%Ni alloy. The occurrence of variant selection is explained in detail using the crystal plasticity model of Bishop and Hill and the Kurdjumov–Sachs transformation relationship. A correlation is established between the slip systems of the former and the rotation axes of the latter. The selection criteria are based on a combination of slip activity, that is, active slip systems, and permissible dislocation reactions. Thus some of the variants selected are associated with slip systems that are active while the remainder are accounted for by the in-plane reaction of active dislocations to form inactive or unstressed dislocations. The variant selection criteria are tested against the experimental findings of Liu and Bunge (Materials Letters, 10(7,8), 336–343, 1991) and found to be in good agreement.

Keywords: Variant selection; Transformation textures; Kurdjumov–Sachs; Bishop and Hill; Slip activity; Dislocation reactions

INTRODUCTION

The austenite-to-ferrite or martensite transformation has been studied extensively and successful models have been proposed by Bain (1924), Kurdjumov and Sachs (1930) (K–S), Nishiyama (1934) and Wassermann (1933) (N–W). All of these are based on rotations about particular axes. Although these models can describe the products formed

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from parents that have not undergone prior deformation, this is generally not the case when dislocations are present. In deformed materials, not all the expected variants are present, and variant selection takes place instead. In other words, the above models only apply to materials that have not undergone prior deformation, while the presence of dislocations is directly related to the occurrence of variant selection.

Slip activity has been employed as a criterion to account for texture inheritance in combination with the resolved shear stresses (i.e. Schmid's law). Both the K–S relationship and Bishop and Hill (1951b) model of crystal plasticity have been used. Four analyses based on the Bishop and Hill plasticity model were put forward by Haslam et al. (1973) that considered martensite nucleation on: (1) the most active slip system, (2) the most active slip plane, (3) all the active slip planes and (4) all active slip systems. Each approach was partially successful in accounting for the product texture.

A habit plane and slip system criterion has also been advanced that relates the habit planes of the variants to the active slip systems of the austenite. Bokros and Parker (1963) and Durlu and Christian (1979) have employed this method. These models use weighting factors based on the relationship between each habit plane and active slip system.

Further models have been proposed, based on one of the transformation laws, i.e. Bain, K–S or N–W, with the aim of predicting transformation textures in the presence of variant selection (Ray and Jonas, 1990). Factors taken into account in these previous models have included grain shape, habit planes, slip activity and residual stress, all of which have been considered to influence the final transformed texture. Nevertheless, no model has yet been proposed that can describe this phenomenon accurately. That is, no previous theoretical treatment has been able to predict the presence or absence of all the observed and missing variants, respectively.

The present variant selection model was deduced by examining the recent work of Liu and Bunge (1991). In their experiments, specimens with a sharp austenitic cube texture were cold rolled to a 10% reduction along different angles with respect to the initial rolling direction of [010]. Following rolling, the transformation to martensite was produced by cooling to −196°C. The five parent orientations, generated by rolling at angles of 0°, 11°, 21°, 31° and 45° to the initial rolling direction, were designated as (001)[0–10], (001)[−1–50], (001)[−2–50], (001)[−3–50] and
(001)[−1−10], respectively. The small amount of deformation applied to the original (cube-oriented) specimens resulted in samples possessing a single component (a slightly rotated cube component) prior to transformation, with enough strain to produce the dislocations that lead to variant selection. The general variant selection model derived from the above observations is also applicable to austenite that contains the fcc rolling texture prior to transformation (Butrón-Guillén et al., 1997).

TRANSFORMATION RELATIONSHIPS

The shearing of the austenite lattice that takes place during the transformation to martensite results in a lattice distortion described as a compression of about 17% along the c-axis of the martensite cell and a uniform expansion of about 12% in the (001) plane. The three transformation models introduced above, those of Bain, K–S, and N–W, are illustrated and compared on the (002) pole figures depicted in Fig. 1.

![Diagram of pole figures illustrating transformation relationships](image)

**FIGURE 1** (002) pole figure illustrating three transformation relationships with the initial cube (001)[100] orientation. The Bain variants are depicted on both pole figures and yield three possible variants. (a) The K–S relationship is shown to be a more precise representation as one Bain variant is surrounded by eight K–S variants resulting in twenty-four possible variants. (b) The N–W relationship is illustrated in relation to the Bain variants and yields twelve possible variants.
In 1924, Bain described the transformation as a 45° rotation about each of the three (100) axes. Three possible products are generated in this way, which are illustrated in Fig. 1(a). The Bain model is now too rudimentary for general use, but it nevertheless provides a good foundation for understanding the more complicated models. In 1930, Kurdjumov and Sachs characterised the austenite-to-ferrite or martensite transformation as involving a ±90° rotation about each of the twelve (112) rotation axes, yielding the twenty-four variants also shown in Fig. 1(a). The K–S relationship corresponds to the following parallelism conditions:

\[
\{111\}_\gamma \parallel \{110\}_\alpha, \\
\langle -101 \rangle_\gamma \parallel \langle 1-11 \rangle_\alpha.
\]

Four possible alternatives exist for the plane parallelism condition and six for the direction condition, yielding twenty-four possible variants. Five years later, N–W proposed yet another correspondence relationship, which can be specified as:

\[
\{111\}_\gamma \parallel \{110\}_\alpha, \\
\langle 1-10 \rangle_\gamma \parallel \langle 101 \rangle_\alpha.
\]

This model was described as involving rotations of 95.27° about a common \(hk1\) axis, where \(hk1 = \langle -1 + \sqrt{2} + \sqrt{3} \rangle\), resulting in the twelve possible variants shown in Fig. 1(b). It should be noted that the K–S and N–W orientations differ by about 5° about the austenite [111] direction.

Of the three models, experimental observations suggest that the present type of transformation is best described by the rotation relationship of K–S. However, the paper by Liu and Bunge that prompted the present research describes the transformation in terms of the N–W relations. The model introduced below will show that, although the pole figures seem to follow the N–W rotations, the K–S relations are in fact the appropriate ones to use to describe the orientation relationships observed.

THE PROPOSED MODEL

As indicated above, the present model was derived using the experimental data reported by Liu and Bunge (1991). It is based on the crystal
plasticity model of Bishop and Hill (1951a,b), also described by Hosford (1994), as well as the K–S transformation relationship. The rate-sensitive slip analysis of Zhou et al. (1991) was employed to determine the amount of slip on each active system.

**LINK Between the Bishop and Hill Slip Model and the Kurdjumov–Sachs Relationship**

In order to explain the occurrence of variant selection in terms of slip activity, a one-to-one relationship was developed between Bishop and Hill (B–H) and K–S. This was based on the analysis of Butrón-Guillén et al. (1996) and is illustrated in Table I. The B–H approach was devised independently of K–S and describes a single crystal as consisting of four octahedral slip planes (see Fig. 2(a)), with three Burgers vectors per plane. Because there are two possible slip directions for each vector, there is a total of twenty-four slip systems. It is important to note that the twenty-four slip systems correspond to the twenty-four K–S variants; for each variant, the K–S rotation axis is perpendicular to the respective slip direction or Burgers vector and lies on the slip plane. This is depicted in Fig. 2(b). As can be seen, each B–H slip system is paired with the corresponding (112) K–S rotation axis.

**Dislocation Reactions**

The limitations of the slip activity models listed above have led researchers to investigate further the appearance of variants that are not called for directly by the slip activity criterion (Abe et al., 1967; Haslam et al., 1973; Davies and Bateman, 1981; Liu and Bunge, 1991; Butrón-Guillén et al., 1998). In the present work, the concept of dislocation

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**Table I**

| Plane or axis (111) | Slipsystemandcorresponding (112) rotation axis |
|--------------------|-----------------------------------------------|
| {111}              |                                              |
| a (111)            | I     II   III | b (111) | I     II   III | c (111) | I     II   III | d (111) |
| (110)              | [011]  [101] [110] | [011]  [101] [110] | [011]  [101] [110] | [011]  [101] [110] |
| (112)              | [211]  [121] [112] | [211]  [121] [112] | [211]  [121] [112] | [211]  [121] [112] |
reactions is used to explain the presence of these additional variants. Basically, *inactive* product dislocations are formed by the in-plane reaction of two active dislocations.

These reactions take place when two Burgers vectors (b) combine to form a product vector (Weertman and Weertman, 1992), leading to the presence of a new Burgers vector not obtained from the slip analysis. This is depicted schematically in Fig. 3. The newly formed vectors, referred to from here on as product vectors, also play a role in the transformation, leading to the appearance of additional variants. However, dislocation reactions are not random events and certain rules must be applied.

On the (111) plane of Fig. 2, all the possible Burgers vectors are $\pm b_1, \pm b_2$, and $\pm b_3$, represented by the two senses of the (110) directions.
and denoted by Bishop and Hill as \( \mathbf{aI} \), \( \mathbf{aII} \) and \( \mathbf{aIII} \) with the respective Burgers vectors: \( \mathbf{b_1} = (a/2)[01\overline{1}] \), \( \mathbf{b_2} = (a/2)[\overline{1}01] \) and \( \mathbf{b_3} = (a/2)[1\overline{1}0] \). Thus the following combinations of parallel dislocations represented by \( \mathbf{b_1} \) and \( \mathbf{b_2} \) can be described:

\[
\begin{align*}
\mathbf{b_1} + \mathbf{b_2} &= (a/2)[01\overline{1}] + (a/2)[\overline{1}01] = (a/2)[-101] = -\mathbf{b_3}, \\
\mathbf{b_1} - \mathbf{b_2} &= (a/2)[01\overline{1}] - (a/2)[\overline{1}01] = (a/2)[1\overline{1}0].
\end{align*}
\]

However, the second reaction cannot in fact occur because this combination results in a higher self-energy. Similar distinctions apply to combinations of \( \mathbf{b_1} \) and \( \mathbf{b_3} \), and \( \mathbf{b_2} \) and \( \mathbf{b_3} \).

When it comes to dislocations travelling on cross-slip related planes and the Burgers vectors are identical and parallel, they will either annihilate each other (if they are of opposite sign) or increase their total self-energy, which is not possible. Finally, Lomer-Cottrell locks can form when reactions take place that involve dislocations on non-cross-slip related and intersecting slip planes. However, these phenomena do not play a role for the five orientations being studied and so are not
TABLE II  In-plane and other dislocation reactions. Here, LC locks are italicised and reactants formed as a resulting cross-slip are shown in normal type

| Reactants | aI | bI | cI | dI | -aI | -bI | -cI | -dI |
|-----------|----|----|----|----|-----|-----|-----|-----|
| aII       | -aIII | -dIII | -aIII | -dIII | *   | *   | *   | *   |
| bII       | -cIII | -bIII | -cIII | -bIII | *   | *   | *   | *   |
| cII       | -cIII | -bIII | -cIII | -bIII | *   | *   | *   | *   |
| dII       | -aIII | -dIII | -aIII | -dIII | *   | *   | *   | *   |
| -aII      | *   | *   | *   | *   | aIII | dIII | aIII | dIII |
| -bII      | *   | *   | *   | *   | cIII | bIII | cIII | bIII |
| -cII      | *   | *   | *   | *   | cIII | bIII | cIII | bIII |
| -dII      | *   | *   | *   | *   | aIII | dIII | aIII | dIII |

considered further here. A table that shows all the possible dislocation reactions that can take place in the present parent orientations is displayed in Table II (Sum et al., 1998). This is based on the work of Butrón-Guillén et al. (1998).

**METHODOLOGY OF TRANSFORMATION**

**TEXTURE PREDICTION**

It is difficult to verify or improve models for the prediction of transformation textures because it is generally not possible to measure the austenite texture prior to transformation directly. This challenge led to the creation of other methods, such as computer simulations of the transformation. Another approach involves the use of materials with metastable fcc phases at room temperature that are transformed to the bcc or bct phase by quenching to cryogenic temperatures. As both phases can be examined at room temperature, the initial and final textures can be measured directly, providing a basis for the construction of a solid model.

The present analysis is exactly of this type and relies on the observations of Liu and Bunge. Their experimental design was based on transformation of an Fe-30\%Ni alloy containing the cube texture after a 10\% rolling reduction was applied at various inclinations to the original rolling direction. Since only a single parent orientation was present in each case, determination of the transformation products was fairly straightforward. Generally, a parent cube texture produces a transformation texture that includes all twenty-four possible variants in the absence of variant selection. However, in the present case, variant selection was observed because of the additional 10\% rolling reduction...
after recrystallisation. The degree of deformation was selected to be low enough for the austenite to continue to display the cube (i.e. recrystallisation) texture and not so high as to convert this into the fcc rolling texture. It was also sufficient to introduce the dislocation density required for variant selection. The transformation textures reported by Liu and Bunge are reproduced here in the form of (200) pole figures and are presented in Fig. 4. (Additional pole figures of the (220) type can be found in the original reference.)

FIGURE 4 Reproduction of the (200) pole figures from Liu and Bunge's experimental transformation textures for the following parent orientations: (a) (001)[−1−50], (b) (001)[−2−50], (c) (001)[−3−50], (d) (001)[0−10] and (e) (001)[−1−10].
The transformation textures were predicted by employing the following sequential steps:

1. All the possible transformation products called for according to K–S for a given parent orientation in the absence of variant selection were first tabulated, together with their associated B–H slip systems and K–S rotation axes.
2. The shear rates for the present strain path (plane strain rolling) were calculated on each applicable slip system; these rates were added to the table described in (1) above.
3. The selection criteria (described in the next section) were then applied; these provided the predicted texture components, also identified on the tables.
4. A pole figure or an ODF was plotted displaying the predicted transformation texture.

In the present work, all twenty-four variants were calculated using K–S for each of the five initial crystallographic orientations. Each variant was linked to its respective rotation axis and possible slip system (step 1). The shear rates were derived from the slip activity programme of Zhou et al. (1991); it assumes that plane strain rolling is taking place and uses a rate-sensitive slip analysis to provide the shears associated with a unit increment of von Mises effective strain (step 2). The variant selection criteria outlined in the next sub-section were then applied (step 3). The five tables generated in this manner for the respective parent textures are presented in Tables III–VII.

The top row of these tables lists all the possible product orientations (in the form of Miller indices) that can be formed from the parent upon transformation. (The Miller indices only provide approximate descriptions of orientations that are specified more accurately by their Euler angles.) The first, second and third columns from the left characterise the twenty-four variants according to the slip systems and rotation axes with which they are associated. The product orientations are labelled as observed or not observed in accordance with the experimental findings. The predicted pole figures that correspond to these tables are illustrated in Fig. 5 (step 4). The filled symbols are the product orientations that have been selected, while the open symbols represent the products that have been eliminated using the present model. For comparison purposes, the actual textures reported in Fig. 4 are also reproduced on these pole figures and depicted in the form of intensity contours.
| Variant No. | Slip system | Rotation axis | Observed  | Not observed |
|------------|-------------|---------------|-----------|-------------|
|            |             |               | (100)[023] | (110)[−110] | (110)[−331] | (110)[−221] | (110)[−114] | (110)[−115] | (110)[001] |
| 1          | −bIII       | −1 −1 −2      |           | R           |             |             |             |             |             |
| 2          | −dIII       | −1 1 2        |           |             | R           |             |             |             |             |
| 3          | −eIII       | 1 −1 2        | R         |             |             |             |             |             |             |
| 4          | −aIII       | 1 1 −2        | R         |             |             |             |             |             |             |
| 5          | dII         | 1 2 1         |           | −0.015      |             |             |             |             |             |
| 6          | bII         | 1 −2 −1       | −0.033    |             |             |             |             |             |             |
| 7          | aII         | −1 2 −1       | −0.033    |             |             |             |             |             |             |
| 8          | cII         | −1 −2 1       | −0.015    |             |             |             |             |             |             |
| 9          | −cI         | −2 −1 −1      |           | −0.36       |             |             |             |             |             |
| 10         | −aI         | −2 1 1        |           |             | −0.82       |             |             |             |             |
| 11         | −bI         | 2 −1 1        |           |             | −0.82       |             |             |             |             |
| 12         | −dI         | 2 1 −1        | −0.36     |             |             |             |             |             |             |
| 13         | bIII        | 1 1 2         |           |             |             | NR          |             |             |             |
| 14         | dIII        | 1 −1 −2       |           |             |             |             | NR          |             |             |
| 15         | cIII        | −1 1 −2       |           |             |             |             |             | NR          |             |
| 16         | aIII        | −1 −1 2       |           |             |             |             |             |             | NR          |
| 17         | −dII        | −1 −2 −1      | 0.015     |             |             |             |             |             |             |
| 18         | −bII        | −1 2 1        | 0.033     |             |             |             |             |             |             |
| 19         | −aII        | 1 −2 1        | 0.033     |             |             |             |             |             |             |
| 20         | −cII        | 1 2 −1        | 0.015     |             |             |             |             |             |             |
| 21         | cI          | 2 1 1         | 0.36      |             |             |             |             |             |             |
| 22         | aI          | 2 −1 −1       | 0.82      |             |             |             |             |             |             |
| 23         | bI          | −2 1 −1       | 0.82      |             |             |             |             |             |             |
| 24         | dI          | −2 −1 1       | 0.36      |             |             |             |             |             |             |

R: reaction product; NR: no reaction takes place.
### TABLE IV  Predicted transformation texture components for the (001)[-2-50] parent orientation

| Variant No. | Slip system | Rotation axis | Observed | Not observed |
|------------|-------------|---------------|----------|-------------|
|            |             |               | (100)[012] | (100)[013] | (110)[-331] | (110)[-221] | (110)[-111] | (110)[-112] | (110)[-113] | (110)[-114] | (110)[-115] |
| 1          | -bIII       | -1 -1 -2      | R        |             |             |             |             |             |             |             |             |
| 2          | -dIII       | -1 1 2        | R        |             |             |             |             |             |             |             |             |
| 3          | -cIII       | 1 -1 2        | R        |             |             |             |             |             |             |             |             |
| 4          | -aIII       | 1 1 -2        | R        |             |             |             |             |             |             |             |             |
| 5          | dIII        | 1 2 1         | -0.026   |             |             |             |             |             |             |             |             |
| 6          | bII         | -1 -2 -1      | -0.14    |             |             |             |             |             |             |             |             |
| 7          | aII         | 1 2 -1        | -0.14    |             |             |             |             |             |             |             |             |
| 8          | cII         | 1 -2 -1       | -0.026   |             |             |             |             |             |             |             |             |
| 9          | -cI         | -2 -1 -1      | -0.16    |             |             |             |             |             |             |             |             |
| 10         | -aI         | -2 1 1        | -0.89    |             |             |             |             |             |             |             |             |
| 11         | -bI         | 2 -1 1        | -0.89    |             |             |             |             |             |             |             |             |
| 12         | -dI         | 2 1 -1        | -0.16    |             |             |             |             |             |             |             |             |
| 13         | bIII        | 1 1 -2        | NR       |             |             |             |             |             |             |             |             |
| 14         | dIII        | 1 -1 -2       | NR       |             |             |             |             |             |             |             |             |
| 15         | cIII        | -1 1 -2       | NR       |             |             |             |             |             |             |             |             |
| 16         | aIII        | -1 -1 2       | NR       |             |             |             |             |             |             |             |             |
| 17         | -dII        | -1 -2 -1      | 0.026    |             |             |             |             |             |             |             |             |
| 18         | -bII        | -1 2 1        | 0.14     |             |             |             |             |             |             |             |             |
| 19         | -aII        | 1 -2 1        | 0.14     |             |             |             |             |             |             |             |             |
| 20         | -cII        | 1 2 -1        | 0.026    |             |             |             |             |             |             |             |             |
| 21         | cI          | 2 1 1         | 0.16     |             |             |             |             |             |             |             |             |
| 22         | aI          | 2 -1 1        | 0.89     |             |             |             |             |             |             |             |             |
| 23         | bI          | -2 1 1        | 0.89     |             |             |             |             |             |             |             |             |
| 24         | dI          | -2 -1 1       | 0.16     |             |             |             |             |             |             |             |             |

R: reaction product; NR: no reaction takes place.
| Variant No. | Slip system | Rotation axis | Observed |         |         |         |         |         | Not observed |
|------------|-------------|---------------|----------|---------|---------|---------|---------|----------|--------------|
|            |             |               | (100)[013] | (110)[−221] | (110)[−332] | (110)[−111] | (110)[−112] | (110)[−113] | (110)[−114] |
| 1          | −bIII       | −1 −1 −2      | *         |         |         |         |         | R        |              |
| 2          | −dIII       | −1 1 2        | R         |         |         |         |         |          |              |
| 3          | −cIII       | 1 −1 2        | R         |         |         |         |         |          |              |
| 4          | −aIII       | 1 1 −2        | R         |         |         |         |         |          |              |
| 5          | dII         | 1 2 1         | −0.019    |         |         |         |         |          |              |
| 6          | bII         | 1 −2 −1       | −0.31     |         |         |         |         |          |              |
| 7          | aII         | −1 2 −1       | −0.31     |         |         |         |         |          |              |
| 8          | cII         | −1 −2 1       | −0.019    |         |         |         |         |          |              |
| 9          | −cI         | −2 −1 −1      | −0.053    |         |         |         |         |          | −0.85        |
| 10         | −aI         | −2 1 1        | −0.053    |         |         |         |         |          | −0.85        |
| 11         | −bI         | 2 −1 1        | NR        |         |         |         |         |          |              |
| 12         | −dI         | 2 1 −1        | NR        |         |         |         |         |          |              |
| 13         | bIII        | 1 1 2         | 0.019     |         |         |         |         |          |              |
| 14         | dIII        | 1 −1 −2       | 0.31      |         |         |         |         |          |              |
| 15         | cIII        | −1 1 −2       | 0.31      |         |         |         |         |          |              |
| 16         | aIII        | −1 −1 2       | 0.019     |         |         |         |         |          |              |
| 17         | −dII        | −1 −2 −1      | 0.053     |         |         |         |         |          |              |
| 18         | −bII        | −1 2 −1       | 0.85      |         |         |         |         |          |              |
| 19         | −aII        | 1 −2 −1       | 0.85      |         |         |         |         |          |              |
| 20         | −cII        | 1 2 −1        | 0.053     |         |         |         |         |          |              |
| 21         | cI          | 2 1 1         | 0.85      |         |         |         |         |          |              |
| 22         | aI          | 2 −1 −1       | 0.85      |         |         |         |         |          |              |
| 23         | bI          | −2 1 −1       | 0.85      |         |         |         |         |          |              |
| 24         | dI          | −2 −1 1       | 0.053     |         |         |         |         |          |              |

R: reaction product; NR: no reaction takes place.
TABLE VI  Predicted transformation texture components for the (001)[0–10] parent orientation

| Variant No. | Slip system | Rotation axis | Observed   | Not observed |
|-------------|-------------|---------------|------------|--------------|
|             |             |               | (100)[011] | (110)[-110] | (110)[001] |
| 1           | –bIII       | –1 –1 2       | R          |              |
| 2           | –dIII       | –1 1 2        | R          |              |
| 3           | –cIII       | 1 –1 2        | R          |              |
| 4           | –aIII       | 1 1 –2        | R          |              |
| 5           | dII         | 1 2 1         | **         |              |
| 6           | bII         | 1 –2 –1       | **         |              |
| 7           | aII         | –1 2 –1       | **         |              |
| 8           | cII         | –1 –2 1       | **         |              |
| 9           | –cI         | –2 –1 1       | –0.61      |              |
| 10          | –aI         | –2 1 1        | –0.61      |              |
| 11          | –bI         | 2 –1 1        | –0.61      |              |
| 12          | –dI         | 2 1 –1        | –0.61      |              |
| 13          | bIII        | 1 1 2         | NR         |              |
| 14          | dIII        | 1 –1 –2       | NR         |              |
| 15          | cIII        | –1 1 –2       | NR         |              |
| 16          | aIII        | –1 –1 2       | NR         |              |
| 17          | –dII        | –1 –2 –1      | *          |              |
| 18          | –bII        | –1 2 1        | *          |              |
| 19          | –aII        | 1 –2 1        | *          |              |
| 20          | –cII        | 1 2 –1        | *          |              |
| 21          | cI          | 2 1 1         | 0.61       |              |
| 22          | aI          | 2 –1 –1       | 0.61       |              |
| 23          | bI          | –2 1 –1       | 0.61       |              |
| 24          | dI          | –2 –1 1       | 0.61       |              |

*Slight slip from Gaussian distribution; **Slight "negative" slip from Gaussian. R: reaction product; NR: no reaction takes place.

Selection Criteria

1. Classical Slip Activity Rule

(a) Select dislocations that undergo positive slip (that have active Burgers vectors).
(b) Eliminate the bs associated with negative slip.
(c) This procedure leads to the selection of 4–8 variants.

2. In-plane Dislocation Reactions

(a) Dislocations with active Burgers vectors react on their glide planes to produce unstressed dislocations.
TABLE VII  Predicted transformation texture components for the (001)[−1−10] parent orientation

| Variant No. | Slip system | Rotation axis | Observed |
|-------------|-------------|---------------|----------|
|             |             | (001)[001]    | (110)[−111] | (110)[−112] |
| 1           | −bIII       | −1 1 2        | R        |
| 2           | −dIII       | −1 1 2        | R        |
| 3           | −cIII       | 1 1 2         | R        |
| 4           | −aIII       | 1 1 2         | **       |
| 5           | dIII        | 1 2 1         | **       |
| 6           | bIII        | 1 2 1         | 0.61     |
| 7           | aIII        | −1 2 −1       | 0.61     |
| 8           | cII         | −1 2 −1       | **       |
| 9           | −cI         | −2 1 1        | **       |
| 10          | −aI         | −2 1 1        | 0.61     |
| 11          | −bI         | 2 1 1         | 0.61     |
| 12          | −dI         | 2 1 1         | **       |
| 13          | bIII        | 1 1 2         | R        |
| 14          | dIII        | 1 1 2         | NR       |
| 15          | cIII        | −1 1 2        | NR       |
| 16          | aIII        | −1 1 2        | R        |
| 17          | −dIII       | −1 2 −1       | *        |
| 18          | −bIII       | −1 2 1        | 0.61     |
| 19          | −cIII       | 1 2 1         | 0.61     |
| 20          | −cI         | 2 1 1         | *        |
| 21          | aI          | 2 1 1         | *        |
| 22          | bI          | −2 1 1        | 0.61     |
| 23          | dI          | −2 1 1        | 0.61     |
| 24          |             |               |          |

*Slight slip from Gaussian distribution; **Slight “negative” slip from Gaussian.

R: reaction product; NR: no reaction takes place.

(b) Sign Rule:

(i) If the shear rates in two systems are unequal, the sign of the system with the larger shear is adopted. The sign of the “weaker” system is then reversed, so that the dislocation line vectors are parallel at the point of contact (see Fig. 3). For example in the case of Burgers vectors +bI and −bII, where +bI and −bII are the “stronger” and “weaker” systems, respectively, this leads to:

\[ bI(\text{large shear}) + (-bII(\text{small shear})) \rightarrow \text{sign change} \]
\[ \rightarrow bI + bII \rightarrow -bIII. \]

(ii) If the shear rates in two systems are equal, both of the possible products (Burgers vectors) are selected. In the above example, this
FIGURE 5 (200) pole figures of the predicted transformation textures (filled symbols) of the following parent orientations: (a) (001)[−1−50], (b) (001)[−2−50], (c) (001)[−3−50], (d) (001)[0−10] and (e) (001)[−1−10]. Open symbols represent K–S variants that are not selected by the present approach.

corresponds to:

1. $\mathbf{b}_I + (-\mathbf{b}_{II}) \rightarrow$ sign change $\rightarrow \mathbf{b}_I + \mathbf{b}_{II} \rightarrow -\mathbf{b}_{III}$, as well as
2. $\mathbf{b}_I + (-\mathbf{b}_{II}) \rightarrow$ sign change $\rightarrow -\mathbf{b}_I + (-\mathbf{b}_{II}) \rightarrow +\mathbf{b}_{III}$.

By taking these in-plane reactions into account, further variants are selected, in addition to the "active slip" ones described above.
RESULTS AND DISCUSSION

By comparing Figs. 4 and 5, it is evident that the textures predicted using the above approach are in excellent agreement with the experimental textures obtained by Liu and Bunge for the five starting orientations. In this section, the slip activity and dislocation reaction criteria are considered individually, first for the “intermediate” cases and then for the two “extreme” parent orientations.

Intermediate Parent Orientations

Here the intermediate parent orientations are (001)[−1−50], (001)[−2−50] and (001)[−3−50].

Slip Activity Variants

The variants with positive shears, considered as the active slip systems, are selected and those with negative slip are eliminated. In the intermediate cases, eight variants are selected. The active slip systems are identical for all the intermediate parent orientations and are: \(aI, bI, cI, dI, -aII, -bII, -cII\) and \(-dII\), with shears that vary as listed in Tables III–V. The negative slip systems are the negatives of the above eight and are thus responsible for eight “absent” orientations.

The first of the intermediate parent orientations is (001)[−1−50] (refer to Table III). Employment of the positive shear criterion leads to the selection of (100)[023] as the transformation component expected in the experimental texture. This orientation is illustrated by a star symbol in Fig. 5(a). The product arises from the following active slip systems and respective shear rates: \(aI\) (0.82), \(bI\) (0.82), \(cI\) (0.36), \(dI\) (0.36), \(-aII\) (0.033), \(-bII\) (0.033), \(-cII\) (0.015) and \(-dII\) (0.015). Similarly, the (110)[−115] and (110)[001] orientations that are associated with the negatives of the above-mentioned slip systems are eliminated and are not in fact experimentally observed. These are denoted by the open square and open trapezoid symbols of Fig. 5(a).

An important point to note in the pole figure is the presence of four “sub-spots” at the cube reflection (centre of the pole figure). (These also appear in the (001)[−2−50] pole figure.) These spots can be seen from Table III to be associated with relatively heavy slip (0.82, 0.82, 0.36 and
0.36) on systems \( aI, bI, cI \) and \( dI \), respectively. By contrast the relatively light slip (0.03, 0.03, 0.02 and 0.02) on systems \(-aII, -bII, -cII \) and \(-dII\), respectively, explains why the sub-spots identified with these systems are much weaker and cannot in fact be distinguished from the background intensity at this location. (Similar remarks apply to the \((001)[-2-50]\) parent, although the differences in the amounts of shear (see below) are somewhat reduced in this case.) Such an explanation, based on relative slip activity, is an alternative to the conclusion that the transformation is taking place according to the \( N-W \) mechanism.

In the second intermediate case, \((001)[-2-50], (100)[012]\) and \((100)[013]\) are selected as the transformed components using the positive slip rule and are represented on Fig. 5(b) by the star symbol once again. The slip systems and shears responsible for these products are: \( aI (0.89), bI (0.89), -cII (0.026), -dII (0.026) \) and \( cI (0.16), dI (0.16), -aII (0.14), -bII (0.14) \), respectively. The \((110)[-113]\) and \((110)[-114]\) components are eliminated as they have the respective negative slips: \(-cI (-0.16), -dI (-0.16) \) and \(-aI (-0.89), -bI (-0.89) \). These components are denoted by the open triangle and open circle symbols, respectively, on Fig. 5(b). This is also clearly shown in Table IV.

The final intermediate \((001)[-3-50]\) parent produces the \((100)[013]\) product orientation (again depicted as the star symbol) when obeying the positive slip rule. The slip systems of interest are once again: \( aI, bI, cI, dI, -aII, -bII, -cII, \) and \(-dII\), with respective shear rates of 0.85, 0.85, 0.053, 0.053, 0.31, 0.31, 0.019 and 0.019. Application of the negative slip rule eliminates the otherwise possible \((110)[-112]\) and \((110)[-113]\) components from the final transformed texture. The symbols used to represent these two orientations are the open diamond and open triangle, respectively. These results are shown in Table V and Fig. 5.

In this case, the four sub-spots observed in the two previous pole figures are replaced by a simple “two-lobed” shape. In terms of slip activity, these lobes can be attributed directly to \((aI \text{ and } -aII)\) on the one hand and \((bI \text{ and } -bII)\) on the other. (Note that the “a” and “b” slip planes are on opposite sides of the B–H pyramid of Fig. 2(a).) That is, the loss of \( cI \) and \( dI \) as significant slip systems is responsible for the disappearance of their associated spots, while the new “spots” attributable to the operation of the \(-aII \text{ and } -bII\) systems merge with those due to their close neighbours, \( aI \) and \( bI \), respectively. These
pairs are adjacent to each other in opposite quadrants of the pole figure of Fig. 1 while the four sub-spots they replace are located in four separate quadrants.

**Dislocation Reaction Approach**

In all three of the intermediate cases, additional symbols appear on the pole figures: these correspond to variants with *unstressed* dislocations and are denoted as “R” (reaction product) or “NR” (no reaction can take place) on Tables III–V. Some of the variants represent orientations that are selected using the dislocation reaction criterion (see below). The remainder represents variants associated with Burgers vectors that cannot be formed according to the present rules.

The reactions that are possible are illustrated in Table II, together with the respective products. The Burgers vectors that result from in-plane reactions are denoted in bold face type and lie along the upper left to lower right diagonal. Here the sign rule from Selection Criterion 2(b)(i) applies to the in-plane dislocation reactions produced from the active Burgers vectors in the intermediate cases. Essentially, the less active Burgers vector undergoes the sign change, whereas the more active one preserves its sign. In all of the three intermediate cases, the following in-plane reactions take place:

\[
(+a_I (\text{large shear})) + (-a_{II} (\text{small shear})) \rightarrow \text{sign change} \rightarrow a_I + a_{II} \rightarrow -a_{III},
\]
\[
(+b_I (\text{large shear})) + (-b_{II} (\text{small shear})) \rightarrow \text{sign change} \rightarrow b_I + b_{II} \rightarrow -b_{III},
\]
\[
(+c_I (\text{large shear})) + (-c_{II} (\text{small shear})) \rightarrow \text{sign change} \rightarrow c_I + c_{II} \rightarrow -c_{III},
\]
\[
(+d_I (\text{large shear})) + (-d_{II} (\text{small shear})) \rightarrow \text{sign change} \rightarrow d_I + d_{II} \rightarrow -d_{III}.
\]

In the case of the (001)[−1−50] parent sample, the (110)[−110] and (110)[−221] orientations, indicated by the filled circle and filled pentagon symbols, respectively, on Fig. 5(a), result from the formation of −c_{III}, −d_{III} and −a_{III}, −b_{III}, respectively, on *unstressed* slip systems and are identified by R on Table III. These reactions are illustrated in Table II. However, the (110)[−331] product (open rectangle) is also classified as an experimentally observed component even though the variants responsible for this orientation are associated with negative shear rates. By the selection criteria listed in the previous section, this component is not in fact selected. It only appears in the observed group
because it lies midway between two predicted components, i.e. (110)[−110] and (110)[−221].

Turning to the (001)[−2−50] parent, it is apparent that the appearance of the (110)[−331] and (110)[−111] transformation components is justified by the dislocation reactions that produce the inactive dislocations (denoted by R on Table IV) associated with the variants of interest (see Table 2). As in the above case, the observed (110)[−221] orientation (open pentagon) is neither a slip activity nor a reaction component. Once again, it is only an apparent and not a true variant, as it arises from the overlap of the neighbouring (110)[−331] and (110)[−111] orientations, illustrated on Fig. 5(b) as the filled square and filled circle, respectively.

The (001)[−3−50] case displays the same characteristics as the previous two “intermediate” parent orientations. The (110)[−221] (filled pentagon) and (110)[−111] (filled circle) components seen on Fig. 5(c) are present as a result of the formation of the unstressed dislocations, −cIII, −dIII and −aIII, −bIII, respectively, marked by R on Table V. The (110)[−332] (open rectangle) is not predicted, but again appears because it lies midway between (110)[−221] and (110)[−111].

The variants that remain and have not been referred to are not selected and do not in fact appear in the experimental transformation textures because no reaction can take place to produce them. These components and their respective variants are illustrated as open symbols (like the negative slip components) in Fig. 5 and are denoted by “NR” in the tables.

**Extreme Parent Orientations**

Here the (001)[0−10] and (001)[−1−10] parent orientations are considered in turn. Variant selection was observed due to the additional 10% rolling reduction applied along the initial [010] rolling direction in the cube material and 45° to it in the rotated cube sample.

**Cube Parent: Slip Activity Variants**

The active slip systems for the starting cube orientation (001)[0−10] are: aI (0.61), bII (0.61), cII (0.61) and dII (0.61). These lead to the selection of the (100)[011] rotated cube transformation component. This orientation was also observed in the experimental texture of Liu and Bunge, as illustrated in Fig. 4(d). The predicted component is depicted by the star
symbol and shown on Fig. 5(d). The (110)[001] orientation represented by the open trapezoid was not observed in the experiments and is eliminated by the negative slip rule (see Table VI and Fig. 5(d)).

In addition, the \(-a_{II}, -b_{II}, -c_{II}\) and \(-d_{II}\) slip systems (marked by the \((*)\) in Table VI) can be considered to carry a slight amount of positive slip due to the Gaussian scatter that is present about the exact cube parent, i.e. the presence of grains with orientations running from the exact cube all the way to the (001)[1\(-5\)0] orientation (see Table III and Fig. 5(a)). In the perfect cube, these systems would not be activated. However, grains with orientations approaching the (001)[1\(-5\)0] (as well as the (001)[1\(-5\)0], (001)[1\(-5\)0] and (001)[150]) will contain the active systems listed in Table III. The slip systems denoted by \((**)\) represent the slight negative shears that exist as a result.

As in the case of the (001)[1\(-5\)0] and (001)[2\(-5\)0] parent orientations, heavy slip on the \(a_{II}, b_{II}, c_{II}\) and \(d_{II}\) systems (see Table VI) is responsible for the four sub-spots that are evident at the rotated cube reflection (centre of the pole figure). The very slight slips on the \(a_{II}, b_{II}, c_{II}\) and \(d_{II}\) systems in the grains that do not coincide perfectly with the cube parent orientation only contribute to the diffuse background intensity in this region.

**Cube Parent: Dislocation Reaction Approach**

The (110)[1\(-1\)0] rotated Goss component was also observed experimentally and is justified in the present approach by the dislocation reaction criterion. The slip systems necessary to produce this orientation are: \(a_{I}, b_{I}, c_{I}, d_{I}, -a_{II}, -b_{II}, -c_{II}\) and \(-d_{II}\). Here the sign rule (Selection Criterion 2(b)(i)) applies and leads to the reaction products \(-a_{III}, -b_{III}, -c_{III}\) and \(-d_{III}\), denoted by "R" in Table VI. This orientation is shown as the filled circle symbol on Fig. 5(d).

**Rotated Cube Parent: Slip Activity Variants**

The (001)[1\(-1\)0] rotated cube parent gives rise to the (100)[001] cube orientation, represented by the filled star on Fig. 5(e). It is a result of the following positive slip activities: \(a_{I} 0.61, b_{I} 0.61, -a_{II} 0.61\) and \(-b_{II} 0.61\) (see Table VII). The \((*)\) seen in this column again represents the slight shears that arise for the \(c_{I}, d_{I}, -c_{II}\) and \(-d_{II}\) slip systems from
the Gaussian scatter that is present about the exact rotated cube orientation, i.e. the presence of grains that run from the rotated cube to the (001)[−3−50] orientation. They are assumed to have shear rates that approach those of the (001)[−3−50] parent (see Table V). The (**) symbol denotes the slight negative slip that is associated with these systems.

Examination of Table V indicates that six systems carry most of the shear in the near-rotated cube case; these are aI/bI, −aII/−bII and cI/dI. (The −cII/−dII systems are only associated with negligible amounts of slip.) Thus the six “lobes” evident at the cube reflection can be considered to be identified with the above six systems.

**Rotated Cube Parent: Dislocation Reaction Approach**

The (110)[−111] and (110)[−112] components are observed via dislocation reactions involving the active Burgers vectors. The (110)[−111] orientation (filled circle) is present from the reactions that take place on the e and d planes. The products −cIII and −dIII marked by R in Table VII arise when the active Burgers vectors (cI, −cII, dI and −dII) react and the sign rule from Selection Criterion 2(b)(i) is applied. Conversely, cIII and dIII do not form as no reaction can take place. These are denoted by NR in Table VII.

The (110)[−112] component is selected by the in-plane reactions of aI, −aII and bI, −bII; these form ±aIII and ±bIII, respectively. In this case, the sign rule of Selection Criterion 2(b)(ii) applies, i.e. the aI, −aII and bI, −bII systems all carry equal shears, and either sign can be adopted for the reaction product as long as the dislocation lines are parallel (Fig. 3). Thus the rule leads to the formation of both sets of products, as shown in Table II. These variants are depicted by R in Table VII and appear as filled diamond symbols on Fig. 5(e).

**Comparison between Predictions and Observations**

The predictions obtained using the selection criteria that were illustrated in Fig. 5 are in excellent agreement with the experimental textures, also depicted on the figure. The slip activity and dislocation reaction variants actually appear in the experimental textures, while those that would be present in the absence of variant selection are eliminated using the classical slip activity rule and the in-plane dislocation reaction criterion.
Another point of significance concerns the various spots and sub-spots present in the pole figures of Fig. 4 and interpreted here as being associated with the slip systems selected by the slip activity rules. Thus the present analysis supports the view that the transformation occurs by the K–S mechanism and not according to the N–W relationship, as concluded by Liu and Bunge.

ODF Representation of the Texture Predictions

The transformation texture predictions obtained using the present model are also illustrated on the $\varphi_2 = 45^\circ$ ODF sections of Figs. 6 and 7. Figure 6(a) depicts the transformation variants chosen for the five parent...
orientations by Selection Criterion 1(a). All these variants are associated with *positive* shears. According to this rule, eight components are selected for each of the parent orientations. These components run inwards along the cube fibre, from $\varphi_1 = 0^\circ$ and $\varphi_1 = 90^\circ$ to the centre ($\varphi_1 = 45^\circ$), where they meet at the transformed rotated cube component. Moving from the edges inward in Fig. 6(a), the diamond symbol represents the cube products while the rectangles depict the (001)[−1−50] products. In both cases, all eight of the slip systems shown are operative.
The first set of triangles that represent the (001)[−2−50] transformation components correspond to the \( \mathbf{aI}, \mathbf{bI} \) and \(-\mathbf{cII}, -\mathbf{dII}\) slip systems, whereas the second set appears due to the positive shears on \( \mathbf{cI}, \mathbf{dI} \) and \(-\mathbf{aII}, -\mathbf{bII}\). The ring symbol represents the components selected for the (001)[−3−50] parent; here again, as in the case of the rotated cube (see below), all eight positive slip systems are identified with a single symbol. Finally, the star symbol located at \( \varphi = 0^\circ \) and \( \varphi_1 = 45^\circ \) is the transformation product of the rotated cube.

The orientations seen on Fig. 6(b) correspond to an approximate \{331\} fibre and are associated with the negatives of the above-mentioned slip systems. Hence these components are predicted not to appear in the final transformation texture. In contrast to Fig. 6(a), however, the symbols only represent single pairs of slip systems.

Figure 6(c) illustrates the transformation products that form from the in-plane dislocation reactions that involve the active Burgers vectors. These orientations form the partial \{110\} fibre that begins at the rotated Goss position and overlaps the opposite partial Goss fibre slightly. This overlap occurs because of the “spread” of the K–S variants about the exact Bain position. (That is, there would be no overlap in the case of an exact Bain transformation.) The reaction Burgers vectors responsible for the cube and intermediate products are \(-\mathbf{aIII}, -\mathbf{bIII}, -\mathbf{cIII}\) and \(-\mathbf{dIII}\). The transformed components for the rotated cube arise from the \(-\mathbf{aIII}, -\mathbf{bIII}, \mathbf{aIII}, \mathbf{bIII}\) and \(-\mathbf{cIII}, -\mathbf{dIII}\) slip systems, see Table VII.

The orientations illustrated on Fig. 6(d) belong to those that are not predicted to appear as part of the transformation texture since they cannot form from dislocation reactions involving the active Burgers vectors. These orientations run along the partial \{110\} fibre that begins at the Goss orientation and overlaps the opposite partial \{110\} fibre (due to the geometry of the K–S transformation, as mentioned above). The results of Fig. 6(a)–(d) are collected and summarised in Fig. 7.

**Practical Implications**

During the hot rolling of austenite, the cube texture generally forms, with an intensity that is dependent on the accumulated strain prior to each cycle of recrystallisation. If the recrystallised austenite undergoes no further straining before transformation, then ferrite (or martensite) components near the rotated cube, Goss and rotated Goss can be
expected to appear, as called for by the Bain relations. However, as can be seen from this work (Fig. 7), if the recrystallised austenite is subjected to small amounts of strain prior to transformation, then the Goss component will be suppressed and only the rotated cube and rotated Goss will appear.

CONCLUSIONS

The present model has been used to predict the textures arising from the transformation of five parent austenite orientations: (001)[0–10], (001)[–1–50], (001)[–2–50], (001)[–3–50] and (001)[–1–10]. These predictions were then compared with the observations of Liu and Bunge on a rolled Fe–30%Ni steel alloy. The following conclusions can be drawn from this work:

(1) The textures predicted using the present variant selection criteria agree very well with the experimental findings of Liu and Bunge. The starting cube orientation is predicted to contain the rotated cube and rotated Goss components, as observed experimentally.
The intermediate parents all have similar transformation textures, with rotations, however, that are proportional to their respective angles of inclination with respect to the initial [010] rolling direction. The rotated cube parent also exhibits a texture that is in agreement with the predictions.

(2) The classical slip activity rule results in the selection of eight variants corresponding to the following active slip systems: +aI, +bI, +cI, +dI, -aII, -bII, -cII and -dII. These are responsible for forming the components of the cube fibre for all five parents defined in terms of Miller indices as (100)[023], (100)[012] and (100)[013] on the pole figures and as the cube fibre on the $\varphi_2 = 45^\circ$ ODF section.

(3) According to the same criterion, the \{331\} fibre on the $\varphi_2 = 45^\circ$ ODF section, and the equivalent near-rotated Goss to the near-Goss reflections on the pole figures, are not selected. This is because they correspond to negative shears on the slip systems responsible for their formation. These are the negatives of the above eight slip systems, i.e. -aI, -bI, -cI, -dI, +aII, +bII, +cII and +dII.

(4) The rotated Goss and near-rotated Goss reflections on the pole figures, which are equivalent to a partial \{110\} fibre on the $\varphi_2 = 45^\circ$ ODF section are selected as being attributable to in-plane dislocation reactions. The unstressed dislocations that form in this way from the active Burgers vectors are -aIII, -bIII, -cIII and -dIII.

(5) Finally, the remaining unstressed slip systems are +aIII, +bIII, +cIII and +dIII. These Burgers vectors cannot form because no reaction can take place given the active Burgers vectors that are available. In the absence of variant selection, they would lead to the appearance of the Goss and near-Goss reflections (or the equivalent partial \{110\} fibre emanating from the Goss corner of the $\varphi_2 = 45^\circ$ ODF section).

(6) Transformation of the present Fe–30%Ni alloy appears to follow the K–S relationship rather than the N–W mechanism that was considered to apply by Liu and Bunge. The appearance of four spots instead of eight for the parent cube, (001)[-1-50], and (001)[-2-50] samples is interpreted here as being due to heavy slip on four of the eight possible slip systems, i.e. one on each of four separate slip planes. In a similar manner, the appearance of the “two-lobed” shape in the cube fibre reflection for the (001)[-3-50] sample has a detailed explanation in terms of a shift to slip on two pairs of adjacent systems, which share a common plane in each case.
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