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Refinement of orientation relations occurring in phase transformation based on considering only the orientations of the variants

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The paper describes a general way to deduce the orientation relation (OR) occurring in phase transformation by considering only the orientations of a sufficient number of variants inherited from the same parent grain. Our current solution, which can be viewed as an optimization scheme using quaternion facilities, differs greatly from previous attempts proposed by other authors. The efficiency of the method is illustrated by searching for the OR determined from the variants of a transformed low-carbon steel.

Keywords: Phase transformations; Variants; Orientation relation determination; Steels

The mechanical properties of a material are strongly dependent on its microstructure, which derives mainly from phase transformation. At room temperature, the inherited phase is formed of variants linked to the parent high-temperature phase by orientation relations (ORs) (e.g. Nishiyama–Wassermann (NW) or Kurdjumov–Sachs (KS) ORs in steel transformation). Improving materials requires effective control of the orientation inheritance and of the variant selection. This implies an accurate knowledge of the parent and inherited microtextures as well as the OR. However, in general, the direct determination of the high-temperature parent microstructures is not easy. Several authors have therefore proposed methods to determine the parent microtexture when the ORs are known [1–3]. In this context, the determination of the representative ORs, which in steels may differ from those of NW or KS, is of particular interest. When a sufficient amount of the parent phase is retained at room temperature, it is possible to deduce a representative OR [4–9]. When this is not the case, Miyamoto et al. [10] briefly present a numerical method for determining the OR occurring in the steel phase transformation. This method uses the orientations of the variants to roughly evaluate the orientation of the parent

austenite grain considering a defined OR (that of NW or of KS). The OR and the estimated parent orientation are then modified so that the sum of the deviations between the recalculated parent from each variant and their average becomes the smallest. When the minimum of the average deviation is reached, the OR and the parent orientation are assumed by the authors to be the best fitting.

We propose an analytical approach to determine the OR from a sufficient number of measured variants inherited from the same parent grain. The solution is quickly obtained analytically and can be adapted to any type of transformation.

Let us start with some brief reminders on the orientation links between parent and inherited orientations occurring in phase transformations. In a parent-to-daughter phase transformation, the orientation of a given daughter variant can be characterized by a rotation g_{vi} which is the product of several rotations (using the notations and conventions given in Ref. [11]):

$$g_{vi} = D_j \cdot \Delta g \cdot P_i \cdot g_0, \quad (1)$$

where g_0 is the rotation characterizing the parent crystal orientation. This orientation makes the sample reference frame parallel to that of the cubic parent. P_i is one of the n_p rotational symmetry elements of the parent phase. OR Δg , which describes the parent-to-daughter transformation, rotates the reference frame of the parent crystal relative to the reference frame of the daughter

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crystal. The choice of a rotation P_i leads to a particular daughter variant. D_j is one of the n_D rotations of the rotational symmetry elements of the daughter lattice. It does not change the orientation of the daughter variant determined by P_i and Δg . Analysis of relation (1) shows that the number of variants does not exceed n_P and can be less (12 for NW and 24 for KS). Conversely, variant g_{vi} can be related to a set of n_D potential parent orientations according to the relation:

$$P_n \cdot \Delta g^{-1} \cdot D_m \cdot g_{vi}, \quad (2)$$

where Δg^{-1} is the inverse OR and P_n and D_m are symmetry elements. Of course, the orientation g_0 is obtained from relation (2) when among the n_P rotational symmetry elements of the parent phase, the symmetry element P_n equals P_i^{-1} , and among the n_D rotations of rotational symmetry elements of the daughter lattice, the symmetry element D_m equals D_j^{-1} . The same type of relation is required irrespective of the variant considered. Consequently, the orientation g_0 corresponds to the unique common orientation shared by all the sets of potential parent (see Ref. [11]) and is expressed by:

$$g_0 = P_{n(i)} \cdot \Delta g^{-1} \cdot D_{m(j)} \cdot g_{vi}, \quad (3)$$

where $P_{n(i)}$ and $D_{m(i)}$ are the specific known symmetry elements for each variant i of the parent and inherited phases. To obtain a unique solution, the number of variants must be sufficient. By considering random choices of variants, one can easily show [1] that 4 different variants out of the 12 in the case of the NW OR always allow the parent orientation to be determined. This number equals 7 (out of 24) in the case of the KS OR. Of course some limited combinations of two specific variants also allow the unique solution to be found.

When the OR is not strict or when the orientations of the variants are determined with errors or are slightly modified by local plastic deformation induced by the transformation itself, relation (3) does not strictly hold. Nevertheless the rotations expressed by $P_{n(i)} \cdot \Delta g^{-1} \cdot D_{m(j)} \cdot g_{vi}$ remain close to each other. Therefore in a first

step, the parent orientation represented by g_0 and $P_{n(i)}, D_{m(j)}$ can be evaluated as in Ref. [11] for a given Δg (NW or KS OR). When the differences between rotations $P_{n(i)} \cdot \Delta g^{-1} \cdot D_{m(j)} \cdot g_{vi}$ are not negligible, this indicates that the chosen OR is not the best representative of the real one. In that case, one can find a statistically more representative OR so that it reduces, on average, the difference between each rotation $P_{n(i)} \cdot \Delta g^{-1} \cdot D_{m(j)} \cdot g_{vi}$. This implicitly leads also to obtaining the best estimate of the parent orientation $\langle g_0 \rangle$ which is simply the mean value of the rotations $P_{n(i)} \cdot \Delta g^{-1} \cdot D_{m(j)} \cdot g_{vi}$ [11], once the best Δg is found.

The search for this best representative OR can be seen as an optimization problem which can be efficiently solved by expressing rotations with quaternions. The product of rotations in relation (3) corresponds to a quaternion Q depending on the OR Δg , the other rotations being fixed and known (see above). For variant i , the corresponding quaternion is $Q^i(\Delta g^{-1})$. It can be seen that reducing the difference between the rotations $P_{n(i)} \cdot \Delta g^{-1} \cdot D_{m(j)} \cdot g_{vi}$ amounts to maximizing the norm of the sum of quaternions $Q^i(\Delta g^{-1})$.

This is illustrated in Fig. 1. The norm of sum of two vectors (the quaternions considered here are unitary

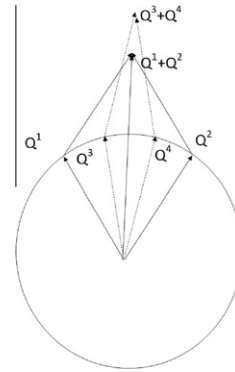


Figure 1. The norm of the sum of two unitary vectors is higher when the two vectors are closer.

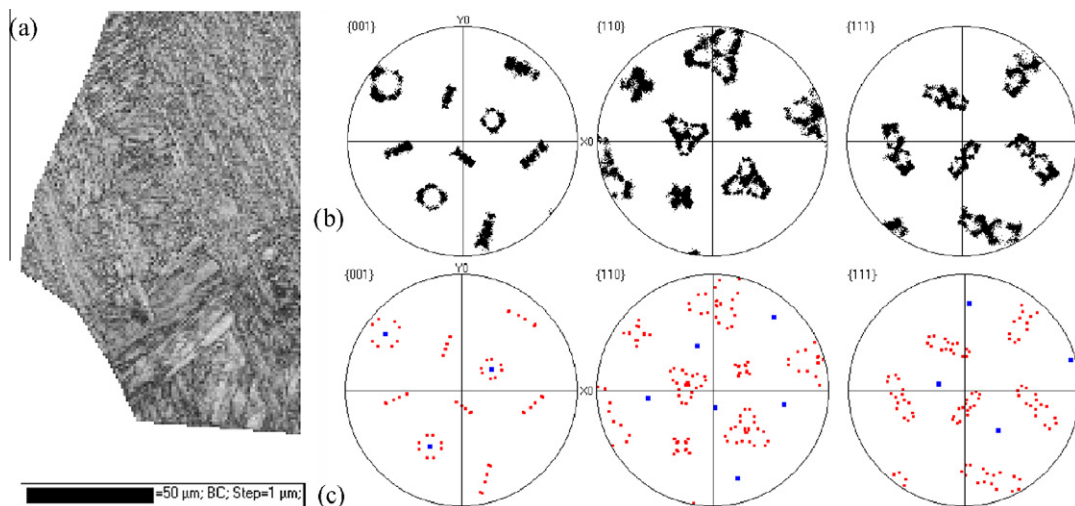


Figure 2. (a) microstructure of the investigated γ transformed grain; (b) orientations of the 14,792 α pixels represented by pole figures; (c) the same pole figures with the calculated parent γ orientation (blue squares) and the recalculated variants (red squares) according to the OR determined. (For interpretation of the references in colour in this figure legend, the reader is referred to the web version of this article.)

vectors of R^4) is higher when the two vectors become closer. At the same time their difference decreases. This result extends irrespective of the number of unitary vectors involved.

Using quaternion properties and multiplication rules [13], the components z_k of a quaternion product $Z = P * Q$ of quaternions $P \equiv (p_0, p_1, p_2, p_3)$ and $Q \equiv (q_0, q_1, q_2, q_3)$ representing a product of rotations can be alternatively expressed by:

$$\begin{aligned} \begin{bmatrix} z_0 \\ z_1 \\ z_2 \\ z_3 \end{bmatrix} &= \begin{bmatrix} p_0 & -p_1 & -p_2 & -p_3 \\ p_1 & p_0 & -p_3 & p_2 \\ p_2 & p_3 & p_0 & -p_1 \\ p_3 & -p_2 & p_1 & p_0 \end{bmatrix} \cdot \begin{bmatrix} q_0 \\ q_1 \\ q_2 \\ q_3 \end{bmatrix} \\ &= \begin{bmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & q_3 & -q_2 \\ q_2 & -q_3 & q_0 & q_1 \\ q_3 & q_2 & -q_1 & q_0 \end{bmatrix} \cdot \begin{bmatrix} p_0 \\ p_1 \\ p_2 \\ p_3 \end{bmatrix} \end{aligned} \quad (4)$$

Thanks to these equivalent writings, each product of rotations such as $P_{n(i)} \cdot \Delta g^{-1} \cdot D_{m(j)} \cdot g_{vi}$ can be represented by a quaternion Q^i whose components are related to the components of the quaternion $X \equiv (x_0, x_1, x_2, x_3)$ representing Δg^{-1} by a relation of type:

$$q_k^i = \sum_{l=1}^4 M_{kl}^i \cdot x_l \quad (5)$$

In this relation, M_{kl}^i are the components of a 4×4 matrix M which are functions of the components of quaternions describing g_{vi} , $P_{n(i)}$ and $D_{m(j)}$. An important point is that a rotation is represented by two opposite quaternions. One has to be aware of this when calculating the components of M .

The search for the most representative Δg^{-1} , expressed in the text above, amounts to maximizing the norm of the sum of quaternions Q^i by finding the convenient unitary quaternion X .

For that purpose, one has to find the components of quaternion X that maximize the expression:

$$\sum_{k=1}^4 \left(\sum_{l=1}^4 \sum_i M_{kl}^i \cdot x_l \right)^2 + \lambda \left(1 - \sum_{l=1}^4 (x_l)^2 \right). \quad (6)$$

This is a classical problem of maximization under constraints (X must be unitary) involving Lagrange multipliers λ . The solution is obtained by analysing the four eigenvalues λ and the corresponding eigenvectors of the 4×4 matrix $A^T A$, the product of the transposed matrix A and matrix A . The components of matrix A are the sum of the corresponding components of matrix M^i calculated from each variant:

$$A_{kl} = \sum_i M_{kl}^i. \quad (7)$$

The analysis of the four eigenvalues λ of matrix $A^T A$ allows conclusions to be drawn on the multiplicity and relevance of the solution. When one eigenvalue is much greater than the three others, the maximization problem has a unique solution. In that case, the unitary eigenvector associated with this highest eigenvalue maximizes

expression (6). It corresponds to the quaternion X_0 representing the best representative inverse OR (Δg_0^{-1}). The multiple solutions arising when several eigenvalues have similar high values and their significances are not discussed in this paper.

Once the best representative solution X_0 is found, the value of the best estimated orientation $\langle g_0 \rangle$ of the parent follows: it corresponds simply to the normalized sum of quaternions $Q^i (\Delta g_0^{-1})$.

To illustrate the efficiency of this method, we have determined the OR and the parent orientation from the α (body-centred cubic) variants of a former γ face-centred cubic grain of a low-carbon steel with a chemical composition (mass%) of 0.2C, 2 Mn, 20 ppm P, Fe balance. The sample was heat-treated at 950 °C for 10 min followed by a water quenching plus a tempering at 300 °C for 5 min. The orientation map was determined by electron backscatter diffraction with a step size of 1 μ m. 14792 pixels were measured on the grain being studied. The Kikuchi pattern quality map (Fig. 2a) gives an idea of its microstructure after transformation. (1 0 0)–(1 1 0)–(1 1 1) pole figures (Fig. 2b) express the orientations of the variants and show that the spread of the OR was not negligible.

In a first step, the parent orientation expressed by Euler angles (Bunge's definition [14]) (125.26°, 35.24°, 20.6°) was evaluated using the KS OR ((1 1 1) $_{\gamma}$ //(1 1 0) $_{\alpha}$ and [1 -1 0] $_{\gamma}$ //[1 -1 1] $_{\alpha}$ corresponding to Euler angles (5.77°, 48.19°, 5.77°)), according to the method described in Ref. [12]. The method proposed in the current paper was then applied to calculate the best representative OR and the best estimated parent orientation.

The highest eigenvalue of the product matrix ($A^T A$) is very close to 1, whereas the three others are very low. This indicates that the solution is unique. The corresponding eigenvector is equal to the quaternion representing Δg_0^{-1} that maximizes the value of expression (6).

The OR Δg calculated with this method is expressed by the following Euler angles $\Delta g \equiv (3.28^\circ, 45.09^\circ, 6.23^\circ)$. This OR and the KS OR differ from 3.8° (2.6° in the case of NW OR ((1 1 1) $_{\gamma}$ //(1 1 0) $_{\alpha}$ and [-2 1 1] $_{\gamma}$ //[-1 1 0] $_{\alpha}$ corresponding to Euler angles 0°, 45°, 9.73°)). Consequently, on average, the (1 1 1) $_{\gamma}$ plane is not exactly parallel to the (1 1 0) $_{\alpha}$ plane (1.38° away), whereas the [1 -1 0] $_{\gamma}$ direction is 2.92° away from the [1 -1 1] $_{\alpha}$ direction.

These values could suggest that the OR determined corresponds to that of GT (Greninger and Troiano [15]) ((1 1 1) $_{\gamma}$ //(1 1 0) $_{\alpha}$ (1°) and [1 -1 0] $_{\gamma}$ //[1 -1 1] $_{\alpha}$ (2.5°) approximated by (-1 -1 -1) $_{\gamma}$ //(-1 -1 0) $_{\alpha}$ and [-17 12 5] $_{\gamma}$ //[-17 17 -7] $_{\alpha}$ according to Ref. [16] cited in Ref. [17]). Nevertheless the corresponding $\Delta g \equiv (3.21^\circ, 46.7^\circ, 7.5^\circ)$ differs from $\Delta g \equiv (3.28^\circ, 45.09^\circ, 6.23^\circ)$ by 2°. At the same time, the calculated parent orientation equal to (126.23°, 34.96°, 20.24°), represented by blue squares on the pole figure in Fig. 2c, differs slightly from the first evaluation (125.26°, 35.24°, 20.6°) by 0.8°. Fig. 2c shows also the good fitting of the 24 variants (red squares) calculated with the calculated representative OR and the experimental ones (Fig. 2b).

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