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Application of Newton's method for precise calculation of parent orientation and orientation relationship from orientations of daughter phase

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ABSTRACT

For any quantitative study on microstructure of a product phase, information on the parent orientation and orientation relationship is essential, yet it is often lost after phase transformation. Even a numerical approach to the problem was proposed elsewhere, a description of the method used for numerical fitting, its efficiency and accuracy has not been reported so far. Here, we address in details the use of Newton's method as one of the fastest convergence techniques for least squares fitting of parent orientation and orientation relationship from EBSD data of the product phase. A robust algorithm with high precision is proposed in a form convenient for programming. Calculation errors, which are evaluated by a novel approach based on simulation of the daughter orientations, are 0.02° for parent orientation and 0.06° for orientation relationship.

1. Introduction

In many alloy systems, phase transformation occurs in a cooperative manner, in which a stable orientation relationship (OR) exists between the parent and product phases. Hence, information on the parent orientation (PO) and OR is essential for a quantitative study on crystallography or morphology of the product phase [1–7]. Recent studies have reported that the microstructure of parent phase affects variant selection and texture in the product phase [2–6], and the OR not only affects morphology of the product phase [7–8] but also controls kinetics of interphase precipitation of carbide in steel [8]. However, information on PO and OR is not readily available in a majority of ferrous alloys, because transformation of the parent phase often completes near room temperature.

In recent decade, several researchers have proposed different methods for finding PO and/or OR indirectly from orientations of the product phase. Their approaches can be classified into three main groups:

1) Averaging approach [9–12]
2) Analytical approach [13–14]
3) Least squares approach [15–17]

The averaging approach was firstly proposed by Humbert [9] for calculation of PO by using a known OR. It involved finding for each daughter orientation a set of parent variants, which would be obtained from the former by a virtual reverse transformation. The mean PO therefore was obtained by averaging orientations of the dominant reversed POs using quaternion algebra. This approach was widely adopted by many researchers since its principle was simple. However, it only allowed approximation of the PO and the solution was sensitive to the choice of initial PO and OR.

Latterly, the analytical approach was introduced by Humbert [13] as a further improvement of the averaging approach for refinement of both PO and OR. It was based on an analytical hypothesis that the best OR should minimize mean distance among the reversely calculated POs. The hypothesis led to an optimization problem involving Lagrange multipliers, which could be solved analytically. Because all the constant coefficients of the function to be optimized were predefined from the choice of initial PO and OR, the solution might also be sensitive on those initial values.

Least squares approach was firstly reported by Miyamoto [16] for determination of both PO and OR from orientations of martensite or bainite in steel. The main idea was least squares fitting of a model of daughter variants to a set of measured daughter orientations, which were inherited from one parent grain. In this approach, the mean PO and OR are reached by the best fit between the model of daughter variants and the measured daughter orientations. The least squares approach is flexible, since the parameters of the objective function can be refined during iteration steps. By this way, the obtained results are less dependent on the initial condition. However, a detailed description of the method used for least squares fitting of PO and/or OR has not

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been addressed by any author so far. Consequently, for many researchers the approach is difficult to reproduce, especially for those who are not familiar with non-linear multivariable optimization.

In nonlinear multivariable optimization, it is important to choose a proper objective function and an efficient and robust method to achieve the solution. Newton's method is one of the fastest convergence techniques for numerical fitting, since it converges on the root quadratically. Near a root, the number of significant digits approximately doubles with each step, so it is also often used to “polish” a root obtained by other methods [18]. Unfortunately, Newton's method requires calculation of secondary derivatives of the objective, which are often unaffordable analytically if the objective is not rationally chosen and simplified.

In this paper, we demonstrate the use of Newton's method for least squares fitting of PO and OR from daughter orientations. Implementation of the method for convenience of programming, efficiency of computation and factors affecting the solution will be addressed in details based on a practical application on steel. Furthermore, a novel approach to evaluate accuracy of the calculation method through simulation of daughter orientations from a standard PO and a well-known OR is also discussed.

2. Calculation Method

For a coherent phase transformation, the orientation of inherited daughter variant is related to the parent orientation by a certain OR as follows [13]:

$$\boldsymbol{g}^{v_l} = \boldsymbol{D}_j.\ \Delta\boldsymbol{g}.\ \boldsymbol{P}_i.\ \boldsymbol{g}_o \tag{1}$$

where $\boldsymbol{g}^{v_l}$ and $\boldsymbol{g}_0$ are orientation matrices of the daughter variant and PO respectively. $\boldsymbol{P}_i$ and $\boldsymbol{D}_j$ are among the rotational symmetry matrices of the parent and inherited phases, respectively. $\Delta\boldsymbol{g}$ is the OR which describes the rotation of parent crystal frame relative to the daughter frame. The number of daughter variants is determined by the parent and daughter crystals symmetries and the OR between them. The topic has been discussed extensively by Cayron in the Ref. [19]. In case of martensitic transformation in steel, the Kurdjumov-Sachs OR has 24 variants of daughter orientations, while the Nishiyama-Wasserman OR has only 12 variants.

Now suppose we have a selected area of inherited phase, which contains N experimentally measured orientations in matrix expression $\boldsymbol{g}_l, l = 1 - N$. In order to find $\boldsymbol{g}_o$ and $\Delta\boldsymbol{g}$, the model of daughter variants $\boldsymbol{g}^{v_l}$ is numerically fitted to the measured orientations $\boldsymbol{g}_l$ by minimizing an objective function, which represents the sum of squared distance between them. The form of objective function depends on the choice of distance function or metric between three-dimensional (3D) orientations. A study has proved that either the rotation angle between two orientations as a geodesic distance on the unit sphere or the Euclidean distance between two unitary quaternions representing the 3D orientations, can be used for this purpose, since those two quantities are equivalent metrics [20].

In this calculation, we used the rotation angle as a metric for building of the objective function. For each measured daughter orientation $\boldsymbol{g}_l$, a pair of symmetry matrices $\boldsymbol{P}_{n(l)}, \boldsymbol{D}_{m(l)}$ is found so that the disorientation matrix $\boldsymbol{O}_l = (\boldsymbol{D}_{m(l)}.\Delta\boldsymbol{g}.\boldsymbol{P}_{n(l)}.\boldsymbol{g}_o).\boldsymbol{g}_l^{-1}$ returns a minimum rotation angle θ_l defined by:

$$\cos(\theta_l) = \frac{1}{2}[Tr(\boldsymbol{O}_l) - 1] \tag{2}$$

where $Tr(\boldsymbol{O}_l)$ is the trace of $\boldsymbol{O}_l$. When θ_l is within a limit of deviation ϑ ($\theta_l \le \vartheta$) we say that the measured orientation $\boldsymbol{g}_l$ is indexed by the variant number $v(l)$, since it is found closest to the daughter variant $v(l)$ determined by $\boldsymbol{P}_{n(l)}$ and $\Delta\boldsymbol{g}$.

The objective function for least squares optimization is therefore

$$f(\Delta\boldsymbol{g}, \boldsymbol{g}_o) = \frac{1}{\widetilde{N}}\sum_1^{\widetilde{N}} \theta_l^2 \tag{3}$$

Note that $\widetilde{N}$ is number of measured daughter orientations (g_l), which satisfy the OR ($\Delta\boldsymbol{g}$) with the parent ($\boldsymbol{g}_o$) within a limit of deviation ϑ ($\theta_l \le \vartheta$). Obviously, $\widetilde{N}$ is equal or less than N and it may change after each iteration step. Under the condition that ϑ is chosen sufficiently small ($\vartheta \le 15^\circ$), $\cos(\theta_l)$ can be quadratically approximated by Taylor series:

$$\cos(\theta_l) = 1 - \frac{\theta_l^2}{2} + O(\theta_l^4),\ (\theta_l\ in\ radian) \tag{4}$$

Using (2) and (4) the objective function in (3) is simplified:

$$f(\Delta\boldsymbol{g}, \boldsymbol{g}_o) = \frac{1}{\widetilde{N}}\sum_1^{\widetilde{N}} 2(1 - cos(\theta_l)) = 3 - \frac{1}{\widetilde{N}}\sum_1^{\widetilde{N}} Tr(\boldsymbol{O}_l) \rightarrow min \tag{5}$$

The objective function using $(1 - \cos(\theta_l))$ instead of ${\theta_l}^2$ is chosen for a sole reason to keep derivations and calculations simple as demonstrated later. It is reasonable to assume that the difference $O({\theta_l}^4)$ can be neglected, as all involved angles are relatively small ($\vartheta \le 15^\circ$). This assumption also implies that a proper initialization is generally required to guarantee small angles right from the start. This point will be elucidated in section 3.

In a previous work [17], we had proposed a strategy to reduce computational work by fitting $\boldsymbol{g}_o$ and $\Delta\boldsymbol{g}$ separately. It was done by initially using a known $\Delta\boldsymbol{g}$, for example the Kurdjumov-Sach (K-S) OR in case of steel then solving Eq. (5) numerically to find $\boldsymbol{g}_o$. Later, $\Delta\boldsymbol{g}$ is refined with a fix of $\boldsymbol{g}_o$, which has been found in the previous step. The refined ORs calculated in a number of parent grains for a given steel are close each other within a deviation of $< 0.5^\circ$ [21]. Therefore, the refined ORs can be used as initial value in any further calculation for the materials of similar composition.

With a fixed $\Delta\boldsymbol{g}$ the objective function in (5) becomes a function of three variables $\boldsymbol{\varphi} = (\varphi_1, \Phi, \varphi_2)^T$, which are three Euler angles in Bunge notation for description of the parent orientation ($\boldsymbol{g}_o$). Analytical expression for $\boldsymbol{g}_o$ as a function of $\boldsymbol{\varphi}$ is

$$\boldsymbol{g}_o(\boldsymbol{\varphi}) = \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix} = \begin{pmatrix} c_1c_2 - s_1s_2c & s_1c_2 + c_1s_2c & s_2s \\ -c_1s_2 - s_1c_2c & -s_1s_2 + c_1c_2c & c_2s \\ s_1s & -c_1s & c \end{pmatrix} \tag{6}$$

where s_1, c_1, s, c, s_2, c_2 are the shorten forms of sine and cosine of $\varphi_1, \Phi, \varphi_2$ respectively.

The cyclic property of the trace of a matrix product, $Tr(\boldsymbol{A}.\boldsymbol{B}.\boldsymbol{C}) = Tr(\boldsymbol{C}.\boldsymbol{A}.\boldsymbol{B})$ for any set of 3×3 matrices $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{C}$ allows us to derive a final form of the objective function in case of a fixed $\Delta\boldsymbol{g}$:

$$f(\boldsymbol{g}_o) = f(\boldsymbol{\varphi}) = 3 - \frac{1}{\widetilde{N}}\sum_1^{\widetilde{N}} Tr(\boldsymbol{O}_l) = 3 - Tr(\overline{\boldsymbol{M}}.\ \boldsymbol{g}_o) \rightarrow min \tag{7a}$$

where $\overline{\boldsymbol{M}} = \frac{1}{\widetilde{N}}\sum_1^{\widetilde{N}} [\boldsymbol{g}_l^{-1}.(\boldsymbol{D}_{m(l)}.\Delta\boldsymbol{g}.\boldsymbol{P}_{n(l)})]$ is a 3×3 matrix. Note that $\overline{\boldsymbol{M}}$ is not a function of $\boldsymbol{\varphi}$, but it is not a true constant throughout the optimization process. If the initial guess of $\boldsymbol{g}_o$ is far from the solution, the parameters $\widetilde{N}$, $D_{m(l)}$ and $P_{n(l)}$ for definition of $\overline{\boldsymbol{M}}$ may change as orientations of the model variants $\boldsymbol{g}^{v_l}$ are affected appreciably by update of $\boldsymbol{g}_o$ on early iteration steps.

For least squares fitting of OR ($\Delta\boldsymbol{g}$), a similar objective function as in Eq. (7a) can be obtained by fixing the PO ($\boldsymbol{g}_o$). In that case the objective function will be

$$f(\Delta\boldsymbol{g}) = 3 - Tr(\overline{\boldsymbol{M}}_{\Delta g}.\ \Delta\boldsymbol{g}) \rightarrow min \tag{7b}$$

where $\overline{\boldsymbol{M}}_{\Delta g} = \frac{1}{\widetilde{N}}\sum_1^{\widetilde{N}} [\boldsymbol{P}_{n(l)}.\ \boldsymbol{g}_o.\ \boldsymbol{g}_l^{-1}.\ \boldsymbol{D}_{m(l)}]$.

Those optimization problems can be solved numerically by application of Newton's method, which is detailed in the appendix A.