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Automated reconstruction of pre-transformation microstructures in zirconium

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An automated reconstruction of the pre-transformation microstructure from the microtexture data of the post-transformation product phase is proposed. The method involves identifying triplets of neighboring product grains with a common variant and linking such neighboring triplets via a generalized misorientation criterion. The approach is non-iterative and extremely efficient computationally. The method was tested successfully for different post-transformation microstructures in zirconium.

Keywords: EBSD; Automated reconstruction; Transformation texture; Zirconium; Phase transformation

The subject of phase transformation in general, and more specifically the topic of variant selection, have been areas of active research for the past several decades [1–3]. Phase transformations are expected to obey certain orientation relationships (ORs) [1,2]. For a variety of reasons, all the variants corresponding to such ORs may not be observed with equal probability [1–13]. This brings us to the topic of variant selection – a method that can be used effectively to elucidate the underlying mechanisms of phase transformations [1–21].

The biggest limitation of any research on microstructural developments through phase transformation arises from the experimental difficulties of viewing both pre- and post-transformation structures [4]. An appropriate heating–cooling stage can provide an alternative [4,5]. However, measurements are never instantaneous and are mostly restricted to the surface. Volumetric measurements using synchrotron radiation are relatively uncommon [9]. Another alternative is to preserve or decorate the high-temperature structures [6]. Such an alternative is specific to a system and is possible only in specific metallic materials.

Recently, serious efforts have been made to convert post-transformation microtexture data to the pre-transformation microstructure [14–22]. Such efforts naturally need the ORs as well as suitable algorithms for the reconstruction. Two different approaches have been used: (i) neighbor-to-neighbor [18–20] and (ii) groupoid [21]. Although the approaches can be used/adopted for any phase transformation, subsequent description is tailored more towards $\beta \rightarrow \alpha$ (body-centered cubic → hexagonal close packed) transformations typical of zirconium (Zr) and titanium (Ti). The OR for such transformation is Burgers [18], where $\{0\,0\,0\,1\}_\alpha // \{1\,1\,0\}_\beta$ and $\langle 1\,1\,\bar{2}\,0\rangle_\alpha // \langle 1\,1\,1\rangle_\beta$. A β grain can transform into 12 crystallographic variants of α, while the inverse transformation of $\alpha \rightarrow \beta$ has six β variants [18]. If one expresses the crystallographic orientation and Burgers transformation in terms of rotation matrices, the effect of inverse transformation on the α orientation is mathematically equivalent to multiplication of its orientation matrix by a suitable transformation matrix or operator. Since there are six equivalent transformation matrices or operators, each product α grain can have six possible β orientations. Both approaches (i) and (ii) are based on this general principle, though the subsequent reconstruction algorithms differ. In (i) clusters of neighboring α grains are identified based on their probability of having a common parent β. The probability is decided firstly by a local (neighbor-to-neighbor) minimization of misorientation of the calculated β variant. Subsequently, the solution is refined by

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the minimization of global misorientation through an iterative Monte Carlo approach [19]. This was historically the first, and relatively simple conceptually, approach used, and was tested with reasonable success in Ti [18–20]. The approach can, however, lead to erroneous reunification of grains belonging to different parents at higher angular tolerances [21]. Arguably in the diffusional transformations the misorientation developments may not approach such high tolerances, but this may not be the case for displacive phase transformations. To circumvent this problem, the second or groupoid approach was proposed [21]. The groupoid structure is formed by the variants and their operators. The method consists of searching a triplet of neighboring product grains, which satisfies groupoid composition with a very low ($\leqslant 3°$) tolerance angle. Then the triplet is made a "nucleus" and is grown by considering neighbors which obey certain conditions of coherence. The process is repeated until no new nucleus can be found. This is an iterative process and expected to be time consuming [22]. With such a background, the need for a faster and more accurate method of automated reconstruction appears warranted. This was the motivation behind the present work. The computational speed would depend on the appropriate conceptualization – simplification without compromising the actual physics. The algorithm is described in the next few paragraphs.

The first step is to process the electron backscattered diffraction (EBSD) data of the product (e.g. hcp α) phase. The following are the necessary steps:

- Raw data needs to be free from wrongly indexed points. If such points exist, appropriate clean-up(s) needs to be conducted. The orientation data representation is reduced to the minimum Euler space required by the symmetry of the product phase to avoid redundancy in orientation description [18].
- A data set is created from the refined EBSD data, containing unique grain IDs $G_{i=1,2,3\ldots}$, average grain orientation and grain IDs of all neighboring grains. A grain, in a standard EBSD program, is identified from the continuous presence of a boundary exceeding a specified misorientation – which was taken in this work as 5°.

The rest of the proposed algorithm (also shown in Fig. 1) can be described in the following steps:

1. Consider a product grain G_i (where $i = 1,2,3\ldots$) has $G_{i+1}, G_{i+2}, \ldots G_{i+N}$ as its neighbors (see Fig. 1a). Figure 1b shows possible triplets containing G_i and its neighbors with the condition that each grain of the triplet is neighbor to the other two. In the limiting case of all the neighbors of the G_i being neighbors to each other, ${}^{N}C_2$ number of triplets are formed. In general, however, the number of triplets will be much smaller.
2. For grains in a given triplet find all possible parent orientations

$$B_{li}^{\beta} = T_{l}^{\alpha\to\beta} G_{i}^{\alpha} \tag{1}$$

where $T_{l=1\ldots6}^{\alpha\to\beta} = D^{-1} S_{l=1\ldots6}^{\alpha}$ and $S_{l=1.6}^{\alpha} = (E_{\alpha}, C_{6z+}, C_{3z+}, C_{21+}, C_{22+}, C_{23+})$ are the hexagonal symmetry operators, D is the matrix representing the Burgers OR for $\beta \to \alpha$ and $i = 1, 2, 3$ are the grain IDs in the selected triplet, B_{li}^{β} are the parent orientations for the product orientation of G_i^{α}.
3. The common solution to all the three grains in a triplet is selected as a potential solution. If there is no such common solution, it is inferred that the grains of the triplet are not from a common parent.
4. These steps are repeated for all triplets of G_i – yielding, say, n potential solutions for G_i. In the ideal case, all the potential solutions of G_i should be identical. However, due to transformation strains and measurement uncertainties there could be misorientations among the potential solutions. In order to assign an "optimum" solution to G_i, the computer program finds the mean solution ($S_{k,l}^{m}$) and the misorientation($\Delta S_{k,l}$) between each pair of the potential solutions: S_k and S_l, where k and l run from 1 to n.

$$S_{k,l}^{m} = mean(S_k, S_l) \quad k \neq l$$

$$\Delta S_{kl} = \mathrm{Cos}^{-1}\left(\frac{(Trace(S_k.S_l^{-1}) - 1)}{2}\right) k \neq l \tag{2}$$

Reject any $S_{k,l}^{m}$ for which $\Delta S_{k,l}$ is more than the user-specified maximum misorientation tolerance ($\delta_{\max}$). The final solution (S_{final}) for G_i is the mean of all $S_{k,l}^{m}$ weighted by $W_{k,l}$ (weighting factor for $S_{k,l}^{m}$.

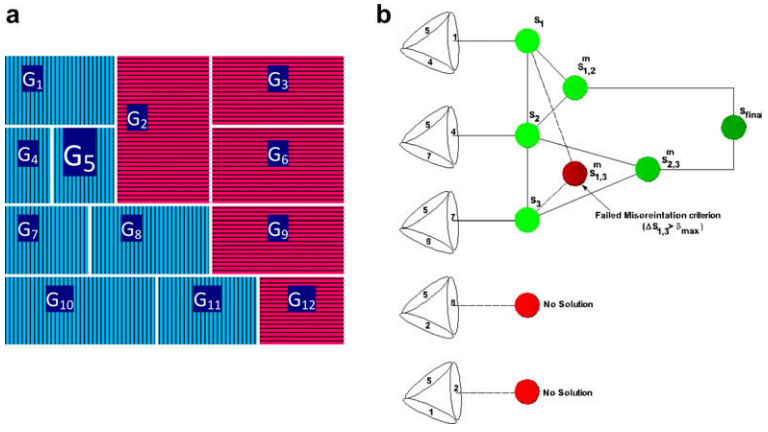

Figure 1. (a) Schematic showing the product α grains. Grains belonging to common parent β are marked with the same color/shade. Subscripts (G_i) indicate the product grain IDs. (b) Adopted algorithm. Let $G_i = 5$. Neighbors of G_5 are G_1, G_2, G_4, G_7 and G_8. The triplets formed by G_5 are [5,1,2], [5,2,8], [5,8,7], [5,7,4] and [5,4,1]. Note that all the three grains of these triplets are neighbors to each other. Triplets either have a common parent variant, i.e. a "potential" solution for the parent β, or "no solution". The next step is to link the "potential" solutions through a generalized misorientation criterion.