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Reconstruction of deformed parent grains from microstructure inherited by phase transformations

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ABSTRACT

The methods used to reconstruct austenite grains from martensite measured by Electron Backscattered Diffraction rely on two assumptions: the orientation relationship and the parent orientation are unique locally. However in presence of an orientation gradient, the second assumption is no longer respected. Therefore in this work, we have first evaluated the deviation to both assumptions which revealed that the presence of an orientation gradient increases the deviation to the second assumption so that it becomes difficult to guaranty a reliable reconstruction. Therefore an adaptation of the method is proposed to better account for the orientation gradient and improve reconstruction results.

Over the last decade, methods have been developed to reconstruct the parent microstructure (e.g., austenite) from EBSD measurements performed at room temperature on its transformation product (e.g., martensite, bainite…) [1–8]. The parent reconstructions offer great advantages over metallographic etching such as Bechet Beaujard [9] or thermal etching [10]. Indeed, their applications require only the acquisition of an EBSD map which is today a widely available characterization technique. Moreover, in addition to the parent grain structure, they also provide the individual orientations of the parent grains which may be used for instance to evaluate their crystallographic texture or to study the variant selection. Two different strategies have been used for fully automated reconstructions: Pixel by pixel reconstructions [7,8] use the data at the pixel level whereas domain based reconstructions [1–6], use average orientations of crystallographic domains identified with a classical grain detection algorithm (e.g. as in [11]). The domain based reconstructions allows saving of computational time in the following steps because the number of domains is much lower than the number of pixels. However some information is lost during averaging which can be damageable when the orientation of the domain contain an orientation gradient like in deformed materials. In this article, the first part explains the assumptions on which domain based reconstructions relies. The second part assess the effect of a deviation to the assumptions. The third part describe briefly the reconstruction method and propose an adaptation to account for orientation gradient. In the last part an application example assess the benefit of the new method.

The domain based reconstruction methods are based on two assumptions. The first assumption is that at any location in the microstructure, a child orientation is related to its parent by a unique orientation relationship (OR). The second assumption is that the parent orientation is unique in a parent grain (or at least in a small neighborhood). Both assumptions have implication for the accuracy of a reconstructed map, especially when an orientation gradient existed before transformation. The objective of this paper is to evaluate the implication of each assumption and to propose an alternative method in the case of the presence of an orientation gradient when the second assumption is not respected anymore (e.g. in a deformed material).

In general, the relation between the orientation of a child crystal $g\alpha_i$ and its parent orientation $g\gamma$ is given by [12]:

$$g\alpha_{i,j} = g\gamma \times P_i \times \Delta g \times C_j \tag{1}$$

where P_i are the rotational symmetry elements of the parent phase and Δg is the OR expressed as a rotation. C_j are the rotational symmetry elements of the child phase and only account for all equivalent rotations describing the same orientation. Conversely, all the potential parent orientations of a given child orientation are given by:

$$g\gamma_{i,j} = g\alpha \times C_i \times \Delta g^{-1} \times P_j \tag{2}$$

From the first assumption, Δg is constant. Even if it was verified by an abundant literature for recrystallized [13] and deformed parent

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grains [14], it is important to assess how experimental data conform to this assumption. According to Eq. (1), an austenite grain with a single orientation transforms into several crystallographic variants, each with a single orientation. Any spread in a martensite lath orientation can therefore be attributed either to measurement errors or to a deviation to the first assumption. The GOS (Grain Orientation Spread) is a relevant metric of the orientation spread in EBSD maps [15]. This indicator is the average angular deviation of all points in a crystallographic domain with respect to its average orientation. Theoretically, this indicator is sensitive to low angle boundaries if the crystallographic domains are not properly defined. Here, to avoid any influence of sub-grain boundaries, the crystallographic domains were identified using a small tolerance angle of 3° and sub-grain boundaries were closed using the ALGrId algorithm down to 1° [16]. The Fig. 1 compares the distribution of GOS for three metallurgical states: an austenite directly measured by EBSD on a stainless steel, a martensite formed from recrystallized austenite grains and an ausformed martensite. The GOS distribution in austenite quantifies directly the measurement error since there is no phase transformation. In general, it depends on measurement parameters but in standard EBSD conditions, the GOS is generally around 0.5°. Then in the martensite formed in a recrystallized austenite, all GOS values above 0.5° characterize the deviation to the first assumption. The GOS distribution is shifted toward higher values with a peak at 1.5° and a tail reaching 4° as confirmed in [17]. This distribution explains why most reconstruction methods use tolerance angles around 3° or above. However, it also shows that it shall not be necessary to use tolerance above 4° if the OR is adequately determined. The data about the ausformed martensite shows that in the presence of an orientation gradient the peak in the GOS distribution stays at 1.5° and the tail is shifted toward higher values.

The second assumption considers that the parent orientation is unique locally. This allows reformulating Eqs. (1) and (2) as follows [18]:

$$\left(g\gamma_{i,j}\right)^{-1} \times g\gamma_{k,l} = P_i \times \Delta g \times C_j \times g\alpha_1{}^{-1} \times g\alpha_2 \times C_k^{-1} \times \Delta g^{-1} \times P_l^{-1} \quad (3)$$

This equation equals the Identity when the two orientations $g\alpha_1$ and $g\alpha_2$ are strictly related to the same parent by the same OR. Any deviation the assumptions (or measurement error) results in a residual rotation of minimum angle θ which can therefore be used to evaluate how the reconstruction method is affected in the presence of an orientation gradient. Here a synthetic example has been designed so that only the second assumption shall influence the results. An austenite grain of 120 × 120 pixels was created with an orientation ($g\gamma = [\varphi_1$: 107°; Φ: 31°; φ_2: 24°]). Then a gradient was introduced by rotating all pixels of the grains depending on their position (x, y) relative to the center of the grain. The rotation angle was 0.3° per unit distance from the grain center (measured in pixels) and the rotation axis was calculated as $\overrightarrow{u} = (\frac{x}{60}; \frac{y}{60}; \sqrt{1-x^2-y^2})$. The initial orientation was chosen because it appears as white in the Inverse Pole Figure color key with respect to Z and reveals clearly the orientation gradient (Fig. 2a). The resulting Grain Orientation Spread (GOS) [15] is 13° which is representative of a highly deformed grain. Then a martensite transformation was simulated by choosing a random child number (i.e., i in Eq. (1)). Then the trace of the corresponding (111) habit plane $\overrightarrow{v_{HP}}$ on the EBSD map was evaluated. Finally, all pixels lying at a distance of 3 pixels from a line parallel to $\overrightarrow{v_{HP}}$ crossing a pixel chosen at random underwent the $\gamma \rightarrow \alpha$ transformation according to Eq. (1). The process was repeated until all pixels were transformed into martensite according to the Greninger Troiano (GT) OR. A cleaning step removed single pixel grains and replaced them by the orientation of one of their neighbors. The result is presented as an IPF map in Fig. 2c.

In domain reconstruction methods, the first step consists in detecting the domains and averaging their orientation. This step performed for the synthetic example is displayed in Fig. 2d. Then to evaluate the deviation to the second assumption at this step, the minimum rotation angle θ was evaluate and is displayed in Fig. 2e and f using a rainbow scale. The corresponding distributions are plot in the graph of Fig. 2g.

For the initial data (Fig. 2e), the θ distribution has a sharp peak at 0.3° because the deviation is only inherited from the orientation gradient of the parent grain at the pixel scale (Fig. 2a). The deviation is much higher for the averaged data (Fig. 1f). In average, they are of 2.8° with a tail reaching 11.8°. Fig. 1h shows that longer domains have the highest deviations. For those domains, the deviation is close to the maximal GOS before averaging. The largest domain has a GOS of 9° which corresponds to the distribution tail in Fig. 1g. Consequently, the tolerance used to find the parent must be increased by the same magnitude as the GOS induced by the gradient in the parent phase but on the length scale of the child domains.

In the original method [1], several domains are used and the most probable parent is the one related to most domains within a tolerance

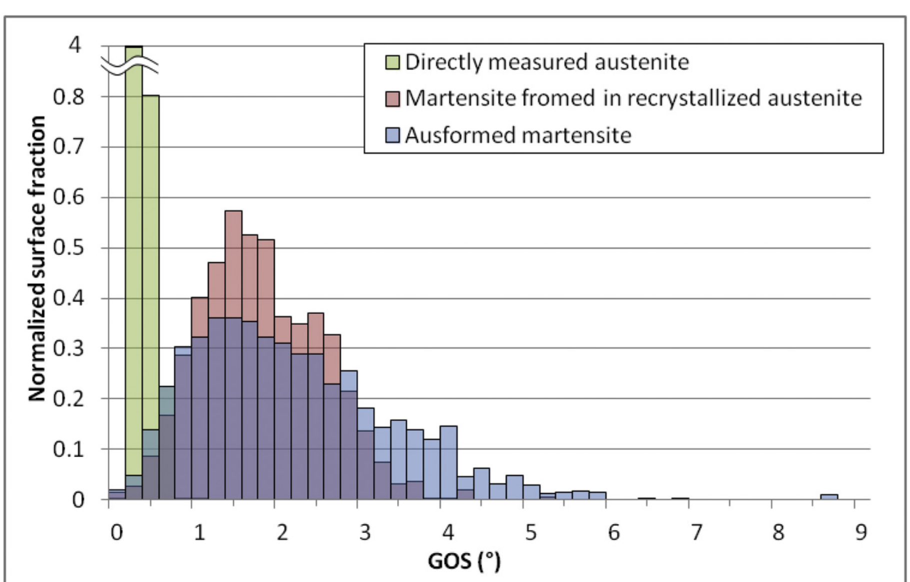

Fig. 1. GOS distribution for three different metallurgical states. The crystallographic domains have been identified so that sub-grain boundaries do not influence the GOS distribution.