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Specific analysis of EBSD data to study the texture inheritance due to the $\beta \rightarrow \alpha$ phase transformation

N. GEY, M. HUMBERT
LETAM CNRS UMR 7078, Université de Metz, Ile du Saulcy, F-57045 Metz Cedex, France
E-mail: GEY@LETAM.sciences.univ-metz.fr

A specific processing of EBSD data is proposed to study the $\beta \rightarrow \alpha$ texture inheritance of α titanium or α zirconium alloys. A non standard misorientation map is calculated to localise the colonies inherited from the same parent β grain. The calculation of the parent orientation from its inherited variants detailed in previous works has been adapted to the data obtained from an automated EBSD analysis. Finally, a method to derive the orientation map of the parent β phase from that of the α inherited phase is proposed. The resulting α and β COMs are used to study some aspects of the variant selection occurring in the $\beta \rightarrow \alpha$ transformation of a T40 sample. © *2003 Kluwer Academic Publishers*

1. Introduction

Hexagonal Close-Packed metals like titanium or zirconium alloys exhibit between 900°C and 1000°C an $\alpha \rightarrow \beta$ phase transformation at heating and a $\beta \rightarrow \alpha$ phase transformation at cooling. These phase transformations influence the microstructure and notably the texture of the material at room temperature. As a matter of fact, the orientations of the inherited α phase depend on the orientations of the high temperature β phase through the Burgers orientation relation and on the variant selection occurring in the $\beta \rightarrow \alpha$ transformation. The Electron Back Scattered Diffraction (EBSD) technique is an adapted tool to study the texture inheritance due to phase transformations and variant selections. Such studies have often been reported for materials such as stainless steels [1–4], Cu-Zn Alloys [5], β-titanium alloys [6] for which the parent and the inherited phases are present at room temperature. Unfortunately, for HCP metals like α titanium or α zirconium alloys, the high temperature parent phase cannot be retained at room temperature. Nevertheless, the variant selection occurring in the $\beta \rightarrow \alpha$ transformation can be studied by a specific analysis of the α inherited orientations [7, 8].

In this contribution, a method of characterising the α inherited microstructures and the $\beta \rightarrow \alpha$ variant selection, using EBSD orientation maps is examined. The characteristic features of the transformation and the inherited microstructure are first briefly recalled. The α variants inherited from the same parent β grain are characterised by specific misorientations linked to the Burgers orientation relation. Therefore, these variants can be systematically identified on the α map by considering the misorientation angles and axes between adjacent measurements. The calculation of the parent orientation from its inherited variants detailed in [7, 8] has then been adapted to process the data obtained from an automated EBSD analysis. This allows to derive the orientation map of the parent β phase from that of the inherited α phase. An illustrative example on a T40 sample shows the efficiency of the method to study some aspects of the variant selection observed in the $\beta \rightarrow \alpha$ transformation.

2. Characterisation of an α inherited microstructure by EBSD

2.1. Type of microstructure and texture inherited from the $\beta \rightarrow \alpha$ transformation

After a β treatment, the α titanium or zirconium alloys exhibit a typical microstructure schematically represented in Fig. 1. It is characterised by α plates (α_{GB}) which preferentially nucleate at β/β grain boundaries, by Widmanstätten α colonies which grow from the α_{GB} and also by α phase which nucleates within the β grains. The alloying elements as well as the treatment conditions strongly influence the size of the α inherited plates, the number of α colonies, and the presence or not of α_{GB} precipitation. For many such alloys, it is not possible to retain the high temperature β phase at room temperature, even by quenching. The only information about the former β microstructure is given by the α_{GB} precipitation contouring the parent β grains when it exists.

Another important feature of the inherited microstructure is that the orientations of the α colonies are often related to the orientation of the parent β grain by the Burgers orientation relation (1).

$$\begin{aligned} &(110)_\beta // (00.2)_\alpha \\ &[\bar{1}1\bar{1}]_\beta // [2\bar{1}.0]_\alpha \end{aligned} \quad (1)$$

This relation can be expressed as a rotation Δg_0. Taking into account this relation and the symmetries of the

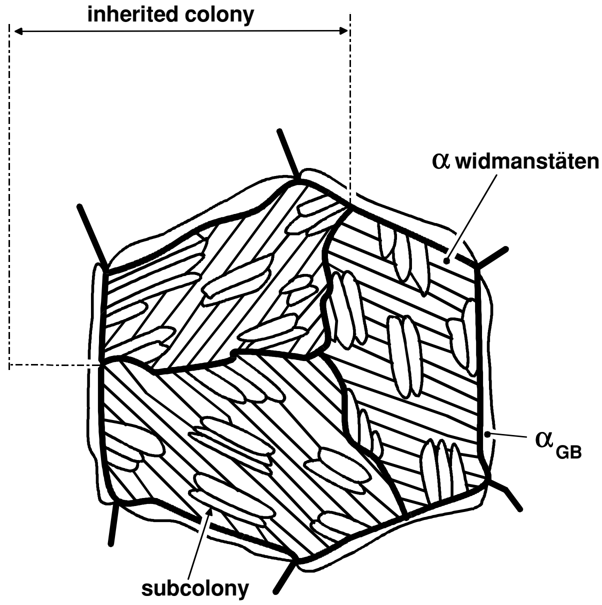

Figure 1 Typical inherited α microstructure.

parent and inherited phases, it can be shown that one parent β grain can give rise to 12 different α orientations, named 'variants' [7, 8]. The orientation of each variant is characterised by 12 rotations, for example for variant i:

$$E \cdot \Delta g_0 \cdot S_i \cdot g_\beta, \ldots H_j \cdot \Delta g_0 \cdot S_i \cdot g_\beta, \ldots$$
$$H_{12} \cdot \Delta g_0 \cdot S_i \cdot g_\beta \quad (2)$$

where $H_1 = E \cdot, \ldots H_i \ldots H_{12}$, are the 12 rotations of the hexagonal symmetry group and S_i one of the 24 rotations of the cubic symmetry group. It is to notice that one of these 12 equivalent rotations is sufficient to characterise the orientation of the ith variant.

Because the cubic symmetry group has 24 rotations ($S_1 = E \cdot, \ldots S_i \ldots S_{24}$) one could conclude that they are 24 variants. This is not the case, because 2 particular sets of 12 rotations derived from ($S_1 = E \cdot, \ldots S_i \ldots S_{24}$) lead to the same final rotations according to the specificity of Δg_0.

A $\beta \rightarrow \alpha$ transformation in which all 12 variants are equally selected generally leads to a smooth inherited texture, because of the multiplication of the orientations. However, due to the metallurgical state of the material before the transformation and the transformation conditions themselves, all variants do not often develop with the same probability. In this case, one speaks of variant selection. This can be at the origin of very sharp inherited α textures.

2.2. Standard EBSD analysis of the inherited α phase

The crystal orientation maps (COM) obtained by EBSD allow the characterisation of the microstructure and the local texture of the inherited phase after the $\beta \rightarrow \alpha$ transformation. In this technique, the local crystallographic orientations are obtained from EBSD patterns, recorded on an ultra-sensitive camera in a SEM. The automatic displacements of either the specimen holder or the electron beam allow to investigate a large and representative area of the sample. The orientations measured at each localisation can then be displayed in a COM with a variety of imaging options. Prior to any analysis, the orientation data have to be corrected. Notably one assigns an orientation coherent with their neighbourhood to the wrongly-indexed pixels and the non-indexed pixels [9, 10].

An EBSD analysis has been performed on a T40 sample (60% cold rolled and β treated). More details about the material and treatment conditions are given in [11]. The results are shown Fig. 2 thanks to a standard COM of the α inherited phase (a) and the (00.2)/(11.0) stereographic projection of the measured orientations (b). The grey level of each pixel in the COM is defined according to the deviation of the measured orientations from the $\langle 11.0 \rangle$//RD fibre (see the colour key of the stereographic projections). The coloured lines display the misorientation angles (θ) between neighbouring pixels. The black lines correspond to the high angle boundaries ($\theta > 15°$) and the white ones to the low angle boundaries ($3° < \theta < 15°$).

The α colonies, schematically described in Fig. 1, can easily be distinguished on the COM. They consist of α plates, having nearly the same orientation. It

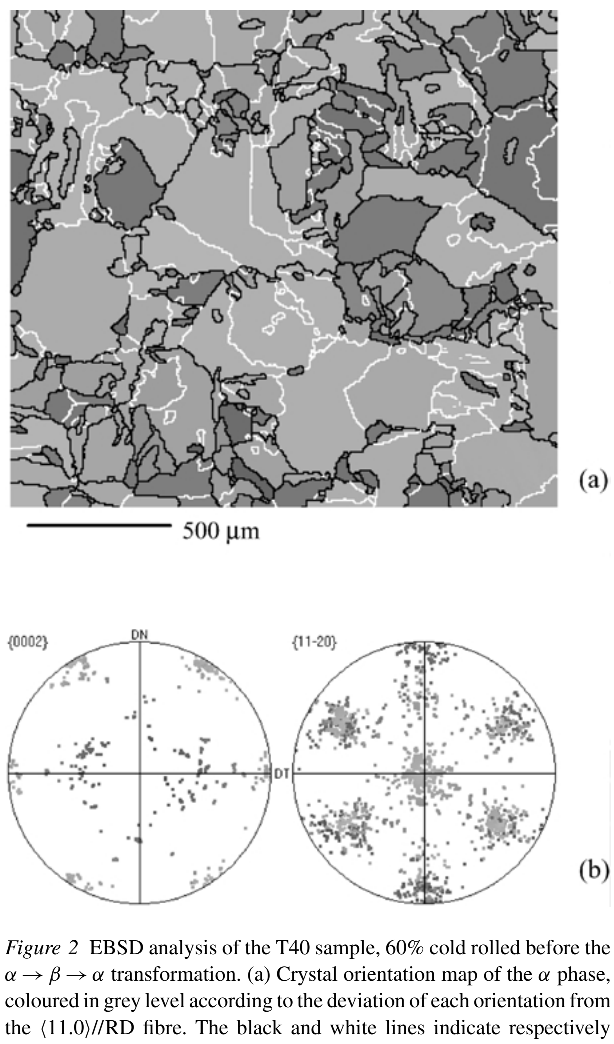

Figure 2 EBSD analysis of the T40 sample, 60% cold rolled before the $\alpha \rightarrow \beta \rightarrow \alpha$ transformation. (a) Crystal orientation map of the α phase, coloured in grey level according to the deviation of each orientation from the $\langle 11.0 \rangle$//RD fibre. The black and white lines indicate respectively misorientation angles between neighbouring pixels higher then 15° and between 3°–15°. (b) The (00.2) and (11.0) pole figures of the measured orientations.

can also be mentioned that some adjacent α colonies are only slightly misoriented, as shown by the white lines in Fig. 2a. In [11, 12], we have clearly shown that cold rolling prior to the $\alpha \rightarrow \beta \rightarrow \alpha$ transformation sequence, leads to a sharp inherited α texture, characterised by a ⟨11.0⟩//RD fibre with a strong reinforcement at the {10.3}/{10.-3}⟨11.0⟩ components. Thus, in the map, 70% of the orientations measured by EBSD are close to these ideal orientations. The calculation of variant selection indexes in [12] also makes clear that this sharp texture is related to a variant selection mechanism in the $\beta \rightarrow \alpha$ transformation. However, information about the parent β microstructure and the variants inherited from each parent grain are not directly visible on such a standard COM. Further investigations about the $\beta \rightarrow \alpha$ texture inheritance and the variant selection require additional information about the parent β microtexture and the colonies inherited from each parent grain. This kind of information can be obtained from the measured data by specific processing not included in the standard codes.

2.3. Identification of variants inherited from the same parent β grain

The first step to study the local variant selection induced by the $\beta \rightarrow \alpha$ transformation is to distinguish the α variants inherited from the same parent β grain on the COM. These variants are generally not recognised as such on the microstructure by considering α_{GB} precipitation. However, they are theoretically characterised by specific misorientations between them, deduced from the Burgers relation. As a matter of fact, two variants (say i and k) inherited from the same β grain have orientations respectively characterised by rotations:

$$\begin{aligned} &E \cdot \Delta g_0 \cdot S_i \cdot g_\beta, \ldots H_j \cdot \Delta g_0 \cdot S_i \cdot g_\beta, \ldots \\ &\quad H_{12} \cdot \Delta g_0 \cdot S_i \cdot g_\beta \\ &E \cdot \Delta g_0 \cdot S_k \cdot g_\beta, \ldots H_j \cdot \Delta g_0 \cdot S_k \cdot g_\beta, \ldots \\ &\quad H_{12} \cdot \Delta g_0 \cdot S_k \cdot g_\beta \end{aligned} \tag{3}$$

Their misorientation is given by rotations:

$$\begin{aligned} &H_j \cdot \Delta g_0 \cdot S_k \cdot S_i^{-1} \cdot \Delta g_0^{-1} \cdot H_n \\ &\quad = H_j \cdot \Delta g_0 \cdot S_p \cdot \Delta g_0^{-1} \cdot H_n \end{aligned} \tag{4}$$

There are $12 * 12$ rotations (j and n run from 1 to 12) expressing the same misorientation between variants i and k. Each of these $12 * 12$ rotations can be expressed as a rotation ω around an axis $\vec{n}$. Among this whole rotation set, the rotation having the minimal rotation angle ω and its corresponding axe is chosen to characterise the misorientation. This calculation has been performed for all the combinations of two variants among the 12 potential ones. As a result, one obtains 5 misorientation types (given in Table I) between variants inherited from the same parent grain.

These specific misorientations can be used to systematically recognise on the α map which variants are related to the same parent grain. For this purpose, the

TABLE I Specific misorientations between α colonies inherited from the same β grain (axis $\vec{n}$ corresponds to one of the symmetrically equivalent rotation axe)

ω	$\vec{n}$
10°529	$\vec{c} = [00.1]$
60°	$\vec{a}_2 = [\bar{1}2.0]$
60°832°	$\vec{d}_1$ at 80°97 from $\vec{c}$ in ($\vec{d}_3$, $\vec{c}$) plane
63°262	$\vec{d}_2$ at 72°73 from $\vec{c}$ in ($\vec{a}_2$, $\vec{c}$) plane
90°	$\vec{d}_3$ at 5°26 from $\vec{a}_2$ in basal plane

experimental misorientation between two neighbouring pixels in the map is compared to the theoretical misorientations given in Table I. When the experimental misorientation between two pixels is close to one of the theoretical misorientations, both pixels are assumed to belong to adjacent colonies inherited from the same β grain. On the contrary, when the experimental misorientation differs from those listed in Table I, both colonies have not the same parent grain. In this case, one reveals the track of a former β/β grain boundary. The allowed tolerance between the experimental and the theoretical misorientations is characterised by the rotation angle τ of the rotation ε which links the experimental and the theoretical misorientations ($\Delta^{\exp} = \varepsilon \cdot \Delta\text{th}$).

The specific misorientation map obtained with the EBSD data of the T40 sample is given in Fig. 3. The white lines characterise misorientations between adjacent measurements matching those of Table I with a tolerance angle τ of 5°. The black lines characterise any other misorientations between adjacent measurements, provided that their misorientation angles are higher than 3°. The misorientation angles lower than 3° have not been considered in this map. Many black lines completely reveal the contours of former β grains and thus give information about their shape and size. Moreover, the variants inherited from each β grain can be identified and used to study the variant selection

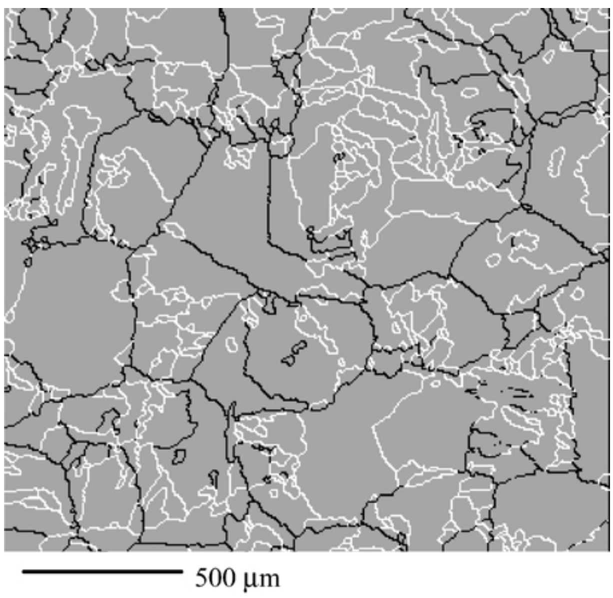

Figure 3 Crystal orientation map of the α phase. The white lines characterise the specific misorientations listed in Table I with a tolerance τ of 5°. The black lines characterise any other misorientations between adjacent measurements, provided that the misorientation angles are higher than 3°.

rules. Nevertheless, some black lines do not draw the entire contour of the parent β grains. This is observed when two neighbouring β grains have specific orientations such as α colonies inherited from two β grains present misorientations close to those listed in Table I. The variation of the tolerance angle τ can somewhat modify the contour lines in the calculated COM.

3. Construction of the parent β COM

3.1. Determination of the parent orientation

The understanding of the mechanisms involved in the $\beta \rightarrow \alpha$ phase transformation does not only require the identification of variants inherited from the same β grain, but also the knowledge of the parent orientation. In [7, 8], a method has been proposed to determine the orientation of a parent β grain from 3 different inherited variants. However, in most of the cases, more than 3 variants are observed within a parent grain. Moreover, an automated EBSD analysis provides nowadays a lot of orientation measurements for a same variant. The method proposed in [7, 8] can thus be adapted to take the whole information contained in a COM into account and to make the determination of the parent orientation more accurate.

If more than 3 variants are identified inside a parent β grain, all combinations of 3 variants can be considered. Each orientation triplet then leads to a calculated parent orientation. The set of resulting β orientations can show some spread, either because the Burgers orientation relation is not strict or because of the orientation measurement accuracy. In such a case, an evaluation of the parent orientation is obtained by averaging the calculated orientations [13]. A COM also contains a large number of orientation measurements for each variant, which generally present some spread. Different calculations can be applied to take into account the whole orientation set per variant, in the determination of the parent orientation. Averaging these orientations can be a solution. Another possibility consists in a random choice of a limited number of orientations for each variant, which are finally used in the calculation. One can also use a more robust method [14] to find the parent orientation from the whole set of inherited variants. The advantages of this new approach are that the number of variants used in the calculation is not limited to 3 and the possible deviation from the strict Burgers relation is better taken into account.

3.2. Automatic construction of the β COM

As detailed previously, the α colonies inherited from the same parent grain can be localised on the α map using a specific misorientation analysis. Moreover, their corresponding orientations can be used to deduce the orientation of their parent β grain. These localisation and orientation calculations are now implemented in a code to reconstruct the β COM from the α inherited one.

For this purpose, it is first necessary to recognise automatically in the α map, all the pixels related to the same parent grain. This can be achieved by adapting a standard EBSD grain reconstruction procedure. In this standard procedure, the user defines a misorientation criteria characterising pixels of a same grain. This criteria is then used to sort out the pixels of the map, according to the grain they belong to [9, 10]. Such a procedure can thus be easily used to reconstruct the parent β grains. As discussed in Section 2.3, the considered β grains correspond to crystallographic domains containing adjacent colonies characterised by specific misorientations between them. Therefore, two adjacent pixels of the α COM are in the same β grain if one of the two following conditions are satisfied:

- if they belong to the same α colony, their relative misorientation angle is lower than a small critical value θc,
- if they belong to adjacent colonies inherited from the same grain, their relative misorientation matches one of those listed in Table I, with a tolerance τ defined by the user.

Introducing these misorientation criteria into a standard EBSD grain reconstruction procedure allows to sort out the orientation measurements of the α map according to the parent β grain they are inherited from. The α orientations identified for each parent grain can then be processed as described in Section 3.1 to deduce their common parent orientation. For each reconstructed grain, the knowledge of the (x, y) positions and the calculated orientation allows to display the β COM.

A successful run of the procedure depends on to the pertinence of the misorientation criteria defining what measurements are related to the same parent grain. As already discussed in Section 2.3, cases exist where neighbouring colonies inherited from two different β grains have misorientations close to those of Table I. These colonies are then automatically assigned to the same parent grain by the codes, although they are inherited from two different grains. In this case, the procedure to calculate the parent grain orientation fails. The user may turn to a semiautomatic procedure so that he has to manually select the α colonies assumed to be inherited from the same parent grain and has to check that their orientations are related to an unique β orientation.

The β COM obtained for the T40 sample is shown in Fig. 4. Because of the specificity of the inherited α orientation distribution, this map has been obtained by using a semiautomatic procedure. Much information about the high temperature β phase can be deduced. First, the β texture can be evaluated from a significant number of calculated β orientations. It can be noticed that the β orientations are mainly around 3 specific texture components ({112}⟨111⟩, {11-2}⟨111⟩ and {100}⟨100⟩ components). One also observes that neighbouring β grains are often highly misoriented, as revealed by the black lines in the β map. Moreover the α and the β COMs allow to investigate the $\beta \rightarrow \alpha$ phase transformation and its variant selection. In particular, it is possible to correlate the spatial features of the β phase and the $\beta \rightarrow \alpha$ variant selection rules as shown in the next section.

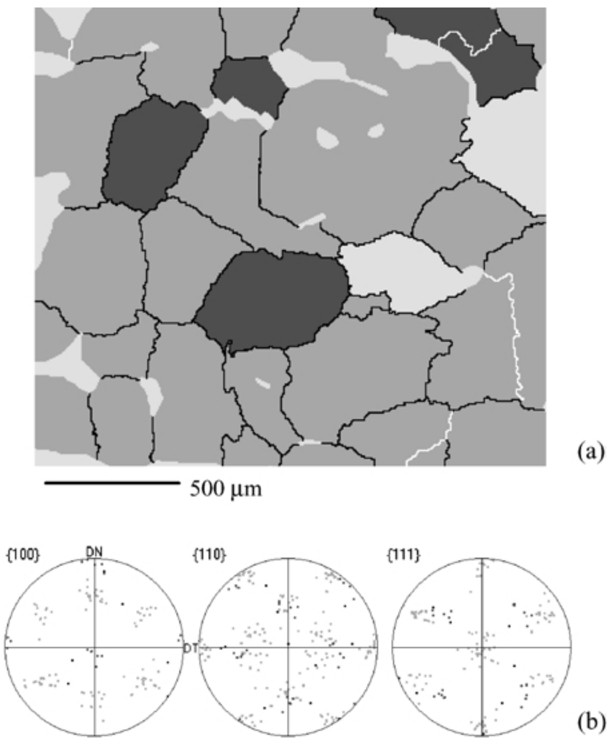

Figure 4 (a) Crystal orientation map of the β phase coloured in grey level according to the deviation of each orientation from the ⟨111⟩//RD fibre. The black and white lines indicate respectively misorientation angles between neighbouring measurements higher then 15° and between 3°–15°. (b) Characteristic pole figures of the calculated orientations.

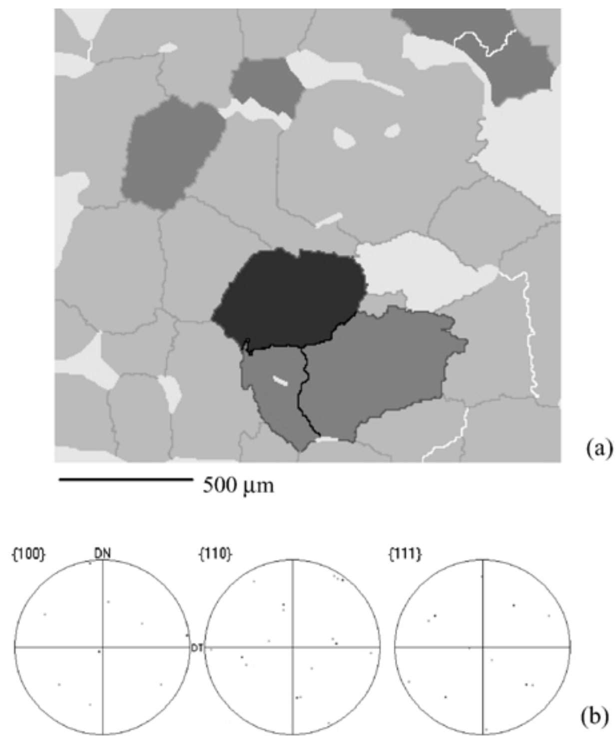

Figure 5 (a) 3 neighbouring grains selected from the β COM in Fig. 4. (b) Characteristic pole figures of the corresponding orientations.

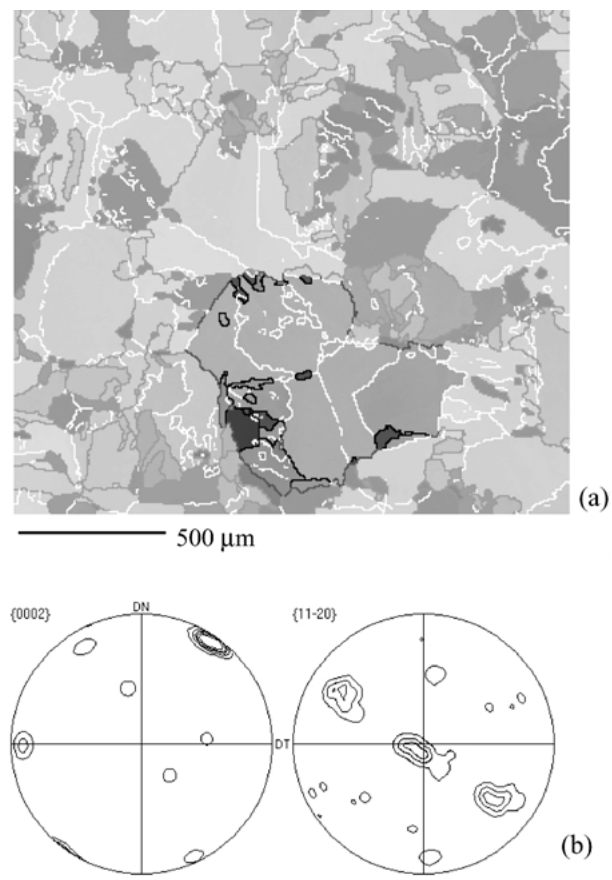

Figure 6 (a) Variants inherited from the 3 selected β grains in Fig. 5. (b) Characteristic pole figures of the corresponding orientations.

4. Application to the $\beta \rightarrow \alpha$ variant selection study: case of the T40 sample 60% cold rolled before the $\alpha \rightarrow \beta \rightarrow \alpha$ transformation sequence

According to the Burgers orientation relation and the symmetries of the α and β phases, a total of 12 distinct α orientations can be inherited from an initial β orientation. There is no variant selection in a parent grain when the volume fraction of each inherited orientation is equal. However, such a distribution is not observed for the T40 sample. In fact, the analysis of the parent β and the inherited α COMs, given in Figs 2 and 4 shows that many β grains have preferentially transformed into a limited number of variants close to the {10.3}/{10-3}⟨11.0⟩ texture components. This variant selection is in agreement with previous results published for this material [12]. In many cases, the α colonies characterised by these orientations are adjacent and misorientated by less than 15° (white lines in Fig. 2). Moreover, they are often inherited from highly misoriented parent grains. This is notably displayed in Figs 5 and 6 which focus on a particular area of the α and β COMs. The 3 selected grains in Fig. 5 belong each to one of the 3 texture components of the high temperature β phase. The inherited variants (Fig. 6) present orientations close to the {10.3}⟨11.0⟩ texture component. This indicates that the transformation preferentially promotes variants (inherited from different β grains) which have close orientations. The specific sharp texture of the parent β phase characterised by a limited number of high density components is so that two neighbouring β grains can statistically transform into variants with nearly the same orientation. In particular, the orientations close to the {10.3}/{10-3}⟨11.0⟩ texture components favoured in the transformation, can be inherited from the 3 different β components.

5. Conclusion

A specific analysis of EBSD data has been developed to study the texture inheritance due to the $\beta \rightarrow \alpha$ phase transformation. It is based on the fact that the variants of the same parent β grain are characterised by a limited number of misorientations between them. Thus, they can be identified with a high probability by a misorientation analysis carried out on the COM of the α phase. After identification, they are used to deduce the parent orientation. This calculation has been implemented to process orientation data obtained with an automatic EBSD analysis. A specific procedure to automatically calculate the parent β COM from that of the α inherited one has been developed. The α and the reconstructed β COMs allowed us to study some aspects of the phase transformation, notably the variant selection occurring in a T40 sample.

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