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Gomes, E; Kestens, LAI

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E Gomes[1] and L A I Kestens[1,2]

[1] Ghent University, Department of Materials Science and Engineering, Technologiepark 903, 9052 Gent, Belgium
[2] Delft University of Technology, Department of Materials Science and Engineering, Mekelweg 2, 2628 CD Delft, The Netherlands

E-mail: Edgar.Gomes@UGent.be

Abstract. Two new methods, one for determining the experimentally observed Orientation Relationship (OR) and another for reconstructing prior austenite phase, are proposed. Both methods are based on the angular deviation of the OR at the grain boundaries. The first algorithm identifies the optimum OR using the misorientation distribution of the entire scan i.e. without manual selection of parent grains. The second algorithm reconstructs the parent phase using a random walk clustering technique that identifies groups of closely related grains based on their angular deviation of the OR.

1. Introduction

Most of the steelmaking process occurs at elevated temperature which, for most steel grades, implies that part of the processing occurs in the austenitic phase. The characterization of the high-temperature austenitic phase is of great value to understand and control the microstructure evolution during the entire production chain. But the direct observation of the austenitic phase is not trivial. It can only be done at elevated temperatures, and therefore, it can only be observed within very specialized *in-situ* equipment like Electron Backscatter Diffraction (EBSD) with a hot stage[1]. Moreover, such sophisticated measurements are always done under simulating laboratory conditions, which are not necessarily representative of the real process.

Alternatively, indirect measurements are done at the room temperature. If, at this temperature, the phase transformation has already completed then the prior austenite microstructure can observed by: (a) optical microscopy with special etching techniques that revel the original grain boundaries[2], (b) reconstruction of Orientation Image Mapping (OIM) obtained with standard EBSD equipment[3, 4, 5, 6, 7]. The latter method identifies and groups product grains derived from a single parent (austenitic) grain. This technique depends on the presence of a specific OR between parent and product phases, and therefore, it only applies to diffusionless phase transformations. This work introduces two new methods aiming to improve the current-state-of-the-art in prior austenite reconstruction.

2. Orientation relationship calculation

One of the main characteristics of martensitic transformations is the presence of a specific OR between parent and product phases. Although there are some theoretical orientation relationships proposed such as the Kurdjumov-Sachs (K-S) or Nishiyama-Wassermann (N-W) correspondences for steels, a more accurate OR can only be derived from experimental data. The available methods[8, 9] for OR identification depend on the manual selection of parent grains, which is time consuming and in some cases, depending on the microstructure, impractical.

The method proposed here can derive the OR from an orientation scan in a fully automated manner and it is based on the misorientation between neighboring grains. There are two possible situations where the OR can be observed. The first one is between a parent grain and its product grain (when still a residual fraction of the parent phase is present in the product microstructure), cf. (1). The second case is between product grains sharing the same parent and involves a double OR transformation, cf. (2). In the ideal conditions that the proposed OR is valid, the angular deviation (ΔOR) is equal to 0.

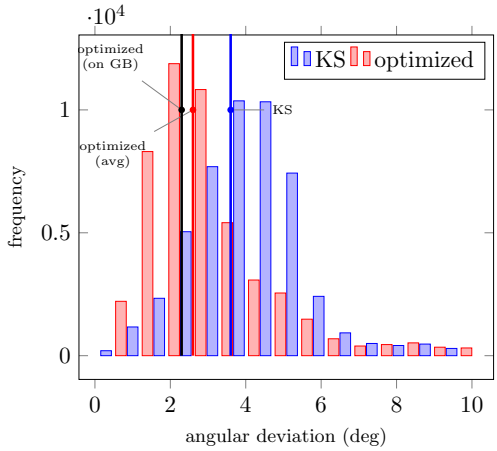

Figure 1. Histogram of angular deviation for KS OR and optimized OR.

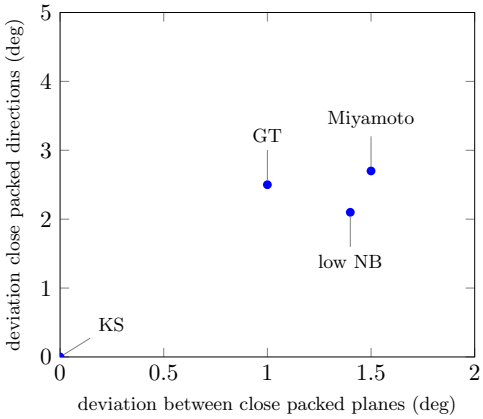

Figure 2. Comparison between optimized OR for low Nb sample and reference value (Miyamoto)[8].

The algorithm finds the optimized OR transformation ($T^{\alpha' \leftrightarrow \gamma}$) that minimizes the average angular deviation for all grain boundaries or for a selected subset of them. The number of grain boundaries exhibiting this OR should be vastly larger than the number of prior parent grain boundaries. This is a reasonable assumption since the martensitic phase transformation produces grain refinement and all the new grain boundaries have misorientations that obey the OR transformation.

$$T_m^{\alpha' \leftrightarrow \gamma} \left(Og^{\alpha'} \right) \left(Og^{\gamma} \right)^{-1} = \Delta OR \qquad T_m^{\alpha' \leftrightarrow \gamma} T_n^{\gamma \leftrightarrow \alpha'} \left(Og_a^{\alpha'} \right) \left(Og_b^{\alpha'} \right)^{-1} = \Delta OR \qquad (1,\ 2)$$

Two strategies were employed in order to calculate the grain boundary misorientations. One is based on the average orientation of both neighboring grains. The other one is based on the orientation in the immediate vicinity of the grain boundary, where only the first layer of orientations at each side of the grain boundary is selected. Slightly different values of OR are obtained by the two strategies due to plastic strain accommodation during phase transformation and associated orientation gradients in bulk of the grains[8].

This new method was validated with a low Nb steel alloy with carbon content around 0.05%. Figure 1 compares the distribution of angular deviation using the theoretical KS OR and the optimized OR, it can be noticed that the distribution shifts to the left, i.e. reducing the

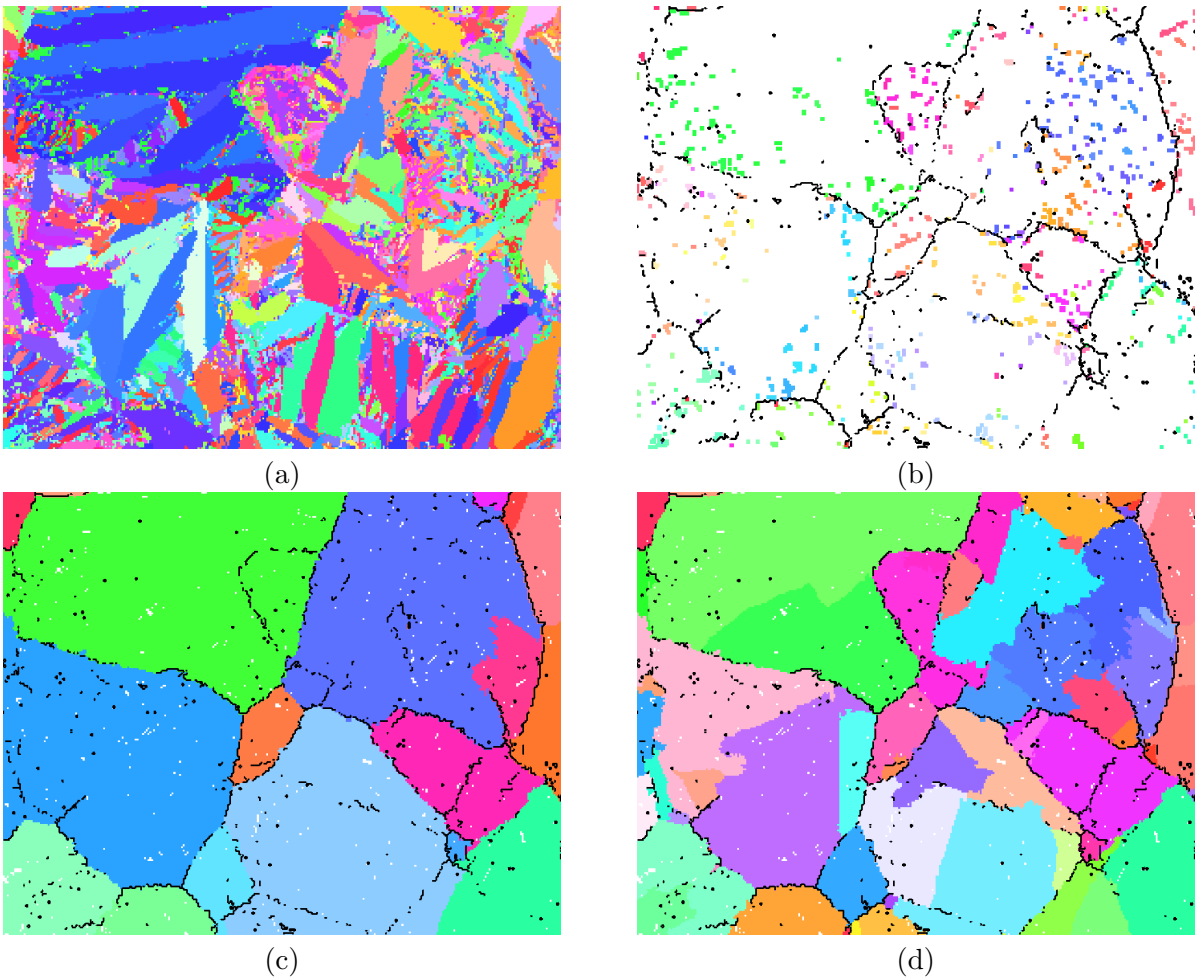

Figure 3. Validation of reconstruction algorithm on Fe-Ni alloy: (a) initial OIM before reconstruction, (b) retained austenite and expected prior austenite GB, (c) reconstruction after the first iteration and (d) second and final step of reconstruction.

overall error, when the optimized OR is used. Better results are obtained when considering orientations in the immediate vicinity of the grain boundary compared to considering grain averaged orientations. Figure 2 compares the optimized OR for the low Nb sample with two theoretical ORs and one reference value[8] that contains comparable amount of carbon. The optimized OR is in good agreement with the reference value.

3. Parent phase reconstruction

A new method, equally based on grain boundary misorientations, is proposed for the parent phase reconstruction. The key concept of this method is the use of a graph clustering algorithm to find groups of closely related grains that originate from a single parent grain. The Markov Clustering algorithm[10, 11] is used because of the following features:

- It is based on the probabilities of random walks through the graph.
- It identifies natural cuts and clusters in the graph without the need to specify threshold values of allowable angular deviations or the necessity to specify a predefined number of clusters

- There is only one parameter that controls the cluster coarsening.
- Excellent noise tolerance.
- Fast calculation time.

In order to use the clustering algorithm, a graph has to be derived from the OIM in the following way: (a) each grain, product or parent, becomes a node in the graph, (b) each grain boundary becomes an edge connecting two neighboring nodes (grains) and (c) each edge receives a value based on the equation (1) or (2), which determines the probability of the two neighboring grains being products of the same parent. Once the graph is constructed, the clusters are determined using the highest level of coarsening. Then each cluster forms a parent grain and its orientation is calculated by an optimization algorithm that minimizes the average angular deviation using the equation (1).

The first iteration described above may result in some of the clusters containing more than one parent grain because of the initial coarsening level. These grains can be identified by its higher average angular deviation, and therefore, they should be further refined by running an extra iteration step with reduced coarsening level. The refinement procedure should be repeated many times until all parent grains have low average error.

A Fe-Ni 29% sample was used to validate the proposed reconstruction method. The OIM after the martensitic phase transformation with still 10% retained austenite is shown in the figure 3a. The expected parent microstructure is visualized in figure 3b by the retained austenite and the traces of high angular deviation ($> 10°$). Figure 3c shows the reconstruction after the first iteration, showing that some reconstructed grains incorporate more than one parent grain. The final microstructure is shown in figure 3d after an extra step of refinement.

A careful look at the figure 3d shows that some unexpected features are visible at twin boundaries in parent grains and some grains are over refined. The current implementation of the reconstruction software is quite simple and does not include any special rule for treating this type of boundaries or for re-merging over-divided clusters.

4. Conclusion

Tolerance error reduction and noise immunity are two fundamental strategies for the success of prior austenite reconstruction. The use of optimized ORs reduces the overall error but the identification by previous techniques requires manual selection of parent grains. The method proposed here identifies an optimized OR, whereby the entire orientation scan is considered and the result is obtained without user intervention.

Markov clustering seems a promising technique for parent grain reconstruction due its noise tolerance and fast calculation time. The present results are satisfactory considering the initial stage of development and the simple implementation. Further work on the special treatment of twin boundaries and cluster re-merging will be done.

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