

Crystallographic Reconstruction of Parent Austenite Twin Boundaries in a Lath Martensitic Steel

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Abstract

The study of post-transformation microstructures and their properties can be greatly enhanced by studying their dependence on the grain boundary content of parent microstructures. Recent work has extended the crystallographic reconstruction of parent austenite in steels to include the reconstruction of special boundaries, such as annealing twins. These reconstructions present unique challenges, as twinned austenite grains share a subset of possible daughter variant orientations. This gives rise to regions of ambiguity in a reconstruction. A technique for the reconstruction of twin boundaries is presented here that is capable of reconstructing $60^\circ \langle 1\ 1\ 1 \rangle$ twins, even in the case where twin regions are comprised entirely of variants that are common between the twin and the parent. This technique is demonstrated in the reconstruction of lath martensitic steels. The reconstruction method utilizes a delayed decision-making approach, where a chosen orientation relationship is used to define all possible groupings of daughter grains into possible parents before divisive decisions are made. These overlapping, inclusive groupings (called clusters) are compared to each other individually using their calculated parent austenite orientations and the topographical nature of the overlapping region. These comparisons are used to uncover possible locations of twin boundaries present in the parent austenite. This technique can be applied to future studies on the dependence of post-transformation microstructures on the special grain boundary content of parent microstructures.

1. Introduction

Many crystalline materials undergo displacive or diffusionless transformations in which the product phase is dependent on the orientation of the parent phase. Various properties of the daughter microstructure are inherited from the parent phase due to this dependence, however the daughter structure typically consumes the parent structure making it difficult to observe how the processing of the parent phase affects the final post-transformation material. The martensite transformation in steel is a common example of this. When the orientation dependence of the daughter phase on the parent phase is known, it may be possible to “reconstruct” the parent phase computationally, identifying parent grains that may have generated the observed daughter grain structure. If this can be done accurately, the pre- and post-transformation structures can be compared directly. This can be of value in improving the understanding of microstructural inheritance in materials such as steel, where it is difficult to observe the history of the pre-transformed phase—including the application of complex loading conditions at austenitic temperatures. Ultimately the crystallographic reconstruction of a parent phase can facilitate optimization of the thermomechanical processing of the pre-transformed structure. [1-3]

Reconstruction of austenite in steel presents unique challenges. Crystallographic reconstruction is based on a known Orientation Relationship (OR) between the two phases, and the quality of the daughter orientation map obtained from electron backscatter diffraction (EBSD) measurements. This information is essential to a parent phase reconstruction, which is often complicated by various



uncertainties. These uncertainties arise in the reconstruction of austenite in steel due to noisy datasets, deviations from a given OR, and other ambiguities [3, 4]. Methods must be developed to deal with these uncertainties. While prior austenite reconstructions in steel can be made difficult by these ambiguities, they can potentially be resolved through a semi-automated delayed-decision making approach detailed here.

Reconstructions depicted in subsequent sections of this work are performed on two martensitic steels. The first EBSD dataset was provided by US Steel and Carnegie Mellon University. The martensitic microstructure is from a seamless tubular steel intended for use as oil country tubular goods. Most of the production parameters are proprietary and the information provided is as specific as possible. The steel composition is similar to AISI 4130, and the product was heat treated as follows: heated to above the austenitizing temperature (>850 °C), then quenched by water sprays, and finally tempered at a temperature between 500 and 700 °C [5]. The second EBSD dataset was provided by ArcelorMittal. It is M1700 steel, a commercially available tempered martensitic sheet steel. Its composition is 0.3 wt% C, 0.45 wt% Mn, 0.01 wt% P, and 0.015 wt% S.

2. Background

Parent phase reconstruction has been performed on various materials and has been applied in the literature by various authors on materials for which an OR can be defined. Germain, Humbert, et al. have performed prior-phase reconstruction on austenite in steel, as well as the beta phase of titanium alloys [3, 6, 7]. Cayron, et al. have developed a method of parent austenite reconstruction in steels that utilizes a groupoid approach, defining mathematical operators that link different daughter variants to each other [1, 8, 9]. Miyamoto, Abbasi, and other authors have proposed methods, and addressed the challenges of prior phase reconstructions in different steels [2, 4, 10]. Central to each of these methods is the definition of the orientation relationship between the parent and daughter phases. Various ORs have been experimentally determined in steels and are well documented in the literature [3, 11, 12]. The determination of which OR is followed has been shown to depend on factors such as material composition, processing of the austenite, and resulting martensite morphology [11, 12]. While ORs are typically expressed as sets of crystallographic planes and directions that are coincident between the two phases, measured ORs are almost always irrational [13]. Different material chemistries will tend towards specific ORs, however; low carbon steels have been shown to exhibit the KS OR, while Fe-Ni systems often exhibit the NW OR [12]. Table 1 lists commonly observed ORs in steel. For martensite, the KS and NW ORs can be seen as “bounding” ORs, where the OR of the formation of lath martensite has been observed to range between the two [12, 13]. Figure 1 demonstrates the resulting set of orientational variants predicted by the KS OR.

Table 1

OR	Parallel Plane	Parallel Direction
Kurdjumov-Sachs (KS)	$\{1\ 1\ 1\}_{\gamma} \parallel \{1\ 1\ 0\}_{\alpha}$	$\langle 1\ 1\ 0 \rangle_{\gamma} \parallel \langle 1\ 1\ 1 \rangle_{\alpha}$
Nishiyama-Wassermann (NW)	$\{1\ 1\ 1\}_{\gamma} \parallel \{1\ 1\ 0\}_{\alpha}$	$\langle 1\ 1\ 2 \rangle_{\gamma} \parallel \langle 1\ 1\ 0 \rangle_{\alpha}$
Greninger-Troiano (GT)	$\{1\ 1\ 1\}_{\gamma} \parallel 1^{\circ}$ from $\{1\ 1\ 0\}_{\alpha}$	$\langle 2\ 1\ 1 \rangle_{\gamma} \parallel 2.5^{\circ}$ from $\langle 1\ 1\ 0 \rangle_{\alpha}$

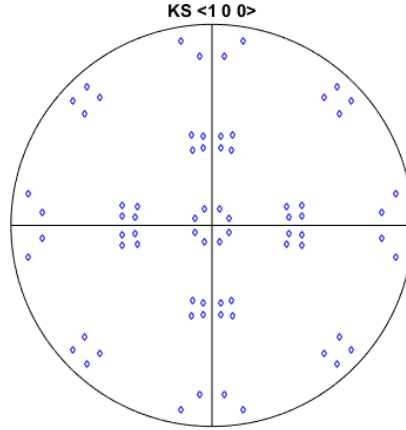


Figure 1: Pole figure centered on [001] demonstrating the $\langle 100 \rangle$ poles of each of the 24 variants of the KS orientation relationship, assuming a parent austenite orientation unrotated from the pole figure's axes.

A common method of parent phase reconstruction is a neighbor-to-neighbor comparison of daughter variants, in search of groupings of daughter grains that have the same parent. Orientation relationships are used in this comparison. For a given parent orientation, a set $\{i\}$ of possible daughter α orientations is defined by an OR according to equation 1. Likewise, a set of possible γ orientations for a single daughter grain can be defined using the inverse of the orientation relationship (represented as a single rotation T_{OR}). The symmetries of each cubic phase are represented by the set of symmetry operators S_i .

$$g_i^\alpha = T_{OR} \cdot S_i^\gamma \cdot g^\gamma \quad g_i^\gamma = T_{OR}^{-1} \cdot S_i^\alpha \cdot g^\alpha \quad (1)$$

Where two daughter grains share a possible parent, they can be grouped together as having possibly originated from a parent austenite grain of that orientation. The two possible parents “overlap” when their misorientation angle ε as defined by equation 2 is within a pre-set tolerance. Groups can be defined for which a single orientation is within tolerance of possible parents for many daughter grains, defining a region of prior austenite. This process is depicted in figure 2. This type of neighbor-to-neighbor comparison using an OR is well outlined in papers by Germain and Humbert [3, 7]. The final reconstruction of a parent austenite grain consists of a “cluster” of daughter grains from the EBSD map, and a collection of possible parent orientations in orientation space - one possible parent for each daughter grain. The orientation of the possible parent is back-calculated by computing the average of the collection of possible parents.

$$Tr(g_2 g_1^T) = 2 \cos(\varepsilon_{12}) + 1 \quad (2)$$

Equation 2: For two orientations g_1 and g_2 , their misorientation is ε_{12}

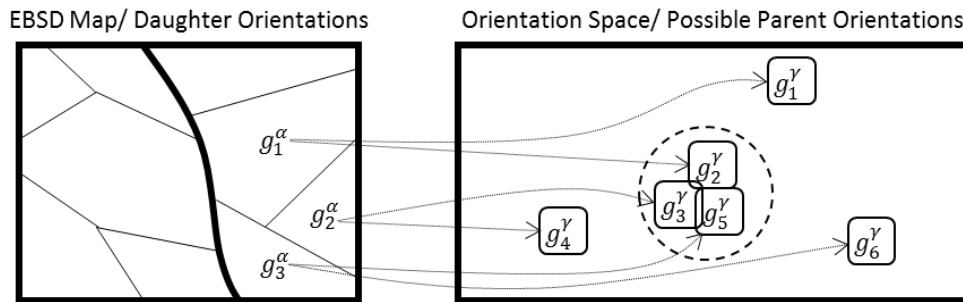


Figure 2: For a daughter grain (left) a set of possible parent orientations (right) is defined using the inverse of an orientation relationship. A viable solution for the grouping of daughter grains is found where each daughter grain has one possible parent within a dense local grouping of possible parents in orientation space. The local grouping of orientations in orientation space is defined by their misorientation as defined in equation 2.

A neighbor-to-neighbor approach to prior austenite reconstruction often leads to ambiguities. The sets of daughter grains belonging to two clusters may not be mutually exclusive; there can be subregions of daughter grains that satisfy the OR for both clusters simultaneously (i.e. each daughter grain in the ambiguous subregion has two possible parents, each fitting with one of the back-calculated parent orientations for the two clusters). When performing a reconstruction, this ambiguous region must be either assigned to one cluster or divided between the two clusters. This process is difficult to automate, and often requires manual decision making [4].

A common cause of ambiguities in the reconstruction of prior austenite in steel is the presence of twin boundaries in the parent austenite. The twin relationship of the two parent crystals results in the theoretical sets of possible daughter orientations having a subset in common. According to the KS OR, two twinned austenite crystals will share 6 of their 24 possible daughter orientations. When the transformation takes place along the twin boundary, the daughter variants that are “selected” to nucleate are often from this common set of 6 variants due to the energetic favorability of having a daughter variant satisfy the OR with both parent austenite orientations simultaneously. These daughter grains are said to satisfy a “double-KS” or “KS-KS” orientation relationship. These ambiguous regions are often very difficult to resolve, as the parent austenite twin boundary is often partially or completely consumed by daughter grains that traverse the twin boundary. Figure 3 demonstrates the often complex morphology of the ambiguous region, as well as the uncertainty as to where the twin boundary actually lies. The orientations of daughter variants for two twinned austenite grains, as predicted by the KS OR, are shown in figure 4. Variants that are common between two twinned austenite orientations are shown to overlap in the pole figure.

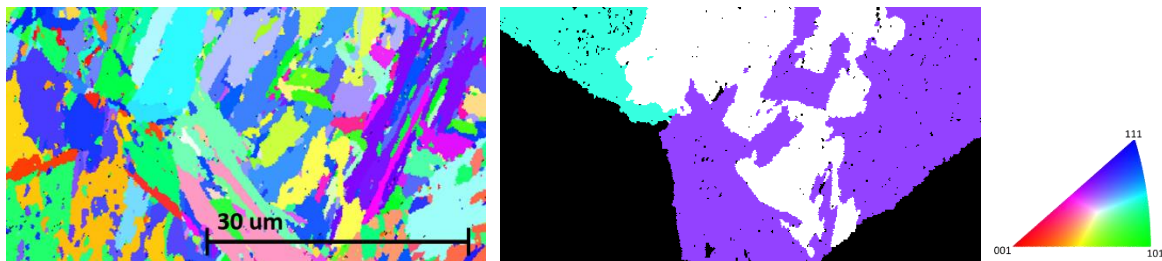


Figure 3: For the martensite grains in the IPF map to the left, two groupings into parent austenite grains can be found and are demonstrated in the IPF map to the right. The region highlighted in white belongs to both clusters. Each martensite grain within the highlighted region satisfies the KS OR with both parent austenite orientations. This EBSD map is a subsection of the data provided by Carnegie Mellon University.

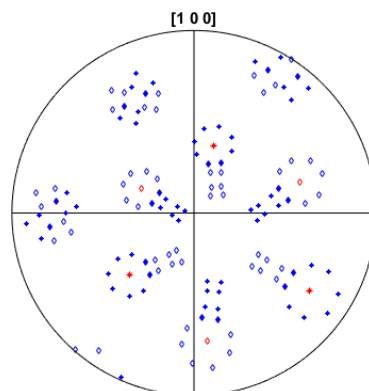


Figure 4: The orientations of the two back-calculated parent austenite grains from figure 3 (red), and their theoretical daughter variants as predicted by the KS OR (blue). Sets of poles belonging to either cluster are differentiated by marker (diamond vs. asterisk). Six variants overlap, as denoted by asterisks and diamond markers overlapping. This suggests that the parent orientations are twinned.

3. Method

The reconstruction method employed here utilizes a neighbor-to-neighbor approach within a delayed-decision making framework. During a reconstruction effort, when an ambiguous region is found, the resolution of that ambiguous region is delayed until after all possible groupings of daughter grains into possible parents have been found. This approach is in contrast to methods that attempt to resolve the ambiguity as they are found (i.e. making a choice of where to assign an ambiguous daughter grain in the moment based on some additional metric). Instead, reconstructed regions are allowed to overlap each other, some groupings completely enveloping others. This provides a list of many possible groupings or “clusters”, with some of the groupings ultimately providing a more insightful view of the pre-transformed structure. This method has significant advantages when reconstructing regions that satisfy a KS-KS relationship.

The core of this reconstruction method lies with the independent “growth” of clusters of daughter grains. Each cluster is started from a seed comprised of 3 daughter grains that share a possible parent orientation (see figure 2). Prior to a reconstruction, all viable seeds for a given region are found by comparing the lists of possible parents for all sets of 3 neighboring daughter grains. Once a seed has been found, the 3 possible parent orientations that are within tolerance of each other are averaged to define a starting PA orientation for the cluster to be grown. Neighboring daughter grains are iteratively added to the cluster if they have a possible parent within a tolerance misorientation of this averaged austenite orientation, which is then re-averaged. This process is repeated until no new neighbors can be added to the cluster. Once this has been achieved, the final parent austenite orientation assigned to the cluster is taken as the average of the collected possible parent orientations- one from each daughter grain that is a member of the cluster. This average is computed as the vector average of the set of collected parent orientations represented as quaternions [14, 15]. This process is described in figure 6, a flowchart outlining the algorithm’s basic logic. Figure 5 depicts the growth of a cluster visually, as neighbor martensite grains are added.

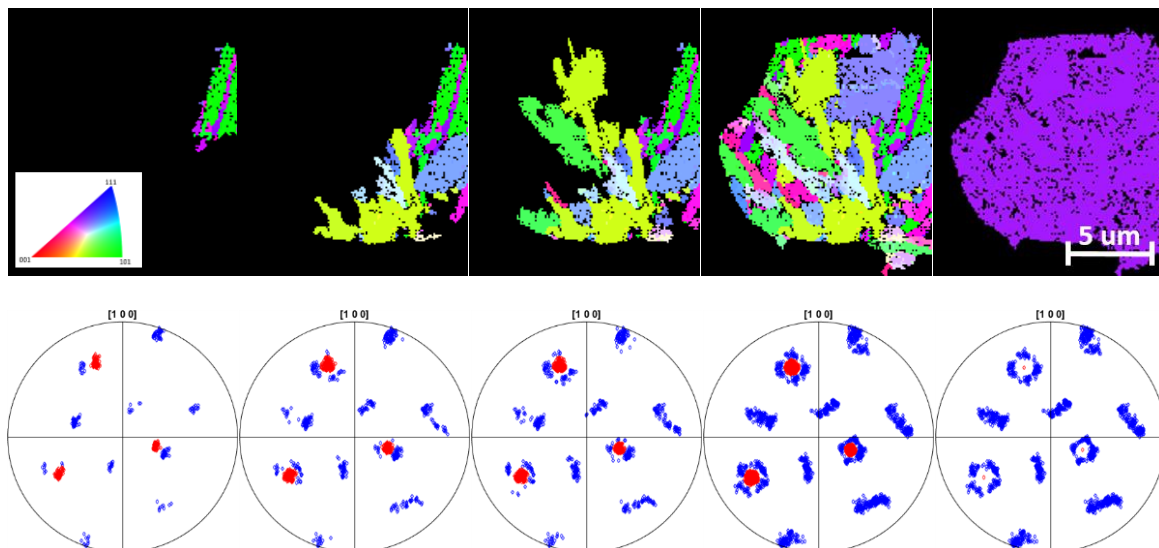


Figure 5: ArcelorMittal M1700 steel, original scan spanning a 14 by 16 μm area at a step size of 0.1 μm . Progressing from left to right- individual stages of the cluster growth algorithm, showing growth of a cluster in the IPF map “space”. The pole figures demonstrate the collection of possible parent orientations (red) in orientation space. As neighboring martensite grains are added to the cluster, their orientations (blue), and their selected possible parents are added to the pole figure. Once no more grains can be added, the group of possible parents are averaged into a single orientation.

Each cluster is grown independently from all other clusters. Any daughter grain that was added to a previous cluster may also be added to a subsequent cluster. By creating an exhaustive list of seeds and

allowing each to grow independently, an extended list of both clusters and ambiguities is created. While each of these ambiguities must be considered, the full list of possible groupings of daughter grains into clusters provides a large dataset that can be explored to find the best reconstruction.

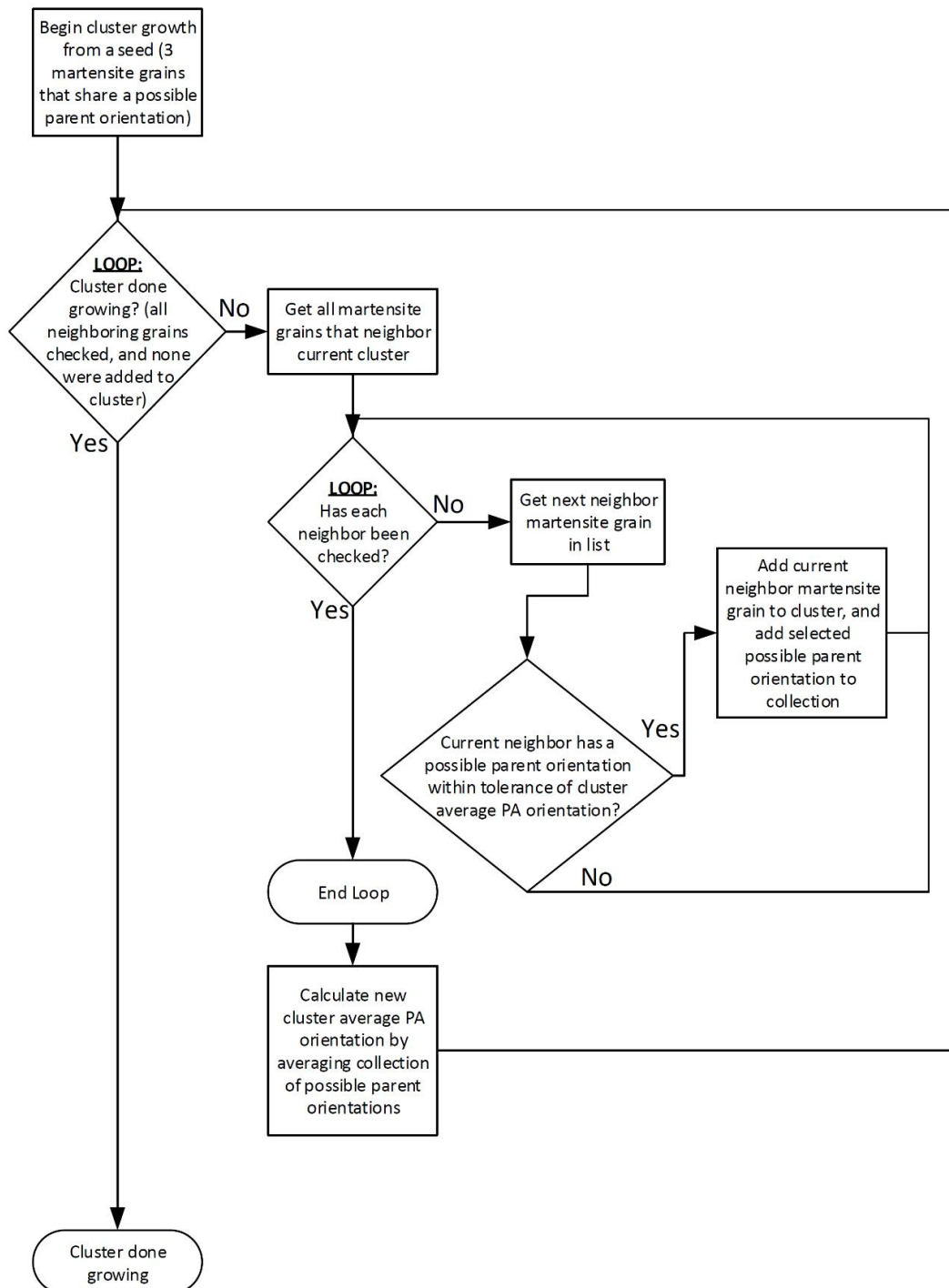


Figure 6: A flowchart describing how a cluster is grown from a "seed"

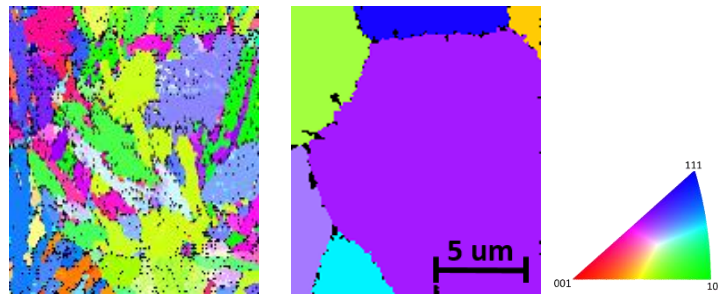


Figure 7: A completed reconstruction of the same region of ArcelorMittal M1700 depicted in figure 5. Each cluster is mutually exclusive and no ambiguities exist.

Various automated and semi-automated methods are used to resolve ambiguities. Ambiguities are classified by the topological relationship between the two overlapping clusters. Some ambiguities are in the form of clusters that are complete subsets of other clusters, where an additional possible austenite orientation can be assigned to that region. Some ambiguities are caused by two clusters with the same set of daughter grains but different parent orientations. These are cases where the set of variants is insufficient for a single unique parent orientation to be calculated. Other ambiguities are caused when daughter grains are erroneously assigned to a neighboring cluster by simply being within tolerance of that clusters calculated parent orientation- which may happen in a noisy dataset. Each of these ambiguities are unique in origin and must be handled in different ways. The determination of the nature of each ambiguity can only be automated to an extent, and often manual intervention is required for their resolution. A delayed decision making process allows the full extent of each ambiguity to be explored. The following sections detail the results of reconstructions containing ambiguities of different types. The approach to resolving them is described.

4. Results

Several reconstructions of martensitic steels demonstrate the different topological natures of ambiguous regions caused by twinning in the parent austenite. The common set of daughter grains belonging to two overlapping clusters as well as the spatial distribution of the clusters within the space of the EBSD map are important factors to consider when assessing the nature of an ambiguity. One cluster may be a subset of another cluster, or they may share a subset. Furthermore, the external boundaries of each cluster (as seen by the human eye) may suggest a relationship not reflected by their topologies. Various reconstructed datasets demonstrate this here.

One such dataset, demonstrated in figure 8b, shows several large clusters with ambiguous regions obscuring the boundaries between the two parents that contain them. In both cases, the calculated parent orientations of the clusters containing the ambiguity can be shown to satisfy the misorientation relationship of a pair of twinned FCC crystals—a 60° rotation about a $\langle 111 \rangle$ axis. From the back-calculated orientations for either overlapping cluster the twinning plane can be defined. In figure 8c, the twinning plane for both ambiguities is plotted where it best fits the existing boundary between the two overlapping clusters. In one case (the leftmost white region), the twinning plane is reasonably well oriented with existing boundary between the two overlapping clusters. In the case of the ambiguity to the right, however, the boundary between both clusters seems to be completely consumed by the ambiguous region. To resolve the ambiguities, the best division of daughter grains was chosen that resulted in a boundary that was both straight and reasonably well oriented with respect to the twinning plane. This example demonstrates the variation in degree of overlap an ambiguity may have with the clusters that define it—an ambiguous region may be evenly distributed between both overlapping clusters, or it may exist mostly to one side of the real parent boundary.

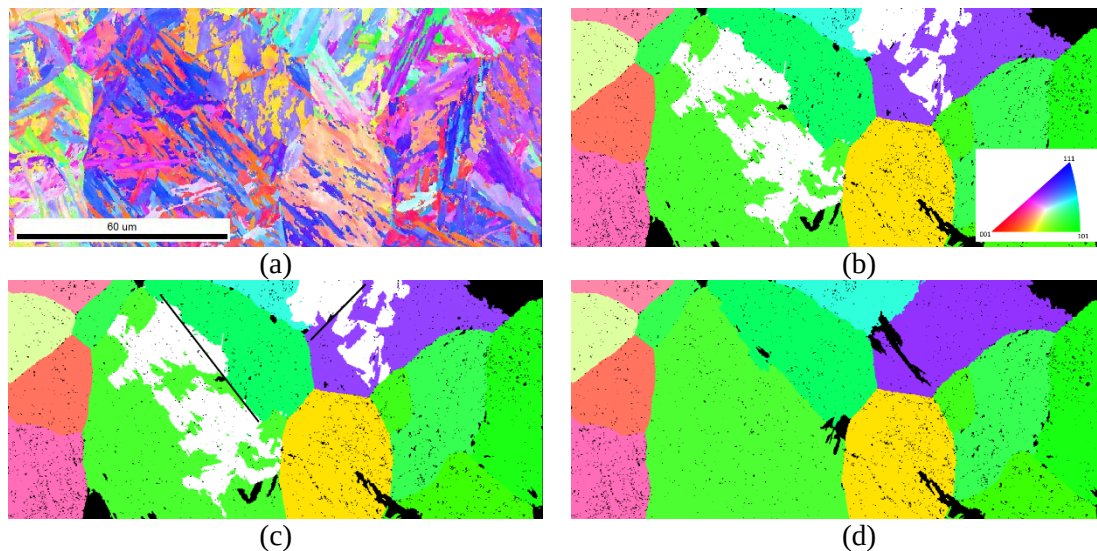


Figure 8: Another, larger subsection of the dataset provided by Carnegie Mellon University. (a) The IPF map of a martensitic steel, as produced by OIM analysis. (b) A reconstruction of the parent structure (IPF map generated in MATLAB), each cluster colored according to its back-calculated parent orientation. Two large ambiguous regions are found, highlighted in white. In both cases, the parent clusters that overlap satisfy the misorientation relationship of two twinned FCC grains to within 2 degrees. (c) The (111) plane that would be the twinning plane (if the two parent grains were indeed twinned) is plotted for each ambiguity. In the case of the left ambiguity, the proposed twinning plane is in good agreement with existing boundary between the two clusters. (d) The ambiguities are split between their clusters according to the best fit with the proposed twinning planes. In this way, other such twins may be found in this dataset.

Another topological case for an ambiguity is when a cluster is found as a complete subset of another cluster. This is demonstrated in figure 9. Here, all the members of the smaller cluster are also members of the larger surrounding cluster. The cluster representing the subset again satisfies the misorientation relationship of a twin with the cluster that contains it. Furthermore, the major axis of an ellipse fitted to the sub-cluster is in close agreement with the orientation of the twinning plane between both clusters' orientations. This suggests the strong possibility that an annealing twin existed within this parent grain, as demonstrated by the sub-cluster stretching across the larger cluster. In this case, each member of the smaller cluster is one of the common variants between the two twinned austenite orientations.

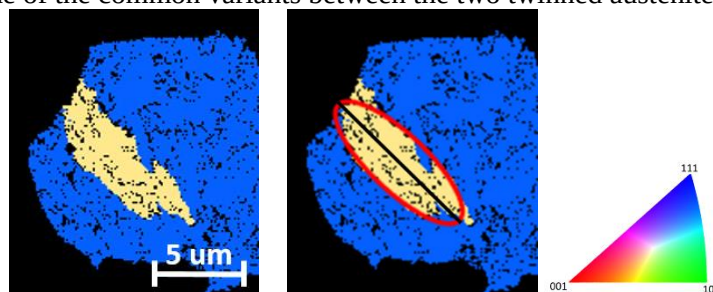


Figure 9: Two clusters found in the M1700 steel, one of which is a subset of martensite grains belonging to the larger cluster. In the case of the smaller cluster, the back-calculated parent orientation satisfies a twin misorientation relationship with the other cluster's orientation to within 3 degrees. The long axis of the cluster (taken as the major axis of a fitted ellipse) is also within 3 degrees of the (111) twinning planes of either austenite orientation.

A final example demonstrates the relationship of two clusters that share a subset, but where one cluster appears to exist only "inside" the physical boundaries of a larger cluster. Figure 10 Shows the larger cluster, and then the superposition of the smaller cluster. There are small sets of daughter grains that

belong to only the smaller cluster, but that are also within the boundary that would form a convex hull around the larger cluster. Again, these two clusters are within a close misorientation of a twin relationship. The smaller cluster appears to suggest the presence of a twin band—this time large enough that some small regions of material within the twin are comprised of variants that were not common between both clusters' orientations, but belonging only to the twinned orientation. The orientation of the twinning plane as plotted is also in agreement with sections of boundary between the two clusters. Of interest is the region not covered by the twin cluster. This region is composed of variants belonging only to the *larger* cluster. This casts doubt on the idea that the twin extended fully across the larger grain.

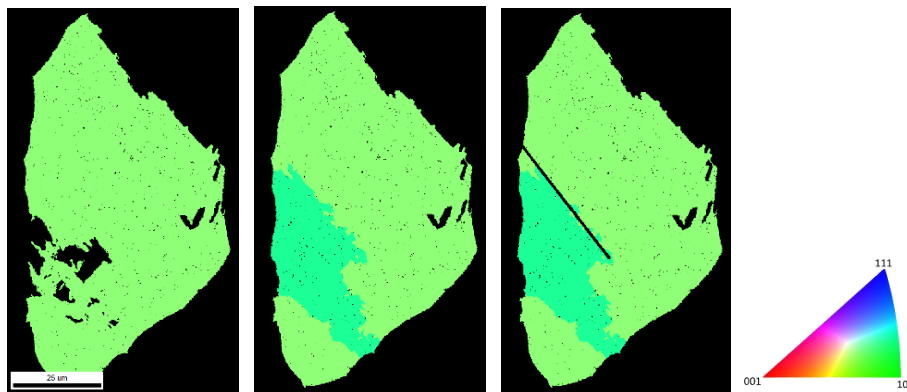


Figure 10: The reconstruction of a large prior austenite grain within the dataset provided by Carnegie Mellon University (IPF created in OIM). Another example of an interior cluster that satisfies a twinned misorientation relationship with the cluster that contains it. The twinning plane is plotted and is shown to be in good agreement with the existing boundary.

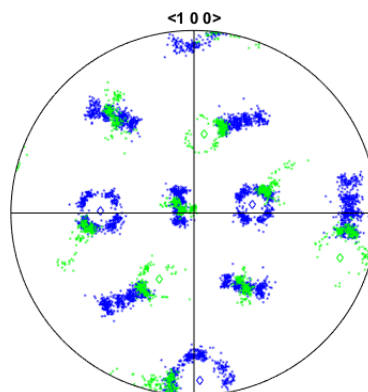


Figure 11: The orientations of the martensite grains plotted for both clusters shown in figure 9. Martensite orientations belonging to the interior clusters are plotted in green, and the orientations belonging to the larger cluster are plotted in blue. The interior cluster contains variants that are not held in common between both twinned cluster orientations.

5. Discussion and Conclusions

The reconstruction of parent austenite was performed here using a cluster growth algorithm within a delayed-decision framework. Many possible groupings of daughter grains into parent clusters are considered, and the nature of the ambiguous overlapping regions are explored. The ambiguous regions caused by the presence of twin boundaries in the parent austenite are of particular interest, and their various topologies and morphologies are demonstrated. While this method of reconstruction is automated, post-processing and interpretation of results is left to semi-automated or manual intervention. The complex nature of each ambiguous region makes it difficult to resolve each one via automated methods, though many ambiguities can potentially be dealt with via automated techniques.

The goal of this method is to explore all possible groupings of daughter grains into possible parent grains. This allows the user to take advantage of the information made available by a full collection of possible groupings, and a full list of ambiguities contained in the data set.

The delayed decision making approach used here was found to have some advantages over a reconstruction that makes assignments prematurely. A cluster growth algorithm that employs a “first come first serve” type approach would be very unlikely to correctly assign members of an ambiguous region to the appropriate cluster. This is demonstrated by the various topologies of the ambiguous regions created by twins, and the different extent to which an ambiguous region may extend into one cluster or the other. Twin bands composed entirely of common variants between both twinned austenite orientations would very likely be missed by a reconstruction method that does not perform a more extensive search of possible groupings. More complex still are the overlapping clusters that have both inclusive and exclusive subsets, but where the nature of their physical boundaries suggest that one cluster is spatially “contained” by the other. Each of these cases demonstrate the advantage a delayed-decision making approach has to exposing the full extent of the ambiguity.

While the reconstruction of twin boundaries is not precise in the sense that it results in a straight boundary, the knowledge of the presence and approximate orientation of the boundary is of great value in a reconstruction attempt. In figure 9, where a large interior twin is demonstrated, there are still questions that must be answered regarding the nature of the boundary between the two reconstructed clusters. The region of the larger cluster that seems as though it should belong to the twin orientation is composed of variants that are *not* common between the two twinned orientations, but only to the larger cluster. Such information must be considered when deciding whether or not an interior cluster truly represents a twin.

Future work will continue to automate specific tasks, as well as study different aspects of the martensite transformation. Reconstructions using this method may shed light into variant selection behaviors. Other nucleation and growth behaviors may be shown to result in similar ambiguities to twins. Variants can be grouped according to the close-packed habit plane on which they form, nucleating and growing in packets. This type of delayed-decision making approach may aid in a study of the formation and size of these packets.

The advantages of this method are demonstrated in the type of information made available to a person performing a reconstruction of parent austenite. The large number of clusters found provide a valuable set of data. Though searching this dataset is only semi-automated and the generation of many clusters can be computationally intensive, the resulting information that is made available is of high value.

6. Acknowledgements

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