Segmentation of 3D EBSD Data for Subgrain Boundary Identification and Feature Characterization

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Abstract

Subgrain structures formed during plastic deformation of metals can be observed by electron backscatter diffraction (EBSD) but are challenging to identify automatically. We have adapted a 2D image segmentation technique, fast multiscale clustering (FMC), to 3D EBSD data using a novel variance function to accommodate quaternion data. This adaptation, which has been incorporated into the free open source texture analysis software package MTEX, is capable of segmenting based on subtle and gradual variation as well as on sharp boundaries within the data. FMC has been further modified to group the resulting closed 3D segment boundaries into distinct coherent surfaces based on local normals of a triangulated surface. We demonstrate the excellent capabilities of this technique with application to 3D EBSD data sets generated from cold rolled aluminum containing well-defined microbands, cold rolled and partly recrystallized extra low carbon steel microstructure containing three magnitudes of boundary misorientations, and channel-die plane strain compressed Goss-oriented nickel crystal containing microbands with very subtle changes in orientation.

Keywords: *Electron Backscatter Diffraction, 3D EBSD, Segmentation, Fast Multiscale Clustering, Subgrain Structures, Kuwahara Filter*

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1. Introduction

1.1 Motivation and Background

Studies of the geometric and crystallographic features of microstructures generated by deformation, annealing, and phase transformation can shed light on both their mechanisms of formation, and how they relate to key properties of the materials. A significant characteristic of many types of deformed metals and alloys is the subgrain structure generated. This structure is regularly investigated by electron backscatter diffraction (EBSD) based on local crystallographic orientation measurements. Since regions belonging to a grain share similar orientations, the grain can be reconstructed and then quantitatively characterized from processed EBSD data [1]. Furthermore, EBSD techniques can produce three-dimensional (3D) crystallographic data for a sample volume, which is necessary to gain a more complete understanding of the structure than can be taken from two-dimensional (2D) data [2, 3]. From a 3D reconstruction, many geometric and crystallographic features may be measured directly, such as grain volume, shape, and the distribution of misorientations across a boundary [4]. Moreover, a 2D study cannot yield the information necessary for a full crystallographic characterization of grain boundaries or the correlation of a specific geometry with crystallographic orientation. This information is straightforward to extract from 3D EBSD data that has been segmented by grains, and any analog can be similarly found from a segmentation based on subgrain structure.

A volumetric EBSD data set that has been segmented into subgrain features can be interrogated for relationships between the detailed microstructure and bulk material properties. However, unlike high angle grain boundaries (HAGBs), the variations between subgrain structures are more subtle in magnitude (low total difference in orientation between subgrains) and spatially

gradual (low point-to-point differences). This makes the identification of subgrain boundaries challenging and, hence, creates a significant obstacle to generating reliable data on the spatial distribution of subgrains within the overall deformation substructure for understanding the mechanisms of subgrain formation.

The identification of features in a 3D EBSD data set may be achieved by grouping points that are not separated by a boundary with misorientation higher than a user-defined threshold. This is a common method in commercial software but fails when applied to subgrain data since there is no threshold angle that identifies the boundaries of interest without being dominated by noise in the sample. Figure 1a-c shows an artificially-constructed volume of orientation data representing a gradual transition between two similar microstructural features. The volume is a cube with 25 voxels per side and 9° corner-to-corner misorientation. The transition occurs linearly along the middle third of the cube diagonal. The data has been made more realistic by contaminating voxels with uniformly distributed noise to add, on average, 0.5° misorientation from its original orientation. This value was selected because, although angular accuracy of 0.01° is possible with high resolution methods, 0.5° is typical for standard methods [5]. Segmentation by thresholding is demonstrated in Figures 1b and c. A threshold angle of 0.5° finds many superfluous boundaries, and a threshold angle of 0.75° finds very few boundaries, all of which are from the added noise. In both cases, noise dominates and no threshold value between improves the situation. We present a robust solution to segmenting 3D EBSD data, which identifies the proper boundary geometry such as that shown in Figure 1d.

The challenges in characterizing fine-scale microstructures have been addressed by Humphreys et al. [6] with a modified Kuwahara filter. This method passes through the data set calculating the average and variance of every neighborhood (*e.g.* 3×3 or $3 \times 3 \times 3$ region). Then every point is replaced with the average value of the neighborhood to which it belongs having the lowest variance. This serves to reduce noise in the data set while preserving edges. Further processing, including multiple passes of the filter, may be carried out before segmenting the data using a misorientation threshold, as described above. While this may be sufficient in many cases, the Kuwahara filter is local in nature, and the final thresholding step may produce too many edges in one region of a data set and not enough in another. Furthermore, the results are unpredictable over spatially gradual boundaries. The Kuwahara filter will be compared to our method below.

1.2 Fast Multiscale Clustering

Fast multiscale clustering (FMC) is a segmentation technique developed for 2D image processing [7]. The method creates a nested partitioning of the data set at many scales. Starting with individual data points at the finest scale, the processes iteratively coarsens the partitioning by combining groups. At each scale in the hierarchy, every group is then scored based on the similarity of points it contains and distinction from neighboring groups. The highest-scoring groups form the final segmentation of the data. FMC uses fuzzy logic in this grouping, so coarse collections are not rigid. That is, a fine-scale group has probabilities of being part of more than one coarse-scale group, and these probabilities are propagated through every scale. The probability of assignment is based on the similarity of a group to certain neighboring groups that are chosen as seeds for the coarser scale. Determining similarity of data requires a metric. For simple color images, this can be a scalar difference between colors, but for application to EBSD

data, the metric is based on misorientation. Here, we adapt FMC to work with a quaternion representation for orientation data, so that misorientations can be calculated efficiently. A detailed description of FMC and its modifications for EBSD data is provided in a 2D setting in ref. [8], and the formulation extends to three dimensions. Although the iteration procedure is probabilistic, selection of the final solution is deterministic, based on the optimal segmentation of groups down to individual data points. Thus, the resulting reconstruction is reproducible over repeated applications of the algorithm. The probabilities are also useful as a measurement of confidence of each point's assignment in the final solution. Maps of this confidence can be produced from the final segmentation data to reveal regions of high and low certainty.

At each scale in the hierarchy, groups inherit properties from the finer scale below, down to the individual data points, all modified by the probability of assignment [9]. The aggregated properties are the group size (volume), the average quaternion orientation, and the variance of orientations within the group. This allows FMC to segment an entire data set with awareness of local and global properties. Another advantage is that the method does not depend on the physical spatial distribution of the data, only on the adjacency of points. Therefore, FMC is not only applicable for 2D situations but easily applied in 3D. In fact, the data points do not have to be located on a regular grid, as is the case after correcting for instrument drift, and neighbors can be selected as any points within a given radius. Finally, since there are fewer groups at coarser scales, FMC has a runtime linear with the number of data points. This is a practical consideration that becomes important for methods applied to large data sets with more than two dimensions.

A misorientation angle between average orientations is not useful on its own when comparing coarse groups containing many data points. The Mahalanobis distance [10] is used to account for additional information. This metric is defined as the pointwise distance between group averages divided by the group variances. This gives groups with low variation naturally less similarity to their neighbors than groups with high variance. Our modified definition for use with EBSD data is the misorientation between the aggregated mean orientations divided by the minimum of the group's variances. The minimum of the variances is used so that a group with a high variance is not assigned a small distance to an entirely dissimilar group. A novel variance aggregation method was developed by the authors [8] since the elements of quaternions are not linearly correlated. While this value of Mahalanobis distance lacks physical significance, it can be scaled at the aggregation step to give sense to closeness and farness, depending on the nature of the data set. The scaling parameter, C_{Maha} , determines the sensitivity of the segmentation [7]. Figure 2 shows segmentations of the artificially-constructed data set using different values of C_{Maha} , along with confidence maps along the diagonal plane. In the more sensitive segmentation with higher C_{Maha} (Figure 2b), the transition region is separate from the two simulated subgrain regions that are uniform in orientation. In both cases, there is less confidence near the boundary and the voxels there have nearly balanced probability of being assigned to either side. The band of higher uncertainty is visibly wider in Figure 2a because the large cluster has larger variance in orientation. This does not, however, necessarily indicate that the second segmentation is more favorable, as one would also expect an inappropriate oversegmentation to have low variation within the groupings. The process by which a C_{Maha} value of 2.5 (Figure 2a) is chosen as optimal is discussed below.

FMC requires several other user-defined values, but fixed values for them have been effective for all data sets examined in 2D and 3D. Hence, FMC has the additional advantage that it can be controlled with a single parameter for application to different EBSD data sets, analogous to the cutoff angle for a thresholding method. While high values of C_{Maha} are effective for subgrain structures, low values are optimal for segmentation of polycrystalline data along high-angle boundaries. This has allowed validation of the method by performing it on data sets for which thresholding is assumed to be effective. Validation in this way is shown in ref. [8] for a 2D slice of 3D polycrystalline data. The entirety of this 3D data set has been subsequently segmented with FMC, providing equally validating results. An additional 3D segmentation is presented in Section 3.2 which identifies the visible grain boundaries in the data.

2. Methods

2.1 Preprocessing

Some spatial preprocessing must be carried out since 3D EBSD data sets are collected in two dimensional sections. Measurement skew and instrument drift are corrected with a bilinear interpolation on each slice [11]. The data are then globally realigned, skewing the points off their regular grid. Points then may be interpolated to a rectangular grid for computational efficiency, but FMC can be performed with any spatial distribution of data points.

2.2 Determining Optimal Sensitivity Parameter C_{Maha}

The sensitivity of the segmentation, controlled by C_{Maha} , should be different based on the nature of the data. Boundaries between clusters in polycrystalline data should be on the distinct grain boundaries without consideration for variation within grains, but subgrain features are only

captured with a more sensitive segmentation. There is no ground truth available for such a segmentation, so the user is responsible for deciding which segmentation to use. Thus, an automated method for determining the optimal value of C_{Maha} has been developed, inspired by similar clustering problems in machine learning [12]. Oversegmentation is characterized by low marginal variance change from splitting existing clusters. Therefore, an “elbow” in a plot of a global variance measure as a function of C_{Maha} indicates a shift from creating clusters that should be distinct towards erroneously breaking these clusters further. Once this elbow is identified, the segmentation created using the associated value of C_{Maha} is selected as optimal.

The contribution of each cluster to the global variance metric is found by computing the variance of misorientations for all points in the cluster from the cluster’s mean orientation. Then these variances are averaged over all clusters, weighted by the clusters’ volumes, into a single global variance metric [8].

2.3 Surface Extraction

When analyzing grain or subgrain volumes, it is often useful to isolate separate faces of an irregular feature. These faces may be defined as regions having similar normal vectors, and, as the FMC method developed operates on orientations, only a small further modification is needed for application to normal vectors. With this modification, a second use of FMC identifies coherent faces from the set of points on the exterior of a cluster.

The voxel locations from a 3D segment are used as the input for a volume reconstruction using tetrahedra. The triangulated boundary surface is used to estimate local normal vectors, and

these are used in the FMC process. As with the main use of FMC, the single C_{Maha} parameter controls the sensitivity of the segmentation of the surface, and the same elbow criterion is used to find the optimal segmentation that separates distinct faces without oversegmenting. It is pertinent to note that it is a straightforward task to identify all of the large clusters in a volume and all of the largest faces on those clusters, making study of many subgrain surfaces possible.

3. Results and Discussion

To demonstrate the utility of FMC for 3D EBSD data, we segment three data sets containing significant microstructural features. In each set, the 2D EBSD scans are globally aligned with a bilinear transformation [13] followed by nearest-neighbor interpolation to a rectangular grid with the same spatial resolution as the original data. The interpolation is done to make the data compatible with MTEX data structures [14], and is not a necessary step in general to perform FMC. The optimal sensitivity parameter is then found and presented along with the resulting segmentation. Finally, we select individual features from these segmentations to demonstrate the FMC surface extraction method.

The FMC segmentations in this section were performed on a Tera multithreaded architecture computer, and each took several hours. While the scalability of runtime is linear with the number of data points, a 3D segmentation is slower than a 2D segmentation with the same number of data points due to the increased connectivity among neighbors. This complexity, along with the fact that an interesting 3D data set requires a large number of points, both contribute to lengthy computations. Additionally, many independent segmentations must be performed if the optimal sensitivity parameter is to be found for a given data set, but these may be done in parallel.

3.1 Microbands in Cold Rolled Aluminum

We first apply FMC to segment microbands in a single grain of cold-rolled (22% reduction) commercial purity aluminum containing 1.1 million data points [13]. Figure 3 shows the EBSD data with inverse pole figure coloring, in which the microbands are visible, as well as its segmentation. The microband structure is captured by the FMC segmentation. The highlighted microbands in Figure 3b are isolated in 3D in Figure 3c to show the nature of the interior of the segmentation.

3.2 Recrystallized Grains in Cold Rolled and Partly Recrystallized Steel

Segmentation of a partly recrystallized extra low carbon (ELC) steel sample containing 350,000 data points [15] illustrates the ability of the FMC method to identify boundaries of different magnitude in the same data set (Figure 4). Here, there are subtle subgrain features, distinct grain boundaries, and a high angle boundary separating α - and γ -fiber regions. The presence of the HAGB separating the regions does not affect the detection of boundaries with smaller misorientation, even those adjacent to it. This is because variance comparisons are done between each neighboring group, rather than with a global standard over the entire data set. The distinct grain boundaries are identified as they would be with a misorientation thresholding segmentation.

3.3 Microbands in Deformed Nickel Single Crystal

Microbands have been isolated in a 3D EBSD data set from a channel die plane strain compressed (35% strain) Goss-oriented nickel single crystal with more than 1.3 million data

points [16]. The data have a standard deviation from the average orientation of only 0.7° . Figure 5 shows the segmented microbands. Identification of these subgrain features would not be attainable with thresholding at any angle. The segmentation in Figure 5b is performed with the optimal C_{Maha} . To show how even more subtle features may be identified, Figure 5c shows a segmentation with a higher C_{Maha} value. This comes with the consequence of oversegmenting the data overall, but specific features of interest may still be used for further analysis.

As an additional validation of the efficacy of the optimal segmentation, 2D sections have been taken in the RD-ND plane, perpendicular to the original EBSD data. The spacing between segment boundaries and the orientation of the bands agrees with TEM images of the microbands within the sample [17]. Both of these observations are from global-scale spatial qualities of the segmentation, which are not considered by the crystallographic orientation-based segmentation method in any way.

This data set also has been segmented with the Kuwahara filter method [6]. The thresholding-based process fails in application to 3D subgrain EBSD data because of the increased difficulty of finding closed boundaries with the additional spatial dimension. What would be considered a closed feature boundary in 2D is often resolved as an internal boundary in 3D. Segmentations of the Kuwahara-filtered data are compared to FMC in Figures 6a and b, using the global variance metric described in Section 2.2. The global variance decreases with increasing sensitivity in both cases (higher C_{Maha} or lower threshold), as expected (Figure 6). However, effective segmentation methods with an adjustable parameter are expected to exhibit decreasing marginal changes in variance, and the segmentations of the Kuwahara-filtered data do not.

Further investigation into the Kuwahara-filtered data reveals that for the range of threshold angles considered, a single, large cluster dominates the segmentation. This cluster occupies about 90% of the entire data set for all but the most dramatic oversegmentations. As the threshold angle is decreased, the smaller clusters are split into progressively further oversegmented pieces while the single large cluster continues to resist significant segmentation. The steep drop in variance in Figure 6b occurs with the separation of a crystallographically-distinct region from the single dominating cluster. Although this region is large compared to the volume removed from the large cluster in previous decrements in the threshold angle, it contains less than 2% of the total remaining volume.

This behavior is further illustrated in Figures 6c and 6d. The two segmentation methods are directly compared, using the total number of clusters produced in each application. With progressively more sensitive FMC applications, regions of distinct orientation are isolated even if point-to-point misorientation is low near their boundaries. On the other hand, the Kuwahara filter method struggles to find closed boundaries satisfying the given threshold angle. Thus the single large region remains unsegmented until the threshold is so low that useful subgrain features are lost. Lastly, we note that applying the Kuwahara filter to a 3D data set is not particularly faster than an FMC segmentation. However, the filter needs to be applied only once before many thresholding segmentations can be carried out.

3.4 Surface Segmentation

The FMC surface extracting method was applied to microbands from the aluminum data set. Figure 7 shows the top microband of Figure 3c, with the entire top and bottom surfaces isolated.

These surfaces can be used for further geometric and crystallographic analysis. FMC is a powerful tool for this application since it can form a full surface from similar components that are separated by a sharp step in the estimated normal vectors.

4. Concluding Summary

The foregoing examples illustrate that fast multiscale clustering is an effective tool for segmenting 3D EBSD data set containing subtle and gradual variations in orientation. The Kuwahara filter, a common technique for segmenting this kind of data in 2D, does not generalize well to three dimensions. To facilitate its use in the materials science community, we have incorporated FMC modified to operate on orientation data into the free open source texture analysis software package MTEX [14], thereby allowing users to take advantage of its existing methods for importing and manipulating data. The algorithm is started by the command `calcGrains` with argument `FMC` as

```
grains = calcGrains(ebsd, 'FMC', C_Maha).
```

All EBSD segmentation described herein has been done with this package. The ability of the method to segment data based on a wide range of boundary magnitudes with linear runtime make FMC a robust method for both 2D and 3D segmentations.

Acknowledgements

This work was supported by the Laspa Fellowship at Harvey Mudd College, the National Science Foundation (DMR-0807240 and DGE-1144153), the Australian Research Council Centre of Excellence for Design in Light Metals (CE05611574), the Harvey Mudd College Department of Engineering and the Electron Microscope Unit at the University of New South Wales. We acknowledge the preliminary FMC work of Cullen McMahon and Brian Soe. We thank Benyue Liu, Donald Bolton and Nasima Afrin for contributions to collection of the aluminum and nickel 3D EBSD data sets, Md. Zakaria Quadir and Nasima Afrin for discussion of the nickel data set, and Wanqiang Xu for the steel data set.

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Figure Captions

Figure 1: (a) A constructed data set; (b) Segmentation with a threshold angle of 0.5° , finding 626 segments, and (c) 0.75° , finding 466 segments. The body has been made translucent and single-voxel segments are removed to display the segments due to noise. (d) Segmentation using fast multiscale clustering produces two clusters with a diagonal boundary.

Figure 2: The constructed data set from Figure 1, segmented with FMC using C_{Maha} values of (a) 2.5 and (b) 5. The associated confidence maps are taken along the highlighted diagonal plane. Darker pixels signify higher uncertainty.

Figure 3: 3D view of the cold rolled aluminum data set: (a) EBSD data; (b) EBSD data with overlaid boundaries of segments (black and white lines) found with the optimal C_{Maha} value of 4.4, and (c) eight selected clusters, indicated with white lines in (b), showing the underlying subgrain structure, including a boundary plane that extends through the entire data set. The inverse pole figure color map shown is used for all figure colorings. (Scale is in microns).

Figure 4: 3D view of the partly recrystallized ELC steel data set: (a) EBSD data using the IPF color map of Figure 3; (b) segmentation with the optimal C_{Maha} value of 3.4, and (c) boundaries from the segmentation colored by local misorientation, showing the HAGB between α - and γ -fiber regions. (Scale is in microns).

Figure 5: 3D view of the nickel data set (a) EBSD data, (b) segmentation with the optimal C_{Maha} value of 6, (c) segmentation with a C_{Maha} value of 7, showing the identification of more subtle features.

Figure 6: Effect of segmentation sensitivity on the global variance measure for 3D nickel data under (a) FMC with C_{Maha} variation (optimal value shown with a solid dot) and (b) Kuwahara-filtered segmentation with threshold angle variation. The threshold angle axis is reversed so that segmentation sensitivity increases to the right. Direct comparison with the total number of clusters using (c) the global variance measure, and (d) the size of the largest cluster produced by each segmentation. Solid dots again indicate the optimal C_{Maha} value. Note that the behavior under a sequence of FMC segmentations is not necessarily monotone, but easily-identifiable trends exist. Unlike thresholding, boundaries that exist at a coarser segmentations may change under more sensitive segmentations.

Figure 7: Two views of a cluster in the segmentation of cold rolled aluminum data. Colors indicate separate extruded surfaces. The top and bottom surfaces are isolated, as well as flat surfaces on the top and side from the boundary faces of the data set.

Figure 1

Figure 2

Figure 3

Figure 4

Figure 5

Figure 6

Figure 7