Clustering Orientations for Texture Analysis

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Driven by advances in sensor, storage, and data handling technology, recent years have seen significant development of techniques used to analyse the information available from scanning transmission electron microscopes. The comparatively large datasets of highly-correlated data are ideal for machine learning, and methods such as statistical decomposition [1] have proved particularly fruitful.

Such techniques often make an implicit assumption that changes in the data are linear, and relate to some linear change in the system. For texture analysis using EBSD or Scanning Precession Electron Diffraction (SPED), such an assumption holds as long as long as the only variations in orientation occur across (potentially overlapping) grain boundaries. Strain within individual grains leads to non-linear variations in the collected signals; machine learning is often unsuitable in such cases.

We have investigated using data clustering, an approximation of distribution fitting, to aid the analysis of orientations and misorientations. Data clustering is particularly useful in contexts where some distance function between two data points can be readily defined. In the case of crystal orientations, this is the angle of the transformation from one orientation to another. The picture is complicated by crystal symmetry: many orientations are symmetrically equivalent, prompting the definition of a fundamental zone of symmetrically-distinct orientations (see Figure 1) [2]. The distance metric must therefore take into account this equivalence, straightforwardly achieved if the orientations are described using quaternions.

One well-known clustering algorithm, DBSCAN, can be used in conjunction with a symmetry-aware distance metric to automatically detect clusters of orientations. DBSCAN is a density-based algorithm and does not require the number of clusters as a parameter [3]. Moreover, clusters found this way are not constrained to particular shapes. This method therefore requires no prior knowledge of the expected distribution of orientations. We envisage using this analysis, or similar approaches, to quickly and easily identify novel orientation or misorientation habits in, for example, deformed microstructures, or to characterise local deformation associated with dislocation networks.

To demonstrate this method, we have reproduced the identification of misorientation habits in deformed Titanium described in [2]. There, clusters were identified about known misorientation relationships. Using quaternion representations of the orientations, misorientations across twin boundaries were calculated and clustered using DBSCAN. The same clusters and misorientation relationships are found, and spurious "noisy" misorientations automatically rejected from the clusters (see Figure 2).

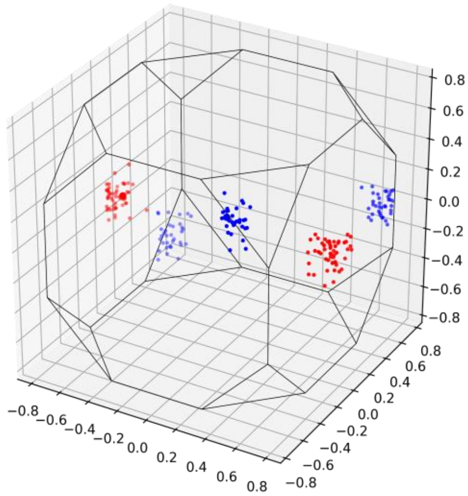

Figure 1: Clusters of orientations of an object with *m-3m* symmetry in an axis-angle projection. The bounding box represents the fundamental zone. Orientations near the edge of the fundamental zone are close in terms of orientation but distant in this projection. Orientation clustering identifies the (two) related primary groups of orientations.

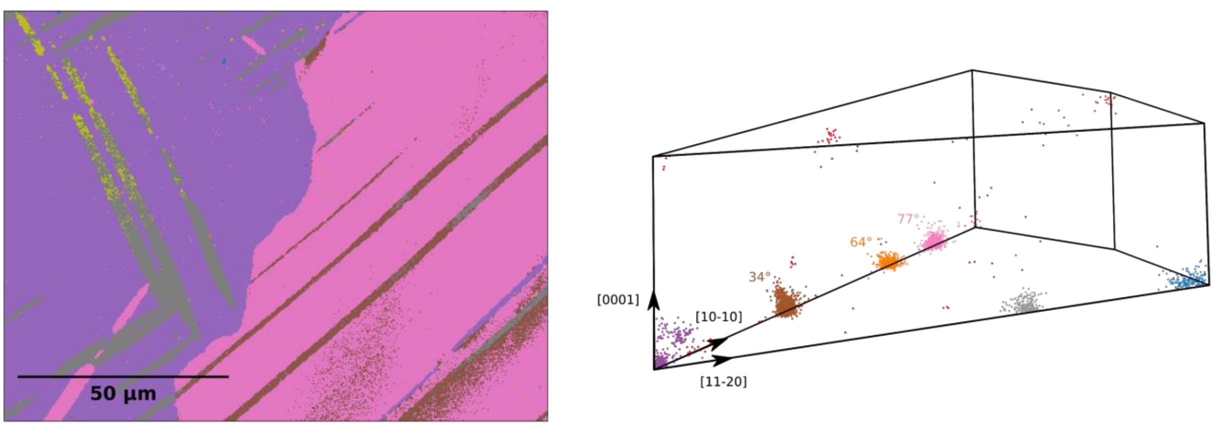

Figure 2: Left: ballistically-tested pure titanium showing a twinned microstructure. Right: clusters of misorientations determined using quaternion representations and DBSCAN. This algorithm can identify 'noisy' points in the data, shown here in red.

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[3] M. Ester, H. Kriegel, J. S, and X. Xu, "A density-based algorithm for discovering clusters in large spatial databases with noise," pp. 226 - 231, 1996.

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