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Inter-phase Relationships Revealed in 3-Dimensional Orientation Spaces

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Spatially resolved orientation mapping is increasingly performed using electron microscopy techniques, including: electron backscatter diffraction, transmission Kikuchi diffraction and scanning precession electron diffraction. The resulting orientation maps contain a wealth of information with crystal phase and orientation specified at each pixel. However, the depth of this data is often underutilized owing to challenges posed by the analysis of such large quantities of data. In the context of understanding complex and multi-phase materials it is important to characterize inter-phase relationships between nanoscale precipitates and the surrounding matrix, which both affect properties and are indicative of formation pathways. Revealing inter-phase relationships requires statistical assessment of the orientation relationship across the phase boundary, the spatial occurrence of particular boundaries and the surfaces of contact at interfaces. Analysis procedures that highlight relationships in both spatial and orientation dimensions are therefore required. Here, we present an approach to revealing inter-phase relationships, based on considering orientation data in 3-dimensional vector spaces constrained to *fundamental zones* defined by the crystal symmetry of both crystals.

Three-dimensional orientation spaces, sometimes referred to as neo-Eulerian mappings, exploit the representation of a (mis-)orientation (or rotation) by an axis of rotation and the angle of rotation about that axis. A 3-vector can therefore be defined by scaling a unit vector parallel to the rotation axis, **v,** by a function of the rotation angle, $f(\omega)$, i.e.

$$\boldsymbol{\rho} = f(\omega)\,\mathbf{v}$$

The scaling function is chosen to convey particular properties on the resulting vector space. At least six such choices with different properties and merit have been suggested [1-3] and the relative merits of these choices are discussed in this work. Fundamental zones for all combinations of crystallographic point groups are considered, generalizing analysis to all crystal symmetries compared to analysis of cubic-cubic or cubic-hexagonal cases that form most of the literature. In all cases, mis-orientations that occur frequently in the data form clusters in the appropriate fundamental zone of the vector space, enabling their identification.

Analysis routines, developed in this work, are demonstrated in a number of examples. A simple case is the consideration of orientation relationships formed between η-phase precipitates (hexagonal, $P6_3/mmc$) and the Ni matrix (cubic, $Fm\bar{3}m$) in the nickel base superalloy 718+, as shown in Figure 1. Clusters in the cubic-hexagonal mis-orientation space reveal preferred orientation relationships, including the well-known Blackburn orientation relationship, as shown in Figure 2. The spatial occurrence of boundaries with this orientation can then be revealed by coloring pixels, where the relationship was observed (Figure 1a). The clustering in the mis-orientation space that indicates a preferred orientation relationship can be assessed in a more systematic manner through the application of clustering algorithms developed to incorporate the crystal symmetry, as shown in Figure 2c.

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A comprehensive approach to revealing inter-phase orientation relationships from orientation mapping data is presented. The approach is based on analysis of the orientation data in 3-dimensional mis-orientation spaces where preferred orientation relationships arise as clusters. These clusters can be extracted using clustering algorithms developed to incorporate the crystal symmetry and the spatial location of boundaries in a particular cluster can then be found. All analysis presented in this work is performed using the MTEX [4] toolbox for Matlab [5].

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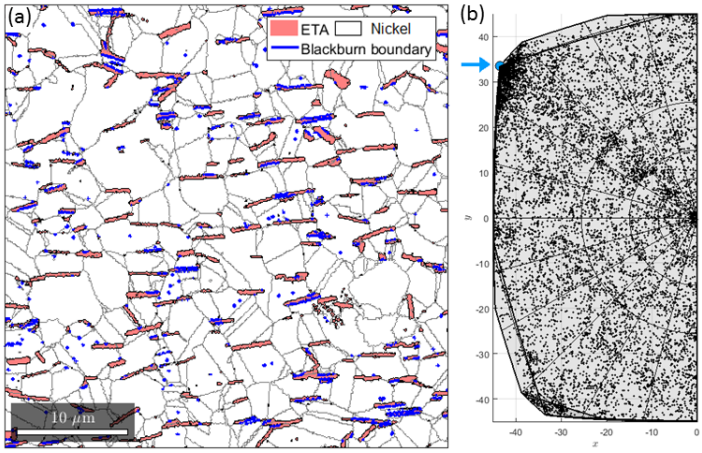

Figure 1. Inter-phase relationship between cubic Nickel matrix and hexagonal η precipitate (a) phase map showing the phases' spatial arrangement and occurrence of the Blackburn orientation relationship (OR); (b) Fundamental zone for cubic-hexagonal symmetry with phase boundary mis-orientations.

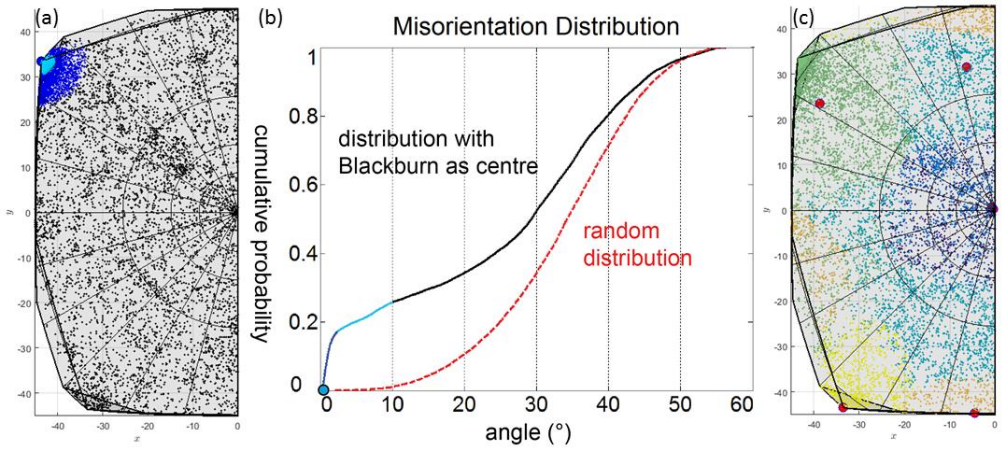

Figure 2. Detailed analysis (a) mis-orientation cluster identified around Blackburn OR; (b) Mis-orientation distribution (cumulative) with Blackburn OR at the center compared with a random distribution showing the significantly higher density. (c) Result of clustering algorithm incorporating crystal symmetry.

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