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Automated Prediction of Pseudo-Symmetry Issues in EBSD

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Pseudo-symmetry (PS) issues arise in the analysis of electron back-scatter diffraction (EBSD) patterns when similarities between patterns for different crystal orientations cause the indexing algorithm to select the incorrect orientation. In inverse pole figure (IPF) maps, the result often appears as grains with a random distribution of two colors instead of a single color. While PS issues are readily recog-nizable in IPF maps, and can be corrected manually by post-processing of the map, the prediction of the occurrence of pseudo-symmetry is not as straightforward. In this contribution, we present a new algorithm capable of predicting for which crystal orientations PS issues may occur.

Using the physics-based forward model described in [1], along with an orientation space sampling approach, and a set of detector parameters, we generate a dictionary $\mathcal{D}$ of simulated EBSD patterns. The dictionary indexing approach [2] is then employed to match the dictionary against itself, i.e., each pattern in $\mathcal{D}$ is compared to all patterns in $\mathcal{D}$ using the dot product as a similarity metric, and the top N dot product values along with the indices of the corresponding patterns are kept. For the set of N best matches, we expect the top match to occur when a pattern is compared to itself; the other $N-1$ matches are generally expected to correspond to orientations that are close to the correct orientation. Hence we compute the disorientation between the top match and the other matches; if all disorientation angles fall below a threshold value, then there is no risk of pseudo-symmetry issues. If, on the other hand, there are matches among the top N for which the disorientation angle is substantially larger than the threshold value, then there is the potential for an indexing algorithm to incorrectly assign this lower ranked orientation to the original pattern.

The algorithm was tested using the $SrTiO_3$ cubic perovskite structure. A total of $333,227$ patterns was simulated for a microscope accelerating voltage of 20 kV, pattern size 480×480, detector pixel size 50 μm, detector tilt $10°$, sample tilt $70°$, and pattern center coordinates $(x^*, y^*, z^*) = (0.5, 0.5, 0.625)$. After binning by a factor of $8\times$, the 60×60 pixel patterns were stored in a dictionary $\mathcal{D}$ and indexed against themselves, keeping the top $N = 20$ matches. In all cases, the top dictionary match was the pattern itself. For all other 19 patterns, the disorientations with respect to the best matching pattern were computed; disorientation angles larger than $4°$ were considered to be due to pseudo-symmetry. Of the $6,664,540$ misorientation angles, 99.35% were smaller than the threshold of $4°$; $40,649$ angles were centered around a value of $45°$, $2,716$ around $60°$, and 171 near the maximum possible misorien-tation angle for cubic symmetry, $62.7994°$. Fig. 1(a) shows the histogram of misorientations using bins of $0.1°$ width; the dashed lines indicate the $4°$ threshold (left) and the maximum cubic misorientation angle (right). The orientations for which pseudo-symmetry is possible (for the given detector param-eters) are shown in four views of the cubic Rodrigues fundamental zone in Fig. 1(b); each blue-gray sphere represents a single orientation. The corresponding misorientations cluster in three regions on the outer surfaces of the cubic misorientation MacKenzie fundamental zone shown in Fig. 1(c). The bottom portion of the figure shows six pairs of pseudo-symmetry related patterns, two pairs for each of the peaks in Fig. 1(a). In each case, a portion of the two patterns is virtually identical and the dif-ferences are typically located near the outer edge of the patterns. For real experimental patterns, in the presence of noise, it is entirely possible

that the Hough-based indexing approach may miss some of the outer Kikuchi bands and incorrectly index the pattern. The DI approach is less sensitive to this issue since it does not make use of feature extraction but instead matches the complete pattern.

Whether or not an experimental pattern will be indexed incorrectly due to a pseudo-symmetry issue depends on many factors. The most important factor is the solid angle of the pattern; the larger the distance between projection center and scintillator, the smaller the portion of the overall EBSD pattern that will be visible on the detector, which increases the probability of mis-indexing. Patterns with a low signal-to-noise ratio are also more prone to mis-indexing, since the Hough peaks corresponding to the bands that would allow for separation of the two PS-related orientations may have too low an intensity to be detected in the Hough transform. Finally, the crystal structure plays an important role; for instance, for tetragonal cells with a c/a ratio close to 1 the Hough-based indexing algorithm may not be able to distinguish between PS-related orientations. We will discuss the PS algorithm as well as its applications to a number of relevant crystal systems [3].

References:

[1] P.G. Callahan and M. De Graef, Microsc. MicroAnal., **19** (2013), p. 1255.

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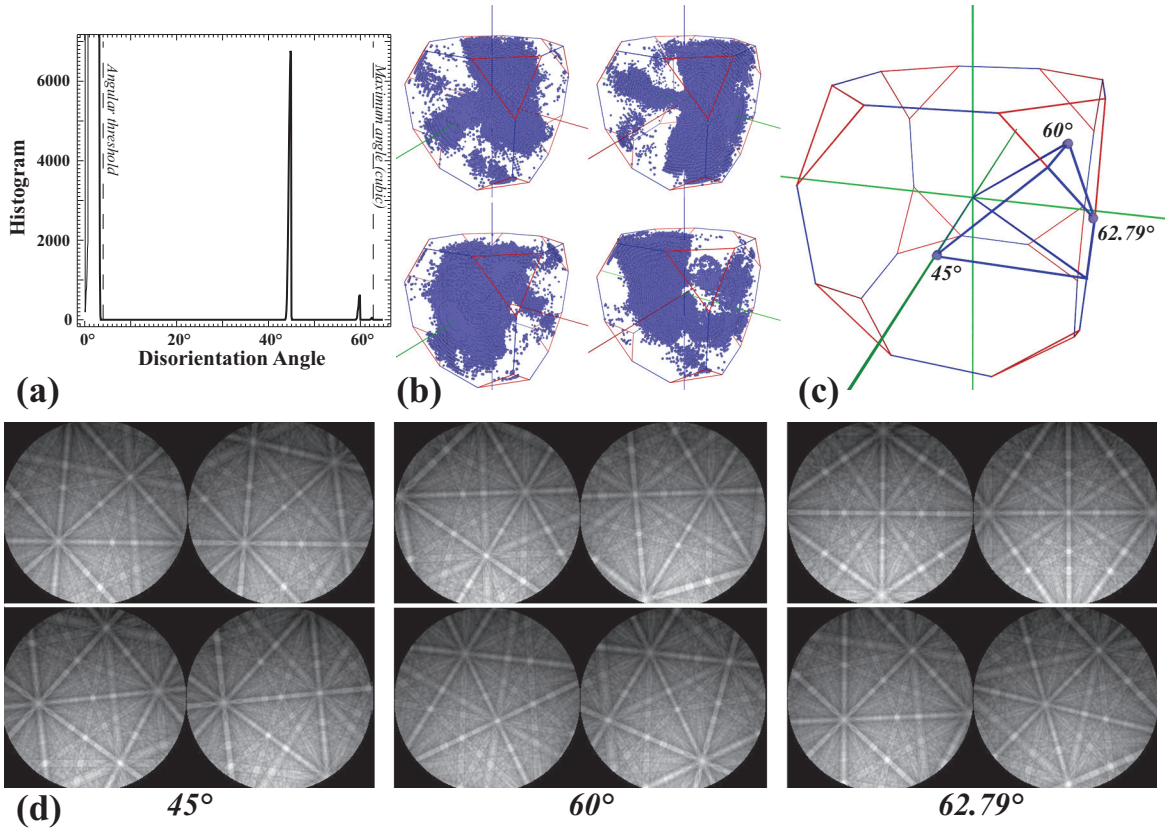

Figure 1. (a) histogram of misorientation angles for the top $N = 20$ matches; (b) four different views of the distribution of grain orientations that potentially give rise to pseudo-symmetry, rendered in the cubic Rodrigues fundamental zone; (c) corresponding disorientation distribution in the cubic Mackenzie cell (outlined in blue); (d) example pattern pairs for each of the disorientation clusters in (c).

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