Triplet Indexing

Introduction

In Orientation Imaging Microscopy (OIM™), indexing is the fundamental process in determining crystallographic orientations from Electron Backscatter Diffraction (EBSD) patterns. The collected orientation measurements become the "raw" data for all subsequent processing, making reliable and accurate indexing the pivotal step for a successful analysis. EDAX has experimented with many indexing methods and found the triplet-voting approach to be the most robust and reliable.

Indexing 101

The bands in an EBSD pattern correspond to crystal lattice planes within the diffracting volume of the sample. The angles between the bands correlate to the angles between the planes. Band widths are related to the spacing between the planes, but are also affected by the accelerating voltage of the electron microscope. Taken together, the spatial arrangement of the bands in a pattern is indicative of the crystal lattice's orientation, relative to the EBSD system geometry.

Hence, the main steps for indexing an EBSD pattern are to detect the bands, measure them, and then compare the measurements to known crystal structure data to find the best fit. Since inter-band angles can be measured more easily and precisely than band widths, given the relatively low resolution images common for automated EBSD, angles are typically preferred over widths for this application. While detecting the bands and having the correct structural information are critical, it is finding the best fit between the two that determines the final solution. For brevity, this review will assume that bands have been accurately detected and the correct structural data for the phase is known. The focus is on the actual process used to derive the most reliable orientation.

It Just Takes Three

The angle between two bands can be compared to a look-up table of interplanar angles and corresponding Miller Indices, hkl's (i.e. the known structural data). Without incorporating the width data, only an hkl pair can be identified, not which member of the pair is associated with which band. On the other hand, if three bands are used, then the indices associated with each band can be uniquely identified using a logic routine. Once the indices of the bands are identified, the corresponding lattice orientation can be determined.

This would seem to imply that a unique orientation solution could be determined using just one triplet of bands. In practice, this is generally not the case for the following reasons.

- Band angle measurements have a degree of uncertainty, so it is necessary to use an angular tolerance or range, to qualify a match. This, and the variance itself, may result in more than one possible orientation solution. Figure 2 shows an example of finding two possible matches, given an angular tolerance of 0.5 degrees.
- False or "rogue" bands could lead to an incorrect solution, or no solution at all. These bands are quite common in overlapping patterns, as they are prevalent near grain boundaries.

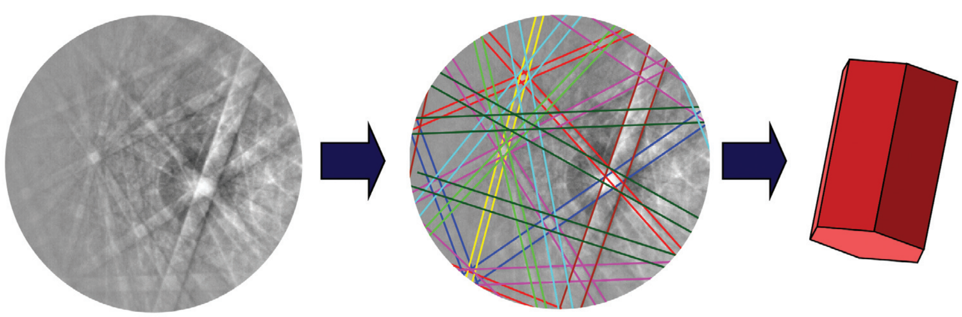
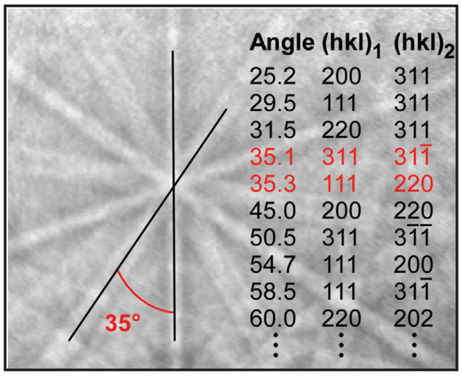


Figure 1. Indexing determines a crystal's orientation information in the EBSD pattern.



Angle	$(hkl)_1$	$(hkl)_2$
25.2	200	311
29.5	111	311
31.5	220	311
35.1	311	$31\bar{1}$
35.3	111	220
45.0	200	220
50.5	311	$3\bar{1}\bar{1}$
54.7	111	200
58.5	111	$31\bar{1}$
60.0	220	202
⋮	⋮	⋮

Figure 2. Matching measured angle to reference structured data.

- If one selects a weak, albeit real band from the pattern, there may not be a match in the look-up table because weakly reflecting planes are often intentionally excluded from the reference data to simplify indexing. It should be noted that these constraints plague all EBSD indexing, not just the triplet method.

Get Out the Vote

To overcome the difficulties described above, EDAX has implemented triplet indexing within a novel voting framework. To begin, all possible combinations of band triplets are determined from the total number of bands. Then, for each triplet, the potential orientations are identified, with each solution getting a vote. When the supply of triplets is exhausted, the votes are tallied and the orientation with the most votes among all candidates is selected as the most probable solution. The voting mechanism opens the door to some very important benefits.

To the Victor

Voting provides the foundation for EDAX's patented Confidence Index (CI). The CI lets you know when you can/can not be confident about results by providing a numerical measure of the indexing solution's accuracy and reliability. The CI is a very powerful tool and is used extensively throughout OIM™. It makes it easier to see when something may have gone wrong, or to determine when and how data might need to be cleaned up.

The voting method also deals very well with rogue and weak bands. For example, assume the green band in Figure 3 happens to be from an overlapping pattern. Any solution involving that band will likely be erroneous. However, all other orientations determined using combinations of the remaining six bands will still be valid and the correct solution can still be found.

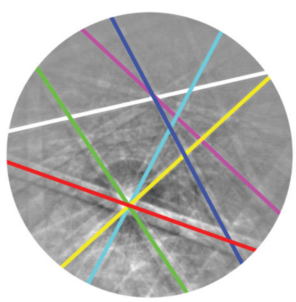
The Alternatives: All (or nothing at all)

How does the triplet-voting procedure compare to other alternatives? For example, what about trying to solve for more than three bands, en masse? As it turns out, increasing the number of bands in this manner soon reaches a point of diminishing returns. Processing additional bands, in an attempt to get more reliable indexing, is computationally more complex and takes longer. A more significant problem is that the more bands one attempts to index at a time, the more difficult it becomes to find a solution that encompasses and satisfies all of them. The result is either a higher indexing failure rate or more zero solutions. This effectively imposes a cap on the number of bands one can use in practice and clearly creates a trade-off between speed and accuracy.

In contrast, bringing more bands into the triplet indexing process simply increases the number of indexing computations, not the complexity of them. Granted, doubling the number of bands used would take longer, but the success rate of finding an index solution is not affected. Because of this, the trade-off between speed and accuracy is significantly minimized.

Conclusion

Triplet indexing, when combined with a voting strategy, improves indexing reliability and accuracy and minimizes trade-off between speed and accuracy. It also provides a foundation for a numerical measure of indexing quality, readily handles false bands, and enables deconvolution of overlapping patterns.



Band Triplets	Indexing Solutions									
	1	2	3	4	5	6	7	8	9	···
	×	×	×							
			×				×			
			×							
	×	×	×	×	×		×			
		×	×	×		×				
		×	×				×	×		
			×			×			×	
			×						×	
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
Σ	4	6	35	5	5	4	8	5	5	···

Figure 3. Voting Mechanism.