Automatic Indexing of Laue Images by Pattern Recognition

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Introduction

One of the key problems in polychromatic x-ray microdiffraction is indexing the overlapping Laue patterns generated by multiple grains. This problem is complicated by deformation of the grains, mosaic spread, or strain gradients that smear the Laue spots. An automated Laue indexing program has previously been described that works well with sharp Laue spots.[1,2] This program is based on matching relative angles between pairs—and then triplets of reflections. However the current algorithm is challenged by weak, diffuse, or smeared spots. We have now demonstrated a new algorithm that is inherently more robust and less likely to miss grains or find false matches. This algorithm is based on a simultaneous matching of all reflections within a Laue pattern to the measured pattern.

Methods and Materials

The new algorithm first finds the positions of the experimental Laue spots in the detector. These positions are turned into absolute angle information, and the strongest spot is chosen and a reasonable guess made as to its index. This guess defines two of the three Eulerian angles for the assumed crystal grain. The anticipated diffraction pattern is then calculated for rotations about the Bragg plane normal defined by the assumed spot index. The correlation function between the theoretical pattern and the observed pattern is calculated and stored. Additional guesses of the strong-reflection index are made, and the correlation calculated for all rotations about the various Bragg plane normals. With the correct index, there is a sharp increase in the correlation between the theoretical and experimental pattern during the diffraction pattern rotation about the Bragg plane normal. This increase is very strong, as all reflections in the pattern line up simultaneously. Because of the high number of simultaneous correlations, the exact angular match between the indexed reflections does not need to be as high as with previous methods. Once the indices of reflections from one grain are found, the Laue spot positions are subtracted from the data, and the image is searched for additional Laue patterns. This process is continued until all grains are detected. This approach is similar to an approach suggested by Sheremet'ev et al.[3] but is shown to be effective in indexing grains with multiple overlapping Laue patterns generated by polychromatic x-ray microdiffraction.

Results

A Laue pattern for which this technique is particularly effective is shown in Fig. 1, this pattern contains 18 spots that are indexed. The indexing time is 30 sec. For the technique described in Ref. 1, this pattern can not be indexed because of the uncertainty in Laue spot position because of the extensive plastic deformation in this grain.

Discussion

The new automated indexing program extends the kinds of samples that can routinely be studied with our so called 3D-x-ray

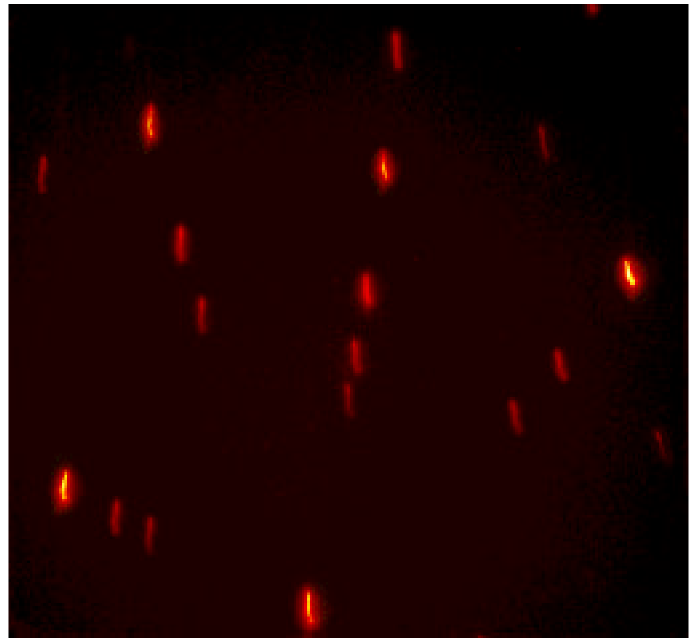

FIG. 1. Polychromatic microdiffraction image of an an approximately (001) iridium grain showing smeared individual Laue spots. These spots were easily indexed with the new routine.

crystal microscope. As illustrated by the example above, the Laue patterns from even highly deformed polycrystalline grains can now be automatically indexed rapidly and robustly.

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References

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