

AUTOMATED LATTICE ORIENTATION DETERMINATION FROM ELECTRON BACKSCATTER KIKUCHI DIFFRACTION PATTERNS

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ABSTRACT

The ability to measure individual orientations from crystallites enables a more complete characterization of the microstructure. A primary obstacle to the use of single orientation measurements is the large investment of direct operator time necessary to obtain a statistically reliable data set. The most viable technique for obtaining individual orientation measurements is electron backscatter Kikuchi diffraction¹ (BKD). Current technology requires an operator to identify a zone axis pair in a BKD pattern². This paper describes research in progress to automate the identification of lattice orientation from BKD patterns by identifying the planes associated with the bands that appear in the patterns. This work considered FCC crystal symmetry.

ORIENTATION IDENTIFICATION

Lattice orientation can be fully determined given the direction of two non-colinear lattice vectors. The information required is knowledge of the family of planes associated with two distinct bands and their interplanar angle. The proposed method for obtaining this information is to detect three bands in a BKD pattern and to identify the family of planes associated with each of the bands from the angles they make with one another. Once this information is available the following procedure can be used to calculate the lattice orientation. See figure 1 for a definition of the parameters used in the procedure.

- (1) Calculate unit plane normal vectors, \hat{n} and \hat{n}' , in the specimen frame \hat{e}_i^s :

$$\hat{n} = \frac{\overline{OP} \times \overline{OQ}}{|\overline{OP} \times \overline{OQ}|}, \quad \hat{n}' = \frac{\overline{OR} \times \overline{OS}}{|\overline{OR} \times \overline{OS}|}$$

- (2) Determine the interplanar angle between these two planes:

$$\cos\theta = |\hat{n} \cdot \hat{n}'|$$

- (3) Identify the family of planes associated with each band:

$$\hat{n} \parallel \{hkl\}, \quad \hat{n}' \parallel \{h'k'l'\}$$

- (4) Select a pair of planes consistent with the interplanar angle:

$$\cos\theta = \left| \frac{hh' + kk' + ll'}{\sqrt{h^2 + k^2 + l^2} \sqrt{h'^2 + k'^2 + l'^2}} \right|$$

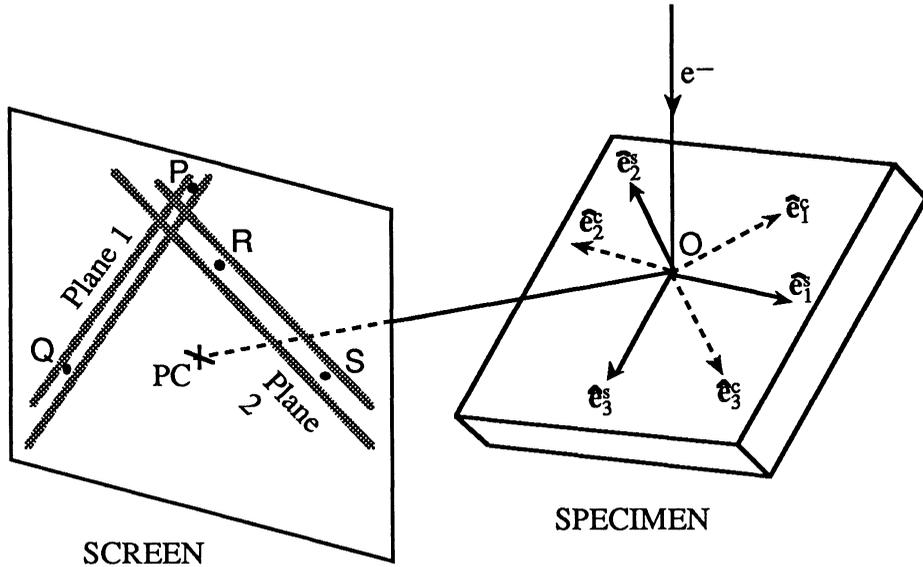


Figure 1. Schematic of the configuration of the BKD system.

- (5) Construct a new orthonormal frame, defined relative to the sample frame:

$$\hat{e}_1^* = \hat{n}, \quad \hat{e}_2^* = \frac{\hat{n} \times \hat{n}'}{|\hat{n} \times \hat{n}'|}, \quad \hat{e}_3^* = \hat{e}_1^* \times \hat{e}_2^*$$

Relative to the crystal frame \hat{e}_i^* the new frame is defined by:

$$\hat{e}_1^* = \frac{(hkl)}{|(hkl)|}, \quad \hat{e}_2^* = \frac{(hkl) \times (h'k'l')}{|(hkl) \times (h'k'l')|}, \quad \hat{e}_3^* = \hat{e}_1^* \times \hat{e}_2^*$$

- (6) Determine two sets of direction cosines according to:

$$g_{ij}^I = \hat{e}_i^* \cdot \hat{e}_j^s, \quad g_{ij}^{II} = \hat{e}_i^c \cdot \hat{e}_j^*$$

- (7) The direction cosines which specify lattice orientation are defined by:

$$g_{ij} = \hat{e}_i^c \cdot \hat{e}_j^s = g_{im}^{II} g_{mj}^I$$

The challenging part of this procedure is to detect three bands and to associate each of them with the correct family of planes.

IMAGE ENHANCEMENT

Several techniques have been explored for improving the quality of the images. These techniques seek to increase the contrast between the bands and the background and to reduce the noise. Both subtraction and division of a background pattern from a BKD pattern have been found to dramatically improve the visibility of bands in experimental patterns. A background image can be created by capturing a diffraction image generated from an uncolumnated electron beam. This is essentially equivalent to the average BKD pattern produced from many grains.

EDGE DETECTION

The primary difficulty in “teaching” the computer to recognize the bands is that of detecting the edges of the bands. The Burns³ edge detection scheme has been found to

lead to good results. As in most edge detection schemes, the Burns algorithm first estimates the gradient of the image by discrete convolution. Pixels with local gradient magnitudes greater than some threshold value are then grouped into regions according to the orientation of their local gradient vectors. This is done by dividing the 360° range of gradient directions into a set of regular intervals. In order to avoid artificial segmentation at the interval boundaries a second overlapping segmentation is created. Each pixel is given two labels, one for each segmentation, according to the intervals into which its gradient vector falls. Adjacent pixels are grouped into regions with the same orientation labels. Every pixel "votes" for one of the two regions to which it belongs according to the number of pixels contained within the regions. Each region is then given a "support" value according to the number of its pixels that voted for it. Regions having support greater than 50% are selected. A line is constructed for each of these regions using a least squares fit of the (x,y) coordinates associated with each pixel in the region. Results from this procedure are shown in figure 2.

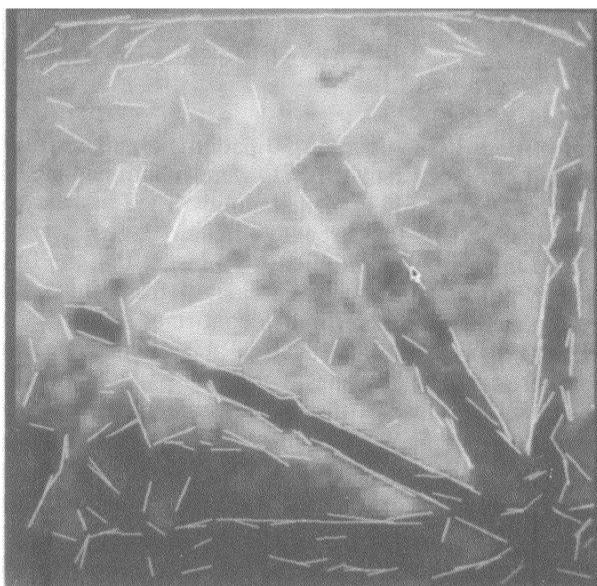


Figure 2. Edges detected on a sample BKD pattern using the Burns Algorithm.

LINE DETECTION

Once the edges have been detected, they need to be linked into lines. A useful tool for performing this linking is the Hough transform. The edges can be parameterized by ρ and θ as shown in figure 3. Each edge detected will fall in a particular bucket of dimension $\Delta\theta \times \Delta\rho$ in ρ - θ space. Buckets containing many edges will correspond to lines. This technique is especially suited to this problem since the lines in the BKD patterns extend across the entire image. The Hough transform of the edges in figure 2 is shown in figure 4 along with the edges corresponding to a peak value in ρ - θ space.

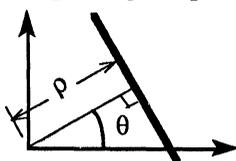


Figure 3. Definition of Hough transform parameters

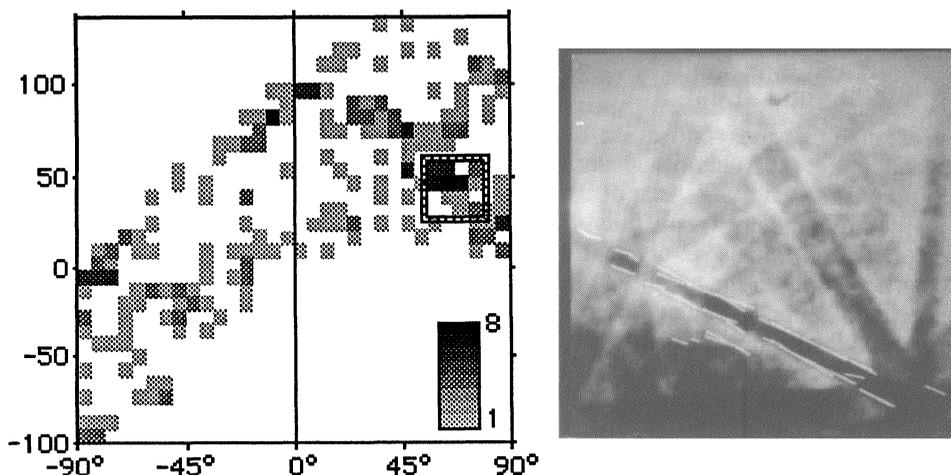


Figure 4. Hough Transform of edges. The edges correspond to the indicated peak.

THREE-LINE ANALYSIS

Using the aforementioned technique on 50 patterns obtained from OFHC copper (FCC) it was found that only four sets of bands were found; namely, those associated with the {111}, {200}, {220} and {113} plane families. The frequency of appearance of bands in the patterns as well as the strength of their edges is a function of their interplanar spacing and their group multiplicity. To insure that the frequency was not influenced by texture, pole figures were calculated from the lattice orientations obtained from the 50 patterns. The pole figures confirmed that the set of orientations represented a random texture. A look-up table of all possible interplanar angles was then constructed for these families of planes.

Once three lines have been fixed by the line detection algorithm the angles between these lines can be found (accounting for the projection). The three angles, θ_i , can be used as a criterion for a search for possible band triplets. For each θ_i a search is made through the table of interplanar angles and a band pair is considered if it falls within $\pm\Delta\theta$ of the experimental angles. Once all possible band pairs have been collected for each of the experimental angles, a check is made to see which sets of band pairs are physically possible. The results of this procedure for several $\Delta\theta$ is shown figure 5. $\Delta\theta$ is directly related to the precision to which the system can be calibrated.

“THICK–THIN” BANDWIDTH ANALYSIS

As demonstrated in the previous section an ambiguity often remains in the choice of a correct band triplet. However, it is clear that some bands in the BKD patterns are thicker than others. If the change in bandwidth as a function of location and orientation in the patterns due to the projection is neglected, the bandwidth is simply inversely proportional to the interplanar spacing. Theoretical results for the four plane families discussed previously are summarized in the following table. Also shown in the table is a label distinguishing “thick” bands from “thin” bands. If the bandwidths are used to categorize the plane families into two groups, the ambiguity in the solution set associated with a band triplet is decreased as shown in figure 5.

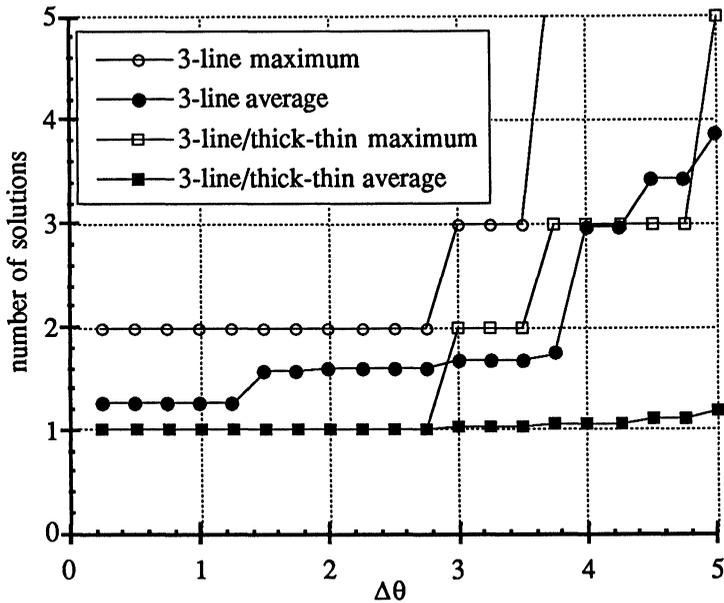


Figure 5. Ambiguity of solutions for the three-line/ "thick-thin" bandwidth analysis.

Current research indicates that recovery of bandwidth information is not likely to be obtained from the Hough transform. However, once the lines have been fixed, the bandwidths may be

Table 1. Bandwidth labels.

(hkl)	d/a	Relative Bandwidth	Label
111	$1/\sqrt{3}$	1	thin
200	$1/\sqrt{4}$	1.15	thin
220	$1/\sqrt{8}$	1.63	thick
113	$1/\sqrt{11}$	1.91	thick

recovered by obtaining band profiles by integration in a window along the line. Results obtained using the method prescribed in figure 6 from the aforementioned 50 BKD patterns are summarized in table 2. The results indicate the feasibility of the proposed "thick/thin" analysis.

Table 2. Experimental bandwidth results.

(hkl)	Minimum - Maximum	Average	Standard Deviation	Relative Bandwidth
111	18 - 27	22.2	2.3	1
200	22 - 28	25.1	1.6	1.13
220	31 - 45	37.4	2.7	1.68
113	35 - 65	44.7	6.3	1.98

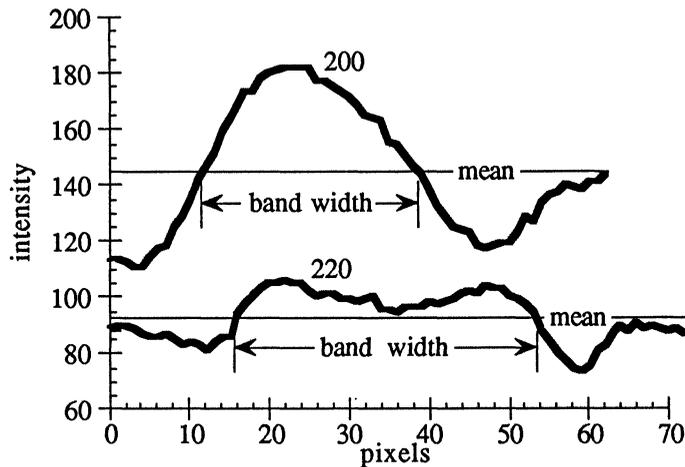


Figure 6. Sample band profiles and proposed bandwidth measurement.

CONCLUSIONS

The results of this and other research indicate that automated identification of lattice orientation from BKD patterns is feasible. However, several problems must be solved. A method of calibrating the system to reduce $\Delta\theta$ to less than 3° is required. Jensen and Schmidt⁴ used a sample holder that enables a calibration sample to be placed next to and in the same plane as the sample of interest. Their results indicate that a $\Delta\theta$ of 1° can be obtained using this configuration.

The Burns algorithm used was a commercial one designed for generic use. A customized version running on an Apple Mac Iici takes 16.3 s. Implemented on a 25 MIP workstation it takes about 1.1 s. Recent advances in technology for obtaining BKD patterns suggest that higher quality patterns are obtainable (e.g., using fiber optics). This can only serve to heighten the capabilities of the edge extraction.

Despite the difficulties mentioned, we are confident that automated BKD pattern analysis will be a viable tool for the characterization of microstructure in polycrystalline materials.

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