Measurement and Mapping of Small Changes of Crystal Orientation by Electron Backscattering Diffraction

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Running head title: (Small Orientation Differences in EBSD)

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Abstract:
We have explored the possibility of measuring small changes of orientation within grains by Electron Backscattering Diffraction (EBSD), in the scanning electron microscope. Conventional orientation maps (using EBSD) index the orientation of each position on the sample separately. This does not give accurate results for small differences of orientation. We have studied methods of measuring small changes in orientation by measuring the change from one EBSD pattern to the next directly, without indexing either. Previous workers have measured the change of position of a zone axis in the EBSD pattern. We have compared this with an alternative method, which we show to be superior, of measuring the shift of the peaks in the Hough transform from one diffraction pattern to the next. This means that we are measuring the change of orientation of sets of crystal planes within the grain, rather than measuring the change of orientation of zone axes. We show that it is possible, with a standard EBSD configuration, to measure the shift of the Kikuchi bands to a precision of about a tenth of a pixel, which corresponds to a change of orientation in the sample of about 0.1 mrad (0.006 degrees).
Keywords:
EBSD, Hough transform, Cross Correlation, Phase Correlation, Orientation Mapping.

1. Introduction:
EBSD has been rapidly developed and widely used in Materials Science in recent years. Its typical usage includes phase identification (Michael, 2001), texture determination (Dingley & Randle, 1992), grain and grain boundary characterization, and strain estimation (Troost et al, 1993, Wilkinson 1996, 2000). However, the conventional orientation mapping function provided by commercial software suffers from low angular precision (worse than 2° in many cases). Even though a lot of progress has been made, strain estimation, especially elastic strain measurement is still a great challenge to the EBSD technique.

Troost and collaborators were the first to measure the elastic strain, in Si$_{1-x}$Ge$_x$ layers on Si(100) structures, using the EBSD technique (Troost et al, 1993). His methods are based on image subtraction to estimate the shift of a zone axis, and using cross correlation to find the accurate value. Wilkinson (Wilkinson 1996, 2000) used a similar approach. In his research, he retracted the camera and scintillater away from the sample to about 3 times of normal distance, pre-filtered the EBSD patterns using a high pass filter and measured the shift of zone axes using cross correlation. Using the measured shift of the zone axis, he calculated the strain in the sample.

We are mostly concerned with detecting the shift of the Kikuchi bands in Hough space (Tao & Eades, 2001). This method can be used to measure the strain and to map small orientation changes at the surface of the sample. In this paper, we describe a method to detect the shift of Kikuchi bands to sub-pixel precision and further use it to map the small orientation changes on a GaN/Sapphire sample. The orientation change measured using this method is far beyond the
angular resolution of conventional EBSD orientation mapping. We also compared our proposed method - measuring the shift of Kikuchi bands in Hough space with the method of measuring the shift of zone axes in image space.

2. Background:

Detecting the shift of a digital image or certain features in an image in a series of similar images is an important and well-studied topic. This kind of problem is often called image matching, image registering or template matching, which is well known as an ill-conditioned problem, since ambiguous solutions may occur. Among all of the methods, cross correlation (or the cross correlation coefficient) and phase correlation (Foroosh, 2001) are conventionally used as criteria. With the usage of appropriate interpolating schemes, both of them can reach a sub-pixel accuracy.

Cross Correlation Coefficient:

The cross correlation coefficient can be understood as the normalized cross correlation; it can eliminate to some extent the effect of the background and a change of contrast between the reference pattern and the target pattern. The physical meaning of the cross correlation coefficient is quite straightforward, illustrated in figure 1, and its definition can be found in most statistics textbooks.

The cross correlation coefficient ranges from –1 to 1. The larger the value, the better the match. The cross correlation coefficient can be calculated directly or through a Fourier transform. The former is fast for small sets of data (equation 1), while the latter is more effective when the dataset is large (equation 2). The cross correlation coefficient is defined as:
\[ r(x,y) = \frac{\sum_{i,j} [(f(i,j) - \bar{f}(i,j)) \times (g(i-x, j-y) - \bar{g}(i-x, j-y))]}{\sqrt{\sum_{i,j} [(f(i,j) - \bar{f}(i,j))^2]} \sqrt{\sum_{i,j} [(g(i-x, j-y) - \bar{g}(i-x, j-y))^2]}} \]  

\[ f(i,j) \text{ is one image (represented by the solid frame in Figure 1a) and } g(i,j) \text{ is the other image (represented by open rectangle in Figure 1b). } x, y \text{ is the relative displacement of the two images.} \]

\[ \bar{f}(i,j) \text{ and } \bar{g}(i-x, j-y) \text{ are the mean values over the solid rectangles in figure 1a) and figure 1b). The core idea is that the two images are displaced, step-by-step, with respect to each other. For each step, } r(x,y) \text{ is evaluated. The best fit of the patterns occurs when } r(x,y) \text{ takes its maximum value.} \]

The cross correlation can be shown to be:

\[ R(x,y) = F^{-1}\{F^*(u,v).G(u,v)\} \]  

\[ F^*(u,v) \text{ is the conjugate of the Fourier transform of } f(i,j), G(u,v) \text{ is the Fourier transform of } g(i,j) \text{ and } F^{-1}\{\} \text{ stands for the inverse Fourier transform. This result is related to the convolution theorem.} \]

With the Fourier transform, if careful attention is paid to normalizing the Fourier transform coefficient, the cross correlation \( R(x,y) \) is normalized to match the cross correlation coefficient, \( r(x,y) \).

**Phase Correlation:**

Phase correlation uses the shift property of the Fourier transform; that is a shift in the spatial domain is equivalent to a phase shift in the frequency domain (Foroosh, 2001).
Let, \( f_2(x, y) = f_1(x-x_0, y-y_0) \)

The relationship between their Fourier transforms can be written as:

\[
F_2(u, v) = F_1(u, v) \exp(-i (ux_0 + vy_0))
\]

Hence, the normalized cross power spectrum is given by

\[
\frac{F_2(u, v)F_1^*(u, v)}{|F_1(u, v)F_1^*(u, v)|} = \exp(-i(ux_0 + vy_0))
\]

If an inverse Fourier transform is performed on equation 5, the right side becomes a Dirac delta function, \( \delta(x-x_0, y-y_0) \), centered at \((x_0, y_0)\). So, the shift \((x_0, y_0)\) can be easily determined. The phase correlation method is notably robust to noise and other false effects and provides a distinct, sharp peak at the point of registration, whereas the standard cross correlation yields broad peaks. However, equation 5 is valid only if the shift \((x_0, y_0)\) is of integer values in the discrete case. Recent research shows that the phase correlation algorithm can be extended to sub-pixel resolution effectively. Experiments show the accuracy for artificial images using this method can reach 1/20th pixel with no difficulty (Foroosh, 2001).

**Proposed Method**

Nowadays, most commercial EBSD systems use the Hough Transform to detect Kikuchi bands (Kreiger Lassen et al., 1992). The Hough transform represents a linear feature in image space by a point in Hough space. So, a Kikuchi band in an EBSD pattern is changed to a “Hough peak” in Hough space. As a result, the shift of a band in the image space \((x,y)\) can be related to a corresponding shift in Hough space \((\rho,\theta)\). Our aim is to measure the shift of the “Hough peak”. In order to improve the precision of the calculation, we choose not to use any convolution mask.
We also revised the standard Hough transform to eliminate artifacts [9]. A brief illustration of our method is shown in figure 2. The method consists following steps:

1). Choose a reference point in the specimen and get a good quality EBSD pattern from this point. This pattern works as the reference pattern (figure 3).

2). Blur* this reference pattern using a large radius Gaussian filter and then subtract it from the original pattern and perform a standard Hough transform.

3). Select an appropriate bright peak in the Hough space as shown in figure 4a and figure 4b. This peak corresponds to one Kikuchi band in the EBSD pattern.

4). Perform a revised Hough transform (no binning, small step size) on the band corresponding to the selected Hough peak only, and save the calculated data of this area as a “template”. The revised Hough transform used is one in which the contribution of the image pixels to the Hough-space pixels is weighted according to their distance from the sampling lines (Tao & Eades, to be published).

5). Shift the beam to a different position and get another EBSD pattern, the target pattern.

6). Perform Gaussian de-blur function for this pattern and do a revised Hough transform for the same area as the reference pattern. In this step again, we use our revised Hough transform with no binning of the EBSD pattern and a small sampling step size.

7). Calculate the cross correlation coefficient for these two Hough peaks, (the one from the reference pattern and the one from the target pattern).

8). Using a curve-fitting method to find the best fit to sub-pixel precision. In our experiment, we chose to use a least square fitting to a parabola.

9). Steps 5 to 8 are then repeated for other points on the sample.

*We found that step 2 is not necessary for many EBSD patterns.
3. Experiments:

The experiments performed can be conveniently divided into two groups. Group a) are trial experiments to test our proposed image processing method. Group b) are the application of this method to map the structure of GaN/Sapphire.

**Trial Experiments**: For these experiments, a single silicon wafer sample, assumed defect free, was used. The principle of these experiments is the following: If the point of impact of the incident electron beam on the sample is displaced, the EBSD pattern moves. This is because the position of the Kikuchi lines is given by the projection of the crystal planes from the generation volume to the phosphor screen. If the point of projection is moved, by moving the beam, the Kikuchi lines move with it.

If the magnification of the microscope is calibrated, the shift of the beam is accurately known and hence the displacement of the Kikuchi lines can be predicted. This value is used to check the accuracy of the shift determined directly from the cross-correlation method on the EBSD patterns.

The experiment was done on a FEI XL30 ESEM with a W filament. The accelerating voltage was 20 kV. A TSL OIM EBSD system with a DigiView CCD camera was used for this research. The beam was shifted in steps as shown in figure 5. At each point, two separate EBSD patterns were captured at different times. All together, we acquired a set of 14 EBSD patterns from 7 points and they were named from **Pattern1a** to **Pattern7b** sequentially. Each EBSD pattern has 987×987 pixels and the data capture time was 21.25s/pattern. We wrote a program to do the large radius Gaussian filtering (Young & van Vliet, 1995) and added the function of measuring the shift of Kikuchi bands into the OIM software. After our revision, the OIM Data Collection software can measure the shift of several bands at the same time. The cross
correlation coefficient was chosen as the criterion. We implemented both ways to calculate the cross correlation coefficient in this program, including calculating the cross correlation coefficient directly (equation 1) and through a Fourier transform (equation 2).

A stand-alone Win32 Program, ShiftDetector, was written and used to detect the shift of zone axes. This program used both the phase correlation and cross correlation coefficient as criteria. Like the revised OIM Data Collection software, both ways to calculate the cross correlation coefficient are implemented (equation 1 and equation 2).

Before the experiments were carried out, the integrity of these two programs was verified by using some artificial images. Experiments showed there are no calculation problems with the programs.

**Application:** After we got positive results from the trial experiments, we applied our shift detection method for Kikuchi bands to map the orientation changes on a GaN/Sapphire structure. The Sample is GaN, grown on sapphire by the technique of lateral epitaxial growth (LEO). It was grown by Dr. Milan Pophirstic using MOCVD at Emcore Inc and provided to us by Drs. Slade Cargill and Eva Campo of Lehigh University. A 2 μm thick GaN buffer layer was first grown on the sapphire substrate, and a 100nm thick SiN_x mask was planted on the buffer layer, in which patterns of windows were produced by lithographic methods. The GaN layer was then grown in the window regions with lateral overgrowth over adjacent masks. The window stripes are along the [11̅00] direction. The growth temperature was 1000°C, growth pressure was 100 Torr and the growth rate was 1.6μm/hr.

The TSL OIM Data Collection software was also modified for this experiment. With our modification, it is possible to store the EBSD pattern for each pixel. In this way, the same
complete data set for a scan could be analyzed after the scan. Then, we selected the first pattern from the dataset as the reference pattern and chose several Kikuchi bands from this reference pattern. The selection process was done in Hough space. We further applied the band shift detection method to every chosen Kikuchi band on each pattern in the dataset. The measured shift value was used to form maps. In theory, the method for the measurement of the shift of Kikuchi bands can be implemented in real time. However, since the EBSD pattern has a relatively low signal to noise ratio, we choose to use a relatively long pattern integration time and to do the analysis offline. A special computer file format (.dan) was defined for the offline mapping process, since the standard image formats lacked flexibility. This map file (.dan) can be tweaked and converted to a .bmp (Bitmap) file using a program DataAnalyzer especially written for this research. The experiments were done on an FEI XL30 ESEM with a Schottkey field emission gun and TSL OIM Data Collection system. The SEM accelerating voltage was 20 kV. Each EBSD pattern has 484×484 pixels. The step size in the scans was 40nm along the horizontal direction and 60nm down the slope. The beam dwell time was about 0.9 second for each point. Careful attention was paid to minimize the hydrocarbon contamination. The captured dataset includes 91×72 patterns.
4. Results and Discussion:

*Shift Measurement in Hough space*

For the hardware configuration in this research, the CCD chip is lens coupled to the phosphor screen, so the actual CCD pixel size is different from the “effective” one. Our estimation shows the effective pixel size is about 35µ.

Using the procedure described in the previous section, we measured the shift of eight Kikuchi bands, marked by the arrows in figure 6. For each target point, we acquired two EBSD patterns, thus we have two sets of measurement data. For the horizontal points in figure 5, **Pattern1a** is used as the reference and the results are listed in Table 1. The largest difference between the values measured from the two patterns captured at the same point is 0.17 pixels, and the average difference is 0.063 pixels.

In this experiment, each selected “Hough peak”, which is used to do the cross correlation, has an angular width (θ) ranging from 10 to 20 degrees. The θ value for the centerline of the Kikuchi band, θ, is listed on the second row in table 1.

Because we could not devise a good way to calibrate the actual pixel size in the EBSD pattern, the shifts were measured only in relative terms by assuming that the correct value was obtained for the largest shift. It was later shown that the value was in good agreement with the estimated pixel size, obtained by measuring the diameter of the phosphor screen. The point is that we can obtain the angular size of one pixel from the pattern calibration, but shifting the beam produces a displacement of the pattern whose size in pixels depends on the (unknown) magnification of the lens coupling from the phosphor screen to the camera.
Approximately, for a horizontal shift of the electron beam, the displacement of the beam (in units of pixels) can be calculated by dividing the shift of the band by \( \cos \theta \). The measured shift of band 1 and band 8 at point 5 are used to calculate the largest horizontal beam shift.

\[
\text{Horizontal Beam Shift} = 0.5 \times (\text{Band1}/\cos \theta_1 + \text{Band8}/\cos \theta_8).
\]  

After the largest beam shift (horizontally) is known, which is 1.38 pixels in this case, we further calculated the shift of the Kikuchi band for each point and compared it with the measured one (averaged over two measurements). The results are listed in Table 2 and figure 7 shows the comparison. The x-axis on this figure stands for the measured shift, while the y-axis is the calculated shift. Every point on the reference line has the same distance to both x and y axes. This figure shows that the measured shifts are in good agreement with the calibrated value, since nearly all the points are clustered around the reference line. The largest discrepancy is 0.145 pixels and the average discrepancy is 0.06 pixels.

The results of this experiment (Table 1 and figure 7) proved: 1). The measured pixel size (32 \( \mu \)) is quite similar to our estimated effective pixel size (35 \( \mu \)). 2). For the same points, the measurement for the patterns captured at different times shows good consistency and their error is less than 0.1 pixel. 3) Our image processing routine could reach sub-pixel resolution when being used to detect the shift of the Kikuchi bands in an EBSD pattern. Our estimate is that an accuracy up to 0.2 pixels can be reached for most bands, which corresponds to angular difference about 0.02 degree. However, it is difficult to give an absolute value on the detection limit of this method, since the results depend on materials, hardware set up, background elimination and some other factors.
However, the measurement for the vertical shift of the electron beam is not as good as that of horizontal shift of electron beam. Table 3 lists the measurement of the shift of the eight Kikuchi bands marked by arrows on figure 6, for the vertical points in figure 5. In this measurement, Point 3a is chosen as the reference pattern. The shift of the Kikuchi bands, in units of pixels, is calculated using the shift of the beam, the $\theta$ value of the Kikuchi band and the measured effective pixel size (32$\mu$). Table 4 lists the average of the two measurements and the results of calculation. Figure 8 shows the comparison between the measurement and the calculation. It is clear that the errors are relatively large between the measurement and calculation and the measurement is systematically smaller than the calculated values. Possible reasons include:

1) The experiment was done under low magnifications, and the sample is highly tilted. So, a shift of the electron beam along the y scanning direction corresponds to a large value of out of focus. As a result, the diffraction volume for Point 6 is quite a lot larger than that of Point 3 and the Kikuchi bands on the EBSD patterns from Point 6 are relatively blurry and wider than those from Point 3. This could be the main reason for the measurement errors.

2) In some cases we observed that the contamination patch was not rectangular, indicating an error in the angle of the scan. This could also lead to larger errors for the measurement of the vertical shifting than that for the horizontal shifting.

3) The error associated with the inaccuracy of the beam shifting has a larger effect (a factor of 3) on vertical points than horizontal points, since the sample is highly tilted (70°).

For shifting the electron beam both horizontally and vertically, errors could also be introduced by the effect of charging and drift, since a long pattern capture time was used in the experiment.
**Shift Measurement in Image space**

In this experiment, we also tested the measurement of the shift of the zone axis, using normal EBSD settings (the distance between the sample and phosphor screen is less than 5cm). The chosen zone axis used for shift measurement is marked by a box in figure 6. The preliminary results showed that neither the cross correlation nor the phase correlation method can detect the shift of the zone axis accurately in most cases. Usually, the shift is invariantly 0 in both x and y directions when no interpolation method is used. A map of the cross correlation coefficient shows that there is a relatively large peak at exactly (0,0), figure 9. This chart also shows the cross correlation coefficient is relatively low even for the maximum value. i.e. the best fit. So is the phase correlation. This suggests the similarity between the selected areas in the two patterns used for comparison is also low.

After checking the calculation for another experiment, in which the electron beam is shifted several pixels from the reference point, we found that, for the cross correlation coefficient, there is a high peak corresponding to a (0,0) shift and there also exists a second peak which could be related to the shift of the selected area, as shown in figure 10. The 3-D display of the phase correlation image also showed these two peaks, the higher peak corresponding to the (0,0) shift and a lower and broader second peak corresponding to the shift of the selected zone axis. Figure 11 shows an image formed by the cross correlation coefficient. The brightest point corresponds to the center of the image, which has an offset from the center of the bright blobs.

If the distance between the first peak and the second peak is small, as in the case of figure 9, the measurement of the shift of the zone axis gives a false answer. On the other hand, even when the first peak and the second peak are separated, the accuracy of the interpolation for the measurement of zone axis could still be affected, since both the cross correlation coefficient and
phase correlation are low and the cross correlation and phase correlation dataset is relatively noisy.

We are not sure of the exact reason for the formation of this (0,0) peak. One possible explanation is the residual background. Since the cross correlation coefficient is a “statistical factor”, all the pixels in the chosen area are features and their effects are counted. The residual background on the EBSD pattern works as a “feature”, and this may cause the high peak at (0,0). In Wilkinson’s research, the distance between the camera and the sample is large and the EBSD pattern covers a small solid angle, so the width of the Kikuchi bands is also large and the chosen zone axis covered more features and less background. He also used very long exposure times to suppress the effect of noise. As a result, the (0,0) peak is not reported in his research. Although he acknowledges seeing such a peak and discarding it as an artifact (private communication).

Our experiment also shows that calculating the cross correlation coefficient directly (without using the Fourier transform) cannot eliminate the center peak. This excludes the possibility that the sharp (0,0) peak is introduced through edge effects in the Fourier transform. Using a Gaussian filter or a high pass filter (Box filter blurred, then subtracted) cannot eliminate the zero shift peak either, at least for the experimental setup in our research. However, the mask size of these filters can affect the relative height between the first peak and the second peak.

Comparison of the shift measurement methods

Our results showed that measuring the small shift of Kikuchi bands in Hough space is more advantageous than measuring the shift of the zone axis in image space for normal EBSD. There are several reasons for this: 1) The former method gave a high cross correlation coefficient value and thus the interpolation is more accurate and meaningful. Figure 10 shows the cross
correlation coefficient from the calculation of the shift of a zone axis, while Figure 12 shows the cross correlation coefficient from the calculation of the shift of a Kikuchi band. Obviously, the method of detecting the Kikuchi band in Hough space gave a larger cross correlation coefficient value than measuring the shift of the zone axis in image space. For most of our experiments, the largest cross correlation coefficient is less than 0.7 when detecting the shift of the zone axis. In most cases, it is less than 0.5. However, the largest cross correlation coefficient for detecting the shift of the Kikuchi band is larger, in most cases it is larger than 0.9.

2). The Hough transform can be understood as an accumulation process, so the effect of noise is suppressed and the effect of “residual background” is minimized since the cross correlation coefficient is calculated only on the peak of the Hough transform corresponding to the Kikuchi band. Figure 13 shows the intensity distribution along line B-B’ for Kikuchi band A in figure 3. Although this figure does show the general shape of the curve, there is a lot of noise. However, if we measure the intensity distribution of band A in Hough space, the effect of noise is suppressed, as shown in Figure 14.

3). Measuring the shift in Hough space doesn’t require any change of the experimental settings, and a much shorter exposure time is needed. Thus mapping is feasible. Besides, the shift of several bands can be measured at the same time when choosing to use the band detection method. By contrast, Wilkinson’s work on the detection of the shift of zone axis required moving the EBSD system and long exposure times. Thus the data could be acquired only at selected points and the EBSD patterns covered a very small solid angle, as a result only a few zone axes are useful.
4). Pre-filtering is not necessary for measuring the shift of the Kikuchi bands in Hough space, while it is necessary for the measurement of the zone axis in image space, according to Wilkinson. Through skipping this step, we can decrease calculation time noticeably.

**Small orientation Mapping**

In this experiment, more than 1GB (Giga byte) of data was captured and analyzed. Figure 15 is the first of the batch of the patterns captured for analysis. It has much better quality than the last pattern in the captured batch, figure 16. The blurriness of figure 16 is caused by hydrocarbon contamination accumulated during the scanning process. Contamination can affect the quality and bring artifacts to the IQ map, to the map of the mean, and to the map of the standard deviation. In order to get rid of the effect of the hydrocarbon contamination, we chose to normalize the generated maps [8]. Figure 17 is a map of the standard deviation of the pattern and figure 18 is a map of the mean of the pattern. Both of these maps show some chevron shapes on the sample, which are missed in the IQ (image quality) map, figure 19, and secondary electron images.

Figures 20, and 21 are the maps generated using the shift of band A and of band B in figure 15. For the first tens of rows of the pixels on the maps, the hydrocarbon contamination didn’t blur the pattern badly and the pattern has less noise. However, as scanning proceeded, the hydrocarbon contamination accumulated, and the measurement of the shift of the Kikuchi band became less accurate. As a result, the bottom part of the generated maps looks nosier than the upper part. Nevertheless, both maps (figures 20, and 21) show features in this nominal single
crystal sample. The features suggest that there could be some orientation fluctuation in this nominally single crystal. There are some regions on this sample, whose orientations are slightly different from each other. However, inside these regions, the orientation is relatively uniform.

Another similar experiment but with a smaller data set (90×32) showed that, more interestingly, the chevron shapes shown on the maps of the mean (figure 22) and standard deviation (figure 23) correspond to the edges of the orientation varying regions on the maps of the shift of Kikuchi bands, figure 24 and 25. The difference between the maximum shift and minimum shift in the shift maps is less than 4 pixels. This corresponds to an orientation difference less than 0.5° degrees. These images suggest that there could be some sub-grain boundaries intersecting the surface of the sample.

**Further Suggestions**

Measuring the shift of the Kikuchi bands can reach sub-pixel accuracy. This fact can be utilized to do “high precision” orientation mapping. The conventional method of orientation mapping relies on indexing the EBSD pattern and then measuring the absolute orientation of the sample. Inevitably, this method suffers from low precision.

As a complement, we propose a way to do it differently. This method is based on the fact that detecting the relative change of the orientation is more accurate than measuring the absolute value. So, high precision orientation mapping could be done this way: First, perform a conventional orientation mapping (or just map the standard deviation), then choose a reference point from each grain, and measure the relative orientation change of all other points in the same grain from this reference point. The orientation changes can be easily calculated using measured shifts of several Kikuchi bands. Finally, using the orientation index of the reference
points and the measured orientation shift for other points, an orientation map, at a higher precision, could be constructed.
5. Summary

a. In this research, we developed an image processing routine, which enables us to measure the shift of Kikuchi bands to sub-pixel precision. This routine is done in Hough space. It is fast, accurate and convenient.

b. We also compared the measurement of shifts of Kikuchi bands with the measurement of shifts of zone axes. Analysis shows that detecting the shift of the Kikuchi bands in Hough space has advantages over detecting the shift of zone axes in image space, at least for normal EBSD settings.

c. The proposed image processing routine can be used for practical mapping. This method has been applied to mapping small changes in orientations in a GaN/Sapphire structure.

d. We also suggest a method to do a high-precision orientation mapping, based on this image processing routine.
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We thank Drexel University for access to their field emission XL30 ESEM, and we are specially appreciative of Dave Von Rohr’s willingness to allow us to install our “home made” software on his machine.

The Fourier transform in this research used the library (.dll) downloaded from: [http://www.fftw.org](http://www.fftw.org).

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**Figure Captions:**

Figure 1. Illustration of the direct calculation of the cross correlation coefficient.

  Figure 1a. The solid square stands for the template window, $f(x,y)$.
  Figure 1b. The solid square inside the green square is $g(x,y)$.

Figure 2. Representation of the band detection method.

Figure 3. EBSD pattern captured from a Si wafer using Noran’s Phase ID system. After Gaussian deblurring, the Hough transform of this pattern is shown in figure 4a. The Hough transform of Band A is inside the frame in figure 4a and figure 4b.

Figure 4a. Hough transform of figure 3 (Gaussian de-blur filtered). The small area (frame) from this reference pattern is the template used to detect the shift of the other patterns.

Figure 4b. An enlarged view of a peak in Hough Space (Figure 4a). Even here the corresponding EBSD pattern is binned. In the program, the cross correlation coefficient is calculated using uncompressed images.

Figure 5. Beam shift pattern used in the trial experiment. The distances between adjacent points are 11 µ. At each point, two EBSD patterns were acquired. For the horizontal points (1,2,3,4, and 5), the first pattern from the first point is used as the reference pattern. For the vertical shifts, the first pattern from point 3 is used as reference pattern.
Figure 6. EBSD pattern captured from a silicon wafer. This pattern served as the reference pattern for the trial experiment. The pattern has 987×987 pixels and the effective pixel size is about 35 µ. The shifts of the bands marked by arrows and of the zone axis marked by the rectangle were measured.

Figure 7. Comparison between the measured and calculated shifts of Kikuchi bands, for horizontal shifts of the beam position. The agreement is good. All of the units are in pixels.

Figure 8. Comparison between the measured and calculated shifts of Kikuchi bands, for vertical shifts of the beam position. The agreement is less good. Reasons for the increased error in this case are discussed in the text.

Figure 9. Plot of the cross correlation coefficient as a function of displacement (in x and y) of the target pattern with respect to the reference pattern, for the case of a zone axis in image space, when the shift of the zone axis is small When measuring the shift of a zone axis, the peak at (0,0) can introduce error. Similar results were obtained from the major zone axis in Figure 6.

Figure 10. Plot of the cross correlation coefficient as a function of displacement of the target pattern with respect to the reference pattern, for the case of a zone axis in image space, when the shift of the zone axis is larger than that of figure 9, the (0,0) peak is higher than the peak sought.
Figure 11. Map of the cross correlation coefficient for detecting the shift of a zone axis. The very small, very bright, point in this figure corresponds to the (0,0) peak, which is different from the center of the broad blob, which corresponds to the pattern shift.

Figure 12. Plot of the cross correlation coefficient as a function of displacement (in $\rho$ and $\theta$) between the target pattern and the reference pattern. In this case, the cross correlation coefficient is calculated for a region of Hough space corresponding to a particular Kikuchi band, in contrast with the previous figures in which the cross correlation coefficient is calculated for a region of the EBSD pattern including a zone axis.

Figure 13. Plot of the intensity along line BB’ in the EBSD pattern in figure 3. It shows the general shape of the profile of Kikuchi band A.

Figure 14. Plot of the intensity variation across Kikuchi band A in figure 3. In this case the intensity is derived from the profile of the corresponding Hough peak. The suppression of noise arises because the Hough peak averages along the whole length of the Kikuchi band.

Figure 15. First pattern in the captured dataset. The sample is GaN; the patterns were obtained at 20kV, see text.

Figure 16. Last pattern in the captured dataset.
Figure 17. Map formed by the normalized mean of the EBSD pattern. At each of the 91x72 pixels the complete EBSD pattern was stored. Off-line processing was used to calculate the mean of each pattern (displayed here) and other quantities displayed in following figures. GaN/Sapphire sample.

Figure 18. Map formed by the normalized and inverted standard deviation of the EBSD patterns. GaN/Sapphire sample.

Figure 19. Normalized IQ map for the same data set as figures 17 and 18.

Figure 20. Map of the shift of band 1 in figure 15.

Figure 21. Map of the shift of band 2 in figure 15.

Figure 22. Map formed by the normalized mean of the EBSD patterns, for a second experiment with 90x32 pixels. GaN/Sapphire sample.

Figure 23. Map formed by the normalized standard deviation, in the second experiment. GaN/Sapphire sample.

Figure 24a. Map formed by the shift of one Kikuchi band. There is a correspondence between the positions of the chevron shapes in figures 22 and 23, and the regions where orientations change in the sample as shown by figures 24 and 25.
Figure 24b. The upper part of figure 24a (where the noise is less because of the absence of contamination) with contrast enhanced.

Figure 25. Map formed by the shift of another Kikuchi band.
Figures:

Figure 1 a. The solid square stands for the template window, \( f(x,y) \).

Figure 1b. The inside solid square is \( g(x,y) \).

Figure 1. Illustration of the direct calculation of the cross correlation coefficient.
*Remove the residual Background from the reference pattern using a Gaussian De-blur Filter. (*Not always necessary)

Perform standard Hough Transform for binned image

Select appropriate areas in Hough Space (The open Rectangle in Figure 4a and Figure 4b)

Do a revised Hough Transform with no binning for the bands which corresponds to the Selected Hough Peak areas, using small sampling steps. (one pixel along the \( \rho \) direction, and about 1/8 degree along the \( \theta \) direction).

Do the operations of Step 1 and Step 4 on the target pattern (The area selected in Step 3 will be used for the target pattern also).

Calculate the Cross Correlation Coefficient between the reference pattern and target pattern (Figure 4).

Use an appropriate curve fitting method to find the shift of the Kikuchi band to sub-pixel resolution.

**Figure 2. Representation of the band detection method**
Figure 3. EBSD pattern captured from a Si wafer using Noran’s Phase ID system. After Gaussian deblurring, the Hough transform of this pattern is shown in figure 4a. The Hough transform of Band A is inside the frame in figure 4a and figure 4b.
Figure 4a. Hough transform of figure 3 (Gaussian de-blur filtered). The small area (frame) from this reference pattern is the template used to detect the shift of the other patterns.

Figure 4b. An enlarged view of a peak in Hough Space (Figure 4a). Even here the corresponding EBSD pattern is binned. In the program, the cross correlation coefficient is calculated using uncompressed images.
Figure 5. Beam shift pattern used in the trial experiment. The distances between adjacent points are 11 µ. At each point, two EBSD patterns were acquired. For the horizontal points (1, 2, 3, 4, and 5), the first pattern from the first point is used as the reference pattern. For the vertical shifts, the first pattern from point 3 is used as reference pattern.
Figure 6. EBSD pattern captured from a silicon wafer. This pattern served as the reference pattern for the trial experiment. The pattern has 987×987 pixels and the effective pixel size is about 35 µ. The shifts of the bands marked by arrows and of the zone axis marked by the rectangle were measured.
Figure 7. Comparison between the measured and calculated shifts of Kikuchi bands, for horizontal shifts of the beam position. The agreement is good. All of the units are in pixels.
Figure 8. Comparison between the measured and calculated shifts of Kikuchi bands, for vertical shifts of the beam position. The agreement is less good. Reasons for the increased error in this case are discussed in the text.
Figure 9. Plot of the cross correlation coefficient as a function of displacement (in x and y) of the target pattern with respect to the reference pattern, for the case of a zone axis in image space, when the shift of the zone axis is small. When measuring the shift of a zone axis, the peak at (0,0) can introduce error.
Figure 10. Plot of the cross correlation coefficient as a function of displacement of the target pattern with respect to the reference pattern, for the case of a zone axis in image space, when the shift of the zone axis is larger than that of figure 9, the (0,0) peak is higher than the peak sought.

Figure 11. Map of the cross correlation coefficient for detecting the shift of a zone axis. The very small, very bright, point in this figure corresponds to the (0,0) peak, which is different from the center of the broad blob, which corresponds to the pattern shift.
Figure 12. Plot of the cross correlation coefficient as a function of displacement (in $\rho$ and $\theta$) between the target pattern and the reference pattern. In this case, the cross correlation coefficient is calculated for a region of Hough space corresponding to a particular Kikuchi band, in contrast with the previous figures in which the cross correlation coefficient is calculated for a region of the EBSD pattern including a zone axis.

Figure 13. Plot of the intensity along line BB’ in the EBSD pattern in figure 3. It shows the general shape of the profile of Kikuchi band A.
Figure 14. Plot of the intensity variation across Kikuchi band A in figure 3. In this case the intensity is derived from the profile of the corresponding Hough peak. The suppression of noise arises because the Hough peak averages along the whole length of the Kikuchi band.
Figure 15. First pattern in the captured dataset. The sample is GaN; the patterns were obtained at 20kV, see text.

Figure 16. Last pattern in the captured dataset.

Figure 17. Map formed by the normalized mean of the EBSD pattern. At each of the 91x72 pixels the complete EBSD pattern was stored. Off-line processing was used to calculate the mean of each pattern (displayed here) and other quantities displayed in following figures. GaN/Sapphire sample.

Figure 18. Map formed by the normalized and inverted standard deviation of the EBSD patterns. GaN/Sapphire sample.

Figure 19. Normalized IQ map for the same data set as figures 17 and 18.
Figure 20. Map of the shift of band 1 in figure 15.

Figure 21. Map of the shift of band 2 in figure 15.

Figure 22. Map formed by the normalized mean of the EBSD patterns, for a second experiment with 90×32 patterns. GaN/Sapphire sample. Only 85×30 pixels are shown here.

Figure 23. Map formed by the normalized standard deviation, in the second experiment. GaN/Sapphire sample.

Figure 24a. Map formed by the shift of one Kikuchi band. There is a correspondence between the positions of the chevron shapes in figures 22 and 23, and the regions where orientations change in the sample as shown by figures 24 and 25.

Figure 24b. The upper part of figure 24a (where the noise is less because of the absence of contamination) with contrast enhanced.

Figure 25. Map formed by the shift of another Kikuchi band.
Tables:

Table 1. Measurement of the shift of the Kikuchi bands for the horizontal beam shifts

<table>
<thead>
<tr>
<th></th>
<th>Band 1</th>
<th>Band 2</th>
<th>Band 3</th>
<th>Band 4</th>
<th>Band 5</th>
<th>Band 6</th>
<th>Band 7</th>
<th>Band 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Center θ</td>
<td>15</td>
<td>33</td>
<td>25</td>
<td>52.5</td>
<td>56.5</td>
<td>101.5</td>
<td>127</td>
<td>166</td>
</tr>
<tr>
<td>Pattern 1b</td>
<td>0.094</td>
<td>0.077</td>
<td>0.003</td>
<td>-0.070</td>
<td>-0.007</td>
<td>0.014</td>
<td>-0.065</td>
<td>0.038</td>
</tr>
<tr>
<td>Pattern 2a</td>
<td>0.345</td>
<td>0.283</td>
<td>0.222</td>
<td>0.068</td>
<td>0.159</td>
<td>-0.065</td>
<td>-0.272</td>
<td>-0.425</td>
</tr>
<tr>
<td>Pattern 2b</td>
<td>0.348</td>
<td>0.318</td>
<td>0.193</td>
<td>0.062</td>
<td>0.110</td>
<td>-0.107</td>
<td>-0.408</td>
<td>-0.317</td>
</tr>
<tr>
<td>Pattern 3a</td>
<td>0.647</td>
<td>0.564</td>
<td>0.587</td>
<td>0.362</td>
<td>0.267</td>
<td>-0.126</td>
<td>-0.557</td>
<td>-0.616</td>
</tr>
<tr>
<td>Pattern 3b</td>
<td>0.709</td>
<td>0.547</td>
<td>0.745</td>
<td>0.265</td>
<td>0.284</td>
<td>-0.198</td>
<td>-0.565</td>
<td>-0.599</td>
</tr>
<tr>
<td>Pattern 4a</td>
<td>0.989</td>
<td>0.866</td>
<td>0.788</td>
<td>0.450</td>
<td>0.501</td>
<td>-0.305</td>
<td>-0.660</td>
<td>-0.921</td>
</tr>
<tr>
<td>Pattern 4b</td>
<td>1.006</td>
<td>1.036</td>
<td>0.939</td>
<td>0.614</td>
<td>0.516</td>
<td>-0.193</td>
<td>-0.668</td>
<td>-1.013</td>
</tr>
<tr>
<td>Pattern 5a</td>
<td>1.405</td>
<td>1.228</td>
<td>1.251</td>
<td>0.761</td>
<td>0.827</td>
<td>-0.276</td>
<td>-0.907</td>
<td>-1.284</td>
</tr>
<tr>
<td>Pattern 5b</td>
<td>1.412</td>
<td>1.251</td>
<td>1.335</td>
<td>0.871</td>
<td>0.882</td>
<td>-0.209</td>
<td>-0.838</td>
<td>-1.257</td>
</tr>
</tbody>
</table>

All the Units are in pixels. From point 1 to point 5, the beam shift distance is about 44µ, which corresponds to 1.38 pixels according to our measurement. So the effective pixel size is about 32µ.
Table 2. Comparison of the measured and calculated shifts of the Kikuchi bands for the horizontal beam shifts.

<table>
<thead>
<tr>
<th>Pattern</th>
<th>Band 1</th>
<th>Band 2</th>
<th>Band 3</th>
<th>Band 4</th>
<th>Band 5</th>
<th>Band 6</th>
<th>Band 7</th>
<th>Band 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>2(C)</td>
<td>0.334</td>
<td>0.290</td>
<td>0.313</td>
<td>0.211</td>
<td>0.191</td>
<td>-0.069</td>
<td>-0.208</td>
<td>-0.336</td>
</tr>
<tr>
<td><strong>Pattern 2(M)</strong></td>
<td><strong>0.346</strong></td>
<td><strong>0.301</strong></td>
<td><strong>0.207</strong></td>
<td><strong>0.066</strong></td>
<td><strong>0.134</strong></td>
<td><strong>-0.086</strong></td>
<td><strong>-0.340</strong></td>
<td><strong>-0.371</strong></td>
</tr>
<tr>
<td>3(C)</td>
<td>0.668</td>
<td>0.581</td>
<td>0.627</td>
<td>0.421</td>
<td>0.382</td>
<td>-0.138</td>
<td>-0.417</td>
<td>-0.672</td>
</tr>
<tr>
<td><strong>Pattern 3(M)</strong></td>
<td><strong>0.678</strong></td>
<td><strong>0.555</strong></td>
<td><strong>0.666</strong></td>
<td><strong>0.313</strong></td>
<td><strong>0.276</strong></td>
<td><strong>-0.162</strong></td>
<td><strong>-0.561</strong></td>
<td><strong>-0.608</strong></td>
</tr>
<tr>
<td>4(C)</td>
<td>1.003</td>
<td>0.871</td>
<td>0.940</td>
<td>0.632</td>
<td>0.573</td>
<td>-0.207</td>
<td>-0.625</td>
<td>-1.007</td>
</tr>
<tr>
<td><strong>Pattern 4(M)</strong></td>
<td><strong>0.998</strong></td>
<td><strong>0.951</strong></td>
<td><strong>0.864</strong></td>
<td><strong>0.532</strong></td>
<td><strong>0.509</strong></td>
<td><strong>-0.249</strong></td>
<td><strong>-0.664</strong></td>
<td><strong>-0.967</strong></td>
</tr>
<tr>
<td>5(C)</td>
<td>1.337</td>
<td>1.161</td>
<td>1.254</td>
<td>0.844</td>
<td>0.765</td>
<td>-0.275</td>
<td>-0.833</td>
<td>-1.342</td>
</tr>
<tr>
<td><strong>Pattern 5(M)</strong></td>
<td><strong>1.408</strong></td>
<td><strong>1.239</strong></td>
<td><strong>1.293</strong></td>
<td><strong>0.816</strong></td>
<td><strong>0.855</strong></td>
<td><strong>-0.243</strong></td>
<td><strong>-0.872</strong></td>
<td><strong>-1.271</strong></td>
</tr>
</tbody>
</table>

(C): Shifts of the Kikuchi bands calculated from the shift of the beam and the angle of the Kikuchi band.
(M): Measured shifts of the Kikuchi band using our image processing routine. The results are the average over two measurements from two different EBSD patterns from the same beam position.
Table 3. Measurement of the shift of the Kikuchi bands for the vertical shifts of the beam.

<table>
<thead>
<tr>
<th></th>
<th>Band 1</th>
<th>Band 2</th>
<th>Band 3</th>
<th>Band 4</th>
<th>Band 5</th>
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<th>Band 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Center θ</td>
<td>15</td>
<td>33</td>
<td>25</td>
<td>52.5</td>
<td>56.5</td>
<td>101.5</td>
<td>127</td>
<td>166</td>
</tr>
<tr>
<td>Pattern 3b</td>
<td>0.074</td>
<td>0.004</td>
<td>0.13</td>
<td>-0.088</td>
<td>0.0278</td>
<td>-0.072</td>
<td>0.002</td>
<td>0.002</td>
</tr>
<tr>
<td>Pattern 7a</td>
<td>-0.234</td>
<td>-0.226</td>
<td>-0.325</td>
<td>-0.393</td>
<td>-0.414</td>
<td>-0.695</td>
<td>-0.381</td>
<td>-0.176</td>
</tr>
<tr>
<td>Pattern 7b</td>
<td>-0.300</td>
<td>-0.190</td>
<td>-0.294</td>
<td>-0.327</td>
<td>-0.393</td>
<td>-0.747</td>
<td>-0.43</td>
<td>-0.054</td>
</tr>
<tr>
<td>Pattern 8a</td>
<td>-0.355</td>
<td>-0.393</td>
<td>-0.149</td>
<td>-0.671</td>
<td>-0.441</td>
<td>-1.241</td>
<td>-0.773</td>
<td>-0.496</td>
</tr>
<tr>
<td>Pattern 8b</td>
<td>-0.461</td>
<td>-0.614</td>
<td>-0.245</td>
<td>-0.916</td>
<td>-0.724</td>
<td>-1.339</td>
<td>-0.992</td>
<td>-0.273</td>
</tr>
</tbody>
</table>

Table 4. Comparison of the measured and calculated shifts of the Kikuchi bands for vertical displacements of the beam.

<table>
<thead>
<tr>
<th></th>
<th>Band 1</th>
<th>Band 2</th>
<th>Band 3</th>
<th>Band 4</th>
<th>Band 5</th>
<th>Band 6</th>
<th>Band 7</th>
<th>Band 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pattern 3</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Pattern 7(C)</td>
<td>-0.244</td>
<td>-0.514</td>
<td>-0.399</td>
<td>-0.749</td>
<td>-0.788</td>
<td>-0.925</td>
<td>-0.754</td>
<td>-0.228</td>
</tr>
<tr>
<td>Pattern 7(M)</td>
<td><strong>-0.267</strong></td>
<td><strong>-0.208</strong></td>
<td><strong>-0.310</strong></td>
<td><strong>-0.360</strong></td>
<td><strong>-0.404</strong></td>
<td><strong>-0.721</strong></td>
<td><strong>-0.406</strong></td>
<td><strong>-0.115</strong></td>
</tr>
<tr>
<td>Pattern 8(C)</td>
<td>-0.488</td>
<td>-1.028</td>
<td>-0.798</td>
<td>-1.499</td>
<td>-1.575</td>
<td>-1.851</td>
<td>-1.509</td>
<td>-0.457</td>
</tr>
<tr>
<td>Pattern 8(M)</td>
<td><strong>-0.408</strong></td>
<td><strong>-0.504</strong></td>
<td><strong>-0.197</strong></td>
<td><strong>-0.794</strong></td>
<td><strong>-0.583</strong></td>
<td><strong>-1.290</strong></td>
<td><strong>-0.883</strong></td>
<td><strong>-0.385</strong></td>
</tr>
</tbody>
</table>