ELABORATION ON THE HEXAGONAL GRID AND SPIRAL TRACE SCHEMES FOR POLE FIGURE DATA COLLECTION

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ABSTRACT

A practical description of the mathematics required to implement the hexagonal grid and spiral trace pole figure data collection schemes is presented. Applying the concepts of stereographic and equal area projections with geometry, spreadsheets were created to calculate the angular settings of the goniometer. Using the generated settings, the hexagonal grid and spiral trace schemes were programmed into the existing X-ray software and employed to collect data for a sample of aluminum foil. The resulting (111) pole figures were similar to those collected with the conventional 5°χ × 5°φ grid. The hexagonal grid has been shown by others to reduce the number of data points and time needed to complete a pole figure, while providing equal area sampling. Although not optimized, the spiral method was also investigated as another alternative to the 5°χ × 5°φ grid.

INTRODUCTION

A four-circle goniometer is usually employed to collect pole figures. Typically the detector (theta axis, θ) is set at the Bragg angle, and the sample (omega axis, Ω) is often set at half the Bragg angle. The desired reflection intensity is measured over a set of sample tilt angles (chi, χ) and azimuthal angles (phi, φ) (see Figure 1). Typically, these data are presented in a pole figure. A pole figure provides a representation of the distribution of a particular set of atomic planes for data acquired through diffraction and is used for analyzing crystallographic texture or preferred orientation. Pole figures are typically constructed from a collection of data points, each with a prescribed χ, φ and measured intensity. The Schulz reflection method [1] with equal angular step increments for χ and φ is commonly employed to acquire the necessary data. Usually a 5°χ × 5°φ grid (see Figure 2) is chosen, i.e., a 5° increment in χ (0° to 80°) and a 5° increment in φ (0° to 355°). However, this equal angular “grid” leads to a non-uniform data density and an inefficient use of time [2].

Pole figure data can be viewed in a variety of ways, including stereographic and equal area projections. Stereographic projections preserve angle measurements but not area proportions, but equal area projections preserve area proportions but not angle measurements [3]. The spiral grid (which is formed on the basis of constant radial angles) is a stereographic projection of a hemisphere with a radius, R, taken as unity. In stereographic projections, the pole opposite the projection plane is connected with a line to any point on the sphere. The line connecting the two is continued onto the projection plane, and their intersection is the projection of the point from the sphere. The projected radial distance, D, of the new point in the plane is found by taking 2Rtan(χ ÷ 2) from the sphere, with φ and magnitude unchanged [3]. On the other hand, the
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hexagonal grid is an equal area projection, which is constructed by taking the point of projection (pole) to be on the projection plane. A circular arc is swung from a point on the sphere to the projection plane with the pole serving as the center of the circle, and the new radial distance is found using \(2R\sin(\chi ÷ 2)\) from the sphere. Each type of projection has distinct advantages, depending on whether the goal is to preserve angle measurements or keep surface areas proportional when projecting from the hemisphere. While data can be displayed using either type of projection, the nature of the grid points may not be preserved. Displayed in stereographic projection, the hexagonal grid will not feature the same layout and equal spacing between data points. Similarly, the spiral grid would be distorted in an equal area projection since the spiral’s angular nature is no longer preserved.

Two alternative data collection schemes, the hexagonal grid [2–4] and spiral trace [5], have been demonstrated previously but only documented tersely. The purpose of this paper is to elaborate on the mathematics needed to implement these schemes so that they may be readily programmed.

**THE HEXAGONAL GRID**

The hexagonal grid data collection scheme removes the over and under sampling at low and high chi values, respectively, that occurs when using equal angular step increments for \(\chi\) and \(\phi\) [2,3]. As an overview, the first step of the hexagonal grid scheme is to select the number of desired data points. This process is initiated by selecting the maximum desired \(\chi_{\text{max}}\) value and the number of equal line segments, \(N\), along the central/east radius [i.e., if \(\chi_{\text{max}} = 90^\circ\), the radius connecting the points (0°, 0°) and (90°, 0°) in polar coordinates (\(\chi\), \(\phi\); see Figure 3). For \(N = 16\), the point spacing is approximately 5° (931 points), typical of the standard 5° × 5° grid [2] (1368 points), but with fewer data points and uniform coverage. For comparison, when \(N = 19\) or \(N = 20\), there are approximately the same number of points on the hexagonal grid as on the standard
Next a hexagonal grid in Cartesian \((x,y)\) coordinates can be created based on the properties of equilateral triangles (see Figure 4) and using the Eqs. (1)–(12). These calculations are split into two parts, with the second resulting from a reflection of Quadrants I and II (sectors of the coordinate system where \(y\) is positive; see Figure 3).

**Figure 3.** Significance of the constant \(N\) in the projected plane. \(D_{\text{max}}\) is represented by the bold arrow.

First and second quadrants encompass Eqs. (1)–(10); the third and fourth, Eqs. (6) and (7), and (11)–(13) (omit points where \(y = 0\)).

\[
\begin{align*}
|y| &\leq D_{\text{max}} = 2\sin(\chi_{\text{max}}/2) \quad (1) \\
|x| &\leq \sqrt{D_{\text{max}}^2 - (y)^2} \quad (3) \\
y_j &\leq \frac{\sqrt{3}D_{\text{max}}}{2N} \cdot j \quad (2) \\
x_{ij} &\leq \begin{cases} \\
\frac{D_{\text{max}} \cdot i}{N} & j \mod 2 = 0 \quad (4) \\
\frac{D_{\text{max}}}{2N} + \frac{D_{\text{max}} \cdot i}{N} & j \mod 2 = 1 \quad (5)
\end{cases} \\
j = 0,1,2,... \\
i = ...,-2,-1,0,1,2,... \\
D_{ij} &\leq \sqrt{(x_{ij})^2 + (y_{ij})^2} \quad (6) \\
\phi_{ij} &\begin{cases} \\
\arctan\left(\frac{y_{ij}}{x_{ij}}\right) & x_{ij} > 0 \quad (8) \\
90^\circ & x_{ij} = 0 \quad (9) \\
\arctan\left(\frac{y_{ij}}{x_{ij}}\right) + 180^\circ & x_{ij} < 0 \quad (10)
\end{cases}
\end{align*}
\]

\[
\chi_{ij} = 2\arcsin\left(\frac{D_{ij}}{2}\right) \quad (7)
\]
\[
\phi_j = \begin{cases} 
\arctan \left( \frac{y_j}{x_{ij}} \right) + 180^\circ & x_{ij} > 0 \\
270^\circ & x_{ij} = 0 \\
\arctan \left( \frac{y_j}{x_{ij}} \right) + 360^\circ & x_{ij} < 0 
\end{cases}
\]  

Equations (1)–(13) are applied as follows. The \(y_j\) values are generated by picking a value for the index \(j\) (\(j = 0\) determines \(y_0\), etc.) and continue until \(y\) is as close as possible to the maximum radial distance, \(D_{\text{max}}\), without exceeding it Eq. (1). The \(y\) values are determined by Eq. (2) based on the height of equilateral triangles with side length \(\frac{D_{\text{max}}}{N}\) (see Figure 4). All the corresponding \(x_{ij}\) values at each \(j\) are then calculated using Eqs. (3)–(5) for specific \(i\) values. In Quadrants I and II, the \(x\) values start at either \(x = 0\) [Eq. (4)] or \(x = \frac{D_{\text{max}}}{2N}\) [Eq. (5)], and the spacing between each value is a multiple of \(\frac{D_{\text{max}}}{N}\), which is calculated by using another index \(i\). The \(x_{ij}\) values alternate between two distinct patterns, depending on whether \(j\) is even or odd. The \(j \mod 2\) notation is used to denote dividing \(j\) by 2 and then reporting the remainder. Any even number, when divided by 2, will have remainder 0 \((j \mod 2 = 0)\); conversely, an odd value of \(j\) will have a remainder of 1 \((j \mod 2 = 1)\). For each fixed value of \(y_j\), the \(x_{ij}\) values can then be determined, up to the boundary of the projected circle with radius \(D_{\text{max}}\) [Eq. (3)]. The values of \(\chi\) and \(\phi\) are then found by transforming each point \((x, y)\) to polar coordinates. Each value of \(D_{ij}\) is equivalent to the length of the hypotenuse of the right triangle formed by \(x_{ij}\) and \(y_j\) [Eq. (6)]. Once \(D_{ij}\) is calculated, \(\chi_{ij}\) can be determined [Eq. (7)]. Each \(\phi_{ij}\) is the arctangent of the ratio \(\frac{y_j}{x_{ij}}\), and it may be necessary to transform from radians to degrees [Eqs. (8)–(10)]. Since the arctangent function is only defined from -90° to 90°, the new points may not lie in the correct quadrant or, in some cases, even be defined. Each point can be rotated to the correct position by adding 0° {when \(x_{ij} > 0\) [Eq. (8)]} or 180° {when \(x_{ij} < 0\) [Eq. (10)]}. When \(x_{ij} = 0\) and \(y_{ij} > 0\), phi must be defined as 90° [Eq. (9)] (to avoid divide by 0 errors). Because of the symmetry of the graph, the points in Quadrants III and IV are 180° rotations [Eqs. (11)–(13)] of all the points in Quadrants I and II (equivalent to a reflection), but points where \(y_j = 0\) must be omitted so they are not duplicated/doubled. The \(D_{ij}\) and \(\chi_{ij}\) values in Quadrants III and IV are the same because of the symmetry [Eqs. (6) and (7)]. Figure 5 shows an example hexagonal grid, and Table I shows some selected calculations.

The hexagonal grid generates points that lie in circles, though the number of points on each circle varies. Thus, similar to the data collection scheme employing the 5° × 5° grid, the hexagonal grid data may be collected by scanning phi at a fixed \(\Omega\) and \(\theta\) (2\(\theta\)) for each specific \(\chi\), beginning at 0 and increasing up to the maximum value.
Table I. Selected hexagonal grid calculations, when $N = 16$ and $\chi_{\text{max}} = 90^\circ$.

<table>
<thead>
<tr>
<th>Quad</th>
<th>$J$</th>
<th>$y_j$</th>
<th>$i$</th>
<th>$\chi_{ij}$</th>
<th>$D_{ij}$</th>
<th>$\chi_{ij}(^\circ)$</th>
<th>$\phi_{ij}(^\circ)$</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>0</td>
<td>0.0000</td>
<td>3</td>
<td>0.2652</td>
<td>0.2652</td>
<td>15.24</td>
<td>0.000</td>
<td>jmod2=0</td>
</tr>
<tr>
<td>I</td>
<td>1</td>
<td>0.0765</td>
<td>3</td>
<td>0.3094</td>
<td>0.3187</td>
<td>18.34</td>
<td>13.898</td>
<td>jmod2=1</td>
</tr>
<tr>
<td>I</td>
<td>3</td>
<td>0.2296</td>
<td>3</td>
<td>0.3094</td>
<td>0.3853</td>
<td>22.21</td>
<td>36.587</td>
<td>jmod2=1</td>
</tr>
<tr>
<td>II</td>
<td>1</td>
<td>0.0765</td>
<td>-3</td>
<td>-0.2210</td>
<td>0.2339</td>
<td>13.43</td>
<td>160.893</td>
<td>jmod2=1</td>
</tr>
<tr>
<td>II</td>
<td>2</td>
<td>0.1531</td>
<td>-3</td>
<td>-0.2652</td>
<td>0.3062</td>
<td>17.61</td>
<td>150.000</td>
<td>jmod2=0</td>
</tr>
</tbody>
</table>

THE SPIRAL TRACE

The spiral is a path of constant angular direction on the hemisphere (like a ship traveling from a pole to the equator with a constant compass direction). The spiral lends itself well to an alternative means of collecting pole figure data because its radius increases more quickly than the $5^\circ \times 5^\circ$ grid with fewer points overall. If equipment was available with such capabilities, then angles $\chi_n$ and $\phi_n$ could be continuously adjusted along the path of the spiral. Since this is not always possible, discrete points of the spiral can be generated using the following equations:

$$\phi_n = \phi_{n-1} + \frac{5\chi_{\text{max}}}{\chi_{n-1}}$$  \hspace{1cm} (14)

$$\chi_n = \begin{cases} 
5^\circ & 0^\circ \\
\phi_{\text{max}} & 0^\circ < \phi < \phi_{\text{max}} \text{ (omit if } \chi < 5^\circ) \\
\chi_{\text{max}} & \phi_{\text{max}} 
\end{cases}$$  \hspace{1cm} (15)

$$b = \frac{\ln(\chi_{\text{max}})}{\phi_{\text{max}}}$$  \hspace{1cm} (16)

Here, we decided to use a logarithmic spiral because when projecting from the reference sphere to the plane, the angles between all points are preserved. A logarithmic spiral always creates the
same angle measure between a radius and a tangent line at any point, which through stereographic projection translates to the same angles on the sphere.

The points of a spiral can be calculated with polar equations, making computation much less complicated. A spiral is an exponential curve in polar form, and most of the \( \chi_n \) values are directly calculated by evaluating \( e^{b\phi} \) [Eq. (16)], where \( n \) represents the term number of the recursively defined sequence [Eq. (14)] not exceeding \( \phi_{\text{max}} \). A spiral is infinite in nature. Since \( e^{b\phi} \) can never be 0, the point \((0^\circ,0^\circ)\) must be separately defined. In order to avoid over sampling at low \( \chi \) values, all points with \( \chi_n \) less than \( 5^\circ \) should be omitted [Eq. (16)]. The points \((5^\circ,0^\circ)\) and \((\chi_{\text{max}},\phi_{\text{max}})\) are added by Eqs. (15) and (17) for consistent starting and ending positions that correspond to the \( 5^\circ \times 5^\circ \) grid. Constant \( b \) is determined by Eq. (18) so that the maximum value of \( \phi_n \) allows the spiral to end very near \( \chi_{\text{max}} \). In order to maintain an approximately equal distance between points on the spiral, the increment by which \( \phi_n \) changes is a function of \( \chi_n \) [Eq. (14)]. At points with low \( \chi \) values, the phi spacing is about \( \chi_{\text{max}} \), and at points with high \( \chi \) values near \( \chi_{\text{max}} \), the phi spacing is only about \( 5^\circ \) [here, as determined empirically with Eq. (14) with the inclusion of 5 in the numerator]. Beginning at \( \chi = 0 \) and increasing \( \chi \) until the maximum is reached will allow for an efficient scan of the spiral grid (see Figure 6).

![Spiral grid](image)

**Figure 6.** Spiral trace with \( \chi \) of \( 0^\circ \) to \( 90^\circ \) and \( \phi \) of \( 0^\circ \) and \( 2520^\circ \) to \( 6480^\circ \) (stereographic projection, 277 points).

**CONVERTING BACK TO THE \( 5^\circ \times 5^\circ \) GRID**

In order to convert the collected data back to the \( 5^\circ \times 5^\circ \) grid (which is the default commonly used in analysis software), a planar interpolation scheme can be used. For every point of the \( 5^\circ \times 5^\circ \) grid, three adjacent points of the hexagonal or spiral grid are used in interpolation. These three points uniquely determine a plane of the form \( ax + by + cz = d \), where \( d \) can be selected to be any constant \((a, b,\) and \( c\) change accordingly). Using a matrix equation, the coefficients \( a, b,\) and \( c\) are determined. Next, the corresponding \( x \) and \( y \) values for the \( 5^\circ \times 5^\circ \) grid point can be substituted into the equation to solve for \( z \), representing the interpolated intensity. This process can be repeated for every point until the \( 5^\circ \times 5^\circ \) grid can be completely reconstructed.
EXPERIMENTAL COMPARISON

Table II lists the details of the experimental conditions for the X-ray measurements. Briefly, a four-axis ($\phi, \chi, \Omega, \theta$) goniometer [6] was employed for the pole figure measurements using Cr$K\alpha$ radiation. Specimen alignment was accomplished using a dial gauge probe that is accurate to ±5 $\mu$m. Here, the relative distance to the center of rotation is known, and the diffracting surface is positioned accordingly.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equipment</td>
<td>Scintag PTS goniometer</td>
</tr>
<tr>
<td></td>
<td>Spellman DF3 series 4.0 kW generator</td>
</tr>
<tr>
<td></td>
<td>Scintag liquid N$_2$-cooled Ge detector</td>
</tr>
<tr>
<td>Power</td>
<td>1.44 kW; 40 kV, 36 mA</td>
</tr>
<tr>
<td>Radiation</td>
<td>Cr, $\lambda K\alpha = 2.28970 \text{ Å}$</td>
</tr>
<tr>
<td>Incidence divergence</td>
<td>0.4°; 1.5 mm pinhole collimator</td>
</tr>
<tr>
<td>Receiving slit acceptance</td>
<td>0.25°; radial divergence limiting parallel plate collimator</td>
</tr>
<tr>
<td>Source to specimen distance</td>
<td>290 mm</td>
</tr>
<tr>
<td>Specimen to back slit distance</td>
<td>290 mm</td>
</tr>
<tr>
<td>Scans</td>
<td>200 to 300 °$\phi$/min</td>
</tr>
</tbody>
</table>

A sample of 13-\(\mu\)m-thick aluminum foil was mounted with rubber cement onto a zero background plate, and data were collected for pole figures using a $5^\circ \chi \times 5^\circ \phi$ grid, hexagonal grid, and spiral trace schemes as described above. Angular settings for the hexagonal grid and spiral trace schemes were programmed into the equipment. The data can be seen in Figure 7, represented graphically with Mathematica software (Wolfram Research, Inc., Champaign, Illinois). All three show the same features. To be clear, we are not suggesting that the spiral scan shown here is an adequate pole figure, just an alternative.

SUMMARY

The mathematics for constructing and implementing the hexagonal grid and spiral trace schemes for pole figure data collection have been elaborated. Experimental measurements of aluminum foil revealed typical rolling textures that compare favorably among the three methods. The hexagonal grid eliminates the over and under sampling of the $5^\circ \chi \times 5^\circ \phi$ grid and uses approximately 30% less points with $N = 16$ and $R = 90^\circ$. The spiral trace scheme has been shown to use over 75% less data points than the $5^\circ \chi \times 5^\circ \phi$ grid, but provides a less complete pole figure as it was not optimized. An option to collect pole figure data using hexagonal grid and spiral trace schemes will be implemented at Oak Ridge National Laboratory using LabVIEW-based data collection code (National Instruments Corporation, Austin, Texas) presently under development. The code will also convert this data back to the conventional $5^\circ \chi \times 5^\circ \phi$ grid.
Figure 7. (111) pole figures of aluminum foil: $5^\circ \chi \times 5^\circ \phi$ grid (top row), hexagonal grid (middle row), and spiral trace (bottom row) schemes displayed as polar plots (left column), equal area (middle row), and stereographic projections (right column).

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REFERENCES