CALCULATION OF MAJOR CRYSTALLOGRAPHIC POLES
ALONG ODF FIBERS PARALLEL TO THE GAMMA FIBER

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ABSTRACT

The mechanical properties of a polycrystalline metal are dependent on the distribution of
grain orientations. The term to describe a preferred distribution of grain orientations in a
metal is called texture. An understanding of a metal’s texture and how it changes as a
function of processing is needed to tailor the properties of the product. A method, based
on the inverse pole figure, was developed by Hosford, et al., in which fiber textures were
described in terms of the relative density of poles within a fixed angle of the <100>,
<110>, and <111> directions. This paper describes a computational tool that extends this
method considerably. This is accomplished by analyzing orientation distribution functions
(ODFs) generated by Los Alamos National Lab’s preferred orientation package (popLA).
This new computational tool calculates the strength of the textures, within a selected
angle, along fibers parallel to the gamma fiber. The program calculates the texture
strength for major crystallographic orientations in either fractional pole density or in units
of times random.

INTRODUCTION

The degree of preferred orientation a crystalline material exhibits, or texture, can have a
great influence on the performance properties of that material. Textures are typically
described as either sheet or wire or a combination of both. The state-of-the-art method
for quantifying textures is the orientation distribution function (ODF). The ODF allows
for the portrayal of grain orientations in polycrystalline materials by using Euler angles
either to characterize the crystallite orientation distributions (COD) or to characterize the
sample orientation distributions (SOD). The projection or average of the COD leads to a
pole figure plotted on the sample axial system, while the projection of the SOD leads to an
inverse pole figure plotted on the crystallographic axial system.

For the case of fiber textured cubic materials, the degree of texture can often be described
by the fraction of poles within a fixed angle of the three major crystallographic directions.
A method that accomplished this was developed by Hosford, et al., in which the fraction of
grains oriented within a specified angle of the <001>, <011>, and <111> crystallographic
directions were determined from the projection of the SOD or inverse pole figure. This
inverse pole figure method proved to be a very useful way to describe and visualize
changes in texture as a function of processing.
This document was presented at the Denver X-ray Conference (DXC) on Applications of X-ray Analysis.

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By applying the inverse pole figure method to discrete sections of the SOD, the strength of the texture in terms of these crystallographic directions can be determined for ODF fibers parallel to the gamma fiber. This provides not only the density of $<001>$, $<011>$, and $<111>$ poles for a given texture, but also describes the density of these along the ODF fiber axis. This allows for a more complete description of the fiber texture for a given processing step. In addition, by modifying the method slightly, the density of poles around a specific [hkl] orientation can be determined along the ODF fiber axis to provide information as to the rotational orientation of those poles about the fiber axis. A computational tool was developed that applied this enhanced inverse pole figure method to the entire SOD and is illustrated by examining the results it produced on some idealized textures and a highly cold worked copper.

**METHODOLOGY**

The computation tool was based on the inverse pole figure method. This method, which quantifies fiber textures in cubic materials, is a numerical procedure that integrates the pole densities existing in an angular range around an [hkl] orientation and gives the fraction of grains that are within that [hkl] orientation. If the SOD is sliced at $\Delta \phi_1$ of $5^\circ$ perpendicular to the $\phi_1$ axis, each of these sections can be thought of as partial inverse pole figures. The projection of all these sections would result in the inverse pole figure. If the inverse pole figure method is applied to these sections, quantitative information about the texture along the ODF fiber axis can be obtained. This concept is illustrated schematically in Figure 1 where the inverse pole figure contains the information from both the SOD sections corresponding to $\phi_1 = 0^\circ$ and $\phi_1 = 90^\circ$.

![Figure 1](image-url)  

**Figure 1** – Schematic illustration showing the relationship between ODF space and the inverse pole figure in Bunge notation.
The application of the inverse pole figure method to SOD sections along the $\varphi_1$ axis also says something about the orientation of the crystallites if one keeps track of the fraction of grains within a specific [hkl] orientation as opposed to the family of <hkl> orientations. Since each section of the SOD is a pole density plot in terms of the two Euler angles $\Phi$ and $\varphi_2$, knowing the corresponding $\varphi_1$ angle for the section, allows for a complete Eulerian description of a ($\Phi, \varphi_2$) pole. This concept is illustrated in Figure 2, which shows the ODF fibers that correspond to the major crystallographic directions for cubic materials (note: the (111) ODF fiber is the gamma fiber).

![Figure 2](image)

**Figure 2** – ODF fibers that correspond to the major crystallographic directions.$^{[2]}$

**PROGRAM SPECIFICS**

The program was written in Visual Basic and utilizes ODF data as determined by Los Alamos National Lab’s preferred orientation package (popLA)$^{[3]}$ for its input. PopLA provides sections of SOD data in 5° increments along the $\varphi_1$ axis in Bunge notation as well as the data for the inverse pole figure. The program allows the angle of encirclement to be specified for each analysis with the default set to 12°. Once initiated, the program calculates the fraction of grains within the <001>, <011>, and <111> directions for each 5° slice of the SOD by dividing the number of grains determined within each <hkl> orientation by the total number of grains determined for the SOD. Once determined, the program plots the <hkl> densities as a function of $\varphi_1$. The projection values are determined by summing the fraction of grains within each <hkl> for each slice of the SOD and displayed. The results from an analysis on a random SOD for an encirclement angle of 12.5° are shown in Table 1 along with the results from a paper by De Angelis, et al.$^{[4]}$ which also determined the fraction of grains within 12.5° of an <hkl> for an ideally random fiber texture.

The program also included a modification to quantify orientation information for the (001) ODF fiber. Examination of Figure 2 shows a unique ODF fiber for each of the specific major crystallographic poles, except the (001). For the (001) there are an infinite number of ODF fibers since $\Phi = 0$ for any $\varphi_2$. For this analysis, the ODF fibers chosen were those
that corresponded to Figure 2, namely at $\phi_2 = 0^\circ$, $45^\circ$, and $90^\circ$ and were identified as
(001c), (001b), and (001a) respectively. This required the need to determine the angle,
$\theta^N$, between these ODF fibers and an arbitrary $\phi_2$ position in addition to the angle between
the fibers and an arbitrary ($\Phi, \phi_2$) orientation. The additional angles were defined as
follows: for (001c), $\theta^N = \Phi$; for (001b), $\theta^N = \lfloor 45 - \Phi \rfloor$; for
(001a), $\theta^N = (90 - \Phi)$. Using these angles, the fraction of the spherical area represented
by an arbitrary ($\Phi, \phi_2$) orientation that lay within the encirclement angle was determined. The
only modification involved using an area ratio instead of a linear ratio for those
orientations that lay partially within the encirclement angle. The fraction of grains within
the encirclement angle of these 3 (001) directions can then be calculated.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
 & F<111> & F<011> & F<001> \\
\hline
De Angelis, et al. & 0.0965 & 0.1428 & 0.0715 \\
Program & 0.0962 & 0.1412 & 0.0701 \\
\hline
\end{tabular}
\caption{Comparison of results for the fraction of grains for the inverse pole figure (projection) for a random sample.}
\end{table}

The fractional value results are normalized by ideally random fractional values giving units
of times random. The ideally random values are obtained by performing the same
computational analysis on a random SOD (see Table 1). For this case the random SOD
was created using popLA from perfectly random theoretical pole figures. The random
SOD input file is independent of the program and can be replaced with any SOD file to
normalize the data.

**EXPERIMENTAL**

Pole figures for a BCC cube, Goss, and cold worked copper texture were analyzed using
popLA to produce SOD data sets. Both the BCC cube and Goss textures were generated
from fabricated pole figure data. The cold worked copper texture was produced by upset
forging a three inch diameter, three inch long cylinder to one inch thick. This was
followed by cold rolling with clockwise rotation of 135° between each pass to a final
thickness of 0.375 inch thick. The sample for analysis was taken about halfway out along
a radial line from the center of the pancaked slab. Each data set was analyzed using the
program as described above to determine the fraction of grains within a 12 degree angle of
the <111>, <011>, and <001> directions. Also the fractions of grains within the specific
crystallographic ODF fibers were also determined for a 12° encirclement angle.

**RESULTS**

The results for the fraction of grain within 12° of the <111>, <011>, and <001> for the
projection or inverse pole figure for the three textures analyzed are shown in Table 2. The
data in Table 2 indicates that all three textures are described basically by one component
or <hkl> orientation. The cube is all <001> and the Goss all <011>. The cold worked
copper also shows predominately a <011> texture component.
Table 2 – Comparison of results for the fraction of grains for the inverse pole figure (projection) for a BCC Cube, Goss, and highly cold worked copper textures.

<table>
<thead>
<tr>
<th>Textures</th>
<th>F&lt;111&gt;</th>
<th>F&lt;011&gt;</th>
<th>F&lt;001&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>BCC Cube</td>
<td>0</td>
<td>0</td>
<td>12.2946</td>
</tr>
<tr>
<td>Goss</td>
<td>0</td>
<td>4.957</td>
<td>0</td>
</tr>
<tr>
<td>Cold Worked Cu</td>
<td>0</td>
<td>4.6761</td>
<td>0.3433</td>
</tr>
</tbody>
</table>

Plots of the fraction of grains within 12° for the major <hkl> crystallographic directions for the textures analyzed are shown in Figure 3. Plots for the major crystallographic ODF fibers for the same textures are shown in Figures 4,5. As shown in Figure 3, the BCC cube has a high density of poles around the <001> at both $\varphi_1 = 0°$ and 90°. It also has a small but almost constant density for $5° < \varphi_1 < 85°$. This small but constant density is a result of the fact that at $\Phi = 0$ for every $\varphi_1$ angle there is a corresponding $\varphi_2$ angle equal to $90-\varphi_1$ that gives a cube orientation. Examination of the data in Figure 3 for the Goss texture show peaks at $\varphi_1 = 0°$ and 90° for the <011> orientation. Inspection of the [hkl] ODF fibers for the Goss texture in Figures 4,5 show zero texture except at $\varphi_1 = 90°$ for the [110] and at $\varphi_1 = 0°$ for the [011] and [101] which is exactly where the Goss texture components are located (see Figure 2). For the highly cold worked copper, it too has a predominately <011> texture component as shown in Figure 3. However, the fraction of grains within the <011> remains almost constant along $\varphi_1$. This is because it is almost a true fiber texture with respect to the <011>, whereas the Goss and Cube are sheet textures. The [hkl] ODF fibers for the copper shown in Figures 4,5 are basically zero except for the <011> type and they are all basically equivalent indicating no preference in one type of <011> orientation over another.

CONCLUSIONS

A computational tool has been created which applies the inverse pole figure method to discrete section of a SOD to determine the fraction of grains within the major <hkl> crystallographic directions as a function of $\varphi_1$. A summation of the values for these slices gives the same information for the inverse pole figure. A modification to the method allows for the quantitative description of individual crystallographic ODF fibers. This allows for the determination of the volume fraction of grains in a specific orientation.

REFERENCES


Figure 3 – Plots of the fraction of grains within 12° of an $\langle hkl \rangle$ orientation for BCC Cube, Goss, and copper cold rolled 90% textures.
Figure 4 – Plots of the fraction of grains within 12° for the crystallographic ODF fibers for BCC Cube, Goss, and 90% cold rolled copper.
**Figure 5** – Plots of the fraction of grains within 12° for the crystallographic ODF fibers for BCC Cube, Goss, and 90% cold rolled copper.