CRYSTALLITE ORIENTATION ANALYSIS FOR ZIRCALOY
APPLICATION OF THREE DIMENSIONAL REPRESENTATION OF TEXTURES

by

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D.E.S., University of Algiers (1977)

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El-khider Si ahmed 1981
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Submitted to the Department of Nuclear Engineering
on January 23, 1981 in partial fulfillment
of the requirements for the degrees of
Master of Science and Nuclear Engineer

ABSTRACT

The procedures for the quantitative characterization of crystallographic textures of Zircaloy have been reviewed. A crystallite orientation distribution function (CODF) has been used to quantify the texture of Zircaloy. The CODF is expanded in series of generalized spherical harmonics and its coefficients are related to the experimental pole figures measurements.

A computer program was written in Fortran IV to compute the CODF from pole figure measurements of any plane. The Fourier coefficients of the associated Legendre functions and the generalized associated Legendre functions have been tabulated to the order of 16 in the case of hcp symmetry. Experimental proof of such theory is given.

The method was applied to generate complete pole figures as well as inverse complete pole figures from CODF. The method of obtaining a CODF from incomplete pole figures was also examined.

Thesis Supervisor: Regis M.N. Pelloux
Title: Professor of Materials Engineering

Thesis Reader: John E. Meyer
Title: Professor of Nuclear Engineering
TO my wonderful parents and family.

The words will never be strong enough to express how grateful I am to you.
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1. INTRODUCTION

In order to characterize an anisotropic polycrystalline material, knowledge of the distribution of crystallite orientation is required.

Zirconium alloys have gained practically universal acceptance as fuel cladding and structural materials in water cooled nuclear reactors. A better understanding of the effects of texture on mechanical properties will aid in the prediction of the in-service behavior of zirconium alloys.

X-ray diffraction measurements afford the best means of studying texture or crystallite orientation. Several methods are currently in use for the quantitative interpretation of diffraction data. The most widely experimental technique used for studying orientation in polycrystals, leads directly to the pole figure representation. The variation of diffracted x-ray intensities is measured as a function of the relative orientation. The examination of pole figures or inverse pole figures will enable us to have a qualitative idea about the preferred orientation.

Since the pole figure gives information about the distribution of plane normals, it does not contain any information about the rotation of the crystallite about these normals. Only two angles are specified rather than three which are required for the full description of preferred orientation.

The angles among the different plane-normals belonging to one crystallite are fixed by the lattice structure of the crystal, and therefore the distribution curves for the plane-normals cannot be completely independent of one another.
The distribution of the crystallographic axes of separate grains of material relative to one another defines the texture of the material. Textures are not always simple and more precise evaluation is needed to better follow the texture during plastic deformation, as well as to predict the mechanical behavior. Viglin [47] suggested that the texture could be described by means of a function describing the distribution of the direction of the crystallographic axis of separate grains.

In recent years methods have been developed which enables determination of the (three-angle) crystallite orientation distribution from several (two-angle) pole figure distributions [43-44].

Detailed work of this research program include:


2. A theory of crystallite orientation distribution function (CODF) for zircaloy.

3. A method of getting CODF for the case of incomplete pole figures.

4. A method of generating pole figures as well as inverse pole figures from CODF.

5. X-ray diffraction measurements.

6. Methods of calculations, including computer programs, leading to the CODF.
2. Background and Literature Survey

2.1 Introduction

The most important applications of zirconium alloys is for fuel cladding in nuclear reactors. The prominent problems arising during normal operation of nuclear reactors include:

- creep;
- irradiation growth;
- hydrogen pick-up; and
- localized failure (possibly stress corrosion cracking).

Both the elastic properties and the plastic deformation behaviour of hexagonal polycrystals are strongly influenced by crystallographic texture. This includes the intrinsic anisotropic nature of individual grains as well as the distribution of grain orientations within a polycrystalline metal. The utilization of zirconium alloys as pressure tubes or as fuel cladding necessitates a degree of creep strength. Irradiation growth and creep depend both on crystallographic orientation. Zirconium is also a strong hydride former. This causes a deteriorating effect on the mechanical behavior. The hydrides are strongly influenced by the crystallographic orientation.

The procedures for fabrication of Zircaloy tubes used as fuel cladding introduce a marked preferred orientation leading to strong anisotropic properties. The non-random distribution of the crystallite orientations over a whole polycrystal is called crystallographic texture, or texture. A better understanding of the texture produced by fabrication requires some knowledge of deformation systems of zirconium alloys. The quantitative texture characterization is done by x-ray diffraction.
The remainder of this chapter contains a discussion on deformation systems of zirconium alloys, texture produced by fabrication and texture measurements by x-ray diffraction.

2.2 Fuel Clad Material in Water Cooled Nuclear Reactors

Zirconium has a low thermal neutron absorption cross section, an advantage for the fuel cladding material in a water nuclear reactor. Moreover, it combines an appropriate water corrosion resistance with adequate mechanical strength at light water reactor operating temperature (280°C to 350°C). In order to improve certain properties, such as general corrosion resistance, reduction of hydrogen pick-up, and strength, small quantities of alloying elements are added to pure zirconium. These are either α-stabilizers, such as tin and oxygen, or β-stabilizers such as niobium. Zircaloy-2 finds its application as fuel cladding for boiling water reactors, because of its corrosion resistance in steam. On the other hand, Zircaloy-4 is used as fuel cladding in pressurized water reactors, because the hydrogen pick-up is less in this alloy. Zirconium-2.5 w/o niobium is used for pressure tubes in CANDU reactors. This alloy has outstanding mechanical properties. The compositions of Zircaloy-2, Zircaloy-4 and Zr-2.5 w/o niobium are presented in Table 1.

2.3 Features of Zircaloy

2.3.1 Crystallography

Pure zirconium exhibits an hexagonal close packed crystal structure (α-phase) up to 862°C. Important planes and directions for hcp crystal structure are presented in Fig. 1. At room temperature the following lattice parameters \((a_0, c_0)\) are reported [1]
<table>
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<tr>
<th>Alloy Element</th>
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<th>Zircaloy-4 wt.%</th>
<th>Zr-2.5 Nb wt.%</th>
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<tr>
<td>Tin</td>
<td>1.20 - 1.70</td>
<td>1.20 - 1.70</td>
<td>-</td>
</tr>
<tr>
<td>Iron</td>
<td>0.07 - 0.20</td>
<td>0.18 - 0.24</td>
<td>0.150</td>
</tr>
<tr>
<td>Chromium</td>
<td>0.05 - 0.15</td>
<td>0.07 - 0.13</td>
<td>0.020</td>
</tr>
<tr>
<td>Nickel</td>
<td>0.03 - 0.08</td>
<td>0.0070</td>
<td>0.0070</td>
</tr>
<tr>
<td>Fe + Cr + Ni</td>
<td>0.18 - 0.38</td>
<td>0.28 - 0.37</td>
<td>-</td>
</tr>
<tr>
<td>Niobium</td>
<td>-</td>
<td>-</td>
<td>2.40 - 2.80</td>
</tr>
<tr>
<td>Oxygen</td>
<td>(a)</td>
<td>(a)</td>
<td>0.09 - 0.13</td>
</tr>
</tbody>
</table>

**TABLE 1**

ZIRCONIUM BASED ALLOYS CHEMICAL COMPOSITIONS


(a) oxygen has a strengthening effect on Zircaloys;
its concentration may be specified
FIGURE 1.
IMPORTANT PLANES AND DIRECTIONS FOR HCP CRYSTAL STRUCTURE
\[ a_0 = 3.23118 \, \text{Å} \text{ and } c_0 = 5.14634 \, \text{Å} \]

The ratio \( \frac{c_0}{a_0} \) resulting is less than the ideal ratio 1.6325 for close packed hard spheres.

\[ \frac{c_0}{a_0} = 1.59271 \quad (2.1) \]

Since Zircaloy contains less than 2 wt % alloying elements the same ratio \( \frac{c_0}{a_0} \) (Eq. 2.1) is assumed.

In Zircaloy, the \( \alpha \)-phase is stable up to 790° C [2]. The small amount of chromium, iron and nickel added to zirconium, to form Zircaloy, form an intermetallic \( \chi \)-phase [3]. The \( \chi \)-phase coexists with the \( \alpha \)-phase from 25° C to 790° C and with \( \alpha \) and \( \beta \) phases from 790° C to 820° C; (\( \beta \) is B.C.C.). In the temperature range 820° C - 950° C the structure consists of \( \alpha \) and \( \beta \) phases [2].

### 2.3.2 Single Crystal Deformation System

The hcp crystal structure has a limited number of easy slip systems. The primary slip system is observed in \( \alpha \)-zirconium [4,5], over the entire temperature range of stability of hcp structure, is \( \{10\overline{1}0\} \langle 2\overline{1}0\rangle \) (Fig. 2a). At elevated temperature basal slip \( \langle 0001 \rangle \) along the \( \hat{a} \) direction \( \langle 2\overline{1}0\rangle \) (Fig. 2b), has been detected [6,7,8], but this slip system is of secondary importance. Other less important, slip systems (Figs. 2b and 2c), have been detected [4]. These are \( \{0\overline{1}1\} \langle 21\overline{0}\rangle \) and \( \{11\overline{2}1\} \langle 2\overline{1}13\rangle \) which require, respectively, complex stressing, elevated temperature, and constraint to occur.

It follows that slip essentially prismatic along the \( \hat{a} \) direction. In order to deform along the \( \hat{c} \) axis without fracturing
FIGURE 2
SLIP SYSTEMS IN ZIRCONIUM

-a

-b

-c
twinning is required. The elements involved in twinning operation are shown in (Fig. 3). Rapperpot [9,10] identified active twin planes in zirconium single crystal as being \{10\bar{1}2\}, \{11\bar{2}1\}, \{11\bar{2}2\} and \{11\bar{2}3\}. In temperature range -195°C to 800°C the predominant twinning systems observed [11], in decreasing order of importance, are respectively \{11\bar{2}1\} with \{10\bar{1}2\}, \{11\bar{2}2\} and \{11\bar{2}3\}. The overall fraction of twinning decreases as the temperature increases. At 800°C the only twins observed are of the type \{11\bar{2}1\}. The mechanism detected which would alloy length reduction along c-axis, below 527°C, is \{11\bar{2}2\} twinning [12]. At temperature above 527°C deformation takes place by combination of \{10\bar{1}1\} twinning and \{10\bar{1}1\} \langle11\bar{2}3\rangle slip system. The observation that the slip plane is \{10\bar{1}1\} agrees with Tenckhoff's data [13]. A list of twins observed in zirconium and zirconium alloys is presented in Table 2 [14].

2.3.3 Polycrystalline Deformation Systems

The deformation mechanisms in polycrystal are not easily predictable as they are in single crystal. This arises from the constraints imposed by grain boundaries and the distribution of the grains with respect to the applied stress. These can have a significant effect on the operating mechanism. Furthermore alloying elements may have a strong effect on the deformation mechanisms.

Reed-Hill [6] reported that for zirconium polycrystalline \{10\bar{1}2\} and \{11\bar{2}1\} twins are formed during tensile deformation along the C-axis, and the twin systems \{11\bar{2}2\} are activated during compression along the C-axis. Figure 4 shows the orientation of the twinning elements. On the other hand, Jensen and Backofen [15]
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<th>$K_1$</th>
<th>$n_1$</th>
<th>$K_2$</th>
<th>$n_2$</th>
<th>S</th>
<th>Stress State Normal to ${0002}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>${10\bar{1}2}$</td>
<td>$&lt;10\bar{1}1&gt;$</td>
<td>${1012}$</td>
<td>$&lt;10\bar{1}1&gt;$</td>
<td>0.167</td>
<td>Tensile</td>
</tr>
<tr>
<td>${1\bar{1}21}$</td>
<td>$&lt;1\bar{1}26&gt;$</td>
<td>${0002}$</td>
<td>$&lt;1\bar{1}20&gt;$</td>
<td>0.630</td>
<td>Tensile</td>
</tr>
<tr>
<td>${1\bar{1}22}$</td>
<td>$&lt;1\bar{1}23&gt;$</td>
<td>${1124}$</td>
<td>$&lt;22\bar{4}3&gt;$</td>
<td>0.225</td>
<td>Compressive</td>
</tr>
<tr>
<td>${10\bar{1}1}$</td>
<td>$&lt;\bar{1}012&gt;$</td>
<td>${1013}$</td>
<td>$&lt;30\bar{3}2&gt;$</td>
<td>0.104</td>
<td>Compressive</td>
</tr>
</tbody>
</table>

**TABLE 2**

TWINNING ELEMENTS IN ZIRCONIUM AND ZIRCONIUM ALLOYS
FIGURE 3
SPATIAL RELATIONSHIPS BETWEEN PLANES
AND DIRECTIONS IN TWINNING
FIGURE 4

COMMONLY OBSERVED TWINNING SYSTEMS IN ZIRCONIUM

\{10\bar{1}2\} TWINNING

TENSILE

K2 AFTER SHEAR

\{10\bar{1}2\}

K1

94.2°

42.9°

42.9°

BASAL PLANE (0002)

TENSILE

\{1\bar{1}21\} TWINNING

TENSILE

K2 AFTER SHEAR

\{1\bar{1}21\}

K1

72.4°

35.2°

BASAL PLANE (0002)

\{11\bar{2}2\} TWINNING

COMPRESSIVE

K2 BEFORE SHEAR

\{11\bar{2}2\}

K1

83.7°

57.8°

BASAL PLANE COMPRESSIVE (0002)
showed that Zircaloy-4, at temperature less than 300°C, does not exhibit any twinning. But, it is found to deform by \(<\vec{c} + \vec{a}\) slip with dislocations confined to thin bands oriented close to \(\{1\overline{2}4\}\). At temperature greater than 300°C deformation occurs by \((10\overline{1}1)\) twinning and \(<\vec{c} + \vec{a}\) slip. In all cases the predominant deformation mechanism is \(<\vec{c} + \vec{a}\) slip. At temperature greater than 525°C, \((0002) <1\overline{1}20>\) is an active slip system [8]. As a summary Table 3 shows the deformation mechanisms, for zirconium and Zircaloy, and the regime at which they have been observed to operate [16].

However, the deformation mechanisms for zirconium and zirconium alloys are function of texture, stress state, composition, temperature and strain rate. This complex dependence yields a highly anisotropic mechanical behaviour.

2.3.4 Overview of Texture Produced by Fabrication

The investigation of the texture of Zircaloy tubing [17-20] showed that no basal poles have been detected in the axial direction of the tube. The basal poles have a strong tendency to be located in the plane perpendicular to the forming, or axial direction. The different directions in tube and plate are shown in Fig. 5. Hobson [21] pointed out that grains with basal poles oriented in the axial direction, will undergo \((10\overline{1}2)\) twinning to end up with an orientation perpendicular to the forming direction.

The method of fabrication Zircaloy tubing consists mainly on three stages, Table 4 [2]. These are: melting stage to assure uniform distribution of alloying elements in the ingot, hot working stage to obtain fine secondary \(\chi\) phase particles and cold working-annealing stage. The cold work contributes to the mechanical
<table>
<thead>
<tr>
<th>TYPE</th>
<th>PLANE</th>
<th>DIRECTION</th>
<th>CRYSTALLOGRAPHIC DESCRIPTION</th>
<th>TEMPERATURE AND STRESS RANGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slip</td>
<td>Prism</td>
<td>a</td>
<td>{10\overline{1}0}&lt;\overline{1}2\overline{1}0&gt;</td>
<td>All Temperatures Lowest Stress System</td>
</tr>
<tr>
<td>Slip</td>
<td>Basal</td>
<td>a</td>
<td>{0001}&lt;\overline{1}2\overline{1}0&gt;</td>
<td>High Temperature</td>
</tr>
<tr>
<td>Slip</td>
<td>Pyramidal</td>
<td>c+a</td>
<td>{10\overline{1}1}&lt;\overline{1}1\overline{2}3&gt;</td>
<td>Intermediate Temperature, High Stress</td>
</tr>
<tr>
<td>Slip</td>
<td>Pyramidal</td>
<td>c+a</td>
<td>{11\overline{2}1}&lt;\overline{1}1\overline{2}3&gt;</td>
<td>High Temperature High Stress</td>
</tr>
<tr>
<td>Twin</td>
<td>Pyramidal</td>
<td>c+a</td>
<td>{10\overline{1}2}&lt;\overline{1}0\overline{1}1&gt;</td>
<td>Intermediate Temperature, c-axis Tension</td>
</tr>
<tr>
<td>Twin</td>
<td>Pyramidal</td>
<td>c+a</td>
<td>{11\overline{2}1}&lt;\overline{1}1\overline{2}6&gt;</td>
<td>Low Temperature c-axis Tension</td>
</tr>
<tr>
<td>Twin</td>
<td>Pyramidal</td>
<td>c+a</td>
<td>{11\overline{2}2}&lt;\overline{1}1\overline{2}3&gt;</td>
<td>Low-Intermediate Temperature, c-axis Compression</td>
</tr>
<tr>
<td>Twin</td>
<td>Pyramidal</td>
<td>c+a</td>
<td>{10\overline{1}1}&lt;\overline{1}0\overline{1}2&gt;</td>
<td>Intermediate-High Temperature, c-axis Compression</td>
</tr>
</tbody>
</table>

**TABLE 3**

DEFORMATION SYSTEMS IN \(\alpha\)-ZIRCONIUM AND ZIRCALOYS
FIGURE 5
DIRECTIONS IN TUBE AND PLATE
<table>
<thead>
<tr>
<th>Stage</th>
<th>Operations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting</td>
<td>Pressing of Zr sponge and alloy additions into briquettes</td>
</tr>
<tr>
<td></td>
<td>Welding of briquettes into electrodes</td>
</tr>
<tr>
<td></td>
<td>Melting High vacuum electric arc</td>
</tr>
<tr>
<td></td>
<td>Remelting Consumable electrode</td>
</tr>
<tr>
<td>Hot Working</td>
<td>Hot forging in upper $\alpha$-range</td>
</tr>
<tr>
<td></td>
<td>Heating to $\beta$-range and quenching</td>
</tr>
<tr>
<td></td>
<td>Extrusion in upper $\alpha$-range</td>
</tr>
<tr>
<td>Cold Working and</td>
<td>Cold rolling</td>
</tr>
<tr>
<td>Annealing</td>
<td>Annealing in upper $\alpha$-range</td>
</tr>
<tr>
<td></td>
<td>Cold rolling</td>
</tr>
<tr>
<td></td>
<td>Annealing</td>
</tr>
<tr>
<td></td>
<td>Final cold rolling 50 - 80%</td>
</tr>
<tr>
<td></td>
<td>Final annealing 475 - 575°C</td>
</tr>
<tr>
<td></td>
<td>Strengthening</td>
</tr>
</tbody>
</table>

**TABLE 4**

PROCESS FLOW SHEET FOR PRODUCTION OF ZIRCALOY TUBING
properties. The cold working steps reduce the tube to the desired dimensions. Picklesimer [22] performed an analysis of the evolution of the texture in various tubing forming operations; this is shown in Fig. 6. Cheadle et al. [23] performed an analysis on how the texture is related to preceding deformation and heat treatment. He concluded that basal poles have a tendency to align themselves parallel to the direction of maximum compressive strain.

The tube reduction is usually specified by the ratio between the wall and diameter reduction, which is called the Q value. The development of the texture is primarily determined by this Q value [24,25]. In zirconium alloy tubing, a texture with basal poles parallel to the radial direction is obtained if the reduction of the wall thickness prevails, which means high wall strain and high Q value. On the other hand, if reduction in the diameter preponderates, which means high circumferential strain and low Q value, a preferred tangential alignment of the basal poles will result.

It should be noted that a texture gradient exists through the wall thickness of the tubes [26,27]. In the usual case of tube reducing processes a compression is applied from the outer surface. Consequently the compressive stress is highest at the outer surface and decreases toward the inner surface. The plastic strain in the radial direction is highest at the outside diameter, thus a strain gradient in the radial direction will result. If the outer diameter is reduced more than the inner diameter, the compressive strain in the tangential direction will be higher at the outer surface than the inner surface of the tube wall. Consequently a strain gradient
FIGURE 6
ANALYSIS OF THE EVOLUTION OF THE TEXTURE IN VARIOUS TUBING FORMING OPERATIONS
in the tangential direction will occur. In both cases a texture variation through thickness will exist.

The anisotropic mechanical properties of Zircaloy tubes are a consequence of their texture. Therefore, the service loads of the tubing will determine which texture is most desirable and can be used to the appropriate application.

2.4 Methods of Texture Measurements

Several methods have been used to obtain the texture on a given sample [28,29,30], but they only give an approximate evaluation of the texture. Measurements of x-ray diffraction afford the best means of studying the crystallite orientation.

Among the methods used in the quantitative interpretation of the x-ray diffraction data, the method which leads to the construction of direct and inverse pole figures will be stressed. In the remaining text the term direct will be omitted.

A pole figure is a map of the statistical distribution of the normals to given \( \{hki\} \) plane of a polycrystalline sample. It depicts the direction of the preferred orientation and the extent of angular deviation from the ideal in a form easily comprehended.

The inverse pole figure is obtained by mathematically "inverting" the x-ray data for a normal pole figure. It will then give a density distribution of the axial direction in a polycrystalline sample on a stereographic projection of the crystal lattice in some chosen orientation.
In order to collect the data which leads to the construction of the inverse pole figure one should perform the following:

- specimen preparation
- measurements of x-ray intensities diffracted by all crystallographic planes parallel to the specimen surface
- data reduction and use of data obtained from random sample to describe the deviation from randomness of the specimen considered.

The construction of the pole figure is obtained after performing the operations described precedently and by

- measuring the variation of the diffracted x-rays intensities, for a chosen crystallographic plane, as function of the relative orientation of the sample with respect to the diffractometer geometry
- reduction of the data by using correction factors and random sample data obtained in the same operating conditions.

2.4.1 Specimen Geometry Considerations

Depending on the type of specimen considered a complete pole figure may be obtained by one or two methods. The procedure for determining the preferred orientation is described in the ASTM Standard E81. This method consists of using a reflection [31] and transmission [32] techniques, which are complementary. The use of these two techniques will lead to the construction of the pole figure. However, the transmission technique is very tedious and time consuming and may lead sometimes to more qualitative data than quantitative [26]. Nevertheless, some methods which do not require transmission methods exist and are related to the specimen geometry. Briefly, these are
- composite specimens from transverse and axial directions will replace the transmission part [33], (Fig. 7)

- a composite specimen cut obliquely at an angle of 54°44' will give a complete pole figure from one quadrant [34], (Fig. 8)

- a cylindrical sample cut from the wall of a tube [35], (Fig. 9), will give nearly a complete pole figure.

However, only reflection methods will be used in the present study to obtain pole figures. In case of tubing a thin sample is cut from the wall of the tube, and then thinned, and unrolled elastically for analysis [26]. The same specimen is used to generate the inverse pole figure.

2.4.2 Inverse Pole Figure Determination

The integrated intensities diffracted by all crystallographic planes parallel to the surface of the specimen are recorded using a diffractometer.

Haris [36] defines a texture coefficient $T_{C_j}$ as being the relative intensity diffracted by the $j^{th}$ crystallographic plane, and it is given by

$$T_{C_j} = \frac{I_j/I_j^0}{\frac{1}{N} \sum_{j=1}^{N} (I_j/I_j^0)} \quad (2-2)$$

where $N$ is the number of reflections considered, $I_j$ is the measured intensity of the $j^{th}$ crystallographic plane and $I_j^0$ is the calculated intensity of the $j^{th}$ crystallographic plane for a random sample. The values of $I_j^0$ have been tabulated for zirconium by Sturken and Duke [37], Table 4.
FIGURE 7
COMPOSITE SPECIMENS FROM TRANSVERSE AND AXIAL DIRECTIONS
FIGURE 8

POSITION OF OBLIQUE PLANE AND STEREGRAPHIC NET FOR DETERMINING ONE QUADRANT OF POLE FIGURE BY REFLECTION

\[ \alpha = \beta = \gamma = 54^\circ 44' \]
FIGURE 9
ROTTING CYLINDER SPECIMEN GEOMETRY
AND STEREORAPHIC NET

(A)

(B)
Note that the intensities $I_j$ and $I_j^0$ are in different arbitrary units but, as it will be shown, it does not affect the relation \((2.2)\).

If instead of calculated intensities $I_j^0$, measured intensities $I_j^{0'}$, in the same operating conditions of $I_j$, are used. The ratio $I_j/I_j^{0'}$ will give the density of the $j^{th}$ pole oriented normally to the surface of the specimen. A texture coefficient is then defined as

$$T_{cj}' = \frac{I_j/I_j^{0'}}{\frac{1}{N} \sum_{j=1}^{N} I_j/I_j^{0'}} \quad (2-3)$$

Theoretically the factor $\frac{1}{N} \sum_{j=1}^{N} I_j/I_j^{0'}$ should be equal to one, but in practice it is slightly greater than unity; this is due to the error introduced in the measurements. Therefore $T_{cj}'$ takes the same significance of the ratio $I_j/I_j^{0'}$ defined earlier. In fact $I_j/I_j^{0'}$ is related to the ratio $I_j/I_j^0$ by a constant $c$ which is affected by the measurements conditions, the units used, etc. This is expressed by

$$\frac{I_j}{I_j^{0'}} = c \frac{I_j}{I_j^0} \quad (2-4)$$

Substitute Eq. (2.4) into Eq. (2.3) to get $T_{cj} = T_{cj}'$. Following the above discussion, it appears that $T_{cj}$ is the density of the $j^{th}$ pole oriented normally to the surface of the specimen.

The inverse pole figure, associated with the normal to the specimen, is plotted on a standard projection of the hcp crystal.
This is done by drawing lines of constant texture coefficients values, $T_{c_j}$. The entire projection is represented by section of $30^\circ$ for symmetry reason, (Fig. 10).

As it will be shown in the next section, the $T_{c_j}$ coefficients are also used to express the variations of the intensities of the pole figure into variation of pole densities in times random units for all orientations.

2.4.3 Pole Figure Determination

The variation of intensities of the $j^{th}$ crystallographic plane as function of the relative orientation of the sample with respect to the diffractometer geometry, is recorded. The collection of the data is done by rotation of the specimen through an angle $\phi$ and tilting along an angle $\alpha$, (Fig.11). These two motions will give a spiral with decreasing pitch, (Fig.12). Only the reflection method developed by Schultz [31] for a flat specimen is used. From this technique data is obtained for $\phi$ as far as $80^\circ$, where $\phi = \frac{\pi}{2} - \alpha$.

X-rays are scattered by the atomic electrons, and the part of scattering which occurs without change in wavelength is of interest. However, the scattering which is due to compton effects results in change in wavelength between incident and scattered waves; this gives rise to an incoherent background. This background should be measured from both sides of the Bragg peak of interest, and subtracted from the measured intensities. Then by using a random sample one can express the variation of the intensities for the textured sample as multiples of random intensities. This is done by the evaluation of the one time random intensity in the units
DEFINITION OF IDEALIZED ORIENTATIONS ON INVERSE POLE FIGURES
FIGURE 12
SPIRAL FOR POLE FIGURE MEASUREMENTS
WITH 5° DECREASING PITCH
(cps) used in the diffraction experiment [38]. It is expressed by

\[(cps)_{\phi=0}^{\text{random}} = \frac{(cps)_{\phi=0} - \text{background (cps)}}{Tc_j}\]  

(2-5)

where \(\phi = \frac{T}{2} - \alpha\)

As \(\phi\) varies a correction factor, due to geometric defocussing, is used. If \(\frac{I\phi}{\phi=0}\) is the latter factor, then the one time random intensity in the units (cps) varies as \(\phi\) varies by the relation

\[(cps)_{\phi}^{\text{random}} = (cps)_{\phi=0}^{\text{random}} \frac{I\phi}{\phi=0}\]  

(2-6)

Equation (2.6) represents a line of iso-intensity. Then, the intensities are expressed as multiples of random intensity; and plotted on polar projection, such as in (Fig.12). Lines of iso-intensity are drawn on the polar projection and converted to an equal area projection, (Fig.13). The factors relating a polar projection to an equal area projection are given in Table 5 [39]. It should be noted that \((cps)_{\phi}^{\text{rand}}\) represent a density of poles, at the values of \(\phi\). Generally, the variation of the pole density, for the \(j^{th}\) crystallographic plane, will be written as

\[q_j(\phi, \delta) = C(\phi, \delta) (cps)_{\phi}^{\text{rand}}\]  

(2-7)
FIGURE 13
EQUALL AREA POLAR PROJECTIONS
<table>
<thead>
<tr>
<th>Tilt Angle, (deg.)</th>
<th>Radii of Latitude Circles on Projection</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Equal-Area</td>
<td>Stereographic</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.125 R</td>
<td>0.085 R</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>0.25 R</td>
<td>0.175 R</td>
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<td>30</td>
<td>0.37 R</td>
<td>0.265 R</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>0.49 R</td>
<td>0.36 R</td>
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</tr>
<tr>
<td>50</td>
<td>0.595 R</td>
<td>0.465 R</td>
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<td>70</td>
<td>0.81 R</td>
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</tr>
<tr>
<td>80</td>
<td>0.905 R</td>
<td>0.84 R</td>
<td></td>
</tr>
<tr>
<td>90</td>
<td>R</td>
<td>R</td>
<td></td>
</tr>
</tbody>
</table>

**TABLE 5**

COMPARISON OF STEREOGRAFIC AND EQUAL-AREA POLAR PROJECTIONS
where \( C(\phi, \delta) \) is the factor multiplicative which depends on \( \phi \) and \( \delta \).

A method of evaluation of the geometric defocussing, 
\[
\frac{I_{\phi}}{I_{\phi=0}},
\]
factor, based on the work of Feng [40], will be outlined in the next section.

2.4.4 Geometric Defocussing Factor

The geometric defocussing is the decrease of the diffracted intensity associated with the increase of the tilt angle \( \phi \). These effects may be minimized by the following factors [41]:

- correct specimen alignment
- decrease the width of the main beam slit
- increase the width of the receiving slit.

Furthermore, the absorption and the effective scattering volume remain constant in the reflection method [31]. For a sample of sufficient thickness, no correction factors are needed [42]; this is because a complete extinction of the x-ray beam by absorption and diffraction will occur.

Feng [40] represents the variation of the geometric defocussing by the relations

\[
\frac{I_{\phi}}{I_{\phi=0}} = 1 - \left[ W \cos \Theta \tan \phi / \Delta (2\Theta) \right] \text{ for } \frac{I_{\phi}}{I_{\phi=0}} \geq \frac{1}{2} \tag{2-8}
\]

and

\[
\frac{I_{\phi}}{I_{\phi=0}} = \Delta (2\Theta) / 4 W \tan \phi \cos \Theta \text{ for } \frac{I_{\phi}}{I_{\phi=0}} \leq \frac{1}{2} \tag{2-9}
\]
where

\[ L \]

is the focal distance of the x-ray unit

\[ \Delta(\theta) \]

is the diffraction line breadth of the reflection considered

\[ W \]

is the width of specimen irradiated by the main beam

\[ \phi \]

is the tilt angle

\[ \theta \]

is the Bragg diffraction angle

\[ \frac{I_{\phi}}{I_{\phi=0}} \]

is the fraction of the \( \phi = 0 \) intensity.

In this study, the curve \( \frac{I_{\phi}}{I_{\phi=0}} \) will be generated experimentally and theoretically by the use of Eqs. (2.8) and (2.9) for the planes (10\( \overline{1} \)0) and (11\( \overline{2} \)0). In the case of plane (0002) this has been done by Knorr [38], (Fig. 14).

2.5 Summary

The most widely used experimental techniques for studying orientation, in polycrystals, lead directly to the pole figure representation. The only examination of pole figure or inverse pole figure will enable us to have only a qualitative idea about the preferred orientation repartition. The pole figure gives information about the distribution of basal plane normals; it does not contain any information about the rotation of the crystallite about these normals. Only two angles are specified rather than three which are required for the full description of preferred orientation. Furthermore, the inverse pole figure is evaluated in approximate manners. However, the angles between the different plane normals belonging to one crystallite are fixed by the lattice structure of the crystal, and therefore the distribution curves for the plane normals cannot be completely independent of one another.
THEORETICAL AND EXPERIMENTAL CURVES FOR
GEOMETRICAL DEFOCUSING OF X-RAY BEAM
FOR THE PLANE (0002)
In recent years, methods [43,44] have been developed which enable determination of the (three-angle) crystallite orientation distribution from several (two-angle) pole figure distributions. The crystallite orientation distribution function (CODF) has found a wide application in case of cubic crystal [45,46]. In the following section the CODF will be developed in the case of Zircaloy material. Moreover, a way of determining pole figure and inverse pole figures from the CODF will be examined.
3. Theory of Crystallite Orientation Distribution Function (CODF)

3.1 Introduction and Statement of the Problem

Various polycrystalline materials with the same chemical composition can be distinguished from one another by the size of the grains and the orientation of the crystallographic axes of various grains relative to one another. The distribution of the crystallographic axes of separate grains of material relative to one another defines the texture of the material. Viglin [47] suggested that the texture could be described by means of a function describing the distribution of the direction of the crystallographic axis of separate grains. Considering that each grain of a polycrystalline specimen is a monocrystal, its orientation can be characterized by the orientation of three unit vectors of crystallographic axes, called $k$, with respect to three unit vectors of coordinate axes, linked with the specimen, called $k_0$.

The relation between $k$ and $k_0$ is

$$k = \hat{g} k_0$$  \hspace{1cm} (3-1)

where $\hat{g}$ is a rotation operator.

The CODF concept may be stated as follows: consider a rotation lying in the range $g$ to $g + dg$, with $dm$ the mass of all grains oriented in the angular range considered, and with $m$ the total mass of the specimen. Then the fraction of grains oriented in the angular range $dg$ can be evaluated if the crystallite orientation distribution function (CODF) is known. Call $F(g)$ the crystallite orientation distribution function (CODF). Since $m = \rho V$ (where $\rho$ is the density and $V$ the volume), one can write:
\[ \frac{dm}{m} = \frac{dV}{V} = F(g) \ dg \]  \hspace{1cm} (3-2)

\( F(g) \ dg \) expresses the probability of having a crystallite oriented in the angular range \( dg \). Note that this formulation is based on a normalization in which \( g \) is integrated over a limited range (to eliminate multiple counts of a single grain).

Therefore the problem is to construct or evaluate the function \( F(g) \). However, this function is not directly measurable, but, as it will be shown in the following sections, it can be evaluated from pole figure measurements, \([43, 44]\). In order to be able to correlate the CODF to pole figure, the basis on which \( F(g) \) is constructed will be given. Preliminary steps include discussion of group theory and matrix representation.

### 3.2 Euler Angles and Choice of Axes

A single direction in a solid may be described by two parameters such as the angles of spherical coordinates. In order to characterize the orientation of a particular crystallite a third parameter is required, to specify the rotational degree of freedom about this direction. This orientation may, therefore, be specified by means of three independent parameters. For that purpose, three angles have been chosen; these are the Euler angles given by \( \Psi, \Theta, \Phi \).

#### 3.2.1 Euler Angles

Consider a Cartesian coordinate system \( (k_0) \) fixed in the specimen and given as \( OXYZ \) in Fig. 15.a. The coordinate axes \( OX, OY, OZ \) are fixed permanently in the specimen. by performing a rotation through an
FIGURE 15

EULER ANGLES
angle $\Psi$ counter clockwise about the Z axis, (Fig. 15.b), with $0 \leq \Psi \leq 2\pi$, a new system of coordinates OX'Y'Z' is obtained. The matrix rotation $R_Z(\Psi)$ which transforms the system OXYZ to OX'Y'Z' is given by:

$$R_Z(\Psi) = \begin{pmatrix} \cos\Psi & \sin\Psi & 0 \\ -\sin\Psi & \cos\Psi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$  \hspace{1cm} (3-3)

This rotation may be represented by the operator $D_Z(\Psi)$. A new rotation is performed through an angle $\Theta$, in a positive sense, about the Y' axis (Fig. 15.c). The angle $\Theta$ is taken in the interval $0 \leq \Theta \leq \pi$. The coordinate system OX'Y'Z' is related to the new coordinate system OX"Y"Z" by the matrix rotation $R_{Y'}(\Theta)$ given by

$$R_{Y'}(\Theta) = \begin{pmatrix} \cos\Theta & 0 & -\sin\Theta \\ 0 & 1 & 0 \\ \sin\Theta & 0 & \cos\Theta \end{pmatrix}$$  \hspace{1cm} (3-4)

This rotation is represented by the operator $D_{Y'}(\Theta)$. Finally a system of coordinates OXYZ is obtained after a rotation of OX"Y"Z" by an angle $\Psi$ in a positive sense around the Z" axis, (Fig. 15.d). The angle is chosen as $0 \leq \Psi \leq 2\pi$.

The matrix $R_{Z''}(\Psi)$ associated with this rotation is given by:

$$R_{Z''}(\Psi) = \begin{pmatrix} \cos\Psi & \sin\Psi & 0 \\ -\sin\Psi & \cos\Psi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$  \hspace{1cm} (3-5)

* In the remainder counter clockwise will be referred as positive sense.
The operator representing this rotation is called $D_2^\Psi$ ($\Psi$).

The new coordinate system OXYZ is related to the fixed system of coordinated OXYZ by:

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = R(\varphi, \theta, \psi) \begin{bmatrix} X \\ Y \\ Z \end{bmatrix}$$

(3-6)

where:

$$R(\varphi, \theta, \psi) = R_2^\varphi (\varphi) \quad R_\psi (\theta) \quad R_\psi (\psi)$$

(3-7)

$x$, $y$ and $z$ refer to the coordinate axes fixed in the crystallite and in the polycrystalline respectively. The product of matrices of Eq. (3-7) leads to:

$$R(\varphi, \theta, \psi) = \begin{bmatrix}
\cos \varphi \cos \theta \cos \psi - \sin \varphi \sin \psi & \sin \varphi \cos \theta \cos \psi + \cos \varphi \sin \psi \\
\cos \varphi \sin \theta \cos \psi + \sin \varphi \cos \psi & -\cos \varphi \cos \theta \sin \psi + \sin \varphi \sin \psi \\
\sin \varphi \cos \theta & -\sin \theta \cos \varphi \\
\sin \theta \sin \varphi & \cos \theta \\
\end{bmatrix}$$

(3-8)

The overall transformation is shown in Fig. (16). Note that $\theta$ is the polar angle of the z axis and $\psi$ is the azimuthal angle of the z axis in the oxyz system. Moreover $\varphi$ specifies the angle between $\text{Oz}$ and $\text{XoZ}$ planes. This will show the possible rotation around the z axis.

3.2.2. Choice of Axes

We select a fixed Cartesian coordinates OXYZ such as the OX, OY, OZ, directions coincident with the rolling direction, transverse direction and normal direction respectively, (Fig. 17.a).
FIGURE 16
OVERALL TRANSFORMATION AFTER ROTATION OF EULER ANGLES
Then we select a system of Cartesian coordinates oxyz fixed in a
crystallite. In the hexagonal close packed (hcp) case, the directions
ox", oy", oz" are perpendicular to the planes (10T0), (1120) and
(0002) respectively, (Fig. 17.b); (for crystallographic notation see
Appendix B). The crystallite orientation is specified by giving the
Euler angles (ψ, Θ, Ψ) defined in Part 3.2.1.

Consider the jth reciprocal lattice factor r_j belonging to a
crystallite. r_j is located by (X_j, η_j) with respect to the crystallite
coordinates oxyz, (Fig. 18.a), and by (ϕ_j, δ_j) with respect to the
sample coordinates OXYZ, (Fig. 18.b). r_j is given by

\[
\begin{align*}
    x &= \sin X_j \cos η_j \\
    y &= \sin X_j \sin η_j \\
    z &= \cos X_j
\end{align*}
\]  \hspace{1cm} (3-9)

and by

\[
\begin{align*}
    X &= \sin ϕ_j \cos δ_j \\
    Y &= \sin ϕ_j \sin δ_j \\
    Z &= \cos ϕ_j
\end{align*}
\]  \hspace{1cm} (3-10)

using Eq. (3.6, 3.9, 3.10) the two sets of angles, (X_j, η_j) and (ϕ_j, δ_j),
are related to each other by

\[
\begin{bmatrix}
    \sin ϕ_j & \cos δ_j \\
    \sin ϕ_j & \sin δ_j \\
    \cos ϕ_j
\end{bmatrix}
= R^{-1}(ψ, Θ, Ψ)
\begin{bmatrix}
    \sin X_j & \cos η_j \\
    \sin X_j & \sin η_j \\
    \cos X_j
\end{bmatrix}
\]  \hspace{1cm} (3-11)

This important relation will find its application in the construction
of the crystallite orientation distribution function.
FIGURE 17
REFERENCE SYSTEM AND FIXED CRYSTALLITE SYSTEM
FIGURE 18
SPHERICAL COORDINATE OF jth RECIPROCAL LATTICE
WITH RESPECT TO a) CRYSTALLITE COORDINATES,
b) TO SAMPLE COORDINATES
3.3 Derivation of the CODF

The probability that \( k \) of an arbitrary grain can be obtained from \( k_0 \) by a rotation lying within the limit \( g \) to \( g + dg \) is expressed as 
\[ F(g) \, dg \] (see Eq. (3.2)). The normalization of \( F(g) \) is expressed as

\[
\int F(g) \, dg = 1 \quad (3-12-a)
\]

This normalization may, for convenience, be performed over angles other than the angles implied by Eq. (3.2).

Since the Euler angles have been taken as the three parameters defining the rotation, it follows that \( F(g) \) is represented by 
\[ F(\Psi, \Theta, \Phi), \] and the limit from \( g \) to \( g + dg \) will correspond to the range \( \Psi \) to \( \Psi + d\Psi \), \( \Theta \) to \( \Theta + d\Theta \) and \( \Phi \) to \( \Phi + d\Phi \). If all the grain orientations are equally probable then \( F(g) \) is set equal to a constant value one. Let \( dg = c \, d\Psi \, \sin\Phi \, d\Phi \, d\Phi \) and use Eq. (3.22) and Euler angles to obtain

\[
F(g)dg = \int \int \int c \, d\Psi \, \sin\Phi \, d\Theta \, d\Psi = 1 \quad (3-12-b)
\]

Therefore 
\[ C = \frac{1}{8\pi^2} \]

or

\[
dg = \frac{1}{8\pi^2} \, d\Psi \, \sin\Phi \, d\Theta \, d\Psi \quad (3-13)
\]

This means that the result of integration is invariant to the rotation of the system of coordinates. Finally for the general case the condition is expressed as:
\[ \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^\pi \int_0^{2\pi} F(\psi', \Theta, \varphi) \, d\psi' \sin\Theta \, d\Theta \, d\varphi = 1 \quad (3-14) \]

3.3.1 Rotation Group

The determinant of the matrix \( R(\psi', \Theta, \varphi) \), given in Eq. (3.8), is equal to +1. In other words, this is the case of pure rotation (see Appendix A). Moreover, it can be verified that the product of two rotation operations \( D(g_1) \) and \( D(g_2) \) can be described as a single rotation operation \( D(g_1 \cdot g_2) \) [48]. This is written as

\[ D(g_1) \cdot D(g_2) = D(g_1 \cdot g_2) \quad (3-15) \]

Furthermore, if \( g_1 \) is the rotation from a number of rotation elements of symmetry, of an hcp crystal in this case, then the grain with crystallographic axes orientation \( k_1 \) given by \( k_1 = g_1 k = g_1 g_0 k_0 \) does not differ physically in its orientation from a grain with \( k = g k_0 \). Mathematically it is expressed by

\[ F(g) = F(g_1 g_0) \quad (3-16) \]

It can be shown [49] (see Appendix A) that the Wigner functions \( D^\ell_{mn}(\psi, \Theta, \varphi) \) are the basis of the representation of the rotation group. Any single value representation can be expressed as a linear combination of the \( D^\ell_{mn}(\psi, \Theta, \varphi) \), where

\[ D^\ell_{mn}(\psi, \Theta, \varphi) = e^{-im\psi} D^\ell_{mn}(0, \Theta, 0) e^{-in\varphi} \quad (3-17) \]
Note that the \( D^\ell_{mn} (\Psi, \Theta, \Phi) \) are also called generalized spherical harmonics, and the functions

\[
D^\ell_{mn} (0, \Theta, 0) = P^\ell_{mn} (\cos \Theta)
\]  

are called the generalized associated Legendre functions, with the condition

\[
\int_0^\pi p^*_{mn} (\cos \Theta) P^\ell'_{m' n'} (\cos \Theta) \sin \Theta \, d\Theta = \frac{2}{2\ell+1} \delta^\ell_{\ell'} \delta^m_{m'} \delta^n_{n'}
\]  

where

\[
\delta_{ij} = \begin{cases} 
0 & \text{if } i \neq j \\
1 & \text{if } i = j 
\end{cases}
\]  

Thus \( F (\Psi, \Theta, \Phi) \) can be expanded on the basis of the generalized spherical harmonics:

\[
F (\Psi, \Theta, \Phi) = \sum_{\ell=0}^{\lambda} \sum_{m=-\ell}^{+\ell} \sum_{n=-\ell}^{+\ell} f^\ell_{mn} e^{-im\Psi} P^\ell_{mn} (\cos \Theta) e^{-in\Phi}
\]

where \( \lambda \) is the degree of the expansion. For simplicity the following conventions are adopted:

\[
w (\Psi, \Theta, \Phi) = \left( \frac{1}{8\pi^2} \right) F (\Psi, \Theta, \Phi)
\]

\[
W^\ell_{mn} = \left( \frac{1}{8\pi^2} \right) \sqrt{\frac{2}{2\ell+1}} f^\ell_{mn}
\]

\[
Z^\ell_{mn} (\cos \Theta) = \sqrt{\frac{2\ell+1}{2}} P^\ell_{mn} (\cos \Theta)
\]
The equation (3.21) is then transformed to:

$$w(\psi, \Theta, \varphi) = \sum_{\ell=0}^{\Lambda} \sum_{m=-\ell}^{+\ell} \sum_{n=-\ell}^{+\ell} W_{\ell mn} e^{-im\psi} Z_{\ell \ell mn} (\cos \Theta) e^{-in\varphi}$$  \hspace{1cm} (3-25)

where $Z_{\ell \ell mn} (\cos \Theta)$ are the normalized generalized associated Legendre functions with the condition that:

$$\int_0^{\pi} Z_{\ell \ell mn} (\cos \Theta) Z_{\ell' \ell' mn'} (\cos \Theta) \sin \Theta \, d\Theta = c_{\ell \ell} \delta_{mm'} \delta_{nn'}$$  \hspace{1cm} (3-26)

The condition of normalization of equation (3.24) is:

$$\int_0^{2\pi} \int_0^{\pi} \int_0^{2\pi} w(\psi, \Theta, \varphi) \, d\psi \sin \Theta \, d\Theta \, d\varphi = 1$$  \hspace{1cm} (3-27)

This last procedure relates the formalism used by Bunge [44] and the one used by Doe [43].

Suppose the function $W(\psi, \Theta, \varphi)$ is known. The coefficients $W_{\ell mn}$ can be evaluated if Eq. (3.25) is multiplied by $e^{im\psi} Z_{\ell' \ell mn'} (\cos \Theta) e^{in\varphi}$, then integrated over all the space. Use Eq. (3.26) to get:

$$\int_0^{2\pi} \int_0^{\pi} \int_0^{2\pi} w(\psi, \Theta, \varphi) e^{im\psi} Z_{\ell' \ell \ell mn'} (\cos \Theta) e^{in\varphi} \, d\sin \Theta \, d\varphi =$$

$$4\pi^2 \sum_{\ell=0}^{\Lambda} \sum_{m=-\ell}^{+\ell} \sum_{n=-\ell}^{+\ell} W_{\ell mn} c_{\ell} \delta_{mm'} \delta_{nn'}$$  \hspace{1cm} (3-28)
Eq. (3.28) is equal to zero if \( m \neq m', l \neq l', n \neq n' \) so:

\[
W_{\ell mn} = \frac{1}{2\pi} \int_{0}^{2\pi} \int_{0}^{\pi} w(\psi, \Theta, \Phi) e^{im\psi} e^{-in\Phi} d\psi \sin\Theta d\Theta
\]

Since the function \( w(\psi, \Theta, \Phi) \) is never known beforehand, the Equation (3.29) cannot be evaluated.

However the pole figures bring information about the distribution of plane normals. The angles between the different plane-normals belonging to one crystallite are fixed by the lattice structure of the crystal. Therefore, the distribution curves for the plane-normals cannot be completely independent of one another. In the following section, a method of calculating the CODF from the pole figure measurements will be derived.

3.3.2 Evaluation of \( W_{\ell mn} \) from Pole Figures

3.3.2.1 Pole Figure Expansion

The crystal is characterized by the directions of the normals to the crystal planes and the angles which the normals make with one another. The simplest method for describing the crystal is to indicate on the surface of a unit sphere the points in which the normals to the crystal planes intersect the surface of the sphere, these are called poles. (More information is given in Section 2.2). The pole figures are presented in two dimensions with the use of stereographic projection. If \( q_j(\phi_j, \delta_j) \) is the density of poles of a plane \( j \), and using information given in Appendix A, this density of poles is expanded
in a series of surface spherical harmonics and it is given by

$$ q_j (\phi_j, \delta_j) = \sum_{\ell=0}^{+\ell} \sum_{m=-\ell}^{+\ell} Q_{\ell m}^j \ P_{\ell m}(\phi_j) \ e^{-im\delta_j} \quad (3-30) $$

where the normalized associated Legendre functions obey

$$ \int_{0}^{\pi} P_{\ell m}(\phi_j) \ P_{\ell' m'}(\phi_j) \sin \chi_j \ d\chi_j = \delta_{\ell \ell'} \ \delta_{mm'} \quad (3-31) $$

the coefficients $Q_{\ell m}^j$ are obtained by multiplying Eq. (3.30) by

$P_{\ell' m'}(\phi_j)e^{im\delta_j}$ and integrating over all the range, $0 \leq \chi_j \leq \pi$ and $\eta_j$ from 0 to $2\pi$, and making use of Eq. (3.31) to get

$$ Q_{\ell m}^j = \frac{1}{2\pi} \int_{0}^{2\pi} \int_{0}^{\pi} q_j(\phi_j, \delta_j) \ P_{\ell m}(\phi_j) e^{im\delta_j} \sin \phi_j \ d\phi_j \ d\eta_j \quad (3-32) $$

Since $q_j(\phi_j, \delta_j)$ can be measured experimentally, the coefficients $Q_{\ell m}^j$ are calculated through the relation given by Eq. (3.32). The next step is to show how the coefficients $Q_{\ell m}^j$ are related to the coefficient $W_{\ell mn}$ of the CODF expansion.

3.3.2.2. Evaluation of $W_{\ell mn}$

We saw in Section 3.3.2.1 that the spherical harmonics give the basis of the representation of the pole density distribution. This means that the spherical harmonic $Y_{\ell m}(\phi_j, \delta_j)$ are the eigen-functions of the reciprocal lattice vector $r_j$ with respect to the simple reference.
The basis of the representation of the pole density \( q_j(\phi_j, \delta_j) \) with respect to the crystalline reference, is obtained by applying the operator rotation \( D(\psi, \theta, \varphi) \) to the eigenfunctions \( \gamma_{lm}(\phi_j, \delta_j) \). This is true since the reference axis fixed in the crystallite is obtained after rotation \( R(\psi, \theta, \varphi) \) of the specimen axes. Use information supplied in Appendix A to get

\[
D(\psi, \theta, \varphi) \gamma_{lm}(\phi_j, \delta_j) = \sum_{k=-l}^{+l} \gamma_{lk}(\phi_j, \delta_j) D_{km}(\psi, \theta, \varphi)
\]  

(3-33)

making use of Eq. (3-11) and (3-33) to write

\[
\gamma_{lm}(\phi_j, \delta_j) = \sum_{k=-l}^{+l} \gamma_{lk}(\phi_j, \delta_j) D_{km}(-\psi, -\theta, -\varphi)
\]

(3-34)

since \( \gamma_{lm}(\phi_j, \delta_j) \) is proportional to \( P_{lm}(\phi_j)e^{im\delta_j} \) and taking into account Eq. (3-17) and (3-24) the equation (3-34) is equivalent to:

\[
P_{lm}(\phi_j)e^{im\delta_j} = \left( \frac{2}{2\ell + 1} \right) \sum_{k=-l}^{+l} P_{lk}(\phi_j)e^{ik\eta_j} Z_{lmk}(\cos \theta)e^{im\psi} e^{ik\varphi}
\]

(3-35)
The goal is to relate the coefficients \( Q_{\xi m}^j \) of the pole figure expansion to the coefficients \( W_{\xi mn} \) of the CODF expansion. This relation is obtained by performing the following steps:

- Multiply both sides of Eq. 3-35 by \( W(\psi, \phi, \varphi) q_j (\phi_j, \delta_j) \)
- Integrate over the whole range of \( \psi, \theta, \varphi, \phi_j, \delta_j \)
- Use Eq. (3-27), (3-29) and (3-32)
- Normalize the density of poles \( q_j(\phi_j, \delta_j) \)

\[
\int_0^{2\pi} \int_0^{\pi} q_j(\phi_j, \delta_j) \sin \phi_j \, d\phi_j \, d\delta_j = 1 \quad (3-36)
\]

The final result is given by

\[
Q_{\xi m}^j = 2\pi \left( \frac{2}{2\ell + 1} \right) \sum_{\ell=-\infty}^{+\infty} W_{\xi mk} P_{\ell k} (\chi_j) e^{i\kappa j} \quad (3-37)
\]

The coefficients \( W_{\xi mn} \) are evaluated through the Eq. (3-37). The number of coefficients to calculate depends on the degree of the expansion considered. However, some simplifications might arise by taking into consideration the symmetry properties of hcp. This is examined in the next section.

3.4 Symmetry Properties

The symmetry considerations of the hcp crystal will allow simplifications of the number of coefficients \( Q_{\xi m} \) and \( W_{\xi mn} \) necessarily for the evaluation of the CODF. The symmetry properties which will be taken into account in the following sections are essentially:

- The fact that the observed x-ray data possess centrosymmetry
(Friedel's law) [50].

- The mirror symmetry and 6-fold rotation axis of the hcp crystal.

3.4.1 Friedel's Law

The integrated intensities of g and -g reflection must be identical, since the quality of reflections from (hk2) and (hk2) cannot be distinguished, it follows that all x-ray diffraction effects are centrosymmetrical. Whether a crystal does or does not have a center of symmetry, its diffraction effects do have a center of symmetry, and hence it is impossible to judge by diffraction effects whether the crystal has a center of symmetry or not. This insertion of a symmetry center into the apparent symmetry of a crystal as judged by x-ray diffraction symmetry is known as Friedel's Law. Therefore, the observed data always possesses centrosymmetry. This can be expressed as:

\[ q(\phi, \delta) = q( -\phi, \delta + \pi) \quad (3-38) \]

Let's expand \( q(-\phi, \delta, \pi) \) and \( q(\lambda, \gamma) \) in series of spherical harmonics

\[ q(\phi, \delta) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} Q_{\ell m} P_{\ell m}(\phi) e^{-im\delta} \quad (3-39) \]

\[ q(-\phi, \delta + \pi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} Q_{\ell m} P_{\ell m}(-\phi) e^{-im(\delta + \pi)} \quad (3-40) \]
Note \[ e^{-im(\delta + \pi)} = (-1)^m e^{-im\delta} \] \hspace{1cm} (3-41)
and \[ P_{\ell m} (-\phi) = (-1)^{\ell+m} P_{\ell m} (\phi) \] \hspace{1cm} (3-42)

Substitute Eq. (3-39), (3-40), (3-41), (3-42) into (3-38) to get

\[ Q_{\ell m} = (-1)^{\ell} Q_{\ell m} \] \hspace{1cm} (3-43)

Equation (3-43) is true only if \( \ell \) is even.

So \( Q_{\ell m} = 0 \) when \( \ell \) is odd.

3.4.2. Reflection Plane

A reflection plane or plane of mirror symmetry is defined as the points on one side of a plane, of symmetry, reflected by identical points on the other side. In the case of hcp symmetry, mirrors perpendicular to z-axis are present. In the first case, the density of poles at the angles \( \pm \phi \) should be the same, or:

\[ q (-\phi, \delta) = q (\phi, \delta) \] \hspace{1cm} (3-44)

By expanding both sides of Equation (3-44) on the basis of the surface spherical harmonics and using Equation (3-42), the following relation will stand

\[ Q_{\ell m} = (-1)^m Q_{\ell m} \] \hspace{1cm} (3-45)

This is true only if \( m \) is an even number.

Therefore

\[ Q_{\ell m} = \begin{cases} 
0 & \text{when } m \text{ is odd} \\
\neq 0 & \text{when } m \text{ is even}
\end{cases} \]

In the case of mirror perpendicular to the x-axis it follows that

\[ q(\phi, \pi - \delta) = q (\phi, \delta) \] \hspace{1cm} (3-46)
By using the same procedure as in equation (3-44) we end up with

\[
Q_{\ell m} = Q_{\ell \bar{m}}
\]

(3-47)

and

\[
W_{\ell \bar{m} \bar{n}} = (-1)^{m+n} W_{\ell m n}
\]

(3-48)

where \(\bar{m}\) and \(\bar{n}\) stands for \((-m)\) and \((-n)\) respectively.

This mirror implies also that the rotation \((\psi', \theta, \varphi)\) and \((\psi, \theta, \pi - \varphi)\) are equivalent. Taking into account Eq. (3-37) we conclude that

\[
W_{\ell mn} = (-1)^n W_{\ell m \bar{n}}
\]

(3-49)

3.4.3 6-fold Rotation Axis

A \(k\)-fold axis of rotational symmetry exists, if a crystal, upon rotation about this axis, assumes a congruent position each time by rotation through an angle \(360\degree / k\). In the case of hcp a 6-fold rotation symmetry around \(z\)-axis is present. In other words the rotation \((\psi', \theta, \varphi)\) and \((\psi, \theta, \varphi + \frac{\pi}{3})\) are equivalent. Therefore

\[
W(\psi', \theta, \varphi) = (\varphi, \theta, \varphi + \frac{\pi}{3})
\]

(3-50)

using Equation (3-25) this traduces to

\[
e^{-i\pi n} = 1
\]

(3-51)

Therefore \(n\) should be multiples of 6.

3.4.4 Consequences of the Symmetry Properties

The symmetry properties of the hcp crystal will simplify drastically the number of coefficients \(W_{\ell mn}\) to evaluate in order to construct the CODF. The consequences of the symmetry can be summarized as follows:

- \(\ell\) and \(m\) are even and \(n\) is a multiple of 6
- the coefficients \(W_{\ell mn}\) are all real and satisfy the following
relations:

\[ W_{\ell mn} = W_{\ell mn} = W_{\ell mn} = W_{\ell mn} \] (3-52)

where \( \bar{m} \) and \( \bar{n} \) stands for \(-m\) and \(-n\) respectively.

- the coefficients \( Q_{\ell m} \) satisfy the relation

\[ Q_{\ell m} = Q_{\ell m} \] (3-53)

- the Space of Euler considered is reduced to the domain of

\[ 0^\circ \leq \psi \leq \frac{\pi}{2} \] 3-54-a
\[ 0 \leq \theta \leq \frac{\pi}{2} \] 3-54-b
\[ 0 \leq \phi \leq \frac{\pi}{3} \] 3-54-c

- since \( \ell, m \) are even and \( n \) a multiple of 6 the normalized associated Legendre functions \( P_{\ell m} \) and the generalized normalized associated Legendre functions \( Z_{\ell mn} \) will satisfy the following properties

\[ P_{\ell m} (\cos \theta) = P_{\ell m} (\cos \theta) \] 3-55a
\[ Z_{\ell mn} (\cos \theta) = Z_{\ell mn} (\cos \theta) \] 3-55-b

From equations (3-52) and (3-55-a) \( q_j(\phi_j, \sigma_m) \) in equation (3-30) is simplified to

\[ q_j(\phi_j, \sigma_j) = \sum_{\ell=2}^{\lambda} \sum_{m=2}^{+\ell} Q^j_{\ell m} P_{\ell m}(\phi_j) \cos m\sigma_j \] (3-56)

where \( \lambda \) is the order of the expansion; \( \ell \) and \( m \) are even.

The coefficient \( Q^j_{\ell m} \) are related to the \( W_{\ell mn} \) coefficient by the Equation 3-37. From equations 3-52 and 3-55-a, Equation 3-57 is written as

\[ Q^j_{\ell m} = 2 \pi \left[ \frac{2}{2\ell+1} \right]^{\frac{1}{2}} W_{\ell m o} P_{\ell o}(\cos \psi) + 2 \sum_{k=6}^{+\ell} W_{\ell m k}(\cos \chi_j) \cos k\phi_j \] (3-57)

with \( k \) a multiple of 6.
Furthermore, the crystallite orientation distribution function (CODF) $W(\psi, \theta, \varphi)$ Eq. (3-25) is expressed by:

$$
W(\psi, \theta, \varphi) = \sum_{Z-0}^L \sum_{m=1}^L \sum_{n=1}^L \sum_{n=1}^L \left\{ W_{m=0} Z_{m=0}^2 \cos m\varphi + W_{m=0} Z_{m=0}^2 \cos n\theta \cos n\varphi \right\}
$$

$$
+ W_{m,n} \left[ (Z_{m,n}^2 + Z_{m,n}^2) \cos n\varphi \cos m\varphi + (Z_{m,n}^2 - Z_{m,n}^2) \sin n\varphi \sin m\varphi \right]
$$

(3-58)

3.5 Determination of the CODF from Incomplete Pole Figure

It has been pointed out in Section 2.4 that the complete pole figure determination normally requires two methods, the reflection and the transmission techniques. These two techniques overlap in the region of $30 \leq \phi \leq 70$ and it is quite difficult to match the data in the overlapping region. In Section 3.3 a method for obtaining a crystallite orientation distribution has been derived by using complete pole figures. The measurements of the pole figure $q_j(\phi_j, \theta_j)$ should be done over $4\pi$ solid angle or a symmetric subregion. If only incomplete pole figures are generated using the back reflection technique, it should be possible to construct the CODF. The use of incomplete pole figure results in the loss of orthogonality relations among the associated Legendre functions, which require integration of the entire domain of the pole figure. Therefore the relations giving $Q_{\ell m}^j$, the coefficients of the pole figure expansion,
as a function of the pole density \( q_j(\phi_j, \delta_j) \) Eq. (3-33) and as function of the texture coefficients \( W_{\ell mn} \) Eq. (3-37), do not hold anymore. In order to evaluate \( W_{\ell mn} \) more complex calculations are required.

Bunge [51] suggested a method for calculating the coefficients \( W_{\ell mn} \). The coefficients \( W_{\ell mn} \) are chosen to minimize the integrals of the square of the difference between the measured pole figure density and the theoretical pole figure expansion. This can be written as:

\[
\sum_j \int_{\phi_1}^{\phi_2} \sin \phi \, d\phi \int_0^{2\pi} \left[ q_j^{\text{meas}}(\phi, \delta) - q_j^{\text{theo}}(\phi, \delta) \right]^2 \, d\gamma = \text{minimum}
\]

(3-59)

where \( q_j^{\text{meas}}(\phi, \delta) \) and \( q_j^{\text{theo}}(\phi, \delta) \) stands for measured and theoretical respectively. \( \phi_1, \phi_2 \) is the interval where the pole figure is measured. Bunge [51] recognized that the measured pole figures are not properly normalized and this is written as

\[
q_j^{\text{meas}}(\phi, \delta) = N_j \hat{q}_j(\phi, \delta)
\]

(3-60)

where \( \hat{q}_j(\phi, \delta) \) are the measured pole figure data and \( N_j \) the normalization factor.

Following Eq. (3-30) and Eq. (3-37) \( q_j^{\text{theo}}(\phi_j, \delta_j) \) can be written as follows:

\[
q_j^{\text{theo}}(\phi, \delta) = 2\pi \sum_{\ell=0}^{+\ell} \left( \frac{2}{2\ell + 1} \right)^{1/2} \sum_{m=-\ell}^{+\ell} P_{\ell m}(\phi) e^{-i m \delta} \sum_{K=-\ell}^{+\ell} W_{\ell m k} \xi_k(\chi_j) e^{im\gamma_j}
\]

(3-61)
Substituting Eq. (3-60) and (3-51) into Eq. (3-59) to get

\[
\sum_{j} \int_{\phi_1}^{\phi_2} \sin \phi \, d\phi \int_{\eta_1}^{\eta_2} \left[ N_j \hat{q}_j(\phi, \delta) - 2 \sum_{\ell=0}^{+\ell} \left( \frac{2}{2 \ell + 1} \right)^{1/2} \sum_{m=-\ell}^{+\ell} P_{\ell m}(\phi) e^{-im\delta} \right. \\
\left. \sum_{k=0}^{+\ell} W_{\ell mk} P_{\ell k}(\chi_j) e^{im\eta_j} \right]^2 \, d\eta = \text{minimum}
\]

(3-62)

Therefore the coefficients \( N_j \) and \( W_{\ell mk} \) should be evaluated such that Eq. (3-62) is minimum. This is done by taking the partial derivatives, with respect to each coefficient \( W_{\ell mk} \) and \( N_j \), equal to zero. We will get a set of equations which can be solved and then the values of \( W_{\ell mk} \) are deduced. In the equation (3-62) the symmetry properties of hcp mentioned in Section 3.4 should be taken into account. This will reduce the number of coefficients \( W_{\ell mk} \) to evaluate.

The normalization of the CODF imposes \( \int \int \int w(\gamma, \theta, \varphi) \sin \theta \, d\theta \, d\varphi = 1 \)

If follows that \( W_{000} = \frac{1}{8 \sqrt{2} \pi^2} \) and has a constant value for textured or untextured material. Considering the symmetry properties developed in Section 3.4 equation (3-57) is reduced to:

\[
q_{\text{theo}}^{j}(\phi, \delta) = \frac{1}{4\pi} + 4 \sum_{\ell=2}^{+\ell} \left( \frac{2}{2 \ell + 1} \right)^{1/2} \sum_{m=-\ell}^{+\ell} P_{\ell 0}(\chi_j) P_{\ell m}(\phi) W_{\ell m 0} \cos m\delta + \\
\sum_{k=0}^{+\ell} W_{\ell 0 k} P_{\ell k}(\chi_j) P_{\ell 0}(\phi) \cos k\eta_j + 2 \sum_{m=1}^{+\ell} P_{\ell m}(\phi) \cos m\delta
\]

(3-63)
Differentiate Eq. (3-62) with respect to $W_{\ell m k}$ and $N_j$ to obtain the following set of equations:

$$
\sum_{j} \left( \frac{2}{2, \ell+1} \right)^{1/2} \int_{\phi_1}^{\phi_2} \sin^2 \phi \int_{0}^{2\pi} \left[ N_j \hat{q}_j(\phi, \delta) - q_j^{\text{theo}}(\phi, \delta) \right] P_{\ell m}(\phi) P_{\ell k}(\chi_j) \cos m \delta \cos k \eta_j \, d\delta = 0
$$

(3-64)

$$
\int_{\phi_1}^{\phi_2} \sin^2 \phi \int_{0}^{2\pi} \left[ N_j q_j(\phi, \delta) - q_j^{\text{theo}}(\phi, \delta) \right] d\delta = 0
$$

(3-65)

In both equations $q_j^{\text{theo}}(\phi, \delta)$ is given by Eq. (3-63). The equations (3-64) and (3-65) may be solved simultaneously to get the coefficients $W_{\ell m k}$ and $N_j$. The number of coefficients $W_{\ell m k}$ that may be obtained depends on the number of measured pole figures $q_j(\chi, \eta)$. More details on the method of evaluating these coefficients are given in Section "Methods of Calculations".

3.6 Summary

Two methods to evaluate the crystallite orientation distribution function have been derived. One method pertains to a complete pole figure, the other to an incomplete pole figure.

In the case of a complete pole figure, the coefficients $Q_j^{\ell m}$ of the pole figure expansion are obtained through the equation (3-33). These coefficients are then substituted into Equation (3-57) to obtain the
three dimensional texture coefficients $\mathcal{W}_{\ell mn}$. Finally, the coefficients $\mathcal{W}_{\ell mn}$ are used in Equation (3-58) to generate the CODF, $W(\varphi, \Theta, \phi)$, for any Euler angles considered.

In the case of incomplete pole figures, the texture coefficients $\mathcal{W}_{\ell mn}$ are obtained from equations (3-63), (3-64) and (3-65). These coefficients are then substituted into Equation (3-58) to obtain the CODF.

The number of pole figures, complete or incomplete, needed to generate the CODF, is a function of the symmetry of the material considered and the degree of the CODF expansion. The symmetry properties reduce the number of coefficients $\mathcal{W}_{\ell mn}$ to evaluate. The details of symmetry effects for hcp materials are supplied in paragraph 3.4.4.

Experimental errors are introduced in pole figure measurements. Even with the reduced number of coefficients $\mathcal{W}_{\ell mn}$ to compute it is advisable to use more pole figures than needed to minimize these errors. More details will be given in Chapter 6.

Some applications of the crystallite orientations distribution function are examined in Chapter 4.
4. Three Dimensional Texture Coefficients. Relation Among CODF, Pole Figure and Inverse Pole Figure.

4.1 Introduction

It has been outlined in Section 3 that the crystallite orientation distribution function (CODF) cannot be measured directly. However, it can be deduced from several pole figures obtained experimentally. The method consists of expanding pole figure and CODF in series of spherical harmonics and generalized spherical harmonics respectively. The coefficients $W_{\ell mn}$ of the CODF expansion can be evaluated from complete or incomplete pole figures. The details of the two methods are given respectively in Sections 3-3 and 3-5. Once these coefficients are calculated the CODF can be generated. Furthermore, the pole figure for any plane as well as the inverse pole figure in any direction can be constructed. The $W_{\ell mn}$ are called three dimensional texture coefficients.

The purpose of this chapter is to examine in detail some possibilities that the three dimensional texture coefficients $W_{\ell mn}$ can offer. This will include the interpretation of the texture coefficients $W_{\ell mn}$; the representation as well as the interpretation of the CODF, and the relations among CODF, pole figure and inverse pole figure.

4.2 Three dimensional Texture Coefficients

The coefficients $W_{\ell mn}$, as they are expressed in Eq. (3-29) represent the value of a certain polynomial of trigonometric function of $\theta$, $\psi$ and $\phi$ averaged over all orientations of crystallites, [42]. As an illustrative example, consider the two coefficients $W_{200}$ and $W_{220}$. From Eq. (3-29) these two coefficients are expressed as:
\[ W_{200} = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^\pi \int_0^{2\pi} w(\psi, \theta, \varphi) Z_{200}(\cos \theta) \sin \theta \, d\theta \, d\psi \, d\varphi \]  
(4-1)

\[ W_{220} = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^\pi \int_0^{2\pi} w(\psi, \theta, \varphi) Z_{220}(\cos \theta) \sin \theta \cos 2\psi \, d\psi \, d\varphi \]  
(4-2)

where

\[ Z_{200}(\cos \theta) = \sqrt{\frac{5}{8}} (3 \cos^2 \theta - 1) \]  
(4-3)

and

\[ Z_{220}(\cos \theta) = \sqrt{\frac{15}{16}} \sin^2 \theta \]  
(4-4)

Therefore Eq.(4-1) brings information about the average value of \( \cos^2 \theta \) 
while Eq.(4-2) gives information about the average value of \( \sin^2 \theta \cos 2\psi \). 
Consequently only the basal pole orientation is included in the coefficients 
\( W_{200} \) and \( W_{220} \). A practical way of interpreting these two coefficients 
would be by introducing two other coefficients \( T_{200} \) and \( T_{220} \) closely 
related respectively to \( W_{200} \) and \( W_{220} \) by:

\[ T_{200} = \frac{1}{3} \left[ \sqrt{\frac{8}{5}} 4\pi^2 W_{200} + 1 \right] \]  
(4-5)

and

\[ T_{220} = 4\pi^2 \sqrt{\frac{16}{15}} W_{220} \]  
(4-6)

After substituting Eqs.(4-3) and(4-4) into respectively Eqs.(4-1) and(4-2) 
and taking into account the normalization of the CODF, Eq.(3-27), \( T_{200} \) and 
\( T_{220} \) are given by:
\[
T_{200} = \int_{0}^{2\pi} \int_{0}^{\pi} \int_{0}^{2\pi} w(\psi, \theta, \varphi) \cos^2 \theta \sin \theta d\theta d\psi d\varphi \quad (4-7)
\]

or

\[
T_{200} = \langle \cos^2 \theta \rangle \quad (4-8)
\]

and

\[
T_{220} = \int_{0}^{2\pi} \int_{0}^{\pi} \int_{0}^{2\pi} \sin^2 \theta \cos 2\psi w(\psi, \theta, \varphi) \sin \theta d\theta d\psi d\varphi \quad (4-9)
\]

or

\[
T_{220} = \langle \sin^2 \theta \cos 2\psi \rangle \quad (4-10)
\]

where \(\langle \rangle\) stands for average value over all crystallites orientations.

The physical meaning of \(T_{200}\) and \(T_{220}\) is well illustrated by Eqs.(4-8) and (4-10). \(T_{200}\) and \(T_{220}\) relate the orientation features of the basal poles as follows:

- \(T_{200} = 1\) and \(T_{220} = 0\) when all the basal poles are exactly parallel to the axial direction
- \(T_{200} = 0\) and \(T_{220} = -1\) when all the basal poles are parallel to the tangential direction
- \(T_{200} = 0\) and \(T_{220} = 1\) when all the basal poles are parallel to the radial direction.

The other coefficients \(W_{2\text{mn}}\) of higher order describe in more detail the deviation from isotropy. However, it should be noted that the normalization of the CODF imposes a constant value of \(\frac{1}{\theta \pi^2 \sqrt{2}}\) to the coefficient \(W_{200}\). For both textured or untextured materials \(W_{200}\) is a constant.
4.3 Representation of CODF and its interpretation

The calculated coefficients \( W_{\ell mn} \) are substituted into Eq.(3-58) to generate the crystallite orientation distribution function. For the symmetry condition stated in paragraph 3.4 it is sufficient to specify \( W(\psi, \theta, \varphi) \) in the region

\[
0 \leq \theta \leq \frac{\pi}{2}, \quad 0 \leq \psi \leq \frac{\pi}{2} \text{ and } 0 < \varphi < \frac{\pi}{3}
\]

The CODF can be represented by two dimensional sections taken at different constant value of \( \varphi \) and where \( \theta \) and \( \psi \) vary in the interval range specified above. An example of such representation is given in Fig.

One way of interpreting the CODF includes the specification of the indices of a crystallographic plane perpendicular to the sheet normal direction and of a crystallographic direction parallel to the rolling direction. This is specified by the crystallographic notation (hki\( \ell \)) [uvtw]. Equations will now be written to find the Euler angles for all crystallites that have the (hki\( \ell \)) plane perpendicular to the sheet normal direction. A second set of equations will define the Euler angles for all crystallites that have the direction [uvtw] parallel to the rolling direction. The first set are given as (see Appendix B):

\[
\begin{bmatrix}
    h \\
    k \\
    i \\
    \ell \\
\end{bmatrix} \begin{bmatrix}
    \sqrt{3} & -1 & 0 \\
    0 & 1 & 0 \\
    \sqrt{3} & 0 & 0 \\
    0 & 0 & c/a
\end{bmatrix} \begin{bmatrix}
    -\sin \theta \cos \varphi \\
    \sin \theta \sin \varphi \\
    \cos \theta
\end{bmatrix}
\]

\[ (4-11) \]

where \((-\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)\) are the components of a unitary vector parallel to the normal direction.
and

\[
\begin{bmatrix}
u \\
v \\
t \\
w
\end{bmatrix}
= \begin{bmatrix}
1/\sqrt{3} & -1/3 & 0 \\
0 & 2/3 & 0 \\
-1/\sqrt{3} & -1/3 & 0 \\
0 & 0 & a/c
\end{bmatrix}
\begin{bmatrix}
\cos \psi \cos \theta \cos \varphi -\sin \psi \sin \varphi \\
-\cos \psi \cos \theta \sin \varphi -\sin \psi \cos \varphi \\
\cos \psi \sin \theta \\
\end{bmatrix}
\tag{4-12}
\]

where \((\cos \psi \cos \theta \cos \varphi -\sin \psi \sin \varphi, -\cos \psi \cos \theta \sin \varphi -\sin \psi \cos \varphi, \cos \psi \sin \theta)\)
are the components of a unitary vector parallel to the rolling direction.

Alternatively the triple \((\psi, \theta, \varphi)\) associated with a given \((hk\ell)\)
[uvtw] system is expressed by:

\[
\cos \phi = \frac{a \ell}{c} \left\{ \left( \frac{4}{3} \right) \frac{(h^2 + k^2 + hk)}{a^2 \ell^2} \right\}^{1/2}
\tag{4-13}
\]

and

\[
\cos \varphi = -\frac{(2h + k)}{2(h^2 + hk + k^2)^{1/2}}
\tag{4-14}
\]

with \(h\) and \(k \neq 0\)

and

\[
\cos \psi = \frac{\left( \frac{cw}{a} \right)}{\left\{ 3(u^2 + uv + v^2) + \frac{c_w^2}{a^2} \right\}^{1/2}} \left\{ \frac{4}{3} \left( k^2 + hk + k^2 \right) + \frac{a^2 \ell^2}{c^2} \right\}^{1/2}
\tag{4-15}
\]

with \(h\) and \(k \neq 0\)

When \(h = k = 0\) the angle \(\phi\) is zero. In this case it is not possible
to specify \(\varphi\) or \(\psi\) alone, but \((\varphi + \psi)\) is given by
\[
\cos (\Psi + \Psi) = \frac{\left(\frac{\sqrt{3}}{2}\right) (2u + v)}{\sqrt{\left\{ 3(u^2 + u^2 + v^2) + \frac{c^2 w^2}{a^2} \right\}}} \quad (4-16)
\]

It should be noted that the values of the Euler angles \( \Psi \) and \( \Theta \), in the case of hcp material, depend on the ratio \( \frac{c}{a} \). Thus the diagrams constructed for the interpretation of CODF, figs. (19) and (20) are valid only in the case of Zircaloy where \( \frac{c}{a} \) is taken equal to 1.59271.

4.4 Relations Among CODF, Pole Figures and Inverse Pole Figures

4.4.1 Calculated Pole Figures

The pole figures are two dimensional "projections" of the three-dimensional crystallite orientation distribution function [52]. Once the \( W_{\ell mn} \) are known it is possible to construct any plane normal orientation distribution. Furthermore, when only incomplete pole figures are available, the complete pole figures can be calculated. The calculated pole figures are obtained by performing the following steps:

- Evaluation of the angles \( \chi_j, \eta_j \) of the plane normal considered, with respect to the axes fixed in the crystallite. \( \chi_j \) and \( \eta_j \) are given by (see appendix B):

\[
\tan \chi_j = \frac{c}{a} \frac{2}{\sqrt{3}} \frac{(h^2 + k^2 + h k)}{L} \quad (4-17)
\]

\[
\tan \eta_j = \frac{k}{2h + k} \quad (4-18)
\]

- the coefficients \( W_{\ell mn} \) are substituted into Eq. (3-57), the coefficients \( Q_{\ell m}^j \) of the pole figure expansion are then calculated.

- finally, the variation of the pole density as function of \( \phi \) and \( \phi \) is then obtained from Eq. (3-56). Note the range of \( \phi \) and \( \phi \) is

\[ 0 \leq \phi \leq \frac{\pi}{2} \quad \text{and} \quad 0 \leq \phi \leq 2\pi \]
4.4.2. Calculated Inverse Pole Figures

The inverse pole figures are also two dimensional "projections" of the crystallite orientation distribution function, [52]. They describe the orientation distribution of particular specimen directions with respect to the crystallographic axes. The inverse pole figure is obtained by averaging \( W(\psi, \theta, \phi) \) with respect to \( \psi \) [43,48]. The inverse pole figure, \( H_{ND}(\theta, \phi) \), of the normal direction is expressed mathematically by

\[
H_{ND}(\theta, \phi) = \frac{1}{2\pi} \int_0^{2\pi} W(\psi, \theta, \phi) \, d\psi
\]  

(4-19)

Substitute the expansion of \( W(\psi, \theta, \phi) \) given in Eq.(3-25) into Eq.(4-18), and using the fact that for \( m \neq 0 \)

\[
\int_0^{2\pi} \cos m \psi \, d\psi = 0
\]

\( H_{ND}(\theta, \phi) \) is given by

\[
H_{ND}(\theta, \phi) = \sum_{\ell = 0}^{\infty} \sum_{n = -\ell}^{\ell} W_{\ell m} Z_{\ell n} (\cos \theta) \cos n \phi
\]  

(4-20)

Equation 4-19 gives only the inverse pole figure in the normal direction. However, an inverse pole figure corresponding to any sample direction can be also calculated from equation (4-19) after a new set of \( W_{\ell m} \) are obtained by a rotation of the sample coordinate system [45]. If the new sample coordinate system \( O_{N}X_{N}Y_{N}Z_{N} \) is obtained by rotation of \( O_{XYZ} \) by \( \alpha, \beta \) and \( \gamma \). These three angles represent the Euler angles as defined in section 3.2.1. Call \( \chi_j' \) and \( \psi_j' \) the polar and azimuthal angles of \( r_j \) (reciprocal lattice vector) with respect to \( O_{N}X_{N}Y_{N}Z_{N} \). The spherical harmonics \( Y_{\ell m}(\chi_j', \psi_j') \) are the eigenfunctions of the reciprocal lattice vector \( r_j \) with respect to the sample coordinates, \( O_{XYZ} \). The eigenfunctions \( Y_{\ell m}(\chi_j', \psi_j') \)
of \( r_j \) with respect to \( OX_N Y_N Z_N \) are obtained after applying the operator rotation \( D(\alpha, \beta, \gamma) \) to the \( Y_{\ell m}(\chi_j, \eta_j) \) to give (see Appendix A):

\[
P_{\ell m}(\chi_j, \eta_j) e^{im\delta_j} = \left( \frac{2}{2\ell + 1} \right) \sum_{k=-\ell}^{+\ell} p_{\ell k}(\chi_j') e^{ik\eta_j'}
\]

\[Z_{\ell m k}(\cos \beta) e^{-im\alpha} e^{-ik\gamma}
\]

(4-21)

After substituting Eq. (4-20) into Eq. (3-37) a new set of coefficients \( W'_{\ell mn} \) are obtained:

\[
W'_{\ell mn} = \left( \frac{2}{2\ell + 1} \right) \sum_{k=-\ell}^{+\ell} W_{\ell mk} Z_{\ell km}(\cos \beta) e^{-ik\alpha} e^{-im\gamma}
\]

(4-22)

For different directions considered the \( W'_{\ell mn} \) will be different. In fact, only three directions are of interest: the Normal Direction (ND), the Rolling Direction (RD), and the Transverse Direction (TD).

The transverse direction is obtained when \( \alpha = 0 \) and \( \beta = \frac{\pi}{2} \). The coefficients of the inverse pole figure will be noted \( W^T_{\ell 0n} \) and given from Eq. (4.21) by

\[
W^T_{\ell 0n} = \left( \frac{2}{2\ell + 1} \right) \sum_{k=-\ell}^{+\ell} W_{\ell 0k} Z_{\ell k0}(0)
\]

(4-23)
The rolling direction is obtained when $\alpha = \beta = \frac{\pi}{2}$ and $\gamma = 0$. The coefficients $W^{R}_{\ell \alpha \gamma}$ of the inverse pole figure in the rolling direction are:

$$
W^{R}_{\ell \alpha \gamma} = \left(\frac{-2}{2 \ell + 1}\right)^{\frac{1}{2}} \sum_{k=-\ell}^{+\ell} W_{\ell \alpha \gamma}^{0k} Z_{\ell \alpha \gamma}^{0k}(0) e^{-i\ell \pi} 
$$

(4-24)

Therefore the inverse pole figure in the rolling and transverse directions are given by Eq. (4-19) after substituting the appropriate coefficients $W_{\ell \alpha \gamma}$ given by Eq. (4-21) and (4-22) respectively.

Methods for gathering the appropriate data will be described in the next section.
FIGURE 19

DIAGRAM OF INTERPRETATION THE CODF FOR ZIRCALOY

AT $\varphi = 0^\circ$
FIGURE 20

DIAGRAM OF INTERPRETATION THE CODF FOR ZIRCALOY

AT $\psi = 30^\circ$
5. EXPERIMENTAL PROCEDURES

This chapter describes the method used in getting the appropriate data leading to the construction of the crystallite orientation distribution function. This will include a description of the experimental instrumentation; specimen preparation; direct and inverse pole figure measurements; and data reduction.

5.1 Experimental Instrumentation

5.1.1 Diffractometer

The essential features of a diffractometer are presented in Figure (22). These are described by the following:

- An x-ray detector is placed on the circumference of a circle centered on the specimen.

- A specimen (S) (Fig. 21) in a form of a flat plate is supported by a table (T) which can be rotated about an axis (O) perpendicular to the plane of drawing.

- The x-ray source (x) is parallel to the diffractometer axis (O)

- (A) and (B) (Fig. 21) are slits which define and collimate the incident and diffracted beams respectively.

- The carriage (E) supports the receiving slits and the counter. (E) may be rotated about an axis (O) and its angular position \( \Theta \) may be read on the graduate scale (K).

The supports (E) and (T) are mechanically coupled so that the rotation of the counter through \( 2\Theta \) degrees is automatically accompanied by a rotation of the specimen through \( \Theta \) degrees.

The intensity of a diffracted beam is measured directly, either by means of the ionization it produces in a gas or by the fluorescence it produces in solid.
FIGURE

SCHEMATIC OF DIFFRACTOMETER
A General Electric Diffractometer is used. The diffractometer axis is vertical and the counter moves in a horizontal plane. The pulse rate is measured as follows: the succession of current pulses is converted into a steady current, which is measured on a counting rate meter calibrated in counts (pulses) per second (c.p.s.). A continuous indication of x-ray intensity is obtained.

The counter is started at $2\theta=30$ and connected to a counting rate meter. The output of this circuit is fed into a fast acting automatic recorder. The counter is then driven at a constant angular velocity through increasing values of $2\theta$. At the same time the paper chart of the recorder moves at a constant speed of one inch per minute, so that distances along the length of the chart are proportional to $2\theta$.

5.1.2 Pole Figure Goniometer

A complete pole figure requires a reflection and a transmission techniques as outlined in Section 2-4. The portion of the latitude $\alpha$ in the range of $0^\circ$ to $70^\circ$ degrees (see Fig. 22) is accessible by the transmission technique. The other portion from $\alpha = 30^\circ$ to $\alpha = 90^\circ$ is obtained by the reflection technique. The angular range in which the two techniques overlap, $30^\circ \leq \alpha \leq 70^\circ$, provides data for placing the intensities on a common basis when the specimen has been studied by both techniques. However, in this study only the reflection technique has been used.

The reflection geometry places the $\alpha$ axis along the cartesian axis x. The specimen plane lies in the equatorial xy plane when $\alpha = 90^\circ$ and (N) is coincident with Y (see Fig.22).

A Siemens pole figure goniometer was used to collect the data.
FIGURE 22

GEOMETRY OF THE REFLECTION AND TRANSMISSION FOR

POLE FIGURE MEASUREMENT
During reflection technique, $\delta$-motion is provided by the vertical circle and $\delta$ motion by the small horizontal azimuth circle in the goniometer. It is possible to scan the pole figure along a spiral path (see Fig. 12) by simultaneous motion about the $\alpha$ and $\delta$ circles.

To suit the precision of counting or degree of resolution desired, adjustments on the Siemens goniometer provide different scanning speed or spirales of different pitches. A spiral pitch of $5^\circ$ (5$^\circ$ increase in $\alpha$ per 360$^\circ$ rotation of $\delta$) is combined with suitable scanning to map the range of $\alpha = 0^\circ$ to $80^\circ$ in 80 minutes.

5.2. Specimen Preparation

A random sample is obtained from a relatively thick layer of zirconium powder (-200 mesh). The reliability of this sample has been checked by comparison of calculated intensities [38], obtained from diffractometer data, against tabulated theoretical values [32], table (6). Specimens for plate are obtained by cutting several pieces of one square inch through the thickness. The faces are polished mechanically through 600 grit SIC paper. Then they are pickled in a solution of 50% $\text{H}_2\text{O}$, 40% $\text{HNO}_3$, 10% HF. Chemical thinning removes also the cold work layers introduced by sample machining.

Specimens for tubing are prepared following the procedure of Tenckhoff and Rittenhouse [28]. Thin foils of one inch length and approximately eight mils wall thickness are cut from the tubing wall. They are chemically thinned in a fluonitric solution, with the composition given above, to about four mils in thickness. These foils are then unrolled elastically and expoxied to a stiff plexiglass backing.

5.3. Inverse Pole Figure

A General Electric diffractometer is used to generate Inverse Pole
<table>
<thead>
<tr>
<th>Reflection</th>
<th>Experimental Intensity, $I(hk\overline{i}l)$</th>
<th>Theoretical Intensity, $I^o(hk\overline{i}l)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(10\overline{1}1)</td>
<td>100.0</td>
<td>100.0</td>
</tr>
<tr>
<td>(0002)</td>
<td>26.1</td>
<td>25.5</td>
</tr>
<tr>
<td>(10\overline{3}0)</td>
<td>23.4</td>
<td>24.3</td>
</tr>
<tr>
<td>(10\overline{1}3)</td>
<td>21.3</td>
<td>17.3</td>
</tr>
<tr>
<td>(11\overline{2}0)</td>
<td>19.7</td>
<td>18.0</td>
</tr>
<tr>
<td>(10\overline{1}2)</td>
<td>17.7</td>
<td>14.6</td>
</tr>
<tr>
<td>(21\overline{3}1)</td>
<td>16.7</td>
<td>12.2</td>
</tr>
<tr>
<td>(20\overline{2}3)</td>
<td>8.6</td>
<td>6.63</td>
</tr>
<tr>
<td>(20\overline{2}2)</td>
<td>4.7</td>
<td>3.12</td>
</tr>
<tr>
<td>(0004)</td>
<td>4.5</td>
<td>2.41</td>
</tr>
</tbody>
</table>

**TABLE 6**

**COMPARISON OF EXPERIMENTAL AND THEORETICAL RELATIVE X-RAY INTENSITY VALUES FOR ZIRCONIUM POWDER STANDARD SPECIMEN[38]**
Figures in the radial direction for the case of tubing, and in the three orthogonal directions for the case of plates. The operating conditions and the method used for the data reduction are described in the following sections.

5.3.1 Operating Conditions

The G.E. diffractometer was used with the following operating conditions:

- CuKα radiation $\lambda = 1.542 \, \text{Å}$
- CuKβ peak eliminated with Ni filter
- X-ray tube voltage of 35 kv and 15 mA filament current
- 2° receiving slit
- 3° the main beam slit
- Scan the region $2\theta = 30^\circ - 141^\circ$
- Scanning rate 2°/min
- Chart recorder 1 inch/min

5.3.2 Data Reduction

The various peaks obtained are identified by their 2θ location, Table 7. The integrated intensity for each peak is then evaluated. This is done by measuring the area under each peak with a planimeter. The average of three or four measurements is taken.

The Texture coefficients Tc(hkilo) are then calculated with the (Eq. 2-2). The peaks {2134} and {1016} overlap, and thus are not considered. Only eighteen reflections are measured.

The Tc(hkilo) values are then plotted on a stereographic projection, (Fig. 10).

5.4 Direct Pole Figure

Pole figures for the planes {0002}, {1010} and {1120}, of the samples
<table>
<thead>
<tr>
<th>(hki )</th>
<th>$2$ (CuKα)</th>
<th>Tilt Angle from (0002) hki£</th>
</tr>
</thead>
<tbody>
<tr>
<td>10̅10</td>
<td>32.00°</td>
<td>90°</td>
</tr>
<tr>
<td>0002</td>
<td>34.84°</td>
<td>0°</td>
</tr>
<tr>
<td>10̅11</td>
<td>36.56°</td>
<td>61.4°</td>
</tr>
<tr>
<td>10̅12</td>
<td>48.02°</td>
<td>42.5°</td>
</tr>
<tr>
<td>11̅20</td>
<td>57.04°</td>
<td>90°</td>
</tr>
<tr>
<td>10̅13</td>
<td>63.60°</td>
<td>31.5°</td>
</tr>
<tr>
<td>11̅22</td>
<td>68.5°</td>
<td>57.8°</td>
</tr>
<tr>
<td>20̅21</td>
<td>69.7°</td>
<td>74.8°</td>
</tr>
<tr>
<td>0004</td>
<td>73.63°</td>
<td>0°</td>
</tr>
<tr>
<td>10̅14</td>
<td>82.5°</td>
<td>24.7°</td>
</tr>
<tr>
<td>20̅23</td>
<td>90.64°</td>
<td>50.7°</td>
</tr>
<tr>
<td>21̅30</td>
<td>93.6°</td>
<td>90°</td>
</tr>
<tr>
<td>21̅31</td>
<td>96.18°</td>
<td>78.4°</td>
</tr>
<tr>
<td>11̅24</td>
<td>100.0°</td>
<td>38.5°</td>
</tr>
<tr>
<td>21̅32</td>
<td>104.03°</td>
<td>67.6°</td>
</tr>
<tr>
<td>10̅15</td>
<td>105.91°</td>
<td>20.2°</td>
</tr>
<tr>
<td>21̅33</td>
<td>117.83°</td>
<td>58.3°</td>
</tr>
<tr>
<td>30̅32</td>
<td>123.09°</td>
<td>70.1°</td>
</tr>
<tr>
<td>20̅25</td>
<td>136.85°</td>
<td>36.3°</td>
</tr>
<tr>
<td>10̅16</td>
<td>140.16°</td>
<td>17°</td>
</tr>
<tr>
<td>21̅34</td>
<td>141.36°</td>
<td>50.6°</td>
</tr>
</tbody>
</table>

**TABLE 7**

**SUMMARY OF DATA PERTINENT TO X-RAY ANALYSIS OF ZIRCONIUM ALLOYS**
considered, were measured.

5.4.1. Operating Conditions

A Siemens pole figure goniometer as described in 5-1-2 is used with the following operating conditions:

- CuKα radiation
- CuKβ is reduced with Ni filter
- The detector is fixed at positions of 2θ equal to 32°, 34.84°, and 57.04°, corresponding to the reflection of the planes {10\overline{1}0}, {0002} and {1\overline{1}20} respectively.
- The beam slits were set at 2mm front and 2mm rear
- The specimen is centered on a moveable carriage with an amplitude of ± 7.5 mm.
- The receiving slits are set at 7.5 mm front and 2mm rear
- δ rotation is 36°/min.
- α rotation is 1°/min.
- Chart recorder 1 inch/min
- The scanning is done in the range of α = 90° to α = 5°
- X-ray tube voltage of 35kv and 15mA filament current
- Careful specimen alignment for each sample

5.4.2. Data Reduction

The background is measured at different α and δ positions. This is usually done at two locations of the Bragg angle 2θ = 40° and 60°. At these positions there are no reflections.

Data is obtained for tilt angle α as far as 10° for the reflection technique. After subtracting the measured background from the measured intensities, the textured sample considered is normalized to the random powder sample, by using Eq.(2-5). Taking into account the geometric
defocussing, lines of constant pole density are drawn using Eq.(2-6). The geometric defocussing is evaluated experimentally using a random sample.

The points where a given pole intensity line intersects the trace of the data chart are located. Finally, these points on the pole figure are connected to give the isointensity contour.
6. Methods Of Calculations

The experimental procedures used for gathering the appropriate data have been described in the preceding chapter. These data points will lead to the construction of the direct and the inverse pole figures. However, only the direct pole figures are of interest since they are used to generate the crystallite orientation distribution function. Nevertheless, the measured inverse pole figures will be compared to those calculated (see section 4.4).

The objective of this chapter is the description of the steps necessary to convert the pole figures data to the crystallite orientation distribution function. This will include the computation methods used leading respectively to:

- the coefficients $Q^j_{\xi m}$ when complete pole figures are used
- the texture coefficients $W_{\xi mn}$
- the CODF $w(\psi, \Theta, \varphi)$
- the calculated inverse pole figures $H(\Theta, \varphi)$ and
- the calculated direct pole figures $a_j(\psi, \Theta)$.

6.1 Bases of Computation

It has been outlined in Section 3.6 that the number of pole figures needed to generate the crystallite orientation distribution is function the degree $\lambda$ of the CODF expansion as well as the symmetry of the material considered. This statement is based on the relation between $Q^j_{\xi m}$ and $W_{\xi mn}$ given by Eq.(3-37). In other words, the number of unknown $W_{\xi mn}$ should not exceed the number of coefficients $Q^j_{\xi m}$ known from the pole figure expansion (see Section 3.3.2.1). In the case of hcp symmetry the number of coefficients $W_{\xi mn}$ to calculate is considerably reduced (see Section 3.4). Equation(3-57) will provide a set of equations relating
$Q_{\ell m}^j$ to $W_{\ell mn}$ in the case of hcp. As an example consider $\lambda$, the degree of the expansion, being taken equal to four and then to ten. Eq. (3-57) will give respectively:

$$Q_{\ell m}^j = 2\pi \left( \frac{2}{2 \ell + 1} \right)^{1/2} \frac{W_{\ell m}^0 \rho \cos \chi_j}{(2 \ell + 1)}$$  \hspace{1cm} (6-1)

with \(0 \leq \ell \leq 4\)

and

$$Q_{\ell m}^j = 2\pi \left( \frac{2}{2 \ell + 1} \right)^{1/2} \left[ \frac{W_{\ell m}^0 \rho \cos \chi_j}{(2 \ell + 1)} \cos \frac{k \chi_j}{2} \right]$$  \hspace{1cm} (6-2)

with \(6 \leq \ell \leq 10\)

where $\chi_j$ and $\eta_j$ are the coordinates of the $j^{th}$ plane normal in the coordinate system oxyz fixed in the crystallite.

It can be seen that Eq. (6-1) will provide a set of 6 equations with 6 unknowns $W_{\ell m}^0$ while Eq. (6-2) will give a set of 15 equations with 30 unknowns. Obviously in the first case only one pole figure is needed and in the second case two pole figures are required. Using the same procedure for different values of $\lambda$, the results given in Table 8 can be verified. It should be noted that for $\lambda = 0$, $W_{000}$ has a constant value fixed by the condition of normalization.

Experimental errors are introduced in pole figure measurements. Therefore, an adequate number of pole figures should be used to calculate the coefficient $W_{\ell mn}$. For this purpose, the crystallite orientation distribution function has been expanded to the order of $\lambda = 16$ and consequently 3 pole figures have been used.

Preliminary steps require the computation of the normalized associated Legendre functions $P_{\ell m}^j (\cos \theta)$ as well as the generalized normalized associated Legendre functions $Z_{\ell mn}^j (\cos \theta)$. For the purpose of the computation, the $P_{\ell m}^j (\cos \theta)$ functions are developed in Fourier series [ ],
<table>
<thead>
<tr>
<th>DEGREE OF THE CODF EXPANSION</th>
<th>NUMBER OF POLE FIGURES REQUIRED</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2 \leq \lambda &lt; 6$</td>
<td>1</td>
</tr>
<tr>
<td>$26 \leq \lambda &lt; 12$</td>
<td>2</td>
</tr>
<tr>
<td>$12 \leq \lambda &lt; 18$</td>
<td>3</td>
</tr>
<tr>
<td>$18 \leq \lambda &lt; 24$</td>
<td>4</td>
</tr>
<tr>
<td>$24 \leq \lambda &lt; 30$</td>
<td>5</td>
</tr>
<tr>
<td>$30 \leq \lambda &lt; 36$</td>
<td>6</td>
</tr>
</tbody>
</table>

**TABLE 8**

Relation between the degree $\lambda$ of the CODF expansion and the number of pole figures required for the computation of $w(\psi, \Theta, \phi)$. 
as follows:

\[ P_{\ell m}(\cos \theta) = \sum_{s=0}^{\ell} a_{\ell ms} \cos(s \theta) \]  \hspace{1cm} (6-3)

with \( \ell, m \) and \( s \) are even

The \( Z_{\ell mn}(\cos \theta) \) functions are also developed in Fourier series [ ], as follows:

\[ Z_{\ell mn}(\cos \theta) = \sum_{s=0}^{\ell} d_{\ell mns} \cos(s \theta) \]  \hspace{1cm} (6-4)

where \( \ell \) and \( m \) are even, \( n \) is a multiple of \( 6 \) and \( s \) is an integer.

The Fourier coefficients \( a_{\ell ms} \) and \( d_{\ell mns} \) of the \( P_{\ell m}(\cos \theta) \) and the \( Z_{\ell mn}(\cos \theta) \) functions respectively are then computed. The method used for such computation and the corresponding computer program are presented in appendix C-1.

Once the coefficients \( a_{\ell ms} \) and \( d_{\ell mns} \) are generated, they are stored in file and will be used for further computation.

6.2 Computation Methods for Texture Coefficients \( W_{\ell mn} \)

Two techniques of computing the coefficients \( W_{\ell mn} \) are described in this section. One is applicable when complete pole figures are generated and the other when incomplete pole figures are generated.

6.2.1 Case of Complete Pole Figures

The mathematical method for getting the coefficients \( W_{\ell mn} \) from complete pole figures has been derived in Section 3.3.2. Taking into account the symmetry considerations of hcp materials, the \( W_{\ell mn} \) are obtained from Eq. (3-57). However, the coefficients \( Q_{\ell m}^j \) given by Eq. (3-32) have to be evaluated in order to compute the \( W_{\ell mn} \) coefficients.

The \( Q_{\ell m}^j \) coefficients are evaluated as follows:
- the x-ray data are collected along a spiral path as shown in Fig.
- The pole figure is drawn on an equal area projection (Fig. ).
- The density of poles \( q_j(\phi, \delta) \) is taken at grid points formed by the intersections of parallels of colatitude \( \phi \) and longitude \( \gamma \).
- The coefficients \( Q_{\xi m}^j \) are then evaluated by numerical integration given by:

\[
Q_{\xi m}^j = \left( \frac{1}{2\pi} \right) \sum_{k_1} \sum_{k_2} q_j(\phi_{k_1}, \delta_{k_2}) \int_{\phi_{k_1} - \frac{1}{2}}^{\phi_{k_1} + \frac{1}{2}} \int_{\delta_{k_2} - \frac{1}{2}}^{\delta_{k_2} + \frac{1}{2}} p_{\xi m}(\cos \phi) \sin \phi \, d\phi \, e^{im\delta} \, d\delta
\]

(6-5)

where \( \phi_{k_1} \), \( \phi_{k_1} \) - \( \frac{1}{2} \), \( \delta_{k_2} + \frac{1}{2} \), and \( \delta_{k_2} - \frac{1}{2} \) are the upper and lower limits of \( \phi \) and \( \delta \) for the \( k_1 \)th and \( k_2 \)th intervals respectively.

The approximation done in Eq. (6-5) is to assume that \( q_j(\phi, \delta) \) is constant in the intervals \((\phi_{k_1} - \frac{1}{2}, \phi_{k_1} + \frac{1}{2})\) and \((\delta_{k_2} - \frac{1}{2}, \delta_{k_2} + \frac{1}{2})\). In this study, the intervals chosen are respectively: \( \Delta \phi = 5^\circ \) and \( \Delta \delta = 6^\circ \).

A computer program for that purpose has been written and presented in Appendix C-2.

Once the coefficients \( Q_{\xi m}^j \) are known, they are substituted into Eq. (3-57) to give the coefficient \( W_{\xi mn} \). Since 3 pole figures have been considered and the order of the expansion \( \lambda = 16 \), the values of \( W_{\xi mn} \) for \( 0 \leq \ell \leq 10 \) are calculated through a subroutine using a least-square method (see Appendix C-3) and for \( 12 \leq \ell \leq 16 \) the \( W_{\xi mn} \) coefficients are solved linearly. An appropriate computer program has been written and presented in Appendix C-3.

6.2.2. Case of Incomplete Pole Figure

The mathematical derivation has been given in Section 3.5, see Eq. (3-64) and (3-65). These two equations are solved simultaneously
to generate the coefficients $w_{mn}$ and $N_j$ of the pole figure normalization. No computer program is presented for this case in this study.

6.3 Computational Methods for CODF, Pole Figure and Inverse Pole Figure

Once the coefficients $W_{\ell mn}$ are known the CODF as well as the direct and inverse pole figures can be generated easily.

6.3.1 CODF

The CODF $W(\psi, \Theta, \varphi)$ is obtained after substituting the calculated coefficients $W_{\ell mn}$ into Eq. (3-58) then $W(\psi, \Theta, \varphi)$ is computed for different fixed values of $\varphi$ in the range $0 \leq \varphi \leq 60^\circ$ and $\Theta$ and $\psi$ varying in the range $0$ to $90^\circ$. A computer program based on Eq. (3-58) has been written and presented in Appendix C-4.

6.3.2 Pole Figure

The direct pole figure is calculated from Eq. (3-56), where the coefficients $Q_{\ell m}^j$ are given by Eq. (3-57) when the $W_{\ell mn}$ are known. The appropriate computer program is presented in Appendix C-3. Note that the pole figure for any plane can be calculated.

6.3.3 Inverse Pole Figure

The mathematical details are given in Section 4.4.2. The same computer program C-4 is used to calculate the inverse pole figure. Depending on the direction chosen the appropriate coefficients $W_{\ell mn}$ are computed as follows:

- Normal directions: the same $W_{\ell mn}$ are used.
- Rolling direction: the $W_{\ell mn}$ are calculated from Eq. (4-23).
- Transverse direction: The $W_{\ell mn}$ are computed from Eq. (4-22).
7. RESULTS AND DISCUSSION

The purpose of this chapter is to give some proof of the theory developed in the previous chapters. The emphasis is put on the accuracy of the results and the reliability of the experimental procedures. The latter is a crucial point since it may be a source of large errors.

In Section 4 some applications of the CODF have been outlined; these are examined and reported in this section. In order to carry a constructive discussion all the results are presented first.

7.1. Presentation of the Results

Three pole figures of a Zircaloy plate sample have been measured experimentally by x-ray diffraction. These are: (10\bar{1}0) Fig. (23), (0002) Fig. (24) and (11\bar{2}0) Fig. (25). Only the back reflection technique developed by Schultz [31] was used to generate the pole figures.

In order to check if the CODF describes exactly the main orientation features of the sample considered, pole figures for the sample planes (0002), (10\bar{1}0) and (11\bar{2}0) have been recalculated from the crystallite orientation distribution function. These are given respectively in Fig. (26), (27) and (28). The methodology followed to calculate pole figures from CODF is given in Section 6.

The crystallite orientation distribution function has been calculated at different values of \( \Psi, \Theta, \) and \( \Phi. \) The CODF is presented by section at constant values of \( \Phi \) and with \( \Theta \) and \( \Psi \) varying from 0 to 90\( ^\circ \). Only three sections taken at constant values of \( \Phi \) of 0\( ^\circ \) and 60\( ^\circ \) respectively presented in Fig. (29), (30).

The inverse pole figure in the normal direction of the sample has been measured experimentally, Fig. (31). The inverse pole figure in the
FIGURE 23

MEASURED (10\text{10}) POLE FIGURE FOR PLATE SAMPLE OF ZIRCALOY
FIGURE 24

MEASURED (0002) POLE FIGURE FOR PLATE SAMPLE OF ZIRCALOY
FIGURE 29

MEASURED (11\overline{2}0) POLE FIGURE FOR

PLATE SAMPLE OF ZIRCALOY.
FIGURE 26
CALCULATED (1010) POLE FIGURE FOR PLATE SAMPLE OF ZIRCALOY
FIGURE 27

CALCULATED (0002) POLE FIGURE FOR PLATE SAMPLE OF ZIRCALOY
FIGURE 28

CALCULATED (11\overline{2}0) POLE FIGURE FOR PLATE SAMPLE OF ZIRCALOY
FIGURE 29
SECTION OF CODF TAKEN AT $\Phi = 0$ FOR PLATE SAMPLE OF ZIRCALOY
FIGURE 30

SECTION OF CODF TAKEN AT $\varphi = 60^\circ$ for PLATE SAMPLE OF ZIRCALOY
same direction has been, also, calculated from the CODF, Fig. (32).

The normalized associated Legendre functions \( P_{\xi m} \) as well as the generalized associated Legendre functions \( Z_{\xi mn} \) are expanded in Fourier series to the sixteenth order (see Appendix C-1). The appropriate Fourier coefficients for the hcp symmetry considered have been calculated and tabulated in Appendix (C-1).

The correcting curves for the geometric defocussing have been generated for the plane \((10\bar{1}0)\) and \((11\bar{2}0)\). These two curves are presented respectively in Figs. (33 and 34). On the same graphs the corresponding theoretical curves Eq. (2-8) and (2-9) have been drawn.

7.2. Discussion of the Results

7.2.1. Measured and Calculated Pole Figures

Good agreement between the measured pole figures Fig. (24-26) and those calculated from the CODF Fig. (27-29) have been obtained. Some differences are recorded for the basal pole figure (0002). The calculated pole figure (0002) shows some high intensities at locations not revealed by measured pole figures. However, the essential features of the pole density are revealed by both pole figures.

It should be noted that incomplete pole figures have been used. Since the pole densities have been recorded for values of tilt angle as far as \(85^\circ\), it appeared logical to consider a gradient of texture toward the outer region of the pole figure. Following this procedure an approximate complete pole figure may be obtained. Using such method the CODF has been generated. This method is not rigorous and leads to some discrepancies between the measured and calculated pole figures.

7.2.2. Inverse Pole Figures

Only one case has been considered. The purpose was to check if the
FIGURE 31
MEASURED INVERSE POLE FIGURE IN THE NORMAL DIRECTION
FIGURE 32

CALCULATED INVERSE POLE FIGURE IN THE NORMAL DIRECTION
FIGURE 33  
THEORETICAL AND EXPERIMENTAL CURVES FOR  
GEOMETRICAL DEFOCUSING OF X-RAY BEAM  
FOR THE PLANE (10\bar{1}0)
THEORETICAL AND EXPERIMENTAL CURVES FOR GEOMETRICAL DEFOCUSING OF X-RAY BEAM FOR THE PLANE (1\bar{1}20)

FIGURE 34
theoretical predictions would meet the experimental results. By comparing Fig.31 and Fig 32, the same features are presented by both methods. However, more details are obtained by the series expansion. This is an important point since the inverse pole figure is usually used to calculate the fraction of basal poles oriented parallel to the reference direction. Experimentally, the details cannot be completely obtained.

7.2.3. Texture Coefficients

Following the above discussion an attempt was made to correlate the texture coefficients \( T_{200} \) and \( T_{220} \) defined by Eq. (4-8, 4-9) and the \( f \)-parameter defined by Kearns 53 has been tried. The values found for the coefficient \( T_{200} \) were close to those found for the \( f \)-parameter. Unfortunately, not enough data was available, therefore no conclusion will be drawn here.

7.2.4. Data accuracy

Pole figures are expressed as multiples of a random sample. If the random sample considered were absolutely random, and if the measured intensities were accurate, the integration of the pole density over all the space should be unity. This integration can be calculated through the computer program presented in C-2. For the three pole figures considered the results were larger than 3. Such deviation from one is attributed to the fact that the measured intensities are too large. Moreover the randomness of the sample considered as random is questionable.

It should be noted that all the measured intensities are corrected for the geometric defocusing and the background intensities. A small error in the measured background intensity may give a large error in the pole density. The geometric defocusing curves for the planes (1010) and (1120) have been evaluated experimentally. Several runs have been
<table>
<thead>
<tr>
<th>Tilt Angle $\phi$</th>
<th>Defocussing Factor $(I\phi/I\phi = 0)^*$</th>
<th>Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.0</td>
<td>0.000</td>
</tr>
<tr>
<td>10</td>
<td>1.0</td>
<td>0.007</td>
</tr>
<tr>
<td>20</td>
<td>0.9988</td>
<td>0.017</td>
</tr>
<tr>
<td>30</td>
<td>0.9889</td>
<td>0.027</td>
</tr>
<tr>
<td>40</td>
<td>0.9364</td>
<td>0.036</td>
</tr>
<tr>
<td>50</td>
<td>0.9206</td>
<td>0.022</td>
</tr>
<tr>
<td>60</td>
<td>0.8356</td>
<td>0.017</td>
</tr>
<tr>
<td>70</td>
<td>0.6367</td>
<td>0.051</td>
</tr>
<tr>
<td>75</td>
<td>0.4496</td>
<td>0.043</td>
</tr>
<tr>
<td>80</td>
<td>0.2415</td>
<td>0.09</td>
</tr>
</tbody>
</table>

**TABLE 9**

Experimental values of the geometric defocussing factor $\left( \frac{I\phi}{I\phi = 0} \right)$ as function of tilt angle $\phi$ for the plane $(11\bar{2}0)$.

* Mean values of 5 runs.
<table>
<thead>
<tr>
<th>Tilt Angle $\phi$</th>
<th>Defocussing Factor $(I\phi/I\phi = 0)^*$</th>
<th>Standard Deviation $\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.0</td>
<td>0.000</td>
</tr>
<tr>
<td>10</td>
<td>.9970</td>
<td>0.014</td>
</tr>
<tr>
<td>20</td>
<td>.9854</td>
<td>0.030</td>
</tr>
<tr>
<td>30</td>
<td>.9556</td>
<td>0.029</td>
</tr>
<tr>
<td>40</td>
<td>.9012</td>
<td>0.08</td>
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<tr>
<td>50</td>
<td>.8196</td>
<td>0.09</td>
</tr>
<tr>
<td>60</td>
<td>.6834</td>
<td>0.09</td>
</tr>
<tr>
<td>70</td>
<td>.4541</td>
<td>0.08</td>
</tr>
<tr>
<td>75</td>
<td>.3017</td>
<td>0.075</td>
</tr>
<tr>
<td>80</td>
<td>.1579</td>
<td>0.09</td>
</tr>
</tbody>
</table>

**TABLE 10**

Experimental values of the geometric defocussing factor $\frac{I\phi}{I\phi = 0}$ as function of tilt angle $\phi$ for the plane (1010)

* Mean values of 5 runs
considered. The geometric defocussing factors have been calculated by taking an average of five values obtained experimentally at different tilt angles $\phi$. The standard deviations presented in table 9 and 10 show that as $\phi$ increases, the scatter of the results increases. Comparisons between experimental geometric defocussing curves and theoretical curves as predicted by Feng 40 are not in good agreement. However, all the curves generated in the range of $0 \leq \phi \leq 65^\circ$ are better described by curves given by:

$$\frac{I_\phi}{I_{\phi=0}} = 1 - Ke^{c\phi}$$

where $K$ and $c$ can be evaluated by a least square method. However, for $\phi$ larger than 65, mean values of the experimental results are more appropriate.

As the Bragg angle increases the defocussing effect decreases. This is well illustrated by Fig (35). Furthermore by comparing table 9 and 10 the scatter of the measured intensities decreases. It follows that as the Bragg angle increases more accurate pole figures may be obtained. This is true as long as there are no overlapping peaks. The diffracted intensities of two peaks may overlap on each other, this can cause serious errors in the experimental measurements. For that purpose some care must be taken when pole figures measurements are performed. The detector should be centered exactly at the maximum of the intensity of the peak considered.

The order of the expansion of the crystallite orientation distribution function has been taken only to the order of 16. In the case of a very sharp texture, the order 16 of the expansion may not be sufficient to
FIGURE 35
COMPARISON OF EXPERIMENTAL CURVES FOR
GEOMETRICAL DEFOCUSING OF X-RAY BEAM
FOR THE PLANE (10\bar{1}0), (0002), (1\bar{1}20).
describe exactly the texture. If the order of the expansion is taken more than 20 the order of magnitude of the coefficients \( W_{\zeta mn} \) will be on the same order of magnitude of the experimental errors. And we should keep in mind that a higher order will lead to longer computations and probably to approximately the same results. Therefore it would be more appropriate to take into account more pole figures than needed to generate the CODF. In that case the coefficients \( W_{\zeta mn} \) will be calculated through a least square method, the experimental errors are then minimized and more accurate results can be obtained.

The CODF has been constructed for \( \phi = 0 \) and \( \phi = 60 \). For these two positions, the CODF exhibits exactly the same features. In other words the symmetry considered in section 3-4 is respected.
8. CONCLUSIONS AND SUGGESTIONS FOR FURTHER WORK

During the fabrication of Zircaloy tubing and plates marked preferred orientations are introduced. Consequently the mechanical properties of such material are anisotropic. In order to predict the mechanical behaviour of Zircaloy tubing used as fuel cladding in light water nuclear reactors, knowledge of the crystallite orientation distribution function is of importance.

It has been pointed in section 2 that creep, irradiation growth, stress corrosion cracking as well as hydride are strongly influenced by Crystallographic texture. The knowledge of the CODF will contribute to a better prediction of the mechanical properties of Zircaloy.

The full description of preferred orientation requires three angles. The goal of this research was to derive such function and to write the appropriate computer program generating it. In order to do so the following steps were performed:

- Review of the procedures for the quantitative characterization of Crystallographic textures of Zircaloy
- Derivation of the crystallite orientation distribution function for Zircaloy.
- A computer program was written in Fortran IV in order to generate the codf.
- A method of getting the codf in the case of incomplete pole figure was also examined.
- Direct applications of the codf were also examined. Furthermore, two texture coefficients of interest for Zircaloy are introduced.

The crystallite orientation distribution function can be generated from several plane normal orientation distributions. Good agreement between the series expansion and the experiments have been recorded.
Following the previous discussion the measured pole figures are not correctly normalized. The main reason for this effect is attributed to the random sample, and the corrected intensities.

The accuracy to which the CODF can be determined is limited only by the experimental error in measuring x-ray intensities over the stereographic coordinates. The order of expansion of the CODF is not required to be greater than 16 or 18. For greater than 20 the order of magnitude of the terms $W_{\text{mn}}$ is on the same order of the experimental uncertainties.

In order to improve the accuracy of the CODF, emphasis should be put on the experimental procedures for gathering the appropriate data.

It has been pointed out that the incomplete pole figure could be used to generate the CODF. The mathematical bases needed for such computation have been given in Section 3-4. The computational methods are much longer than for the case of complete pole figures. However, in the case where only incomplete pole figures are generated, such methods will allow the computation of complete pole figures which are required for the quantitative characterization of crystallographic textures. Some more work should be done on using that method.

Since inverse pole figures can be generated from the codf, a better evaluation of the f-parameter can be performed. An attempt to correlate the f-parameter with the texture coefficients $T_{200}$ and $T_{220}$ should be tried.
MATHEMATICAL APPENDIX
A.1. Legendre Functions

The Legendre differential Equation is given by

\[ (1-x^2) \frac{d^2 y}{dx^2} - 2x \frac{dy}{dx} + \ell (\ell +1)y = 0 \]  

(A-1)

The points \( x = \pm 1 \) are regular singular points. The solution under a series expansion can be written as

\[ y = \sum_{m=0}^{\infty} c_m x^m = c_0 + c_1 x + c_2 x^2 \ldots \]  

(A-2)

After substituting Eq. (A-2) in Eq. (A-1), a recurrence relation between the coefficients \( c_r \) is obtained. This is

\[ \frac{c_m + 2}{c_m} = \frac{(m + \ell + 1)(m - \ell)}{(m+2)(m+1)} \]  

(A-3)

Two sets of coefficients are obtained whether \( m \) is odd or even. We note also that

\[ \lim_{m \to \infty} \frac{c_m + 2}{c_m} = 1 \]  

(A-4)

A solution \( y(x) \) which is finite, in the interval \(-1 \leq x \leq 1\), is required with \( n \) as an integer. The resulting solution is a polynomial which, when normalized by the condition \( y(1) = 1 \), is known as Legendre polynomial \( P_\ell(x) \).

For any non-negative integer \( n \), even or odd the polynomial

\[ P_\ell(x) = k \sum_{r=0}^{\ell} (-1)^r \frac{(2 \ell - 2r)}{(\ell - r) r} \frac{x^{\ell - 2r}}{(\ell - 2)!} \]  

(A-5)

is solution of Legendre's equation. The constant \( k \) is determined by the normalization condition.

It should be noted that \( P_\ell(x) \) can be written also as

\[ P_\ell(x) = \frac{k}{\ell !} \left( \frac{d}{dx} \right)^\ell \sum_{r=0}^{\ell} (-1)^r \frac{\ell !}{(\ell - r) r} x^{2\ell - 2r} \]  

(A-6)

or

\[ P_\ell(x) = \frac{k}{\ell !} \left( \frac{d}{dx} \right)^\ell (x^2 - 1)^\ell \]  

(A-7)
It is convention to impose the normalization.

\[ P_{\ell}(1) = 1 \quad \text{for all } \ell \]  \hspace{1cm} (A-8)

After the derivatives have been calculated we get

\[ P_{\ell}(1) = \frac{K_{\ell}}{\ell!} \ell! \quad 2^\ell = 2^\ell K_{\ell} \]

so

\[ K_{\ell} = \frac{1}{2^\ell} \]  \hspace{1cm} (A-9)

the resulting expression

\[ P_{\ell}(x) = \frac{1}{2^\ell \ell!} \left( \frac{d}{dx} \right)^\ell (x^2 - 1)^\ell \]  \hspace{1cm} (A-10)

is called the Rodrigues' Formula for the Legendre polynomials.

Consider the integral defined by

\[ I_{mn} = \int_{-1}^{+1} P_m(x) P_n(x) dx \]  \hspace{1cm} (A-11)

Where \( P_m(x) \) and \( P_n(x) \) are given by Eq. (A-10).

After integrating \( n \) times by part the following conclusions are reached.

\[
I_{mn} = \begin{cases} 
0 & \text{if } m < n \\
\frac{2}{2n + 1} & \text{if } m = n
\end{cases} \]  \hspace{1cm} (A-12)

Thus Eq. (A-11) is written as

\[
\int_{-1}^{+1} P_m(x) P_n(x) dx = \frac{2}{2n + 1} \delta_{mn} \]  \hspace{1cm} (A-13)

where

\[ \delta_{mn} = \begin{cases} 
0 & \text{for } m \neq n \\
1 & \text{for } m = n
\end{cases} \]

if a function \( f(x) \) is continuous and has a finite number of maxima and minima, or if it has in addition a finite number of jump discontinuities,
then the function \( f(x) \) can be expanded in the interval \(-1 \leq x \leq 1\) in series of Legendre polynomials such as

\[
\begin{align*}
f(x) &= \sum_{\ell=0}^{\infty} C_{\ell} P_{\ell}(x) \\
(A-14)
\end{align*}
\]

After multiplying both sides of Eq.\( (A-14) \) by \( P_{m}(x) \) and integrating from \(-1\) to \(+1\) and using Eq.\( (A-13) \) the coefficients \( C_{m} \) can be evaluated as follows:

\[
C_{\ell} = \frac{2\ell + 1}{2} \int_{-1}^{+1} P_{\ell}(x) f(x) \, dx
\]

\[
(A-15)
\]

the Legendre polynomial \( P_{\ell}(x) \) are calculated from Eq.\( (A-10) \). Some values of \( P_{\ell}(x) \) are presented below:

\[
\begin{array}{ll}
\ell = 0 & P_{0}(x) = 1 \\
\ell = 1 & P_{1}(x) = x \\
\ell = 2 & P_{2}(x) = \frac{3x^2 - 1}{2} \\
\ell = 3 & P_{3}(x) = \frac{5x^3 - 3x}{2}
\end{array}
\]

When normalized these values are multiplied by the factor

\[
\sqrt{\frac{2\ell + 1}{2}}
\]

**A.2. Associated Legendre Functions**

The associated Legendre functions are solutions of the following differential equation

\[
(1-x^2) \frac{d^2v}{dx^2} - 2x \frac{dv}{dx} + \left[ \ell (\ell + 1) \frac{m^2}{1-x^2} \right] v = 0
\]

\[
(A-16)
\]

Note if \( m = 0 \) Eq.\( (A-16) \) is reduced to Eq.\( (A-1) \).

Let \( y = v \left(1-x^2\right)^{m/2} \), the equation \( (A-16) \) is then reduced to

\[
(1-x^2) \frac{d^2v}{dx^2} - 2x (m+1) \frac{dv}{dx} + \left[ \ell (\ell + 1) - m(m+1) \right] v = 0
\]

\[
(A-17)
\]

By taking \( v \) under the form of series expansion
\[ v = \sum_{r=0}^{\infty} C_r x^r \]  \hspace{1cm} (A-18)

A recurrence relation for the coefficients \( C_r \) is obtained as:

\[ \frac{C_r + 2}{C_r} = \frac{(r + m - \ell)(r + m + \ell + 1)}{(r + 2)(r + 1)} \]  \hspace{1cm} (A-19)

A bounded solution exists only if \( r \) and \( m \) are such that one series terminates after some term \( x^r \). This condition is:

\[ \ell - m = r = \text{an integer} \geq 0 \]  \hspace{1cm} (A-20)

Usually in physical applications \( r \) and \( m \) are both integers. It may be verified that \( y \) is then simply at constant times equal to

\[ P_\ell^m(x) = (1 - x^2)^m \left( \frac{d}{dx} \right)^m P_\ell(x) \]  \hspace{1cm} (A-21)

which is called an associated Legendre function. The orthogonality-normalization integral for associated Legendre function is

\[ \int_{-1}^{+1} P_\ell^m(x) P_{\ell'}^m(x) \, dx = \frac{(\ell + m)!}{(\ell - m)!} \frac{2}{2\ell + 1} \delta_{\ell \ell'} \]  \hspace{1cm} (A-22)

where

\[ \delta_{\ell \ell'} = \begin{cases} 0 & \text{if } \ell \neq \ell' \\ 1 & \text{if } \ell = \ell' \end{cases} \]

the Associated Legendre functions with \( m \) fixed, are also a complete set of orthogonal functions. An arbitrary function \( f(x) \) on the interval \( -1 \leq x \leq +1 \) may be expanded in a series of the form

\[ f(x) = \sum_{\ell=m}^{\infty} c_\ell P_\ell^m(x) \]  \hspace{1cm} (A-23)

Some values of associated Legendre polynomials are calculated
through Eq.(A-21). These are

\[ \ell = 0 \quad m = 0 \quad P_{00}(x) = P_0(x) = 1 \]
\[ \ell = 1 \quad m = 0 \quad P_{10}(x) = P_1(x) = x \]
\[ m = 1 \quad P_{11}(x) = \sqrt{1 - x^2} \]
\[ \ell = 2 \quad m = 0 \quad P_{20} = P_2(x) = (3x^2 - 1)/2 \]
\[ m = 1 \quad P_{21} = 3x \sqrt{1 - x^2} \]
\[ m = 2 \quad P_{22} = 3 (1 - x^2) \]

When the normalized associated Legendre functions are used the
associated Legendre functions are multiplied by \( \sqrt{(\ell - m)!/2} \) \( \sqrt{(\ell + m)!} \) and
the right hand side of Eq.(A-22) is only equal to \( \delta_{\ell \ell'} \).

A.3. Spherical Harmonics

Consider the Laplace equation in spherical coordinates
\[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \varphi^2} = 0 \]  
(A-24)

we can look for the solution under the form
\[ \psi(r, \theta, \varphi) = R(r) \Theta(\theta) \Phi(\varphi) \]

The substitution of Eq.(A-25) into Eq.(A-24) gives the following set of
equations.
\[ \frac{d^2 \phi}{d\varphi^2} + m^2 \phi = 0 \]  
(A-26)
\[ \frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d \Theta}{d\theta} \right) + \left[ n(n+1) - \frac{m^2}{\sin^2 \theta} \right] \Theta = 0 \]  
(A-27)
\[ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) - \left( \frac{n(n+1)}{r^2} \right) R = 0 \]  
(A-28)

Equation A-26 has a solution \( \phi = e^{im\varphi} \) and Eq. (B-5) is the
differential equation for the associated Legendre function. The combined
\( \Theta (\theta) \phi (\varphi) \) are known as spherical harmonics and are written as
\[
Y_{\ell m}(\theta, \varphi) = \Theta_{\ell m}(\theta) \phi_{m}(\varphi)
\]  
(A-29)

These functions are eigen functions for the two dimensional surface
of the sphere, being mutually orthogonal. Any function which is continuous
and with its derivatives to the second order or the sphere may be expanded
in an absolutely and uniformly convergent series in terms of the spherical
harmonics. If \( g(\theta, \varphi) \) is this function we can write
\[
g(\theta, \varphi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} C_{\ell m} Y_{\ell m}(\theta, \varphi)
\]  
(A-30)

\[
\int_{0}^{2\pi} \int_{0}^{\pi} Y_{\ell m}(\theta, \varphi) Y_{\ell' m'}(\theta, \varphi) \sin \theta d\theta d\varphi = \delta_{\ell \ell'} \delta_{mm}
\]  
(A-31)

the \( Y_{\ell m}(\theta, \varphi) \) can also be expressed as
\[
Y_{\ell m}(\theta, \varphi) = (-1)^m \frac{1}{\sqrt{2\pi}} \left[ e^{im\varphi} P_{\ell m}(\cos \theta) \right]
\]  
(A-32)

where \( P_{\ell m}(\cos \theta) \) are the normalized associated Legendre functions.

The coefficients \( C_{\ell m} \) of Eq.(30)are obtained after multiplying both
sides of Eq.(30)by \( Y_{\ell m}^*(\theta, \varphi) \) and integrating over all the space
\[
C_{\ell m} = \int_{0}^{2\pi} \int_{0}^{\pi} g(\theta, \varphi) Y_{\ell m}^*(\theta, \varphi) \sin \theta d\theta d\varphi
\]  
(A-33)


A.4.1. Definition

The concept of group is a generalization of the properties of a large
number of systems of mathematical interest; such systems as the set of all
permutations of \( n \) objects, the set of all rotations of a rigid body, etc.
The strict definition of group is a set of objects, which are the elements of the group, among which one kind of operation is defined, called multiplication. This multiplication specifies, for every two elements of the group, a third element of the group, the product which must exhibit the following characteristics.

- associativity \((AB)C = A(BC)\)
- unit element \(EA = AE = A\)
- every element \(A\) has reciprocal noted \(A^{-1}\)

The number of elements in a group constitute its order.

A-4.2. Group Representation Theory

If we can assign to each element of the group an operator \(T(x)\) in some linear space \(L\) in such a way that the product of any two elements of the group corresponds to the product of the operators, that is

\[
T(x_1) \cdot T(x_2) = T(x_1 x_2)
\]

(A-34)

The operator \(T(x)\) is called a representation of the group. The operators \(T(x)\) are often expressed in terms of square matrices. The dimensionality of the representation is the same as that of the matrix. By choosing a definite coordinate system in the space \(R^n\), each transformation \(T(x)\) corresponds to a square non singular matrix. The orthogonal unit vectors which establish this coordinate system are called the basis of the representation.

For example, let us consider the set of all sufficiently well behaved functions on the surface of a sphere. The spherical harmonics form a complete orthogonal set. Therefore, a given function may be represented by a vector in function space whose basis vectors are the spherical harmonics.
If the coordinate system is replaced by another which is obtained from the first coordinate system by a transformation $s$, then the group element will be represented by the transformation
\[ S T(x) S^{-1} \]  
(A-35)

In the example considered previously a rotation of the sphere will induce linear transformations in this function space; these will give a representation of the rotation group.

If we consider a representation based on a space $R$, this representation is called irreducible if $R$ contains no subspace other than itself and the null space which is invariant under the transformation $T(x)$ representing the group $G$. The representation of degree $2\ell + 1$ whose basis is the set of spherical harmonics is irreducible.

A.4.3. The Rotation Group in Three Dimensions and Generalized Spherical Harmonics

The group of all real linear homogeneous transformation on an $n$-dimensional space which preserve the distance between two points, such as rotations and reflections about the origin, is called the orthogonal group $O(n)$. It corresponds to the set of all real $n \times n$ orthogonal matrices.

The group $O(3)$ of real orthogonal in three dimensions is a three parameter group. It consists of all transformations with real coefficients which leave
\[ x^2 + y^2 + z^2 \] invariant.

The matrix $A$ of an orthogonal transformation must satisfy
\[ AA^t = 1 \]
\[ A^t = \text{transpose of } A \]

since
\[ \det A^t = \det A \]

so

\[ \det A^t A = (\det A)^2 = 1 = \det A = \pm 1 \quad (A-38) \]

In the case of \( \det A = +1 \) this will correspond to pure rotations.

Any rotation of a rigid body may be symbolized by three real numbers as the Euler angles chosen previously.

The operators \( D(g) \) form a continuous group which is isomorphic to the continuous group of rotations \( g \). This means that if \( g = g_1 \cdot g_2 \), then

\[ D(g) = D(g_1) \cdot D(g_2) \quad (A-39) \]

The representation of the group of operators \( D(g) \) is the group of matrices with \( 2\ell + 1 \) lines and columns each.

\( D_{\ell mn}(g) \) is a function of the rotation \( g \), in our case the rotation will be specified by the Euler angles.

The statement that \( 2\ell + 1 \) functions \( f_{\ell m}(\psi, \theta) \) for the basis of the representation of the group of operator \( D(g) \) means that the application of the operator \( D(g) \) to any of \( 2\ell + 1 \) functions \( f_{\ell m}(\psi, \theta) \) gives a linear combination of these \( 2\ell + 1 \) functions, so

\[ f_{\ell m}(\psi', \theta') = D(g) \cdot f_{\ell m}(\psi, \theta) = \sum_{n=-\ell}^{+\ell} D_{\ell mn}(g) \cdot f_{\ell, n}(\psi, \theta) \quad (A-40) \]

The function \( D_{\ell mn}(g) \) are called the generalized spherical functions.

In the basis of spherical functions \( \varphi_{\ell m}(\psi, \theta) \) \( D_{\ell mn}(g) \) are written as

\[ D_{\ell mn}(\psi, \theta, \varphi) = e^{i m \varphi} \varphi_{\ell mn}(\cos \theta) e^{i n \varphi} \quad (A-41) \]

In a case of \( g \) is a rotation of radius vector \( r \) for a fixed system of axes we replace in the right hand side \( \psi \) by \( -\psi; \theta \rightarrow -\theta; \varphi \rightarrow -\varphi \)

The functions \( D_{\ell, m, n}(g) \) are orthogonal and obey the following
\[ \int D_{\ell mn}'(g) D_{\ell' m' n'}(g) \, dg = \frac{2}{2\ell + 1} \delta_{\ell\ell'} \delta_{mm'} \delta_{nn'} \]  \hspace{1cm} (A-42)

Due to that any function \( F(g) = F(\psi, \theta, \varphi) \) can be expanded in generalized spherical harmonics functions as follows:

\[ F(g) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} \sum_{n=-\ell}^{+\ell} C_{\ell mn} D_{\ell mn}(g) \]  \hspace{1cm} (A-43)

Note \( D_{0,0,0}(g) = 1 \)

This section is concluded by listing some properties of the generalized associated legendre functions \( P_{\ell mn}(x) \). These are:

\[ P_{\ell, m, n,}(x) = P_{\ell, n, m}(x) \]

\[ P_{\ell mn}(x) = P_{\ell, mn}(x) \]

\[ P_{\ell mn}(1) = S_{m, n} \]

\[ P_{\ell mn}(-1) = (-1)^{\ell} S_{m, -n} \]

\[ P_{\ell m0}(x) = P_{\ell m}(x) \]

\[ P_{\ell 00}(x) = P_{\ell}(x) \]
- B -

CRYSTALLOGRAPHIC INDICES
B.1. Indices of Directions

The primitive unit cell of hcp is defined by a 3-axis system based on the vectors \( \hat{a}_1, \hat{a}_2 \) and \( \hat{c} \) (Fig. B-1-a). Any direction \( \hat{d}_3 \) will have 3 indices U, V, W, given by

\[
\hat{d}_3 = U\hat{a}_1 + V\hat{a}_2 + W\hat{c}
\]  

(B-1)

The angles between the vectors \( \hat{a}_1, \hat{a}_2 \) and \( \hat{c} \) are respectively:

\( (\hat{a}_1, \hat{c}) = (\hat{a}_2, \hat{c}) = 90^\circ \) and \( (\hat{a}_1, \hat{a}_2) = 120^\circ \) (Fig. B-1-a).

The indices U, V, W based on the 3-axis system are known as Miller indices.

Instead of the above coordinate system, a Cartesian coordinate system is defined by 3 unit vectors \( \overrightarrow{0x}, \overrightarrow{0y}, \overrightarrow{0z} \) with \( (\hat{a}_1, \overrightarrow{0x}) = 30^\circ \),

\( (\hat{a}_2, \overrightarrow{0y}) = (\hat{c}, \overrightarrow{0z}) = 0^\circ \) (Figures B-1-b and B-1-c). The indices \( x, y, z \) in the oxyz system of coordinates are related to the Miller indices U, V, W by:

\[
\begin{bmatrix}
x \\
y \\
a
\end{bmatrix} = \begin{bmatrix}
\frac{\sqrt{3}}{2} & 0 & 0 \\
-\frac{1}{2} & 1 & 0 \\
0 & 0 & \frac{c}{a}
\end{bmatrix} \begin{bmatrix}
U \\
V \\
W
\end{bmatrix}
\]  

(B-2)

where a and c are the lattice parameters of the hexagonal close packed structure considered.

However in the case of hcp, it is customary to represent a direction by 4-indices \( u, v, t, w \) based on 4-axis system with vectors \( \hat{a}_1, \hat{a}_2, \hat{a}_3 \) and \( \hat{c} \) (Fig. B-1-d). Since \( (\hat{a}_1, \hat{a}_2) = (\hat{a}_2, \hat{a}_3) = (\hat{a}_3, \hat{a}_1) = 120^\circ \) the vector \( \hat{a}_3 \) is redundant and related to \( \hat{a}_1 \) and \( \hat{a}_2 \) by
\[ \hat{a}_3 = - (\hat{a}_1 + \hat{a}_2) \]  \hspace{1cm} (B-3)

In such a system a direction \( \hat{d}_4 \) is given by

\[ \hat{d}_4 = u\hat{a}_1 + v\hat{a}_2 + t\hat{a}_3 + w\hat{c} \]  \hspace{1cm} (B-4)

with the impose condition

\[ u + v + t = 0 \]  \hspace{1cm} (B-5)

The indices \( u, v, t, w \) based on the 4-axis hexagonal system are known as Miller-Bravais indices \( [uvtw] \). A direction will be represented by [uvtw].

By substituting Eq. (B-3) into Eq. (B-4) and equating the result to Eq. (B-1), relations between Miller indices \( U, V, W \) and Miller-Bravais indices \( u, v, t, w \) are obtained, these are:

\[ U = u - t; \quad V = v - t; \quad W = w \]  \hspace{1cm} (B-6)

or

\[ u = \frac{1}{3} (2U - V) \]  \hspace{1cm} (B-7-a)

\[ v = \frac{1}{3} (2V - U) \]  \hspace{1cm} (B-7-b)

\[ t = - (u + v) \]  \hspace{1cm} (B-7c)

\[ w = W \]  \hspace{1cm} (B-7-d)

Furthermore, \( u, v, t, w \) can be related to the indices \( x, y, z \) in the system of Cartesian coordinates \( oxyz \). Use Eqs. (B-7) and (B-2) to get
\[
\begin{bmatrix}
x \\
y \\
z
\end{bmatrix} = 
\begin{bmatrix}
\sqrt{3} & \frac{\sqrt{3}}{2} & 0 & 0 \\
0 & \frac{3}{2} & 0 & 0 \\
0 & 0 & 0 & \frac{c}{a}
\end{bmatrix}
\begin{bmatrix}
u \\
v \\
t \\
w
\end{bmatrix}
\] (B-8)

or

\[
\begin{bmatrix}
u \\
v \\
t \\
w
\end{bmatrix} = 
\begin{bmatrix}
\frac{1}{\sqrt{3}} & -\frac{1}{3} & 0 \\
0 & \frac{2}{3} & 0 \\
-\frac{1}{\sqrt{3}} & -\frac{1}{3} & 0 \\
0 & 0 & \frac{a}{c}
\end{bmatrix}
\begin{bmatrix}
x \\
y \\
z
\end{bmatrix}
\] (B-9)

B.2. Indices of Planes

The usual method of determining the indices of a plane is done by performing the following steps:

- determine the intercepts of the plane on the respective axes of the direct lattice in multiples of fraction of the unit distance along each axis.

- then take the reciprocals of these values, reduced to the smallest integer having the same ratio. These values will constitute the Miller indices \( (hkl) \) of the plane. If the Miller-Bravais indices \( (hki\ell) \) are used, the condition \( i = -(h + k) \) is imposed.

The direct lattice is based on system of axes \( 0a_1a_2a_3c \) as described in B-1. The indices \( (hki\ell) \) can be also expressed in the orthogonal system of axes \( oxyz \) (Fig. B-1-b and c). Call \( X, Y, \) and \( Z \) the indices of a plane in the \( oxyz \) system of reference. Using the definition of the
indices \((hkl)\) it follows that
\[
(\frac{1}{X})/(1/h) = \cos 30^\circ; \quad (\frac{1}{X})/(1/k) = -\sin 30^\circ; \quad (1/y)/(1/k) = 1
\]
and
\[
(1/2)/(1/\ell) = \frac{c}{a}. \quad \text{In better form this is written as:}
\]
\[
\begin{bmatrix}
  X \\
  Y \\
  Z
\end{bmatrix}
= \begin{bmatrix}
  2/\sqrt{3} & 1/\sqrt{3} & 0 & 0 \\
  0 & 1 & 0 & 0 \\
  0 & 0 & 0 & a/c
\end{bmatrix}
\begin{bmatrix}
  h \\
  k \\
  i \\
  \ell
\end{bmatrix}
\]
\text{(B-10)}
or
\[
\begin{bmatrix}
  h \\
  k \\
  i \\
  \ell
\end{bmatrix}
= \begin{bmatrix}
  \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\
  0 & 1 & 0 \\
  \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\
  0 & 0 & c/a
\end{bmatrix}
\begin{bmatrix}
  X \\
  Y \\
  Z
\end{bmatrix}
\]
\text{(B-11)}

The normal of the \(j\)th plane (Fig. B-1-d) can be specified by 2 angles \(\chi_j\) and \(\eta_j\) (spherical coordinates) with respect to oxyz (coordinate system
fixed in the crystallite). \(\chi_j\) and \(\eta_j\) are given by:
\[
\tan \chi_j = \frac{\sqrt{x^2 + y^2}}{z}
\]
\text{(B-12)}
and
\[
\tan \eta_j = \frac{y}{x}
\]
\text{(B-13)}

Using Equation (B-10), Eq. (B-12) and (B-13) can be written as:
\[ \tan \chi_j = \frac{c}{a} \frac{2}{3} \frac{(h^2 + k^2 + hk)^{\frac{1}{2}}}{L} \]  

(B-14)

and

\[ \tan \eta_j = \frac{k \sqrt{3}}{2h + k} \]  

(B-15)
- C -

COMPUTER PROGRAMS
C.1. Fourier Coefficients for the Normalized Associated Legendre Functions $P_{\ell m}(\cos \theta)$ and the Generalized Associated Legendre Functions $Z_{\ell mn}(\cos \theta)$.

C.1.1 Introduction

For the purpose of the computation the $P_{\ell m}(\cos \theta)$ as well as the $P_{\ell mn}(\cos \theta)$ are developed in fourier series according to

$$P_{2\ell, 2m}(\cos \theta) = \sum_{s=0}^{\ell} a_{2\ell, 2m, 2s} \cos(2s\theta) \quad (C-1-1)$$

and

$$Z_{2\ell, 2m, 2n}(\cos \theta) = \sum_{s=0}^{\ell} c_{2\ell, 2m, 2n, s} \cos(s\theta) \quad (C-1-2)$$

The integrated associated Legendre functions $\int P_{2\ell, 2m}(\cos \theta) \sin \theta d\theta$ are also used to compute the coefficients $Q_{\ell m}^j$ of the pole figure expansion. Using Eq.(C-1-1) we can show that:

$$\int P_{2\ell, 2m}(\cos \theta) \sin \theta d\theta = \sum_{s=0}^{\ell} b_{2\ell, 2m, (2s+1)} \cos(2s+1)\theta \quad (C-1-3)$$

The remainder of this Appendix contains the formulae used to compute the Fourier coefficients $a_{2\ell, 2m, 2s}$, $b_{2\ell, 2m, 2s+1}$, and $c_{2\ell, 2m, 2n, s}$; a computer program; and tables of these coefficients for a degree of expansion $\lambda$ as far as $\lambda = 16$.

C.1.2 Formulae

C.1.2.1. $a_{2\ell, 2m, 2s}$ Coefficients

The Fourier coefficients of the normalized associated Legendre functions are calculated according to the following formulae
\[ a_{2 \ell, 2m, 2s+2} = \frac{2 \ell (2 \ell + 1) - 4s^2 - 8m^2}{\ell (2 \ell + 1) - (s+1)(2s+1)} \cdot a_{2 \ell, 2m, 2s} - \]
\[ - \frac{\ell (2 \ell + 1) - (s-1)(2s-1)}{\ell (2 \ell + 1) - (s+1)(2s+1)} \cdot a_{2 \ell, 2m, 2s-2} \]  
(C-1-4)

The first few terms are given by:

\[ a_{2 \ell, 0, 0} = (2 \ell + 1)^\frac{1}{2} \left[ 4 - \frac{2 \ell}{(\ell)!^2} \right]^2 \]  
(C-1-5)

\[ a_{2 \ell, 2m+2, 0} = \left( \frac{(2 \ell + 2m+1)(2 \ell - 2m)}{(2 \ell - 2m-1)(2 \ell + 2m+2)} \right)^\frac{1}{2} a_{2 \ell, 2m, 0} \]  
(C-1-6)

and

\[ a_{2 \ell, 2m, 2} = \frac{2 \ell (2 \ell + 1) - 8m^2}{\ell (2 \ell + 1) - 1} \cdot a_{2 \ell, 2m, 0} \]  
(C-1-7)

C.1.2.2. \textit{b}_{2 \ell, 2m, 2s+1} coefficients

Since the associated Legendre functions can be developed into Fourier series Eq. (C-1-1), the integrated associated Legendre functions

\[ I = \int p_{2 \ell, 2m}(\cos \theta) \sin \theta d\theta \]  
(C-1-8)

can be evaluated easily. This is done by performing the following steps

(1) substitute Eq. (C-1-1) into Eq. (C-1-8)

(2) integrate and put the terms with the same factor \( \cos (2s+1)\theta \)
to get

\[
I = \left( \frac{1}{2} a_{2\ell,2m,2} - a_{2\ell,2m,0} \right) \cos \Theta + \sum_{s=1}^{\ell-1} \frac{1}{2(2s+1)} \left( a_{2\ell,2m,2s+2} - a_{2\ell,2m,2s} \right) \cos (2s+1) \Theta - \frac{1}{2(2\ell+1)} a_{2\ell,2m,2\ell} \cos (2\ell+1) \Theta \quad (C-1-9)
\]

(3) introduce the coefficients \( b_{2\ell,2m,2s+1} \) defined as follows:

for \( s = 0 \)

\[
b_{2\ell,2m,1} = \frac{1}{2} a_{2\ell,2m,2} - a_{2\ell,2m,0} \quad (C-1-10)
\]

for \( s = 1, \ell-1 \)

\[
b_{2\ell,2m,2s+1} = \frac{1}{2(2s+1)} (a_{2\ell,2m,2s+2} - a_{2\ell,2m,2s}) \quad (C-1-11)
\]

and

for \( s = \ell \)

\[
b_{2\ell,2m,2\ell+1} = -\frac{1}{2(2\ell+1)} a_{2\ell,2m,2\ell} \quad (C-1-12)
\]

where the coefficients \( a_{2\ell,2m,2s} \) are given by Eqs. (C-1-4 to C-1-7).

(4) substitute Eqs. (C-1-10 to C-1-12) into Eq. (C-1-9) to get Eq. (C-1-3).

### C1.2.3. \( c_{2\ell,2m,2n,s} \) Coefficients

The following formulae are used to compute the coefficients \( c_{2\ell,2m,2n,s} \):
for s pair:
\[ c_{2\ell,2m,2n,2s} = \frac{(a_{2\ell,2m,2s})(a_{2\ell,1n,2s})}{a_{2\ell,0,2s}} \] (C-1-13)

for s impair
\[ c_{2\ell,2m,2n,2s+1} = \frac{1}{2} \ a_{2\ell,0,0} \ \frac{(d_{2\ell,2s+1,2m})(d_{2\ell,2s+1,2n})}{(a_{2\ell,2m,0})(a_{2\ell,2n,0})} \] (C-1-14)

with
\[ d_{2\ell,2s+1,2i} = (2\ell-2s-1)^{\frac{1}{2}}(2\ell+2s+2)^{\frac{1}{2}} a_{2\ell,2s+2,2i} - (2\ell+2s+1)^{\frac{1}{2}}(2\ell-2s)^{\frac{1}{2}} a_{2\ell,2s,2i} \] (C-1-15)

where i stands for m or n.

C.1.3. Computer Program

A computer program written in FORTRAN IV is given here. This program computes the values of the Fourier coefficients of \( P_{\ell m}(\cos \Theta) \), \( Z_{\ell mn}(\cos \Theta) \) and \( P_{\ell m}(\cos \Theta) \sin \Theta d\Theta \), according to method presented in Section C-1-2. This program takes into account the consequences of the symmetry properties of hcp material. Consequently, it has the following restrictions:

\[ \ell = 0,2,4... \text{ even} \]
\[ m = 0,2,4... \text{ even} \]
\[ n = 0,6,12... \text{ multiple of 6.} \]

However, it can be adapted to other symmetry by making appropriate changes on \( \ell \), \( m \) and \( n \).

The input data is only the degree of expansion used

Input \( \frac{\lambda}{2} \) (Integer) Format I3
The Fourier coefficients are only computed once. The output is divided into three parts and saved in three different files for further computations.

- The first file stores the Fourier coefficients $a_{2\ell,2m,2s}$ of the normalized associated Legendre functions. These coefficients which constitute the first part of the output of the program are presented in Table C-1. The $a_{2\ell,2m,2s}$ are used for the computation of the $W_{\lambda mn}$ coefficients of the CODF expansion as well as for the calculated pole densities $q_j(\phi,\delta)$.

- The second file stores the coefficients $b_{2\ell,2m,2s}$ of the integrated normalized associated Legendre functions, (See Eq.(C-3)). These coefficients as shown in Table C-2 constitute the second part of the output of the program. The $b_{2\ell,2m,2s}$ are only used to compute the coefficients $Q_{\lambda,m}$ of the pole figure expansion.

- Finally, the third file stores the Fourier coefficients $c_{2\ell,2m,2n,s}$ of the generalized associated Legendre functions. The $c_{2\ell,2m,2n,s}$ presented in Table C-3 form the third part of the program output. These coefficients are used for the computation of the CODF and the inverse pole figures.
<table>
<thead>
<tr>
<th>L₂</th>
<th>N₂</th>
<th>S₂</th>
<th>A</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0.7071067695 × 10⁰</td>
<td>0.7071067695 × 10⁰</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0.3952846530 × 10⁰</td>
<td>0.1185653901 × 10⁰</td>
</tr>
<tr>
<td>0</td>
<td>2</td>
<td>0.4841228222 × 10⁻²</td>
<td>0.4841228222 × 10⁻²</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>0.2983107270 × 10⁻²</td>
<td>0.6629124747 × 10⁻²</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>0.3144470725 × 10⁻²</td>
<td>0.4192562630 × 10⁻²</td>
</tr>
<tr>
<td>0</td>
<td>4</td>
<td>0.4159744784 × 10⁻²</td>
<td>0.5546356825 × 10⁻²</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>0.2489155586 × 10⁻³</td>
<td>0.5228085770 × 10⁻³</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>0.2551239000 × 10⁻³</td>
<td>0.4337105800 × 10⁻³</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>0.2794741180 × 10⁻³</td>
<td>0.1397370590 × 10⁻³</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>0.3764098470 × 10⁻³</td>
<td>0.5676133200 × 10⁻³</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>0.3764098470 × 10⁻³</td>
<td>0.5676133200 × 10⁻³</td>
</tr>
</tbody>
</table>

This table gives the values of the Fourier coefficients of the normalized associated Legendre functions represented here by 'A'.
\[ A = -0.25611785 \times 10^{-5} \]

\[ L_2 = 12 \]
\[ M_2 = 0 \]

\[ S_2 = 0 \]
\[ A = 0.179919839 \times 10^0 \]
\[ 0.364512792 \times 10^0 \]
\[ 0.379706550 \times 10^0 \]
\[ 0.409835364 \times 10^0 \]
\[ 0.467211964 \times 10^0 \]

\[ S_2 = 10 \]
\[ L_2 = 12 \]
\[ M_2 = 2 \]

\[ A = 0.181084360 \times 10^0 \]
\[ 0.348058165 \times 10^0 \]
\[ 0.303766943 \times 10^0 \]
\[ 0.222109255 \times 10^0 \]
\[ 0.844017428 \times 10^0 \]

\[ S_2 = -0.168502183 \times 10^0 \]
\[ -0.9706166 \times 10^0 \]
\[ L_2 = 12 \]
\[ M_2 = 2 \]

\[ A = 0.164818408 \times 10^0 \]
\[ 0.297629486 \times 10^0 \]
\[ 0.956091879 \times 10^0 \]
\[ -0.19041921 \times 10^0 \]
\[ -0.465166142 \times 10^0 \]

\[ S_2 = 10 \]
\[ L_2 = 12 \]
\[ M_2 = 2 \]

\[ A = -0.516851362 \times 10^0 \]
\[ 0.594374429 \times 10^0 \]

\[ S_2 = 0 \]
\[ L_2 = 12 \]
\[ M_2 = 8 \]

\[ A = 0.192012960 \times 10^0 \]
\[ 0.209468334 \times 10^0 \]
\[ -0.183284238 \times 10^0 \]
\[ -0.447197656 \times 10^0 \]
\[ -0.180043900 \times 10^0 \]

\[ S_2 = 10 \]
\[ L_2 = 12 \]
\[ M_2 = 6 \]

\[ A = 0.663313734 \times 10^0 \]
\[ 0.254254563 \times 10^0 \]

\[ S_2 = 0 \]
\[ L_2 = 12 \]
\[ M_2 = 8 \]

\[ A = 0.205013281 \times 10^0 \]
\[ 0.745502742 \times 10^0 \]
\[ -0.419345223 \times 10^0 \]
\[ -0.168525540 \times 10^0 \]
\[ 0.597289441 \times 10^0 \]

\[ S_2 = 12 \]
\[ L_2 = 12 \]
\[ M_2 = 10 \]

\[ A = -0.360325079 \times 10^0 \]
\[ 0.714347395 \times 10^0 \]

\[ S_2 = 0 \]
\[ L_2 = 12 \]
\[ M_2 = 10 \]

\[ A = 0.231286122 \times 10^0 \]
\[ -0.132163490 \times 10^0 \]
\[ -0.413010795 \times 10^0 \]
\[ 0.550689835 \times 10^0 \]
\[ -0.319394719 \times 10^0 \]

\[ S_2 = 10 \]
\[ L_2 = 12 \]
\[ M_2 = 8 \]

\[ A = 0.941152522 \times 10^0 \]
\[ -0.115007350 \times 10^0 \]

\[ S_2 = 0 \]
\[ L_2 = 12 \]
\[ M_2 = 12 \]

\[ A = 0.329201194 \times 10^0 \]
\[ -0.548916071 \times 10^0 \]
\[ 0.343072160 \times 10^0 \]
\[ -0.152475973 \times 10^0 \]
\[ 0.457412439 \times 10^0 \]

\[ S_2 = 10 \]
\[ L_2 = 12 \]
\[ M_2 = 0 \]

\[ A = -0.830769772 \times 10^{-2} \]
\[ 0.520966535 \times 10^0 \]

\[ S_2 = 0 \]
\[ L_2 = 14 \]
\[ M_2 = 0 \]

\[ A = 0.977505450 \times 10^0 \]
\[ 0.337333333 \times 10^0 \]
\[ 0.317607421 \times 10^0 \]
\[ 0.366918420 \times 10^0 \]
\[ 0.400274105 \times 10^0 \]

\[ S_2 = 14 \]
\[ L_2 = 14 \]
\[ M_2 = 2 \]

\[ A = 0.460315081 \times 10^0 \]
\[ 0.590145330 \times 10^0 \]

\[ S_2 = 0 \]
\[ L_2 = 14 \]
\[ M_2 = 2 \]

\[ A = 0.167886796 \times 10^0 \]
\[ 0.326877779 \times 10^0 \]
\[ 0.296552070 \times 10^0 \]
\[ 0.242274818 \times 10^0 \]
\[ 0.157047788 \times 10^0 \]

\[ S_2 = 10 \]
\[ L_2 = 14 \]
\[ M_2 = 2 \]

\[ A = 0.220252891 \times 10^0 \]
\[ -0.220248 \times 10^0 \]
\[ -0.9 \times 10^0 \]
TABLE C-2

This table gives the values of the Fourier coeff.
of the integrated normalized associated Legendre
functions, represented here by "B".

<table>
<thead>
<tr>
<th>L2=</th>
<th>B2=</th>
<th>N2=</th>
<th>B=</th>
<th>L2=</th>
<th>N2=</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0</td>
<td>2</td>
<td>0.353555368E+00</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>2</td>
<td>0.187642267E+00</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
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<td>2</td>
<td>0.726184189E+00</td>
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<tr>
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<td>0.331439997E-01</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>2</td>
<td>0.106215722E+00</td>
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</tr>
<tr>
<td>0</td>
<td>0</td>
<td>2</td>
<td>0.693290713E+00</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>2</td>
<td>0.124487057E-01</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>2</td>
<td>0.382686071E-01</td>
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<td>4</td>
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<tr>
<td>0</td>
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<td>2</td>
<td>0.299157236E+00</td>
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</tr>
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<td>0</td>
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<td>0.165835755E-00</td>
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<td>4</td>
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<tr>
<td>0</td>
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<td>2</td>
<td>0.353941850E-02</td>
<td>0</td>
<td>8</td>
</tr>
</tbody>
</table>
The following table gives the values of the Fourier coefficients of the generalized associated Legendre functions. These are represented here by $c$.

<table>
<thead>
<tr>
<th>$L$</th>
<th>$M$</th>
<th>$N$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.707106769D+00</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
<td>0.395284653D+00</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>0</td>
<td>0.484122822D+00</td>
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<tr>
<td>4</td>
<td>0</td>
<td>0</td>
<td>0.290310727D+00</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>0</td>
<td>0.314447072D+00</td>
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<td>4</td>
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<td>0.415974478D+00</td>
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<tr>
<td>6</td>
<td>0</td>
<td>0</td>
<td>0.740975860D+00</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>6</td>
<td>0.370409847D+00</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>0</td>
<td>0.255123900D+00</td>
</tr>
<tr>
<td>S =</td>
<td>8</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-----</td>
<td>---</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C =</td>
<td>0.0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>L = 8 ; M = 8 ; N = 0</th>
</tr>
</thead>
<tbody>
<tr>
<td>S = 0</td>
</tr>
<tr>
<td>C = 0.353278051D+00</td>
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</table>

<table>
<thead>
<tr>
<th>L = 8 ; M = 8 ; N = 6</th>
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</thead>
<tbody>
<tr>
<td>S = 0</td>
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<tr>
<td>C = 0.418125856D+00</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>L = 1 ; M = 2 ; N = 3</th>
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<tbody>
<tr>
<td>S = 0.222999770D+01</td>
</tr>
<tr>
<td>C = -0.354773337D+00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>L = 5 ; M = 6 ; N = 7</th>
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</thead>
<tbody>
<tr>
<td>S = -0.764102555D+00</td>
</tr>
<tr>
<td>C = -0.764102555D+00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>L = 0</th>
</tr>
</thead>
<tbody>
<tr>
<td>S = 0</td>
</tr>
<tr>
<td>C = 0.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>L = 10 ; M = 0 ; N = 0</th>
</tr>
</thead>
<tbody>
<tr>
<td>S = 0.196243767D+00</td>
</tr>
<tr>
<td>C = 0.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>L = 10 ; M = 0 ; N = 6</th>
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</thead>
<tbody>
<tr>
<td>S = 0</td>
</tr>
<tr>
<td>C = 0.216401330D+00</td>
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</tbody>
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<table>
<thead>
<tr>
<th>L = 10 ; M = 2 ; N = 0</th>
</tr>
</thead>
<tbody>
<tr>
<td>S = 0</td>
</tr>
<tr>
<td>C = 0.198052410D+00</td>
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<table>
<thead>
<tr>
<th>L = 10 ; M = 2 ; N = 6</th>
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</thead>
<tbody>
<tr>
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<tr>
<td>C = 0.190600777D+00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>L = 5 ; M = 6 ; N = 7</th>
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</thead>
<tbody>
<tr>
<td>S = -0.272033042D+00</td>
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<tr>
<td>C = -0.141910156D+00</td>
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</table>

<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>S = 0.996484947D-01</td>
</tr>
<tr>
<td>C = 0.152673893D+00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>L = 0</th>
</tr>
</thead>
<tbody>
<tr>
<td>S = 0</td>
</tr>
<tr>
<td>C = 0.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>S = 0.146501614D+01</td>
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<tr>
<td>C = 0.146580161D+01</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>S = 0</td>
</tr>
<tr>
<td>C = 0.204025094D+00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>L = 10 ; M = 4 ; N = 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>S = 0</td>
</tr>
<tr>
<td>C = 0.224919320D+00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>L = 5 ; M = 6 ; N = 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>S = 0.392696452D+00</td>
</tr>
<tr>
<td>C = 0.116078208D+01</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>S = 0.343871823D+00</td>
</tr>
<tr>
<td>C = 0.408921891D+00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>L = 0</th>
</tr>
</thead>
<tbody>
<tr>
<td>S = 0</td>
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The table contains rows with values for L, M, and N, with some values being 0 and others being non-zero numbers.
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C DIMENSION Y1(11), Y3(11), Y5(11), Z1(2), Z5(11), KQE(11), D(9, 9, 9, 18),
C 1A(10, 10, 10), E(10, 10, 10)
C DOUBLE PRECISION Y1, Y3, Y5, XI, X2, 55, 56, S51, S56, X6, FACT, A, D, TIC, TAC
C INTEGER S2

C HERE STARTS THE COMPUTATION OF THE FOURIER COEFFICIENTS OF THE C NORMALIZED ASSOCIATED LEGENDRE FUNCTIONS, AND THE INTEGRATED C NORMALIZED ASSOCIATED LEGENDRE FUNCTIONS

C READ(5, 100) L
C Y1(1) = SQRT(0.5)
C A(1, 1, 1) = Y1(1)
C WRITE(6, 130) Y1(1)
C Z1(1) = 0.5
C DO 5 J = 1, L
C L5 = 1 + LMAX
C L2 = 2 * (L1 - 1)
C X1 = FACT(L1)/(FACT(L1) + 2)
C X2 = SQRT(FLOAT(L1) - 1)
C Y1(L1) = ((XI/4.)**((FLOAT(L1) - 1.))**2.)*X2
C A(L1, 1, 1) = Y1(L1)
C Y3(L1) = Y1(L1)
C Y5(L1) = Y1(L1)
C DO 6 L = 12*n, L1
C L3 = 12
C M1 = L3 - 1
C U1 = 0 + (FLOAT(M1)**2.)*Y5(L1)
C Y5(L1) = (FLOAT(L1)*(L1 + 1))**2./((FLOAT(L1 + 1)/(L1 + 1)))**2.*Y3(L1)
C A(L1, L3, 1) = Y5(L1)
C Z5(L1) = 0.5
C DO 6 L = 1, L1
C L3 = 13
C IF(L10, LE, 1) GOTO 9
C S41 = FACT(L1 - 1 + L2 + 1) - 6.
C S51 = FACT(L1 + L2 + 1) - 4./S41
C S51 = FACT(L1 + L2) + S51
C Y5(L1) = S51 + Y5(L1)
C A(L1, L3, 2) = Y5(L1)
C Z5(L1) = 0.2*FLOAT(L5(L1) - Y5(L1 - 1))
C IF(L10, LE, 2) GOTO 9
C DO 7 J = 3, L110
C L3 = 13
C S3 = (FLOAT(LS2)**2.)*2.
C LS2 = 2*(L51 - 1)
C S3 = FLOAT(LS2)**2.
C LS2 = (L1 - 1 + L2 + 1 - L51 + L52 + 1)
C S3 = FLOAT(L1 + L2 + 1)**2. - S3*UM/FACT(LS4)
C LS2 = FLOAT(L1 - 1 + L2 + 1 - L51 - L52 + 1)/FACT(LS4)
Y5(L51+1)=Y5(L51)=S5+Y5(L51-1)
A(L1,L1+1)=Y5(L51-1)
Z5(L51)=1/(2.*(FLOAT(L2)+1.*)(Y5(L51-1)-Y5(L51-2))
7 CONTINUE
9 CONTINUE
M2=M1+1
U3=FLOAT((L2+M2+1-1)/(L2-M2-1+1))
X6=SORT(U3)
Y3(LM1+1)=X6+Y3(LM1)
A(L1,L1+1)=Y3(LM1+1)
A(L1,L1+1-)=Y3(LM1+1)
Z5(L1)=1/(2.*(FLOAT(L1)+1.))
J1=J1+L10
J2=J1
J3=L1
IF(L110.GE.5) GOTO 14
GOTO 15
14 J2=0
J3=0
15 CONTINUE
WRITE(6,140) L2,M2,(S2,S2+2,J2,2)
WRITE(32,140) L2,M2,(S2,S2+2,J2,2)
WRITE(32,160) (Z5(M),M=1,J3)
WRITE(6,150) (Y5(M),M=1,J3)
IF(L110.GE.5) GOTO 13
GOTO 6
13 CONTINUE
WRITE(6,170) (S2,S2+10,J1,2)
WRITE(32,170) (S2,S2+10,J1,2)
WRITE(6,150) (Y5(M),M=6,J1)
WRITE(32,160) (Z5(M),M=6,J1)
6 Y5(L1)=Y3(LM1+1)
5 CONTINUE
C HERE STARTS THE COMPUTATION OF THE FOURIER COEFFICIENTS OF THE
C GENERALIZED ASSOCIATED LEGENDRE FUNCTIONS
C
WRITE(31,500) ITITLE
DO 20 120=1,LMAX
J1=J1+1
J10=J1-1
DO 21 121=1,J1
J2=J2+1
DO 22 122=1,J1,3
J3=J3+2*(J3-1)
DO 23 123=1,J1,2
J=J+1
DO 24 144=1,J1/2+1
K=J4=J4+1
DO 25 144=1,J4+1
DI(J1,J2,J3,J444)=A(J1,J2,J444)*A(J1,J3,J444)/A(J1,1,J444)
IF(J22.EQ.0) GOTO 30
20 CONTINUE
21 CONTINUE
22 CONTINUE
23 CONTINUE
24 CONTINUE
25 CONTINUE
C
DUT00560
DUT00570
DUT00580
DUT00590
DUT00600
DUT00610
DUT00620
DUT00630
DUT00640
DUT00650
DUT00660
DUT00670
DUT00680
DUT00690
DUT00700
DUT00710
DUT00720
DUT00730
DUT00740
DUT00750
DUT00760
DUT00770
DUT00780
DUT00790
DUT00800
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DUT01010
DUT01020
DUT01030
DUT01040
DUT01050
DUT01060
DUT01070
DUT01080
DUT01090
DUT01100
KK2+10
11 $F4 = F4 + DBLE(FLOAT(KK2))$
FACT = F4
RETURN
12 FACT = 1.0 DO
RETURN
END
C.2. Computer Program for the Coefficients $Q_{\ell m}^j$

C.2.1. Bases of the Computation

The coefficients $Q_{\ell m}^j$ are computed according to Eq. (6.10), written as:

$$Q_{\ell m}^j = \frac{1}{2\pi} \sum_{k_1=1}^{N_1} \sum_{k_2=2}^{N_2} q_j(\phi_{k_1}, \sigma_{k_2}) \int_{\phi_{k_1} - \frac{1}{2}}^{\phi_{k_1} + \frac{1}{2}} \int_{\sigma_{k_2} - \frac{1}{2}}^{\sigma_{k_2} + \frac{1}{2}} p_{\ell m}(\cos \phi) \sin \phi d\phi \cos m \sigma d\sigma \quad (C-2-1)$$

where:

- $N_1$ and $N_2$ are respectively the number of points considered in the domain of integration of $\phi$ and $\sigma$
- $\phi_{k_1 - \frac{1}{2}}$, $\phi_{k_1 + \frac{1}{2}}$ are the lower and upper limit of the interval considered for the angle $\phi$
- $\sigma_{k_2 - \frac{1}{2}}$, $\sigma_{k_2 + \frac{1}{2}}$ are the lower and upper limit of the interval considered for the angle $\sigma$
- $q_j(\phi_{k_1}, \sigma_{k_2})$ is the pole density at the position $(\phi_{k_1}, \sigma_{k_2})$

In Appendix C.1 the method for computing the integrated associated Legendre functions has been outlined. The Fourier coefficients $b_{2\ell,2m,2s}$ are used for the computation of the $Q_{\ell m}^j$ coefficients as follows:

$$\int_{\phi_{k_1} - \frac{1}{2}}^{\phi_{k_1} + \frac{1}{2}} p_{\ell m}(\cos \phi) \sin \phi d\phi = -2 \sum_{s=0}^{\ell} b_{2\ell,2m,2s} \left( \sin(2s+1) \frac{K}{2} \right) \left( \sin(2s+1) \phi_{k_1} \right) \quad (C-2-2)$$

where the coefficients $b_{2\ell,2m,2s}$ are given by Eq. (C-1-10-C-1-13) and $K$ is defined as:
\[ K = \phi_{k_1+\frac{1}{2}} - \phi_{k_1-\frac{1}{2}} = \frac{\pi}{N_1} \]

It can be shown that

\[ \int_{\delta_{k_2 - \frac{1}{2}}}^{\delta_{k_2 + \frac{1}{2}}} \cos m\delta d\delta = \frac{2 \cos m\delta_{k_2} \sin \left( \frac{mH}{2} \right)}{m} \quad (C-2-3) \]

where \( H \) is defined by:

\[ H = \delta_{k_2 + \frac{1}{2}} - \delta_{k_2 - \frac{1}{2}} = \frac{2 \pi}{N} \quad (C-2-4) \]

\( q_j(\phi_{k_1}, \delta_{k_2}) \) is the pole density at the angular position \( \phi_{k_1} \) and \( \delta_{k_2} \). This is measured experimentally.

**C.2.2. Computer Program**

A computer program based on Eq. (C-2-1) has been written in Fortran IV and presented at the end of this appendix.

Basically, this program has four parts:

- The \( q_j(\phi_{k_1}, \delta_{k_2}) \) are read first and appropriate indices are put.
- Then the coefficients \( b_{2\ell}, 2m, 2s \) are read and the Equation (C-2-2) is then computed for each value of \( \phi_{k_1} \) considered.
- The Equation (C-2-3) is also computed for each value of \( \delta_{k_2} \).
- Finally, the results are taken and put together in Eq. (C-2-1). The latter is then computed and the \( Q_{\ell m} \) are generated.

As input this program needs to know:
(1) First Line
- \( N = \) the number of pole figures considered with the format I3.

(2) Second Line
- \( N_1, N_2 \) Format I3
- \( F \) the number of spaces left to fill the last line of each set
  of data: format I3
- \( \phi_1, \delta_1, H, K \) format FS.2

(3) Next Lines
Then at the beginning of set of data the plane considered the
following must be specified
- \( \text{Ititle: the type of specimen considered} \)
- \( h,k,\ell: \) Miller indices of the plane considered with the format
  3I3.
- The values of the \( Q_j(\phi,\delta) \) written as follows
  8 values per line with the format F5.2.

It is evident that the input data contains also the values of the
\( b_{2\ell}, 2m, 2s+1 \) calculated by the previous computer program (C-1). These
values are added when all the points \( q_j(\phi,\delta) \) are entered.

As an output the program gives the values of the coefficients \( Q_{\ell m} \).
These values are stored in a file for further calculations.
THIS COMPUTER PROGRAM COMPUTES THE
CONSIDERATIONS OF THE WAVE PATTERN EXPANSION.
THESE COEFFICIENTS ARE CALLED IN THE TEXT Q(L,M)
THESE COEFFICIENTS ARE STORED IN A FILE
FOR FURTHER COMPUTATION.
THE INPUT NEEDS THE FOURIER COEFFICIENTS OF
THE NORMALIZED INTEGRATED ASSOCIATED LEGENDRE FUNCTIONS
A AND THE POLE DSNSITY AT DIFFERENT LOCATIONS PHI AND ETA
FOR FURTHER DETAILS SEE APPENDIX C-2

DIMENSION A(3,39),B(3,64),Q(3,39,64),SNK(3,39,66),SIG(3,39,66),
152(10),G(10),A1(3),B1(3),H(3),K(3),U(3,39,70),SUMI(3,39),
2SUMI(3,63),RNOR(3),RDNR(3)
INTEGER E1,0,D1,S2,E3,D5,F1,D6,E30
REAL K,KN
DOUBLE PRECISION Y,X,0.2,ALPHA,BETA,G,TOT,KS1,PHI,
121,ALPHA2,SNK,TSIG
COMMON Z(11,11,11)
C
READ(5,100) N200
WRITE(6,100) N200
DO 50 J36=1,N200
N=J36
READ(5,160) ITITLE
READ(5,200) N1,N2,F1,A1(N),B1(N),H(N),K(N)
WRITE(6,200) N1,N2,F1,A1(N),B1(N),H(N),K(N)
A(N,1)=A1(N)
B(N,1)=B1(N)
E3=(N2+F1)/8-1
DO 10 110=1,N1
10 J10=110
DO 19 J16=1,E3
19 J16=J16+1
J17=J10+7
19 READ(5,300) (U(N,J10,1),1=J16,J17)
E30=E3
READ(5,300) (U(N,J10,1),1=E30,N2)
DO 312 19=1,N2
J9=19
U(N,J9+J2)=U(N,J10,J9)
U(N,J9+J2)=U(N,J10,J9)
312 U(N,38-J10,J9+30)=U(N,J10,J9+30)
10 CONTINUE
50 CONTINUE
READ(5,400) L
WRITE(6,400) L
LMAX=L+1
DO 2 12=1,LMAX
12=L12
READ(5,700) L2
B(J6,J44+1)=B(J6,J44)+H1

44 CONTINUE
SCUK(J6,J4+1,D6+1)=SIG(J6,J4,D8+1)*X*SDUK(J6,J4,D6+1)
A(J6,J4+1)=A(J6,J4)+K1

4 CONTINUE
ROR(D6)={1./ROR(D6)}
WRITE(6,1200) ROR(D6)
Q(J6,L99,M99)=(SDUK(J6,D5,D6+1)*(-2./3.14I592654))*(ROR(D6))

30 CONTINUE
L44=L99
L2=L99-1
IF(L99.GT.5) GOTO 31
GOTO 32

31 L44=6
L2=B
GOTO 32

32 CONTINUE
WRITE(31,1100) (M4,M4+2,L22,2)
WRITE(31,1200) Q(J6,L99,1,I=1,L44)
IF(L99.GT.5) GOTO 33
GOTO 20

33 L33=L99-1
WRITE(31,1400) (M4,M4+10,L33,2)
WRITE(31,1200) Q(J6,L99,1,I=6,L99)

20 CONTINUE

6 CONTINUE

C CFORMATS STATEMENTS
C
100 FORMAT (I3)
160 FORMAT (2X,A50)
200 FORMAT (3(I3),4(F4,2))
300 FORMAT (1X,B(F6,4))
400 FORMAT (14)
700 FORMAT (123,12)
800 FORMAT (123,12)
900 FORMAT (9X,I10,11B17,11B17,11B17)
1000 FORMAT (3X,5D17.9)
1050 FORMAT (4X,4I14)
1100 FORMAT (1X,'Mx=',15X,'O',4(I17))
1200 FORMAT (1X,'Q=',5D17.9)
1300 FORMAT (1X,'L=',12)
1400 FORMAT (1X,'Mx=',5I17)

STOP
END

DCOUBLE PRECISION FUNCTION KSI(N11,N12,K,P)
REAL K
COMMON Z(11,11,1.)
DOUBLE PRECISION ALPHA,BETA,TOT,G(10),Z
G(1)=0.0 DO
DO 66 66 166=1,N11
JG6=166
JG6=2+(JG6-1)
ALPHA=SIGN((FLOAT(JG6+1))*P)
BETA=SIGN((FLOAT(JG6+1))*(K/2.))
TOT=Z(N11,N12,JG6)+ALPHA+BETA
66 CONTINUE

66 G(J66+1)=G(J66)+TOT
KSI=G(211+1)
RETURN
END
DOUBLE PRECISION FUNCTION PHI(N33,H,R)
DOUBLE PRECISION ALPHA2
IF(I33.EQ.1) GOTO 36
S=FLOAT(N33-1)
ALPHA2=((COS(S*R))*(SIN((S*H)/2.))/S
PHI=ALPHA2
RETURN
36 PHI=H
RETURN
END
C.3. Computer Program for the $W_{\xi mn}$ Coefficients and Calculated Pole

Figures

A computer program written in Fortran IV is presented here. This program computes the $W_{\xi mn}$ coefficients and it can also generate the pole figure of any plane.

The computation of the coefficients $W_{\xi mn}$ is based on Eq. (3-57), once the coefficients $Q_{\xi m}$ are known. Two subroutines belonging to the computer library have been used. These are: a least squares subroutine called LLSQF, and subroutine LINV3F for the solution of linear equations.

Since the order of the expansion has been taken to $\lambda = 16$, it is necessary to have at least three different sets of coefficients $Q_{\xi m}$. The subroutine LLSQF is used for $0 \leq \varphi \leq 10$ and for $12 \leq \varphi \leq 16$ the subroutine LINV3F is used. It should be noted that this is true only when $\lambda \leq 16$ and when 3 pole figures are used. If, for example, more than 3 pole figures are used for the same $\lambda = 16$ order of expansion only the subroutine LLSQF should be used. The computed coefficients $W_{\xi mn}$ are stored in a file and can be used for further computations.

It is desired the pole figure $q_{j}(\phi, \delta)$ for the $j^{th}$ plane can be generated from the three dimensional texture coefficients $W_{\xi mn}$. The following steps are performed during the computation of the $q_{j}(\phi, \delta)$ for a given (hki\ell) plane.

1. The spherical coordinates $X_j$ and $\eta_j$ of the plane normal with respect to the crystallite reference system are calculated.

2. The normalized associated Legendre function $P_{\varphi m}(\cos X_j)$ are then generated.

3. The $Q_{\xi m}^j$ are then computed from the $W_{\xi mn}$ coefficients Eq. (3-57).
(4) These coefficients are then plugged into Eq. (3-56) to get the pole density distribution $q_j(\phi, \delta)$.

The $q_j(\phi, \delta)$ are calculated for the values of:

$\phi = 0, 5, 10, \ldots, 90^{\circ}$

and

$\delta = 0, 6, 12, \ldots, 360^{\circ}$

The $W_{mn}$ are also generated using the 3 first steps described earlier. However, the third step is different in the sense that instead of computing the $Q_{2m}^j$, the $W_{mn}$ are computed.

The input should contain:

First line:
- KJ: This number specifies whether or not calculated pole figures are wanted. Format I3
  - KJ = 0 means that the calculated pole figures are not desired
  - KJ = 1 means that the calculated pole figures are desired

Next line:
- KN = the number of pole figures: Format I3
  - hkl: indices of the plane for which the pole figure will be generated. The format used is 3I3

Next lines:
- The next lines contain: the Fourier coefficients $a_{2p,2m,2s}$ of the normalized associated Legendre function; and the output of the program C-2, these are the $Q_{2m}$ coefficients and the corresponding indices hkl.

The output of this program will be:
- $W_{nm}$ coefficients stored in a file
- The $q_j(\phi, \xi)$ appearing at the terminal or printer
THIS COMPUTER PROGRAM COMPUTES THE COEFFICIENTS OF THE C.O.D.F.
EXPANSION W(L,M,N). THE OUTPUT IS STORED IN A FILE FOR FURTHER
COMPUTATION.

DIMENSION Y(10,10,10)
INTEGER K,IA,IP(2),MIER,1J0B,52(10),K1(6),K2(6),K3(6),LU(6),LB(6)
REAL D1,D2,CMAREA(19),THETA(6),UN(6),PHI(6),UL(6),HIC(6),H(2)
DOUBLE PRECISION Y,QU(10,10,10),C(10,10,10),B(6),CPF(63),CPF2(63),
1A[NV13,3],Q2(10),P(10,10,10),X(3),A(3,3),K1(20),XX2(20),XX3(20),
2PQG1,XX4(10),XX5(10),XX6,XX7(10),XX8(10),PFG2,WP(10,10,10),
3XX5(10),XX6(10),XX7(10,10,10),OS(10,10),XXX1,XXX2,CPF(30,65),PD,
4XX9(10,10,10)

C READING OF THE FOURIER COEFFICIENTS OF THE NORMALIZED
C INTEGRATED ASSOCIATED LEGENDRE FUNCTIONS

C READ(5,200) L
WRITE(6,200) L
LMAX=L+1
DO 1 L=1,LMAX
J=L+1
READ(5,300) L2
L1=(L2/2)+1
L200=L11
DO 2 L=1,L11
J2=12
READ(5,300) M2
M1=(J2/2)+1
IFI(L1200,GE,5) GOTO 210
GOTO 220
210 L1200=5
220 READ(5,500) (S2(J),J=1,L1200)
READ(5,600) (Y(L11,M11,J),J=1,L1200)
IFI(L11,GT,5) GOTO 230
GOTO 220
230 READ(5,500) (S2(J),J=6,L11)
READ(5,600) (Y(L11,M11,J),J=6,L11)
32 CONTINUE
IFI(J2,EQ,L11) GOTO 2
READ(5,300) L6
2 CONTINUE
L6
1 CONTINUE
C READ OF J AND Q(J,2L,2M)
DL=(1.59271+2.)/SQRT(3.)
READ(5,700) J
L=TE(34,700) J
DD 3 13=1,J
J3=J3
READ(5,800) K1(J3),K2(J3),K3(J3)
LU(J3)=K1(J3)++*1K2(J3)++*2K1(J3)++*1K2(J3)
IF(K3(J3),EQ,0) GOTO 301
UL(J3)=(SORT(FLOAT(LU(J3))))/FLOAT(K3(J3))
THETA(J3)=ARCCOS(SQRT(1./(UL(J3)+DL+2.)))

TAX00010
TAX00020
TAX00030
TAX00040
TAX00050
TAX00060
TAX00070
TAX00080
TAX00090
TAX00100
TAX00110
TAX00120
TAX00130
TAX00140
TAX00150
TAX00160
TAX00170
TAX00180
TAX00190
TAX00200
TAX00210
TAX00220
TAX00230
TAX00240
TAX00250
TAX00260
TAX00270
TAX00280
TAX00290
TAX00300
TAX00310
TAX00320
TAX00330
TAX00340
TAX00350
TAX00360
TAX00370
TAX00380
TAX00390
TAX00400
TAX00410
TAX00420
TAX00430
TAX00440
TAX00450
TAX00460
TAX00470
TAX00480
TAX00490
TAX00500
TAX00510
TAX00520
TAX00530
TAX00540
TAX00550
GOTO 302
301 THETA(J3) = ARCOS(0.0)
302 CONTINUE
IF (K1(J3).EQ.0) GOTO 196
198 LB(J3) * 2 * K1(J3) * K2(J3)
IF (LB(J3).EQ.0) GOTO 303
UK(J3) = FLOAT(K2(J3))/FLOAT(2 * K1(J3) * K2(J3))
HIC(J3) = (3.0 + 0.5) * UK(J3)
PHI(J3) = ARCOS(SQRT(1./(HIC(J3)**2 + 1.)))
GOTO 304
303 PHI(J3) = ARCOS(0.0)
GOTO 304
196 CONTINUE
IF (K2(J3).EQ.0) GOTO 197
GOTO 198
197 PHI(J3) = 0.0
304 CONTINUE
WRITE(34,800) J3
WRITE(34,1500) THETA(J3), PHI(J3)
DO 4 14 = 1, LMAX
J3 = 14
READ(5,900) Q(J3, J4, M), M = 1, J4
DO 5 15 = 1, J4
J5 = 15
F1 = SQRT(2./((2.*FLOAT(J5-1)+1.)))
F2 = 2.*3.141592654*F1
C(J3, J4, J5) = Q(J3, J4, J5)/F2
5 CONTINUE
4 CONTINUE
3 CONTINUE
C COMPUTATION OF P(2L, 2M, (COS(THETA(J))))
DO 6 16 = 1, 3
J6 = 16
P(J6, 1, 1) = Y(1, 1, 1)
DO 7 17 = 2, LMAX
J7 = 17
DO 8 18 = 1, J7
J8 = 18
G2(1) = 0.0 DB
DO 9 19 = 1, J7
J9 = 19
G2 = (FLOAT(J9-1))+THETA(J6)
G1 = COS(G)
G2(J9+1) = G2(J9) + G1*Y(J7, J8, J9)
9 CONTINUE
P(J6, J7, J8) = G2(J7+1)
WRITE(34, 800) J34, J7, J8
WRITE(34, 1200) P(J6, J7, J8)
8 CONTINUE
7 CONTINUE
6 CONTINUE
C COMPUTATION OF W(L, M, N) FOR G < L < 4
DO 10 11 = 1, 3
J10 = 11
DO 11 111 = 1, J10
J11=I11
DO 12 I12=1,3
J12=I12
A(J12,1)=P(J12,J10,1)
R(J12)=C(J12,J10,J11)
12 CONTINUE
C LEAST SQUARE METHODS SUBROUTINE
IA=3
M=3
N=1
TOL=0.0
KBASIS=0
CALL LLSQF(A,IA,M,N,B,TOL,KBASIS,X,H,IP,IER)
WRITE(31,1000) (B(I),I=1,3)
WRITE(31,1100) KBASIS
WRITE(31,1200) TOL
WRITE(33,1300) X(1)
W(J10,J11,1)=X(1)
C END OF SUBROUTINE
11 CONTINUE
10 CONTINUE
IF(LMAX.EQ.4) GOTO 55
L39=6
GOTO 56
55 CONTINUE
L39=4
56 CONTINUE
C COMPUTATION OF W(L,M,N) FOR 6<L<10
DO 13 L13=4,L39
J13=I13
DO 14 I14=1,J13
J14=I14
DO 15 I15=1,13
J15=I15
A(J15,1)=P(J15,J13,1)
G=2.*COS(6.*PHI(J15))
A(J15,2)=G-P(J15,J13,4)
A(J15,3)=C(J15,J13,J14)
C LEAST SQUARE METHOD
IA=3
M=3
N=2
TOL=0.0
KBASIS=0
CALL LLSQF(A,IA,M,N,B,TOL,KBASIS,X,H,IP,IER)
WRITE(31,1400) (B(I),I=1,3),KBASIS,TOL
WRITE(33,1500) (X(L),L=1,2)
W(J13,J14,1)=X(1)
W(J13,J14,4)=X(2)
C END OF SUBROUTINE
14 CONTINUE
13 CONTINUE
IF(LMAX.EQ.4) GOTO 58
C COMPUTATION OF W(L,M,N) FOR 12<L<16
DO 16 L16=7,9
16 CONTINUE
J16=116
DO 17 I17=1,J16
J17=117
DO 18 I18=1,3
J18=119
A(J16,1)=P(J18,J16,1)
G5=2.*COS(6.*PHI(J18))
A(J18,2)=G5*P(J18,J16,4)
G6=2.*COS(12.*PHI(J18))
A(J18,3)=G6*P(J18,J16,7)
B(J18)=C(J18,J16,J17)
16 CONTINUE
C HERE COMES SUBROUTINE SOLUTION LINEAR
N=3
J4=3
J3=3
D1=-1.0
CALL LIN3F(A,B,J4,B,N,1A,D1,D2,WKAREA,IER)
WRITE(31,1600) IER
WRITE(33,1700) (B(J),J=1,3)
W(J16,J17,1)=B(1)
W(J16,J17,4)=B(2)
W(J16,J17,7)=B(3)
C END OF SUBROUTINE
17 CONTINUE
16 CONTINUE
58 CONTINUE
865 CONTINUE
C COMPUTATION OF THE Q(L,M) COEF. FROM THE W(L,M,N) COEF.
X7(1,1,1)=0.0 DO
DO 333 J33=1,3
J3=1333
DO 20 J20=1,LMAX
J20=120
X5(J20)=[2.*3.141592654*SQRT(2./(FLOAT(2+J20)-1.))]
DO 21 J21=1,J20
J21=121
X7(J20,J21,1)=0.0 DO
DO 22 J22=1,J20,3
J22=122
X6(J22)=COS((2.*(FLOAT(J22)-1.)*PHI(J3))
X5(J20,J21,J22)=W(J20,J21,J22)+X6(J22)*P(J3,J20,J22)
IF(J22.GE.4) GOTO 24
X7(J20,J21,J22)=X7(J20,J21,J22)+X5(J20,J21,J22)
GOTO 22
24 X7(J20,J21,J22+3)=2.*X9(J20,J21,J22)+X7(J20,J21,J22)
22 CONTINUE
IF(J20.GT.4) GOTO 40
GOTO 41
40 CONTINUE
IF(J20.GT.7) GOTO 42
GOTO 43
41 J29=4
GOTO 45
43 J29=7
42 J29=10.
45 QS(J20, J21)*XS(J20)*X7(J20, J21, J29)
WRITE(35, 2200) J20, J21, QS(J20, J21)
21 CONTINUE
20 CONTINUE

C HERE COMES THE CALCULATED POLE FIGURES

POT=(3.141592654/180.)
TILT=0.0
LM=LMAX
DO 25 J25=1, LMAX
J25=125
TOLT=(TILT/POT)
WRITE(6, 2300) TOLT
XX2(1)=0.0 DO
XX3(1)=0.0 DO
DO 130 I1=1, LMAX
J1=I1
J2=I2
XX1(J2)*=(COS(2.*FLOAT(J2)-1.)*TILT))*Y(J1, J2)
130 XX2(J2+1)=XX2(J2)+XX1(J2)
XX3(J1+1)=XX2(J1+1)+QS(J1, J1)+XX3(J1)
PFG1=XX3(LMAX+1)
XX1=XX1
PFG1
WRITE(37, 2100) XXX1
CPF1(J25)=XXX1
ETHA=0.0
DO 26 I26=1, LMAX
J26=I26
XX6(1)=0.0 DO
XX7(1)=0.0 DO
XX5(1)=0.0 DO
DO 132 I1=2, LMAX
J1=I1
J2=I2
DO 134 I3=1, J1
J3=I3
XX4(J3)=COS(2.*(FLOAT(J3)-1.)*TILT))*Y(J1, J2, J3)
XX5(J3+1)=XX5(J3)+XX4(J3)
XX6=2.*COS(2.*(FLOAT(J2)-1.)*ETHA)
XX7(J2)=XX7(J2-1)+XX5(J1+1)+XX6+QS(J1, J2)
132 XX8(J1)=XX3(J1-1)+XX7(J1)
PFG2=XX8(LMAX)
XX2=PFG2
WRITE(37, 2100) XXX2
CPF1(J26)=XXX2
ETHA=ETHA+6.0
CPF(J25, J26)=CPF1(J26)+CPF2(J25)
IF(CPF(J25, J26), LT, 0) GOTO 290
290 GOTO 26
26 CONTINUE
WRITE(6, 2400) K1(J3), K2(J3), K3(J3)
WRITE(6,2100) (CPF(J25,1),I=1,61)
25 TILT=TILT+5.*PQT
333 CONTINUE
C FORMATS STATEMENTS
200 FORMAT(15)
300 FORMAT(123.12)
500 FORMAT(4X,114,118,3117)
550 FORMAT(4X,4114)
600 FORMAT(3X,5D17.9)
700 FORMAT(1X,13)
800 FORMAT(1X,13,13,13)
900 FORMAT(1X,/,3X,5D17.9)
1000 FORMAT(1X,3F12.6)
1100 FORMAT(15)
1200 FORMAT(1X,D17.9)
1300 FORMAT(1X,D17.9)
1400 FORMAT(1X,3D17.9,14,D17.9)
1500 FORMAT(1X,2D17.9)
1600 FORMAT(1X,D17.9)
1700 FORMAT(1X,3D17.9)
2100 FORMAT(1X,6(F10.6,2X))
2200 FORMAT(2X,14,14,5X,D17.9)
2300 FORMAT(20X,'PHI=',F5.2,'DEGREES')
2400 FORMAT(4X,'CALCULATED POLE FIGURE FOR THE PLANE:','(3I3,')')
STOP
END
C.4. Computer Program for the CODF and the Inverse Pole Figures

Once the coefficients $W_{mn}$ are known the CODF as well as the inverse pole figure in any direction can be computed. The computer program leading to such computation is given at the end of this appendix. This program has been written in Fortran IV.

The bases of the computation for the CODF are given by Eq. (C-1-2, 3-58) and the inverse pole figures by Eq. (C-1-2, 4-19 and 4-20).

The program works basically on the input of the values of the Fourier coefficients $d_{2n,2m,2n,s}$ generated by the program C-1 and the values of the $W_{mn}$ coefficients generated by the program C-3. However, at the beginning of the input the following parameter should be included.

- $K$: Format I3. $K$ can take the following values:
  - $K = 1$ if only the CODF is wanted
  - $K = 2$ if only inverse pole figures should be computed
  - $K = 3$ if both CODF and inverse pole figures should be calculated

The following should be specified only if $K = 2$ or 3:

- $N$: Format I3. The value of $N$ specifies the number of inverse pole figures to compute -

- $\alpha, \beta, \gamma$: Format F10.5. These are the Euler angles of the directions where the inverse pole figure should be computed.

  ex: $\alpha = 0.0$, $\beta = 0.0$, $\gamma = 0.0$. will correspond to the normal direction

  $\alpha = 0.0$, $\beta = 90.0$, $\gamma = 0.0$. will correspond to the transverse direction

  $\alpha = 90.0$, $\beta = 90.0$, $\gamma = 0.0$ will correspond to the rolling direction.
The output depending on the value of $K$ will be:

if $K = 1$ the values of $w(\Psi, \Theta, \Phi)$ of the CODF with:

- $\Phi = 0, 10, 30$
- $\Psi = 0, 5, 10, \ldots, 90^\circ$
- $\Theta = 0, 5, 10, \ldots, 90^\circ$

if $K = 2$ the values of $H(\Theta, \Phi)$ of the inverse pole figure with:

- $\Phi = 0, 5, 10, \ldots, 30$

and $\Theta = 0, 5, \ldots, 90^\circ$

if $K = 3$ both outputs will be obtained.
C THIS COMPUTER PROGRAM COMPUTE THE CRYSTALLITE ORIENTATION
C DISTRIBUTION FUNCTION AS WELL AS THE INVERSE POLE FIGURE.
C
DIMENSION ALPHA(3), BETA(3), GAMA(3), K(20)
DOUBLE PRECISION W(9,9,8), D(9,9,9,18), CDF2(10), CDFO(10),
CDF3(10), C1(10), CDF1(10), X(118), X2(18), TOT(19), TOT2(19),
22Z(9,9,7), C2(7), C22(7), C11(9), YO1(7), ZI(9,9,7),
3Y1(7), Y2(7), Y3(7), CDFO(7), Y5(9), CDF2(9), CDF3(9), Y4(9)
REAL INVVPN(10)
READ(5,1001) K1, N
IF (K1.EQ.1) GOTO 41
DO 100 1 = 1, N
J = 1100
READ(5,1002) ALPHA(J), BETA(J), GAMA(J)
100 CONTINUE
41 CONTINUE
C READ OF THE COEF. OF THE CDF EXPANSION.
READ (5,1003) L
LMAX = L + 1
DO 101 1 = 1, LMAX
I1 = 1101
DO 102 1 = 1, 11
I2 = 1102
READ (5,1004) (W(I1, I2, I), I = 1, 11, 3)
102 CONTINUE
101 CONTINUE
C READ OF THE FOURIER COEF. OF THE Z(L,M,N)
DO 103 1 = 1, LMAX
J1 = 1103
J2 = (J1 - 1) + 1
DO 104 1 = 1, J1
J2 = 1104
DO 105 1 = 1, J1
J3 = 1105
READ (5, 1005) K6, K7, K8
IF (J1.EQ.1) GOTO 42
IF (J1.EQ.1) GOTO 42
J115 = J11
GOTO 43
42 J115 = 1
43 CONTINUE
DO 106 1 = 1, J115, 4
J26 = 1106
IF (J115 .LT. 5) GOTO 44
J26 = 1106
IF (J115 .LT. 5) GOTO 44
GOTO 45
44 J27 = J115
45 READ (5, 1006) (K(J), J = J26, J27)
READ (5, 1007) (D(J1, J2, J3, J), J = J26, J27)
106 CONTINUE
105 CONTINUE
104 CONTINUE
103 CONTINUE
PHI = 0.0
C0DF2(1)=0.0 D0
INVPHI(1)= 0.0 D0
DD 11 I11=1,4
K1=111
PSI= 0.0
DD 10 I:2=1,10
K2=112
THETA= 0.0
DO 1 I1=1,10
J1=11
DD 2 J2=1,LMAX
J2=12
CDF2(1)=0.0 D0
CDFD1(1)=0.0 D0
CDFD2(1)=0.0 D0
CDFD3(1)=0.0 D0
J2=2+1(L2-1)+1
DO 3 I3=1,J2
J3=13
C1(J3)=COS(2.*FLOAT(J3)-1.)*PSI
CDF1(1)=0.0 D0
DD 4 J4=1,J2,3
J4=14
T01(1)= 0.0 D0
T02(1)= 0.0 D0
DD 5 I5=1,J22
J5=15
X1(J5)=COS((FLOAT(J5)-1.)*THETA)
X2(J5)=COS((FLOAT(J5)-1.)*(THETA+3.141592654))
T03(J5)=T01(J5)+T02(J5)+J2(J3,J4,J5)*X1(J5)
T04(J5)=T05(J5)+T06(J5)+X2(J5)
CONTINUE
Z1(J2,J3,J4)=T01(J2+1)
Z2(J2,J3,J4)=T02(J2+1)
IF(J4. EQ.1) GOTO 4
IF(J3. EQ.1) GOTO 4
C2(J4)=COS(2.*FLOAT(J4)-1.)*PHI
C3(J4)=SIN(2.*FLOAT(J4)-1.)*PHI
C4(J3)=SIN(2.*FLOAT(J3)-1.)*PSI
Y01(J4)=2.*W(J2,J3,J4)+Z1(J3,J4)+C2(J4)
CDFD(J4)=CDFD(J4-3)+Y01(J4)
Y1(J4)=Z1(J2,J3,J4)+Z2(J2,J3,J4)
Y2(J4)=Z2(J2,J3,J4)-Z1(J2,J3,J4)
Y3(J4)=Y1(J4)+Y2(J4)+C1(J3)
Y4(J4)=Y2(J4)+C1(J3)+C2(J4)
CD1(J4)=2.*W(J2,J3,J4)+Y3(J4)+Y4(J4)
CDF1(J4)=CDF1(J4-3)+CDFD(J4)
CONTINUE
IF(J3. EQ.1) GOTO 40
CONTINUE
IF(J2. GE. 4) GOTO 36
GOTO 37
CONTINUE
IF(J2. GE. 7) GOTO 38
J3=4
CONTINUE
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