X-Ray Diffraction
METE 416 and Graduate Students
Reciprocal Lattice
( Taken from various section of the Cullity Text and Consolidated)
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Appendix 1 in Cullity

Appearance of Diffraction Spots in Reciprocal Space (Actual Representation on Film and How to Interpret the patterns)

Real Lattice

Reciprocal Lattice Representation
Not to scale
Reciprocal Lattice Concepts (Cont’d)

Real Crystal Lattice

→
a_1 = x – direction Vector in Real Space
→
a_2 = y – direction Vector in Real Space
→
a_3 = z – direction Vector in Real Space

Reciprocal Lattice

\[ b_1 = \frac{a_2 \times a_3}{a_1 \cdot a_2 \times a_3} \]
\[ b_2 = \frac{a_3 \times a_1}{a_1 \cdot a_2 \times a_3} \]
\[ b_3 = \frac{a_1 \times a_3}{a_1 \cdot a_2 \times a_3} \]
Volume of the Unit Cell (Real Space): $a_1 \cdot a_2 \times a_3$

\[
\begin{align*}
\vec{b}_1 &= \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \\
\vec{b}_2 &= \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3} \\
\vec{b}_3 &= \frac{\vec{a}_1 \times \vec{a}_3}{\vec{a}_1 \cdot \vec{a}_2 \times \vec{a}_3}
\end{align*}
\]
**DEFINITION OF RECIPROCAL LATTICE VECTOR**

*Reciprocal lattice vector is defined as Vector: $H_{hkl}$*

\[ \vec{H}_{hkl} = h \vec{b}_1 + k \vec{b}_2 + l \vec{b}_3 \]

**Magnitude of the Reciprocal lattice vector $H_{hkl}$**

\[ \therefore H_{hkl} = \frac{1}{d_{hkl}} \]
Real and Reciprocal Lattice Representation

Reciprocal Lattice Representation of 010, and 110
Not to scale

Reciprocal Lattice Representation Of 020 and 220
Not to scale
Reciprocal Lattice Concepts (Cont’d)

Real Crystal Lattice

We will look at more details – please see the next page.

Reciprocal Lattice

Figure 2-6 Two-dimensional lattice, showing that lines of lowest indices have the greatest spacing and the greatest density of lattice points.

Figure 2-7 Illustration of crystal lattices (left side) and corresponding reciprocal lattices (right side) for a cubic system (top) and an hexagonal system (bottom).
Another View - Reciprocal Lattice Concepts (Cont’d)
Reciprocal Lattice (Concepts)

Real Crystal Lattice

4Å

110

210

Normal Representation of Coordinates in Reciprocal Lattice

Units: Å⁻¹ or nm⁻¹

Different Orientation of Reciprocal Lattice

Choose a Convenient Scale

For 110 Plane: \[ \frac{b}{a} = \frac{l}{l = \frac{1}{2.82 Å}} = 0.25 Å⁻¹ \]

Similarly measure d - space For 210 Plane and find the b value for 210 in Å⁻¹
Real Space – Unit Cell

Real Lattice Crystal Plane

Reciprocal Space – Unit Cell

Reciprocal Lattice Points

Each Point Represents a Crystal Plane

Reciprocal Lattice Concepts – Construction of Reciprocal Lattice
Reciprocal Lattice Indexing

Each Point (small yellow circle) Represents a Plane in Real lattice
Reciprocal Lattice and X-ray Diffraction

- The large yellow circle is called “Ewald Circle” and may contain all the spots which will diffract.

\[
\text{Radius} = \frac{1}{\lambda_{SWL}}
\]

- This is the Upper Limit of the Spots that will diffract

- If the Circle touches a spot then that plane or spot will appear on the film

Shaded (Blue) Small Circle represents Spots will not be observed due to Film with AgBr emulsion limitations (lower Limit)
Reciprocal Lattice and X-ray Diffraction

- The Blue Circle touches the 440, -4-40, and 800 spots and these will diffract.

\[ \text{Radius} = \frac{1}{\lambda} \]

- If the Circle touches a spot then that plane or spot will appear on the film.

\[ \frac{1}{\lambda_{Ag \text{ Edge}}} = 10 \]

\[ \frac{1}{\lambda_{SWL}} = 3-10 \]
The new Circle touches the 510, 5-10, and spots and these will diffract.
Reciprocal Lattice Representation of Non-Orthogonal Lattices

Monoclinic Unit Cell

101 in Real Space

90°
Reciprocal Lattice in Three Dimensions (Reference: Prof. Barrett’s Text)

Reciprocal Space – Non Conventional Coordinates

Real Space – Non Conventional Coordinates

\[ h - k l = 1 - 2 n \]
Reciprocal Lattice Construction for TEM Image (Spots)

\[ \frac{1}{\lambda} = 25.8 \text{ A} \]

**Real Crystal Lattice:**
2 - 5 Angstroms (LP)

Diffracts from:
0.5 to 0.2 Angs. in Reciprocal Lattice Using 100kV

\[ \lambda \approx \sqrt{\frac{150}{\text{kV}}} \]

\[ = \sqrt{\frac{150}{100}} = 0.387 \text{ Angstroms (A)} \]

**Radius Vector**
\[ = \frac{1}{\lambda} \]

\[ = \frac{1}{0.387} = 25.8 \text{ A}^{-1} \]

..use this to a Scale
Reciprocal Lattice For Powder Camera Concepts (Cont’d)

Number of Lattice Points

\[ n = \left( \frac{4}{3} \pi \right) \left( \frac{2}{\lambda} \right) \]

\[ v = \text{ReciprocalVolume} \]

\[ n = \frac{32 \pi V}{3 \lambda^3} \]
\[ \overrightarrow{OA} = p \cdot a_1 + q \cdot a_2 + r \cdot a_3 \]

\[ \phi_{O'A'} = \frac{\delta_{OA}}{\lambda} (2\pi) \]
corresponding reciprocal lattice has a unit cell defined by the vectors $b_1$, $b_2$, and $b_3$, where

$$b_1 = \frac{1}{V} (a_2 \times a_3), \quad (1)$$

$$b_2 = \frac{1}{V} (a_3 \times a_1), \quad (2)$$

$$b_3 = \frac{1}{V} (a_1 \times a_2), \quad (3)$$

and $V$ is the volume of the crystal unit cell. This way of defining the vectors $b_1$, $b_2$, $b_3$ in terms of the vectors $a_1$, $a_2$, $a_3$ gives the reciprocal lattice certain useful properties which we will now investigate.

Consider the general triclinic unit cell shown in Fig. A1-3. The reciprocal-lattice axis $b_3$ is, according to Eq. (3), normal to the plane of $a_1$ and $a_2$, as shown. Its length is given by

$$b_3 = \frac{|a_1 \times a_2|}{V}$$

$$= \frac{\text{(area of parallelogram OACB)}}{\text{(area of parallelogram OACB)(height of cell)}}$$

$$= \frac{1}{OP} = \frac{1}{d_{001}},$$

since $OP$, the projection of $a_3$ on $b_3$, is equal to the height of the cell, which in turn is simply the spacing $d$ of the (001) planes of the crystal lattice. Similarly, we find that the reciprocal lattice axes $b_1$ and $b_2$ are normal to the (100) and (010) planes, respectively, of the crystal lattice, and are equal in length to the reciprocals of the spacings of these planes.

By extension, similar relations are found for all the planes of the crystal lattice. The whole reciprocal lattice is built up by repeated translations of the unit cell by the vectors $b_1$, $b_2$, $b_3$. This produces an array of points each of which is labeled with its coordinates in terms of the basic vectors. Thus, the point at the end of the
b₁ vector is labeled 100, that at the end of the b₂ vector 010, etc. This extended reciprocal lattice has the following properties:

1. A vector \( \mathbf{H}_{hk\ell} \) drawn from the origin of the reciprocal lattice to any point in it having coordinates \( hkl \) is perpendicular to the plane in the crystal lattice whose Miller indices are \( hkl \). This vector is given in terms of its coordinates by the expression

\[
\mathbf{H}_{hk\ell} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3.
\]

2. The length of the vector \( \mathbf{H}_{hk\ell} \) is equal to the reciprocal of the spacing \( d \) of the \( (hkl) \) planes, or

\[
H_{hk\ell} = \frac{1}{d_{hk\ell}}.
\]

The important thing to note about these relations is that the reciprocal-lattice array of points completely describes the crystal, in the sense that each reciprocal-lattice point is related to a set of planes in the crystal and represents the orientation and spacing of that set of planes.

Before proving these general relations, we might consider particular examples of the reciprocal lattice as shown in Figs. A1–4 and A1–5 for cubic and hexagonal crystals. In each case, the reciprocal lattice is drawn from any convenient origin, not necessarily that of the crystal lattice, and to any convenient scale of reciprocal angstroms. Note that Eqs. (1) through (3) take on a very simple form for any crystal whose unit cell is based on mutually perpendicular vectors, i.e., cubic, tetragonal, or orthorhombic. For such crystals, \( \mathbf{b}_1, \mathbf{b}_2, \) and \( \mathbf{b}_3 \) are parallel, respectively, to \( \mathbf{a}_1, \mathbf{a}_2, \) and \( \mathbf{a}_3 \), while \( b_1, b_2, \) and \( b_3 \) are simply the reciprocals of \( a_1, a_2, \) and \( a_3 \). In Figs. A1–4 and A1–5, four cells of the reciprocal lattice are shown, together with two \( \mathbf{H} \) vectors in each case. By means of the scales shown, it may be verified that each \( \mathbf{H} \) vector is equal in length to the reciprocal of the spacing of the corresponding planes and normal to them. Note that reciprocal lattice points such as
Fig. A1–4 The reciprocal lattice of a cubic crystal which has $a_1 = 4 \text{ Å}$. The axes $a_3$ and $b_3$ are normal to the drawing.

Already Covered- please see previous slides
nh, nk, nl, where n is an integer, correspond to planes parallel to (hkl) and having 1/n their spacing. Thus, \( H_{220} \) is perpendicular to (220) planes and therefore parallel to \( H_{110} \), since (110) and (220) are parallel, but \( H_{220} \) is twice as long as \( H_{110} \) since the (220) planes have half the spacing of the (110) planes.

Other useful relations between the crystal and reciprocal vectors follow from Eqs. (1) through (3). Since \( \mathbf{b}_3 \), for example, is normal to both \( \mathbf{a}_1 \) and \( \mathbf{a}_2 \), its dot product with either one of these vectors is zero, or

\[
\mathbf{b}_3 \cdot \mathbf{a}_1 = \mathbf{b}_3 \cdot \mathbf{a}_2 = 0.
\]

The dot product of \( \mathbf{b}_3 \) and \( \mathbf{a}_3 \), however, is unity, since (see Fig. A1-3)

\[
\mathbf{b}_3 \cdot \mathbf{a}_3 = (b_3) \text{ (projection of } \mathbf{a}_3 \text{ on } \mathbf{b}_3) = \frac{1}{(OP)} (OP) = 1.
\]

In general,

\[
\mathbf{a}_m \cdot \mathbf{b}_n = 1, \quad \text{if } m = n, \quad (4)
\]

\[
= 0, \quad \text{if } m \neq n. \quad (5)
\]

The fact that \( \mathbf{H}_{hkl} \) is normal to \( (hkl) \) and \( H_{hkl} \) is the reciprocal of \( d_{hkl} \) may be proved as follows. Let ABC of Fig. A1-6 be part of the plane nearest the origin in the set \( (hkl) \). Then, from the definition of Miller indices, the vectors from the origin to the points A, B, and C are \( \mathbf{a}_1/h, \mathbf{a}_2/k, \) and \( \mathbf{a}_3/l \), respectively. Consider the vector \( \mathbf{AB} \), that is, a vector drawn from A to B, lying in the plane \( (hkl) \). Since

\[
\frac{\mathbf{a}_1}{h} + \mathbf{AB} = \frac{\mathbf{a}_2}{k},
\]
then

$$AB = \frac{a_2}{k} - \frac{a_1}{h}.$$ 

Forming the dot product of $H$ and $AB$, we have

$$H \cdot AB = (hb_1 + kb_2 + lb_3) \cdot \left( \frac{a_2}{k} - \frac{a_1}{h} \right).$$

Evaluating this with the aid of Eqs. (4) and (5), we find

$$H \cdot AB = 1 - 1 = 0.$$ 

Since this product is zero, $H$ must be normal to $AB$. Similarly, it may be shown that $H$ is normal to $AC$. Since $H$ is normal to two vectors in the plane $(hkl)$, it is normal to the plane itself.

To prove the reciprocal relation between $H$ and $d$, let $n$ be a unit vector in the direction of $H$, i.e., normal to $(hkl)$. Then

$$d = ON = \frac{a_1}{h} \cdot n.$$ 

But

$$n = \frac{H}{H}.$$ 

Therefore

$$d = \frac{a_1}{h} \cdot \frac{H}{H}$$

$$= \frac{a_1}{h} \cdot \frac{(hb_1 + kb_2 + lb_3)}{H}$$

$$= \frac{1}{H}.$$ 

Fig. A1-6   Relation between reciprocal-lattice vector $H$ and crystal plane $(hkl)$. 

Taken or scanned from “X-ray Diffraction,” Cullity, 2nd Ed. Addison Wesley 1174, text
Used purely as a geometrical tool, the reciprocal lattice is of considerable help in the solution of many problems in crystal geometry. Consider, for example, the relation between the planes of a zone and the axis of that zone. Since the planes of a zone are all parallel to one line, the zone axis, their normals must be coplanar. This means that planes of a zone are represented, in the reciprocal lattice, by a set of points lying on a plane passing through the origin of the reciprocal lattice. If the plane \((hkl)\) belongs to the zone whose axis is \([uvw]\), then the normal to \((hkl)\), namely, \(H\), must be perpendicular to \([uvw]\). Express the zone axis as a vector in the crystal lattice and \(H\) as a vector in the reciprocal lattice:

\[
\text{Zone axis} = ua_1 + va_2 + wa_3, \\
H = hb_1 + kb_2 + lb_3.
\]

If these two vectors are perpendicular, their dot product must be zero:

\[
(ua_1 + va_2 + wa_3) \cdot (hb_1 + kb_2 + lb_3) = 0, \\
hu + kv + lw = 0.
\]

This is the relation given without proof in Sec. 2–6. By similar use of reciprocal-lattice vectors, other problems of crystal geometry, such as the derivation of the plane-spacing equations given in Appendix 3, may be greatly simplified.
A1-4 DIFFRACTION AND THE RECIPROCAL LATTICE

The great utility of the reciprocal lattice, however, lies in its connection with diffraction problems. We shall consider how x-rays scattered by the atom O at the origin of the crystal lattice (Fig. A1–7) are affected by those scattered by any other atom A whose coordinates with respect to the origin are $pa_1$, $qa_2$, and $ra_3$, where $p$, $q$, and $r$ are integers. Thus,

$$\mathbf{OA} = pa_1 + qa_2 + ra_3.$$ 

Let the incident x-rays have a wavelength $\lambda$, and let the incident and diffracted beams be represented by the unit vectors $S_0$ and $S$, respectively. $S_0$, $S$, and $\mathbf{OA}$ are, in general, not coplanar.

To determine the conditions under which diffraction will occur, we must determine the phase difference between the rays scattered by the atoms O and A. The lines $Ou$ and $Ov$ in Fig. A1–7 are wave fronts perpendicular to the incident beam $S_0$ and the scattered beam $S$, respectively. Let $\delta$ be the path difference for rays scattered by O and A. Then

$$\delta = uA + Av$$

$$= Om + On$$

$$= S_0 \cdot \mathbf{OA} + (-S) \cdot \mathbf{OA}$$

$$= -\mathbf{OA} \cdot (S - S_0).$$
Fig. A1–7 X-ray scattering by atoms at \( O \) and \( A \). After Guinier [G.10].

The corresponding phase difference, in radians, is given by

\[
\phi = \frac{2\pi \delta}{\lambda}
\]

\[
= -2\pi \left( \frac{S - S_0}{\lambda} \right) \cdot OA.
\]

(6)

Diffraction is now related to the reciprocal lattice by expressing the vector \( (S - S_0)/\lambda \) as a vector in that lattice. Let

\[
\frac{S - S_0}{\lambda} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3.
\]
This is now in the form of a vector in reciprocal space but, at this point, no particular significance is attached to the parameters $h$, $k$, and $l$. They are continuously variable and may assume any values, integral or nonintegral. Equation (6) now becomes

$$\phi = -2\pi(hb_1 + kb_2 + lb_3) \cdot (pa_1 + qa_2 + ra_3) = -2\pi(hp + kq + lr).$$

A diffracted beam will be formed only if reinforcement occurs, and this requires that $\phi$ be an integral multiple of $2\pi$. This can happen only if $h$, $k$, and $l$ are integers. Therefore the condition for diffraction is that the vector $(S - S_0)/\lambda$ end on a point in the reciprocal lattice, or that

$$\frac{S - S_0}{\lambda} = H = hb_1 + kb_2 + lb_3,$$

where $h$, $k$, and $l$ are now restricted to integral values.
Both the Laue equations and the Bragg law can be derived from Eq. (7). The former are obtained by forming the dot product of each side of the equation and the three crystal-lattice vectors \( \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3 \) successively. For example,

\[
\mathbf{a}_1 \cdot \left( \frac{\mathbf{S} - \mathbf{S}_0}{\lambda} \right) = \mathbf{a}_1 \cdot (\mathbf{h} \mathbf{b}_1 + \mathbf{k} \mathbf{b}_2 + \mathbf{l} \mathbf{b}_3) = h,
\]

or

\[
\mathbf{a}_1 \cdot (\mathbf{S} - \mathbf{S}_0) = h\lambda. \tag{8}
\]

Similarly,

\[
\mathbf{a}_2 \cdot (\mathbf{S} - \mathbf{S}_0) = k\lambda. \tag{9}
\]

\[
\mathbf{a}_3 \cdot (\mathbf{S} - \mathbf{S}_0) = l\lambda. \tag{10}
\]

Equations (8) through (10) are the vector form of the equations derived by von Laue in 1912 to express the necessary conditions for diffraction. They must be satisfied simultaneously for diffraction to occur.

As shown in Fig. A1–7, the vector \( \mathbf{S} - \mathbf{S}_0 \) bisects the angle between the incident beam \( \mathbf{S}_0 \) and the diffracted beam \( \mathbf{S} \). The diffracted beam \( \mathbf{S} \) can therefore be considered as being reflected from a set of planes perpendicular to \( \mathbf{S} - \mathbf{S}_0 \). In fact, Eq. (7) states that \( \mathbf{S} - \mathbf{S}_0 \) is parallel to \( \mathbf{H} \), which is in turn perpendicular to the planes \((hkl)\). Let \( \theta \) be the angle between \( \mathbf{S} \) (or \( \mathbf{S}_0 \)) and these planes. Then, since \( \mathbf{S} \) and \( \mathbf{S}_0 \) are unit vectors,

\[
(\mathbf{S} - \mathbf{S}_0) = 2 \sin \theta.
\]

Therefore

\[
\frac{2 \sin \theta}{\lambda} = \frac{\mathbf{S} - \mathbf{S}_0}{\lambda} = H = \frac{1}{d},
\]

or

\[
\lambda = 2d \sin \theta.
\]
The conditions for diffraction expressed by Eq. (7) may be represented graphically by the “Ewald construction” shown in Fig. A1–8. The vector \( \mathbf{S}_0 / \lambda \) is drawn parallel to the incident beam and \( 1/\lambda \) in length. The terminal point \( O \) of this vector is taken as the origin of the reciprocal lattice, drawn to the same scale as the vector \( \mathbf{S}_0 / \lambda \). A sphere of radius \( 1/\lambda \) is drawn about \( C \), the initial point of the incident-beam vector. Then the condition for diffraction from the \((hkl)\) planes is that the point \( hkl \) in the reciprocal lattice (point \( P \) in Fig. A1–8) touch the surface of the sphere, and the direction of the diffracted-beam vector \( \mathbf{S}/\lambda \) is found by joining \( C \) to \( P \). When this condition is fulfilled, the vector \( \mathbf{OP} \) equals both \( \mathbf{H}_{hkl} \) and \( (\mathbf{S} - \mathbf{S}_0)/\lambda \), thus satisfying Eq. (7). Since diffraction depends on a reciprocal-lattice point touching the surface of the sphere drawn about \( C \), this sphere is known as the “sphere of reflection.”

Our initial assumption that \( p, q, \) and \( r \) are integers apparently excludes all crystals except those having only one atom per cell, located at the cell corners. For if the unit cell contains more than one atom, then the vector \( \mathbf{OA} \) from the origin to “any atom” in the crystal may have nonintegral coordinates. However, the
Number of Lattice Points

\[ n = \left( \frac{4}{3} \pi \right) \left( \frac{2}{\lambda} \right)^v \]

\( v = \text{Reciprocal Volume} \)

\[ n = \frac{32 \pi V}{3 \lambda^3} \]
Rotating Crystal Camera Schematic of Spots from Crystal Planes

\[ n\lambda = d = a \cos \phi \]  

\[ n\lambda = e + d = a \cos \theta + a \cos \phi \]
Stereographic Projection

X-Ray Diffraction Assignment No. ____

Determination of Orientation of Single Crystal
And
Indexing of A Back Reflection Laue Pattern

-Submitted by-

Name: ___________________
Date: _________________
Determine the orientation of a Ba

Given:
(a) B.R. Laue Film
(b) Greninger Chart
(c) Wulff Net
(d) Standard Projection for the C

Procedure:

1. Coincide the center of the Grenin the Laue Pattern; vertical line d line via thumb tack.

2. Read off the $\gamma$ and $\delta$ angles for al Greninger chart.

<table>
<thead>
<tr>
<th>Point No.</th>
<th>$\gamma$</th>
<th>$\delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td></td>
<td></td>
</tr>
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<td>9</td>
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<tr>
<td>4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Determine the orientation of a Back reflected Al Laue Pattern.

Given:
(a) B.R. Laue Film
(b) Greninger Chart
(c) Wulff Net
(d) Standard Projection for the Cubic system

Procedure:

1. Coincide the center of the Greninger chart with the center of the Laue Pattern; vertical line drawn through the center of the line via thumb tack.

2. Read off the $\gamma$ and $\delta$ angles for all the points using the Greninger chart.

3. Place a transparent sheet on the Wulff Net and draw the trace of the circle on to the tracing paper.

4. Record all the (Laue) points on the tracing paper in a manner shown in Figure 8-4 page 238. (Set the Wulff Net such the North Pole faces the left.)

5. Once all the points are transferred form the Greninger chart to the Stereograph join the longitudes and terminate them at the end of the circle. Figure 8-6, P-240.

6. Next find the POLE for a particular zone in which there are several points representing the crystal plane (on an arc).

7. Repeat for all the zones and mark them P_A, P_B, P_C, P_D, P_E FOR THEIR CORRESPONDING TRACES OF A, B, C, D AND E, respectively.
Determine the orientation of a Back reflected Al Laue Pattern.

Given:
(a) B.R. Laue Film
(b) Greninger Chart
(c) Wulff Net
(d) Standard Projection for the Cubic system

Procedure:

1. Coincide the center of the Greninger chart with the center of the Laue Pattern; vertical line drawn through the center of the line via thumb tack.

2. Read off the γ and δ angles for all the points using the Greninger chart.

3. Place a transparent sheet on the Wulff Net and draw the trace the circle on to the tracing paper.

4. Record all the (Laue) points on the tracing paper in a manner shown in Figure 8-4 page 238. (Set the Wulff Net such the North Pole faces the left.

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7. Repeat for all the zones and mark them P_A, P_B, P_C, P_D, P_E FOR THEIR CORRESPONDING TRACES OF A, B, C, D AND E, respectively.
NEXT_STEP_IS_INDEXING

8. Al has an FCC structure and the standard projection for CUBIC 001 and 011 are given; we use trial and error method and label the points using 001 CUBIC projection.

9. It can be noted that in the Laue film all the zone cross point 5. This must be a major pole and if we assume this to be 001 pole then locate the other pole normal to it using face normals.

10. Suppose the angle between:
   1. $P_A$ and $P_B = 90^\circ$
   2. $P_A$ and $5' = 90^\circ$
   3. $P_B$ and $5 = 90^\circ$

There are two possibilities of indexing of the poles.

No.1

$5' = 001, P_A = 010, P_B = 100$

{100}

No.2

$5' = 001, P_A = 110, P_B = -110$

{100} {110}

Compare your results from the No.1 choice with the standard projection.
then \( P_E \) must be 110 pole lying mid-way between \( P_A \) and \( PB \) at 45° angle. (This turns out to be a wrong assumption.)

Then try choice No.2

Check the angle from 5'-a and 5'-b. These should equal 55° and \( a-b= 71° \).

Go to table 2-3 in the test on page 75 and check if these angles are correct. It turns out that this assumption is incorrect.

11. Now suppose we want to know what the Miller indices of pole 11; the steps are:
   a. Measure the angle between 5' and 11' which should =35°.
   b. Using Table (P75) in the 001 column find the corresponding plane for a 25° angle it should turn out to be 112. In a similar manner other poles may be found.

12. Finally the crystal is \( \gamma=18° \) and \( \delta=13.5° \) from the true 001 pole.
Fig. 8–1 Intersection of a conical array of diffracted beams with a film placed in the back-reflection position. C = crystal, F = film, Z.A. = zone axis.
**Direction Cosines**

\[ p, q \text{ and } r \]

\[ p = \cos \rho \cdot \frac{d}{a / h} \]

\[ q = \cos \sigma \cdot \frac{d}{b / k} \]

\[ r = \cos \tau \cdot \frac{d}{c / l} \]

**Ratio** \[ h:k:l = p.a : q.b : r.c \]

**Miller** Indices Are in the same ratio of Direction cosines.
GRENINGER CHART

\[ \begin{align*}
\tan \mu &= \frac{FN}{FO} = \frac{CF \tan \delta}{CF \sin \mu} = \frac{\tan \delta}{\sin \mu} \\
\tan \sigma &= \frac{ON}{OC} = \frac{FN \cdot 1}{CF \cos \gamma} = \left( \frac{CF \tan \delta}{\sin \mu} \right) \left( \frac{1}{CF \cos \gamma} \right) \\
&= \frac{\tan \delta}{\sin \mu \cos \gamma}
\end{align*} \]

\[ OS = OC \tan \theta \]

Film to Specimen distance.
Position of $x$ and $y$ can be determined if $S$ and $\beta$ are known.

1. $\sin \theta$ is unknown for $x$ (also $s$)
   But $S$ and $\beta$ are known from plane normals.

2. $\phi$ can also be calculated.
Fig. 8–4 Use of the Greninger chart to plot the pole of a reflecting plane on a stereographic projection. Pole $l'$ in (b) is the pole of the plane causing diffraction-spot $l$ in (a).
Fig. 3-5 (a) Transmission and (b) back-reflection Laue methods.
Standard Projection on (001) Cubic Lattice Plane (After Prof. Barrett)

Fig. 2-37. Standard (001) projection of a cubic crystal, after Barrett [1,7].
Preparation of Stereographic Projection for the Exercise

Using the Laue Film of Al Single Crystal Given to you
### Table 2-3
Interplanar Angles (in degrees) in Cubic Crystals between Planes of the Form \((h_1k_1l_1)\) and \((h_2k_2l_2)\)

<table>
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<th>(h_1k_1l_1)</th>
<th>100</th>
<th>110</th>
<th>111</th>
<th>210</th>
<th>211</th>
<th>221</th>
<th>310</th>
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<td>30</td>
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<td>24.1</td>
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<td>43.1</td>
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<td>11.3</td>
<td>36.9</td>
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Largely from R. M. Bozorth, Phys. Rev. 26, 390 (1935); rounded off to the nearest 0.1°. A much longer list is given on p. 120-122 of Vol. 2 of [G.11].
Standard Projection on (001) and 011 Cubic Lattice Plane
Wulff Net to Represent the Poles
Preparation of Stereographic Projection for the Exercise  Using the Laue Film of Al Single Crystal Given to you
Standard Projection of Cubic Crystals—Another View
This will end the Sterography and Reciprocal Lattice