X-Ray Diffraction
METE 416 and Graduate Students
Chapter 4
Diffraction II – Intensities of Diffracted Beams
Instructor
Prof. Dhanesh Chandra
Room LMR 468, LMR Building,
Phone: 784-4960,
e-mail: dchandra@unr.edu

Metallurgical and Materials Engineering Division
University of Nevada, Reno

Fundamentals of Structure Factor Calculations

Scattering from a loose electron.

Atoms in Lattice
Intensities of Diffracted Beams

1. Effects of arrangement of Atoms in the lattice
2. Scattering Electrons in an Atom
3. Scattering from an Atom
4. Scattering By a Unit Cell
5. Structure Factor Calculations - Diffracted Intensity Prediction
6. Applications to Polycrystal Diffraction
7. Multiplicity Factor
8. Lorentz factor
9. Absorption Factor - applicable to Film Cameras
10. Temperature factor
11. Overall Intensities of Diffraction Peaks. taking into account all the above mentioned factor
12. Examples of Intensity calculations
### Guinier X-ray Diffraction Film

<table>
<thead>
<tr>
<th>Step</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empty cell</td>
<td></td>
</tr>
<tr>
<td>a Li₃N RT</td>
<td></td>
</tr>
<tr>
<td>Hydriding 150C</td>
<td></td>
</tr>
<tr>
<td>Hydriding 200C</td>
<td></td>
</tr>
<tr>
<td>Hydriding 250C</td>
<td></td>
</tr>
<tr>
<td>De-hydriding 250C</td>
<td></td>
</tr>
<tr>
<td>De-hydriding 200C</td>
<td></td>
</tr>
<tr>
<td>De-hydriding 320C</td>
<td></td>
</tr>
<tr>
<td>De-hydriding 350C</td>
<td></td>
</tr>
</tbody>
</table>

Each strip shows XRD patterns at one temperature.

- LiND₂ + Li₂ND
- α Li₃N
- LiD
- Li₂ND

Neutron Diffraction Pattern

- 0°
- Time

Guinier X-ray Diffraction Film
1. Position of Atoms in a Unit cell Make a big difference in the Diffracted Beam Intensity and Positions

Figure 4-1 (a) Base-centered and (b) body-centered orthorhombic unit cells.

001 Diffracts

002 Diffracts

Diffraction from the (001) planes of scatterers in (a) base-centered and (b) body-centered orthorhombic lattices.

- D. Chandra
Scattering of X-rays By an Electron – J.J. Thomson Intensity Equation

1. Consider an Electron at Point “O” Scattering X-rays

2. Intensity of X-rays at Point P at a distance “r” scattered by an electron of mass “m” is Given by J.J. Thomson Equation

Angle \( yOP = \alpha = 90^\circ \)

\[ \alpha = \frac{\pi}{2} - 2\theta \]
Scattering of X-rays By an Electron – J.J. Thomson Intensity Equation (Cont’d)

$I = I_o \left( \frac{\mu_o}{4.\pi} \right)^2 \cdot \left( \frac{e^4}{m^2 \cdot r^2} \right) \cdot \sin^2 \alpha = I_o \left( \frac{K}{r^2} \right) \cdot \sin^2 \alpha$

So Intensity is dependent on $1/r^2$ distance

$I_o = $ Intensity of Incident Beam

$\mu_o = 4.\pi \times 10^{-7} \ m.\ kg.\ C^{-2}$

$K = \left( \frac{\mu_o}{4.\pi} \right)^2 \cdot \left( \frac{e^4}{m^2} \right) = \text{Constant}$
Assume That a unpolarized X-ray beam has an Vector "E" in yz Plane

It resolves as : $E_y$, and $E_z$, and $E_y = E_z$, since the direction is perfectly random

$E^2 = E_y^2 + E_z^2$

and $\frac{1}{2}E^2 = E_z^2 = E_y^2$

$I \propto \text{Energy}$

$I_{o_y} = I_{o_z} = \frac{1}{2} I_o \quad \ldots \ldots \text{Finally}$

In y-direction, the Intensity of X-rays ($I_{py}$)

$I_{py} = I_{o_y} \cdot \frac{K}{r^2} \cdot \sin^2 \alpha = I_{o_y} = \frac{K}{r^2} \quad \ldots \ldots \text{as } \alpha = 90; \text{and } \sin 90 = 1$

---

**Figure 4-4** Elastic collision of photon and electron (Compton effect).
Polarization Factor (Cont’d)

\[ I_{py} = I_{oy} \cdot \frac{K}{r^2} \cdot \sin^2 \alpha = I_{oy} = \frac{K}{r^2} \text{...................as } \alpha = 90 \text{; and } \sin 90 = 1 \]

\[ I_{pz} = I_{oz} \cdot \frac{K}{r^2} \cdot \sin^2 2\theta \]

**But**, Intensity of X-rays at Point P

\[ I_p = I_{py} + I_z \]

\[ I_p = I_o \cdot \frac{K}{r^2} \left( \frac{1 - \cos^2 2\theta}{2} \right) \]

**Polarization Factor**:

\[ \left( \frac{1 - \cos^2 2\theta}{2} \right) \]
Energy Absorbed in an Elastic Recoil of an Electron- Compton Effect

\[ \Delta \lambda (A) = \lambda_2 - \lambda_1 = 0.0486 \sin^2 \theta \]

Notes on Compton effect ...a different type .. Called “Incoherent scattering.”

1. Compton Effect is related to loosely Bonded electron such delocalized electrons in Metals.

2. If the incoming X-rays have an \( E = h \nu_1 \) which can also be expressed in terms of wavelengths (\( \lambda \)).

Then there is certain amount of energy absorbed during elastic recoil and the resultant \( E = h \nu_2 \) or has longer wavelength=\( \lambda_2 \)
Compton Effect

Arthur Compton – Uni. of Chicago. used to Conduct Low Temperature Physics. Ex: Phase Diagrams of CO-Ar gases at very low temperatures.

Prof. Charles Barrett (renowned Physicist/Metallurgist was Dr. Compton’s Graduate Student) …was a Metallurgy Prof. at Uni. of Denver in 1970’s.

If the atom (in turn bound electrons with in an atom) are periodic, then there is coherent scattering of X-rays, which leads to giving strong diffracted beams. Incoming beam \( \lambda_1 \) = outgoing diffracted beam \( \lambda_2 \).
What is the real meaning of Compton Effect??

Scattering from loose electron.

Note the size of Free Electron is shown much larger than atom for clarity

- D. Chandra
Comparison of Coherent and Incoherent Scattering

Coherent Scattering

Incoherent Scattering

Scattering from loose electron
Intensities of Diffracted Beams

1. Effects of arrangement of Atoms in the lattice
2. Scattering Electrons in an Atom
3. Scattering from an Atom
4. Scattering By a Unit Cell
5. Structure Factor Calculations - Diffracted Intensity Prediction
6. Applications to Polycrystal Diffraction
7. Multiplicity Factor
8. Lorentz factor
9. Absorption Factor - applicable to Film Cameras
10. Temperature factor
11. Overall Intensities of Diffraction Peaks. taking into account all the above mentioned factor
12. Examples of Intensity calculations

03/06/2006
MSE 416 and Graduate Students
- D. Chandra
Scattering from An Atom involves many electron bound within the Atom

Path Difference: \(CB - AB'\)

Completely In Phase & scatter in the plane

1. Nucleus is large is relatively heavy, and cannot oscillate when an X-ray strikes it

2. Electrons do excited and oscillate when struck by X-Rays…note there is no momentum of electron and the electron is bound within the parent atom

3. Scattering is directional

Case shown in Red X-ray Paths:

Path Difference: \(CB - AD\)

Somewhat out of Phase with along wave front \(YY'\)

Figure 4-5 X-ray scattering by an atom.
Atomic Scattering (Form Factor) is dependent on the angle of Scattering

Atomic Scattering Factor ($f$)

$$f = \frac{\text{Amplitude of the Wave Scattered by an Atom}}{\text{Amplitude of the Wave Scattered by one electron}}$$

There are Table in the Back of the Book that give these values
In forward direction:

$$f = Z \ (\text{Atomic Number} = \text{No. of electrons Scattering})$$

Ex: Cu No. of Electrons = 29 = At. No.

Scattering Factor, $f = 29$ at $\theta = 0^\circ$

usually represented as $\left(\frac{\sin \theta}{\lambda}\right)$

But drops to about $f = 10 @ \left(\frac{\sin \theta}{\lambda}\right) = \sim 0.65$

Figure 4-6 The atomic scattering factor of copper.

and Graduate Students
- D. Chandra
Summary of Scattering Coherent (for diffraction) and also Incoherent Like Compton Effect

Figure 4.7 Effects produced by the passage of x-rays through matter, after Henry, Lipson, and Wooster [G.15].
Intensities of Diffracted Beams

1. Effects of arrangement of Atoms in the lattice
2. Scattering Electrons in an Atom
3. Scattering from an Atom
4. Scattering By a Unit Cell
5. Structure Factor Calculations- Diffracted Intensity Prediction
6. Applications to Polycrystal Diffraction
7. Multiplicity Factor
8. Lorentz factor
9. Absorption Factor- applicable to Film Cameras
10. Temperature factor
11. Overall Intensities of Diffraction Peaks. taking into account all the above mentioned factor
12. Examples of Intensity calculations
Scattering From a Unit Cell

- Scattering from atoms assembled in a Unit Cell in some order…
  i.e Scattering from all electrons that are bound to all the atoms in the Unit Cell

- In this section we want to Calculate the Intensity of a particular diffracted beam scattered by (100) plane.

- To do this we need to know the POSITIONS OF ATOMS in a Unit Cell

- Also BRAGS”S LAW is assumed to be satisfied

- In some cases Bragg’s law is satisfied but diffraction will not occur due to arrangement of atoms…i.e Intensity of the beam is dependent on the position of atoms in the Unit Cell
For the Calculation of Intensity we first draw a arbitrary unit cell with many atoms such as shown in the 2-Dimensional drawing.

First we evaluate only the atoms (shown in Purple color) in the Unit Cell.

We will calculate the Path difference in the that the Diffracted X-rays have to take to emerge form the atoms.

Path Difference = NC + MC… i.e extra distance traveled by X-rays.

Path Difference between: 1' and 2' is MCN

$$\delta_{1'2'} = MCN = 1\lambda = 2d_{h00} \sin \theta$$

But, $$d_{h00} = \frac{a}{h}$$

This will be completely in phase.
What do we mean by path Difference of X-rays

Extra Path (Exactly One wavelength, $\lambda=1$)
That the X-rays have to take for Diffracting
Effect of Addition of a New Atom B on Intensity of (h00) Plane

Figure 4-8 The effect of atom position on the phase difference between diffracted rays.
If a new Atom “B” is added to the Unit cell we need to evaluate the effect of this addition of new atom on the intensity of a Bragg Peak.

Addition of New Atom (B) in the Unit cell

$\delta_{r3'} = \text{RBS} = \left( \frac{AB}{AC} \right) \cdot \lambda$

$\delta_{r3'} = \text{RBS} = \left( \frac{x}{a/h} \right) \cdot \lambda$

Please Note: $\frac{x}{a} = u$

as inuvw position of atom in unit cell

$\frac{\text{RBS}}{\text{MCN}} = \frac{AB}{AC}$

$\therefore \frac{AB}{AC} \cdot \text{MCN} = \frac{AB}{AC} \cdot 1 \lambda$
The path Difference Term Includes Wavelength

We need to find another way to describe the Path Length Independent of The wavelength.

We use “Phase Difference” (φ) for this purpose.

Definition:

\[ φ = \left( \frac{δ}{λ} \right) \cdot 2π. \text{Radians} \]

\[ δ = \text{Path Difference} \]

Going Back to the Equation: Path Difference (δ₁,₃) due to addition of Atom"B":

\[ φ_{1,3} = \left( \frac{δ_{1,3}}{λ} \right) \cdot 2π \]

But

\[ δ_{1,3} = \text{RBS} = \left( \frac{x}{a/h} \right) \cdot λ \]

\[ \frac{x}{a} = u \]

∴ \[ φ_{1,3} = 2π.h.\left( \frac{x}{a} \right) = 2π.h.u \]
Phase Difference Definition and Relation to Atom Coordinate

In 3 Dimensions:
\[ \phi = 2\pi (h.u + k.v + l.w) \]

\(uvw\) → are Atom Coordinates

\(hkl\) → is Crystal Plane

- One can move this atom B around within the Unit cell and observe the effect on the intensity of a plane.
- The atom B need not be in the (hkl) plane in question, it could be anywhere.
Intensities of Diffracted Beams

1. Effects of arrangement of Atoms in the lattice
2. Scattering Electrons in an Atom
3. Scattering from an Atom
4. Scattering By a Unit Cell
5. Structure Factor Calculations - Diffracted Intensity Prediction
6. Applications to Polycrystal Diffraction
7. Multiplicity Factor
8. Lorentz factor
9. Absorption Factor - applicable to Film Cameras
10. Temperature factor
11. Overall Intensities of Diffraction Peaks. taking into account all the above mentioned factor
12. Examples of Intensity calculations

03/06/2006 MSE 416 and Graduate Students - D. Chandra
We wish to obtain Intensity $I \propto A^2$

Note: $E_1$ and $E_2$ are reinforcing but somewhat out of phase.

Net Intensity is higher than $E_1$ or $E_3$ for the same case.

In this case $\phi$ and $A$ are different and $\lambda$ is the same for both.

\[
\vec{E}_1 = A_1 \cdot \sin(2\pi \nu - \phi_1)
\]
\[
\vec{E}_2 = A_2 \cdot \sin(2\pi \nu - \phi_2)
\]
We Introduce **Analytical Solution** to solve the Intensity and Phase difference Issue

Consider a Vector, \( A = \) Amplitude of the Wave
\[ A = (a + ib) \]

Next:
Write the Power Series:
\[ e^{ix} = \cos x + i \cdot \sin x \]

\[ A e^{i\phi} = A \cos \phi + i \sin \phi \ldots \text{in terms of Phase difference} \]
but \( I \propto A^2 \)

Going Back to the Scattering of X-rays from atoms:
We can express Scattered wave as ..in term of hkl, uvw, and Phase Difference \( (\phi) \):
\[ A e^{i\phi} = f \cdot e^{2\pi i (hu + kv + lw)} \]
Structure Factor Calculations

We can express a Resultant of waves scattered by Atoms in a Unit cell:

$$|F| = \frac{\text{Amplitude of Wave Scattered by all Atoms in Unit Cell}}{\text{Amplitude of Wave Scattered by one electron}}$$

**For Example:** If we have two atoms of Cu \((u_1, v_1, w_1)\) and Ni \((u_2, v_2, w_2)\)

We can Write Structure Factor \((F)\) for a particular Plane \((hkl)\):

$$F_{hkl} = f_{Cu} \cdot e^{2\pi i (hu_1 + kv_1 + lw_1)} + f_{Ni} \cdot e^{2\pi i (hu_2 + kv_2 + lw_2)}$$

A more generalized Expression may be Written for all atoms, \((u_1, v_1, w_1), (u_2, v_2, w_2), \ldots, (u_n, v_n, w_n)\) in a Unit cell as Follows:

$$F_{hkl} = f_1 \cdot e^{2\pi i (hu_1 + kv_1 + lw_1)} + f_2 \cdot e^{2\pi i (hu_2 + kv_2 + lw_2)} + f_3 \cdot e^{2\pi i (hu_3 + kv_3 + lw_3)} + \ldots + f_n \cdot e^{2\pi i (hu_n + kv_n + lw_n)}$$

$$F_{hkl} = \sum_{n=1}^{N} f_n \cdot e^{2\pi i (hu_n + kv_n + lw_n)}$$

Structure Factor Allows Calculations of Intensity of Peak
Examples of Structure Factor Calculations

CASE No.1: Simple Cubic

→ One Atom / Unit Cell.....located at Origin

\( u,v,w = 0,0,0 \)

\[ F_{hkl} = f \cdot e^{2\pi i (hu_1 + kv_1 + lw_1)} = f \cdot e^{2\pi i (h.0_1+k.0+1.0)} \]

Pl. Note: \( e^{\pi i} = -1 \), \( e^{3\pi i} = -1 \)............for odd powers

and \( e^{2\pi i} = +1 \), \( e^{4\pi i} = +1 \)............for even powers

and \( e^0 = 1 \)

\[ F = f \cdot e^{2\pi i(0)} = f \cdot 1 \]

\[ \therefore F^2 = f^2 \]

All Planes reflect....no restrictions
CASE No.1: BCC

→ 2 Atoms / Unit Cell.....located at Origin \((u, v, w = 0, 0, 0)\)

and \(u, v, w = \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\)

\[ F_{hkl} = f \cdot e^{2\pi i (h \cdot 0 + k \cdot 0 + l \cdot 0)} + f \cdot e^{2\pi i [h \cdot (1/2) + k \cdot (1/2) + l \cdot (1/2)]} \]

\[ F_{hkl} = f \cdot \left[ 1 + e^{\pi i (h + k + l)} \right] \]

\( F = 2f \) when \((h + k + l)\) is even \quad Ex : \((hkl = 110)\). = 1 + 1 + 0 = 2

\( F^2 = 4f^2 \)

\( F = 0 \) when \((h + k + l)\) is odd \quad Ex : \((hkl = 111)\). = 1 + 1 + 1 = 3

\( Pl.\) Note : \(e^{\pi i} = -1\) \quad \(e^{3\pi i} = -1\)............for odd powers

and \(e^{2\pi i} = +1\) \quad \(e^{4\pi i} = +1\)............for odd powers

and \(e^0 = 1\)
CASE No. 3: FCC

→ 4 Atoms / Unit Cell.....located at

\[ u,v,w = 0,0,0 \quad u,v,w = \frac{1}{2}, \frac{1}{2}, 0 \quad u,v,w = \frac{1}{2}, 0, \frac{1}{2} \quad u,v,w = 0, \frac{1}{2}, \frac{1}{2} \]

\[ F_{hkl} = f [e^{2\pi i(0)} + e^{2\pi i(h/2+k/2)} + e^{2\pi i(k/2+l/2)} + e^{2\pi i(h/2+l/2)}] \]

\[ F_{hkl} = f [1 + e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(h+l)}] \]

Conditions Under which Peak will appear assuming Bragg's law is obeyed.

If the h, k, l are unmixed (111), (200), (220).

\[ F_{111} = f [1 + e^{\pi i(1+1)} + e^{\pi i(1+1)} + e^{\pi i(1+1)}] \]

\[ F_{111} = f [1 + e^{2\pi i} + e^{2\pi i} + e^{2\pi i}] \ldots \ldots (Note: e^{2\pi i} = +1) \]

\[ F = 4.f \]

\[ F^2 = 16.f \]
CASE No. 3: FCC (Cont'd)

→ 4 Atoms / Unit Cell.....located.

If the h, k, l are unmixed (111), (200), (220).

\[ F^2 = 16f^2 \]

If the h, k, l are mixed (210), (012),

\[ F_{012} = f \left[ 1 + e^{\pi i(0+1)} + e^{\pi i(1+2)} + e^{\pi i(0+2)} \right] \]

\[ F_{111} = f \left[ 1 + e^{\pi i} + e^{3\pi i} + e^{2\pi i} \right] \ldots \ldots \left( \text{Note: } e^{2\pi i} = +1, \text{and, } e^{\pi i} = e^{3\pi i} = -1 \right) \]

\[ F_{111} = f \left[ 1 - 1 - 1 + 1 \right] \]

\[ F = f \cdot (0) \]

F = 0 or \( F^2 = 0 \) .....No Intensity even though the Braggs law is Obeyed
Structure Factor Calculations for Special Structures such as NaCl

CASE No. 4 : NaCl Structure with FCC Bravais lattice

→ 4 Atoms of Na + 4 Atoms of Cl / Unit Cell.....located at FCC

Bravais lattice Positions

\[
F_{hkl} = \left[ 1 + e^{\pi i(0+1)} + e^{\pi i(1+2)} + e^{\pi i(0+2)} \right] \left[ f_{Na} + f_{Cl} \cdot e^{\pi i(h+k+l)} \right]
\]

If the h, k, l are mixed for mixed (210), (012),

F = 0 or \( F^2 = 0 \) .....No Intensity even though the Braggs law is obeyed

Case No. 1 : (h + k + l) is even (110), (200), (220).

\[
F_{hkl} = 4 \left[ f_{Na} + f_{Cl} \cdot e^{\pi i(h+k+l)} \right]
\]

\[
F_{hkl} = 4 \left[ f_{Na} + f_{Cl} \cdot e^{\pi i(1+1+0)} \right] = 4 \left[ f_{Na} + f_{Cl} \right] \text{ .... if (h + k + l) is even Ex :110}
\]

\[
F^2_{hkl} = 16 \left[ f_{Na} + f_{Cl} \right]^2
\]

Case No. 2 : (h + k + l) is odd (111), (300), (120).

\[
F_{hkl} = 4 \left[ f_{Na} + f_{Cl} \cdot e^{\pi i(h+k+l)} \right]
\]

\[
F_{hkl} = 4 \left[ f_{Na} + f_{Cl} \cdot e^{\pi i(1+1+1)} \right] = 4 \left[ f_{Na} - f_{Cl} \right] \text{ .... if (h + k + l) is even Ex :110}
\]

\[
F^2_{hkl} = 16 \left[ f_{Na} - f_{Cl} \right]^2
\]
1. Effects of arrangement of Atoms in the lattice
2. Scattering Electrons in an Atom
3. Scattering from an Atom
4. Scattering By a Unit Cell
5. Structure Factor Calculations- Diffracted Intensity Prediction
6. Applications to Polycrystal Diffraction
7. Multiplicity Factor
8. Lorentz factor
9. Absorption Factor- applicable to Film Cameras
10. Temperature factor
11. Overall Intensities of Diffraction Peaks. taking into account all the above mentioned factor

12. Examples of Intensity calculations
Calculation of Intensity of an X-Ray Peak from a Polycrystalline or Powder sample

Factors Affecting the Intensity of the Diffracted Beam

1. Structure factor (F)
2. Absorption factor (A)
3. Temperature factor ($e^{-M}$)
4. Multiplicity Factor ($p$)
5. Lorentz Polarization Factor (LP) Rotation and geometry of Crystal

$\theta \quad d_{001} = 4A$

$22.6^\circ$
Intensities of Diffracted Beams

1. Effects of arrangement of Atoms in the lattice
2. Scattering Electrons in an Atom
3. Scattering from an Atom
4. Scattering By a Unit Cell
5. Structure Factor Calculations - Diffracted Intensity Prediction

6. Applications to Polycrystal Diffraction

7. Multiplicity Factor

8. Lorentz factor

9. Absorption Factor - applicable to Film Cameras

10. Temperature factor

11. Overall Intensities of Diffraction Peaks. taking into account all the above mentioned factor

12. Examples of Intensity calculations

03/06/2006
MSE 416 and Graduate Students
- D. Chandra
Maximum Intensity

\[ I_{B_{\text{Max.}}} \propto \frac{1}{\sin \theta_B} \]

Maximum Intensity

\[ B \propto \frac{1}{\cos \theta_B} \]

\[ I_{B_{\text{Max.}}} \cdot B = \frac{1}{\sin \theta_B \cdot \cos \theta_B} \]

\[ I_{\text{Int.I}} = \frac{1}{\sin 2\theta_B} \]
Difference in path length, $\delta$:

$\delta_{1,2'} = AD - CB$ for atoms on the same planes

$\delta_{1,2'} = a \cdot \cos \theta_2 - a \cdot \cos \theta_1$

$\delta_{1,2'} = a \left[ \cos(\theta_B - \Delta \theta) - \cos(\theta_B + \Delta \theta) \right]$

$\delta_{1,2'} = 2a \cdot \Delta \theta \cdot \sin \theta_B$

Condition for zero diffraction of beam
Factor No. 2 Geometrical Factor  
Crystal Oriented at or near Bragg Angles

1. For Particular (hkl) ON is normal to the plane
2. The $\Delta \theta$ for the Plane is high for the High Angle and low for the low angle.
3. This occurs even if the crystals are oriented randomly (or not oriented)
4. If there are DN crystals favorably oriented to diffract out of N crystals
5. Then Fraction of Crystals favorably oriented = $X$
6. Peaks broader @ High Angles

$$X = \frac{\Delta N}{N} = \frac{\text{Surface Area of the Strip}}{\text{Surface area of the sphere}}$$

$$X = \frac{\Delta N}{N} = \frac{r \Delta \theta \cdot [2\pi \cdot r \cdot \sin(90^\circ - \theta_B)]}{4\pi \cdot r^2}$$

$$\frac{\Delta N}{N} = \frac{\Delta \theta \cdot \cos \theta_B}{2}$$

Low for High Angles: Intensity Low
Factor No. 3 Geometrical Factor
Circumference of Diffracted line in a Debye Scherrer Film

1. Compare Integrated Intensity of the diffracted lines

2. \( L = \text{Length of Diffracted Line (Circumference)} \)

3. \( L = 2\pi R \sin \theta_B \)  
   \( R = \text{radius of the Camera} \)

Relative Intensity between lines of two planes, for Example:

Rel. Int. (111) And (110) /unit Length

Rel. Int. \( \propto \frac{1}{\sin^2 \theta_B} \)
Combined Equation for Geometrical Factor Of a Debye Scherrer Film Bragg Line

Combining All Geometrical factors:
1. Crystal Rotation
2. No. of Crystals Oriented
3. Length of the Diffracted Line

We can write an equation called:

Lorentz Factor = \left( \frac{1}{\sin 2\theta} \right) \cdot \cos \theta \cdot \left( \frac{1}{\sin 2\theta} \right)

LFactor = \frac{\cos \theta}{\sin^2 2\theta} = \frac{1}{4\sin^2 2\theta \cdot \cos \theta}
1. Effects of arrangement of Atoms in the lattice
2. Scattering Electrons in an Atom
3. Scattering from an Atom
4. Scattering By a Unit Cell
5. Structure Factor Calculations - Diffracted Intensity Prediction
6. Applications to Polycrystal Diffraction
7. Multiplicity Factor
8. Lorentz factor (Cont’d)
9. Absorption Factor - applicable to Film Cameras
10. Temperature factor
11. Overall Intensities of Diffraction Peaks. taking into account all the above mentioned factor

12. Examples of Intensity calculations
Recall Polarization Factor for Trig. factors

\[
\text{Polarization Factor} = \frac{1}{2} \left( 1 + \cos^2 2\theta \right)
\]

Now we can write an Combined Polarization factor:

\[
\text{Lorentz Polarization Factor} = \frac{1}{4 \sin^2 \theta \cos \theta}
\]

\[
\text{LFactor} = \frac{\cos \theta}{\sin^2 2\theta} = \left( \frac{1 + \cos^2 2\theta}{\sin^2 2\theta \cos \theta} \right) \cdot \frac{1}{8}
\]

*Given In Appendix 12*
Intensities of Diffracted Beams

1. Effects of arrangement of Atoms in the lattice
2. Scattering Electrons in an Atom
3. Scattering from an Atom
4. Scattering By a Unit Cell
5. Structure Factor Calculations - Diffracted Intensity Prediction

6. Applications to Polycrystal Diffraction
7. Multiplicity Factor
8. Lorentz factor
9. Absorption Factor - applicable to Film Cameras
10. Temperature factor
11. Overall Intensities of Diffraction Peaks. taking into account all the above mentioned factor

12. Examples of Intensity calculations

03/06/2006 MSE 416 and Graduate Students - D. Chandra
Absorption Factor for a Debye Camera

Applies to Debye and other Cameras

It is related Mass absorption Coefficient \((\mu/\rho)\) of the material.

For Heavy metals there is significant Effect at low angles: Intensities appear to be lower than they actually are!!
Absorption Effects in a Diffractometer - Diffracted Beam Intensity

Diffraction from a flat plate: incident and diffracted beams have a thickness of 1 cm in a direction normal to the plane of the drawing.

\[ I_D = \int_{x=0}^{x=\infty} dI_D = \frac{I_o \cdot a \cdot b}{2 \cdot \mu} \]

\( \mu, a, b \) are constants..a varies somewhat with angle

Assumes Infinite thickness:

\[ t = \frac{3.45 \sin \theta}{\mu} \]

Ex:

"Ni Powder" with Cu - K\( \alpha \) @ approx. \( \theta = 90^\circ \)
Density of the Compact = 0.6 of the density of solid (\( \rho = 8.9 \text{ g/cc} \))
Thus, \( \mu = 261/\text{cm} \)
\( t = 1.32 \times 10^{-2} \text{ cm} \).
Intensities of Diffracted Beams

1. Effects of arrangement of Atoms in the lattice
2. Scattering Electrons in an Atom
3. Scattering from an Atom
4. Scattering By a Unit Cell
5. Structure Factor Calculations - Diffracted Intensity Prediction

6. Applications to Polycrystal Diffraction
7. Multiplicity Factor
8. Lorentz factor
9. Absorption Factor - applicable to Film Cameras
10. Temperature factor
11. Overall Intensities of Diffraction Peaks. taking into account all the above mentioned factor

12. Examples of Intensity calculations

03/06/2006 MSE 416 and Graduate Students - D. Chandra
Temperature on Intensities of the Bragg Peaks

Atomic Scattering Factor @ T = f = f_o e^{-M}

F_o = Scattering when the atom is at rest......these are values a Tabulated in Appendix 10.

Debye Model Gives us:

\[ M = \frac{6. \lambda^2 T}{m k \Theta^2} \left[ \phi(x) + \frac{x}{4} \right] \left( \frac{\sin \theta}{\lambda} \right)^2 \]

Where \[ x = \frac{\Theta}{T} \]

\[ m = \text{Mass of Vibrating Atom} \]
Appendix 13

Data for Calculation of the Temperature Factor

Values of $\phi(x) = \frac{1}{x} \int_{x,0}^{x} \frac{\xi}{e^{\xi} - 1} d\xi$ as a Function of $x$

<table>
<thead>
<tr>
<th>$x$</th>
<th>0</th>
<th>0.1</th>
<th>0.2</th>
<th>0.3</th>
<th>0.4</th>
<th>0.5</th>
<th>0.6</th>
<th>0.7</th>
<th>0.8</th>
<th>0.9</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.000</td>
<td>0.975</td>
<td>0.951</td>
<td>0.928</td>
<td>0.894</td>
<td>0.860</td>
<td>0.839</td>
<td>0.818</td>
<td>0.787</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.778</td>
<td>0.758</td>
<td>0.739</td>
<td>0.721</td>
<td>0.703</td>
<td>0.686</td>
<td>0.669</td>
<td>0.653</td>
<td>0.637</td>
<td>0.622</td>
</tr>
<tr>
<td>2</td>
<td>0.607</td>
<td>0.592</td>
<td>0.578</td>
<td>0.565</td>
<td>0.552</td>
<td>0.539</td>
<td>0.525</td>
<td>0.514</td>
<td>0.503</td>
<td>0.491</td>
</tr>
<tr>
<td>3</td>
<td>0.480</td>
<td>0.470</td>
<td>0.460</td>
<td>0.450</td>
<td>0.440</td>
<td>0.431</td>
<td>0.422</td>
<td>0.413</td>
<td>0.404</td>
<td>0.396</td>
</tr>
<tr>
<td>4</td>
<td>0.388</td>
<td>0.380</td>
<td>0.377</td>
<td>0.366</td>
<td>0.359</td>
<td>0.352</td>
<td>0.345</td>
<td>0.339</td>
<td>0.333</td>
<td>0.327</td>
</tr>
<tr>
<td>5</td>
<td>0.321</td>
<td>0.313</td>
<td>0.310</td>
<td>0.304</td>
<td>0.299</td>
<td>0.294</td>
<td>0.289</td>
<td>0.285</td>
<td>0.280</td>
<td>0.276</td>
</tr>
<tr>
<td>6</td>
<td>0.271</td>
<td>0.267</td>
<td>0.263</td>
<td>0.259</td>
<td>0.255</td>
<td>0.251</td>
<td>0.248</td>
<td>0.244</td>
<td>0.241</td>
<td>0.237</td>
</tr>
</tbody>
</table>

For $x$ greater than 7, $\phi(x)$ is given to a good approximation by $(1.642x)$. (From [G.1].)

Debye Temperatures

James [G.19, p. 221] gives the following values of the characteristic Debye temperature $\Theta$ for some cubic metals:

<table>
<thead>
<tr>
<th>Metal</th>
<th>$\Theta$ (K)</th>
<th>Metal</th>
<th>$\Theta$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>390</td>
<td>Ta</td>
<td>245</td>
</tr>
<tr>
<td>Ca</td>
<td>230</td>
<td>Pb</td>
<td>88</td>
</tr>
<tr>
<td>Cu</td>
<td>320</td>
<td>Fe</td>
<td>430</td>
</tr>
<tr>
<td>Ag</td>
<td>210</td>
<td>Co</td>
<td>410</td>
</tr>
<tr>
<td>Au</td>
<td>175</td>
<td>Ni</td>
<td>400</td>
</tr>
<tr>
<td>Zr</td>
<td>485</td>
<td>Pd</td>
<td>275</td>
</tr>
<tr>
<td>Mo</td>
<td>380</td>
<td>Ir</td>
<td>285</td>
</tr>
<tr>
<td>W</td>
<td>310</td>
<td>Pt</td>
<td>230</td>
</tr>
</tbody>
</table>

- D. Chandra
Typical Effects on the Bragg Peak Intensities

- Temperature effects on the Peaks are not very profound at reasonable temperatures.
- They generally effect the High angle peak at very high temperatures. Difficult to access this effect.

Applications to of Structure Factor Calculations To Polycrystals
Temperature Factor

Figure 4-22 Effect of thermal vibration of the atoms on a powder pattern. Very schematic, see text.
Intensities of Diffracted Beams

1. Effects of arrangement of Atoms in the lattice
2. Scattering Electrons in an Atom
3. Scattering from an Atom
4. Scattering By a Unit Cell
5. Structure Factor Calculations - Diffracted Intensity Prediction

6. Applications to Polycrystal Diffraction

7. Multiplicity Factor
8. Lorentz factor
9. Absorption Factor - applicable to Film Cameras
10. Temperature factor
11. Overall Intensities of Diffraction Peaks. taking into account all the above mentioned factor

12. Examples of Intensity calculations
Final Intensities of the Diffracted Peaks From Polycrystalline Materials

Approx. Intensity of Bragg Peak from a Debye Scherrer Camera:

\[ I = |F|^2 \cdot p \left( \frac{1 + \cos^2 2\theta}{\sin^2 2\theta \cdot \cos \theta} \right) \]

LP Factor Given In Appendix 12

Exact Intensity of Bragg Peak from a Debye Scherrer Camera:

\[ I = |F|^2 \cdot p \left( \frac{1 + \cos^2 2\theta}{\sin^2 2\theta \cdot \cos \theta} \right) \cdot A(\theta) \cdot e^{-M} \]

Exact Intensity of Bragg Peak from a Diffractometer:

\[ I = |F|^2 \cdot p \left( \frac{1 + \cos^2 2\theta}{\sin^2 2\theta \cdot \cos \theta} \right) \cdot e^{-M} \]
## Intensities of Diffracted Beams

1. Effects of arrangement of Atoms in the lattice
2. Scattering Electrons in an Atom
3. Scattering from an Atom
4. Scattering By a Unit Cell
5. Structure Factor Calculations - Diffracted Intensity Prediction

6. Applications to Polycrystal Diffraction

7. Multiplicity Factor
8. Lorentz factor
9. Absorption Factor - applicable to Film Cameras
10. Temperature factor
11. Overall Intensities of Diffraction Peaks. taking into account all the above mentioned factor

12. Examples of Intensity calculations
Consider a Debye-Scherrer Pattern

\[ I = \left| F^2 \right| \cdot p \left( \frac{1 + \cos^2 2\theta}{\sin^2 2\theta \cdot \cos \theta} \right) \cdot A(\theta) \cdot e^{-M} \]

Steps to be Followed:
1. We know the Structure of Cu = FCC, and crystal plane that diffract in Appendix
2. \( \lambda = 1.542 \) (Cu - K\(\alpha\))
3. \( a = 3.615 \) Angstroms

\[ \frac{\lambda^2}{4a^2} = 0.0455... \text{gives values of } \sin^2 \theta \]

We also need \( \frac{\sin \theta}{\lambda} \) for Lorentz Polaization Factor
Sample Calculation for Cu Metal

<table>
<thead>
<tr>
<th>Line</th>
<th>hkl</th>
<th>h^2 + k^2 + l^2</th>
<th>sin^2θ</th>
<th>sin θ</th>
<th>θ</th>
<th>sin θ/λ (Å^-1)</th>
<th>fCu</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>111</td>
<td>3</td>
<td>0.1365</td>
<td>0.369</td>
<td>21.7°</td>
<td>0.24</td>
<td>&gt;2.1</td>
</tr>
<tr>
<td>2</td>
<td>200</td>
<td>4</td>
<td>0.1820</td>
<td>0.427</td>
<td>25.3</td>
<td>0.27</td>
<td>20.9</td>
</tr>
<tr>
<td>3</td>
<td>220</td>
<td>8</td>
<td>0.364</td>
<td>0.603</td>
<td>37.1</td>
<td>0.39</td>
<td>16.8</td>
</tr>
<tr>
<td>4</td>
<td>311</td>
<td>11</td>
<td>0.500</td>
<td>0.707</td>
<td>45.0</td>
<td>0.46</td>
<td>14.8</td>
</tr>
<tr>
<td>5</td>
<td>222</td>
<td>12</td>
<td>0.546</td>
<td>0.739</td>
<td>47.6</td>
<td>0.48</td>
<td>14.2</td>
</tr>
<tr>
<td>6</td>
<td>400</td>
<td>16</td>
<td>0.728</td>
<td>0.853</td>
<td>58.5</td>
<td>0.55</td>
<td>12.5</td>
</tr>
<tr>
<td>7</td>
<td>331</td>
<td>19</td>
<td>0.865</td>
<td>0.930</td>
<td>68.4</td>
<td>0.60</td>
<td>11.5</td>
</tr>
<tr>
<td>8</td>
<td>420</td>
<td>20</td>
<td>0.910</td>
<td>0.954</td>
<td>72.6</td>
<td>0.62</td>
<td>11.1</td>
</tr>
</tbody>
</table>

Sample Intensity Calculations

<table>
<thead>
<tr>
<th>Line</th>
<th>F^2</th>
<th>ρ</th>
<th>1 + cos^2 2θ</th>
<th>sin^2θ cos θ</th>
<th>Relative integrated intensity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>7810</td>
<td>8</td>
<td>12.03</td>
<td></td>
<td>7.52 × 10^5</td>
</tr>
<tr>
<td>2</td>
<td>6990</td>
<td>6</td>
<td>8.50</td>
<td></td>
<td>3.56</td>
</tr>
<tr>
<td>3</td>
<td>4520</td>
<td>12</td>
<td>3.70</td>
<td></td>
<td>2.01</td>
</tr>
<tr>
<td>4</td>
<td>3500</td>
<td>24</td>
<td>2.83</td>
<td></td>
<td>2.38</td>
</tr>
<tr>
<td>5</td>
<td>3230</td>
<td>8</td>
<td>2.74</td>
<td></td>
<td>0.71</td>
</tr>
<tr>
<td>6</td>
<td>2500</td>
<td>6</td>
<td>3.18</td>
<td></td>
<td>0.48</td>
</tr>
<tr>
<td>7</td>
<td>2120</td>
<td>24</td>
<td>4.81</td>
<td></td>
<td>2.45</td>
</tr>
<tr>
<td>8</td>
<td>1970</td>
<td>24</td>
<td>6.15</td>
<td></td>
<td>2.91</td>
</tr>
</tbody>
</table>

- D. Chandra
Sample Calculation for Cu Metal

<table>
<thead>
<tr>
<th>Column No. 2:</th>
<th>(hkl) Plane</th>
</tr>
</thead>
<tbody>
<tr>
<td>Column No. 3:</td>
<td>h² + k² + l²</td>
</tr>
<tr>
<td>Column No. 4:</td>
<td>sin²(\theta) = 0.1365</td>
</tr>
<tr>
<td>Column No. 6:</td>
<td>value of (\theta) (need to calculate the L-P factor)</td>
</tr>
<tr>
<td>Column No. 7:</td>
<td>sin(\theta/λ) (need to calculate the Atomic Scattering Factor, f)</td>
</tr>
<tr>
<td>Column No. 8:</td>
<td>At. Scattering factor (f)</td>
</tr>
</tbody>
</table>

\[ \sin^2 \theta = \frac{\lambda^2}{4a^2}(h^2 + k^2 + l^2) \]

\(\lambda = 1.542\) Angstrom = 0.1542 nm

\(Cu: \) Lattice Parameter: \(a_{FCC} = 3.615\) Angstrom = 0.3615 nm

\[ \therefore \frac{\lambda^2}{4a^2} = 0.0455 \]

Then, we can find the \(\sin^2 \theta\) which is in the Column No.4

Interpolate the value from the Table

<table>
<thead>
<tr>
<th>(\sin \theta/\lambda)</th>
<th>0.0</th>
<th>0.1</th>
<th>0.2</th>
<th>0.3</th>
<th>0.4</th>
<th>0.5</th>
<th>0.6</th>
<th>0.7</th>
<th>0.8</th>
<th>0.9</th>
<th>1.0</th>
<th>1.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>29</td>
<td>25.9</td>
<td>21.6</td>
<td>17.9</td>
<td>15.2</td>
<td>13.3</td>
<td>11.7</td>
<td>10.2</td>
<td>9.1</td>
<td>8.1</td>
<td>7.3</td>
<td>6.6</td>
</tr>
</tbody>
</table>
Sample Calculation for Cu Metal

Applications to of Structure Factor Calculations To Polycrystals
Sample Intensity Calculations

- D. Chandra
Sample Calculation for Cu Metal (Cont’d)

<table>
<thead>
<tr>
<th>Line</th>
<th>$F^2$</th>
<th>$\rho$</th>
<th>$\frac{1 + \cos^2 2\theta}{\sin^2\theta \cos\theta}$</th>
<th>Relative integrated intensity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>7810</td>
<td>8</td>
<td>12.03</td>
<td>7.52 x 10^5</td>
</tr>
<tr>
<td>2</td>
<td>6990</td>
<td>6</td>
<td>8.50</td>
<td>3.56</td>
</tr>
</tbody>
</table>

Column No. 9: Structure factor ($F$) for FCC $\rightarrow F^2 = (4f)^2 = 16f^2$ (see page 139)

Column No. 10: Multiplicity $p=6$ for 200 plane from Appendix 12 (see next Page)

Column No. 11: Lorentz Polarization Factor (L.P)

Column No. 12: Use Eq. 4-19 $\rightarrow I = \left| F^2 \right| \rho \left( \frac{1 + \cos^2 2\theta}{\sin^2\theta \cos\theta} \right)$

Column No. 13: Normalized to the First Intensity of 10: $(7.52\times10^5 / 7.52\times10^5)\times10 = 10$

$(3.56\times10^5 / 7.52\times10^5)\times10 = 4.7$

$(2.01\times10^5 / 7.52\times10^5)\times10 = 2.7$
## Appendix 12

### Atomic Scattering Factors (f) for Cu Scatterer

**Form Factor** …… we need \( \sin \theta / \lambda \)

<table>
<thead>
<tr>
<th>( \sin \theta / \lambda ) (Å(^{-1}))</th>
<th>0.0</th>
<th>0.1</th>
<th>0.2</th>
<th>0.3</th>
<th>0.4</th>
<th>0.5</th>
<th>0.6</th>
<th>0.7</th>
<th>0.8</th>
<th>0.9</th>
<th>1.0</th>
<th>1.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>29</td>
<td>25.9</td>
<td>21.6</td>
<td>17.9</td>
<td>15.2</td>
<td>13.3</td>
<td>11.7</td>
<td>10.2</td>
<td>9.1</td>
<td>8.1</td>
<td>7.3</td>
<td>6.6</td>
</tr>
</tbody>
</table>

Interpolate the value from the Table ……just Cu values are traced here.
Explanation of Column Listing on the Last Page

written down in this column in order of increasing values of \((h^2 + k^2 + l^2)\), from Appendix 10.

Column 4: For a cubic crystal, values of \(\sin^2 \theta\) are given by Eq. (3-10):

\[
\sin^2 \theta = \frac{\lambda^2}{4a^2} (h^2 + k^2 + l^2).
\]

In this case, \(\lambda = 1.542 \text{ Å} \) (Cu \(K\alpha\) and \(a = 3.615 \text{ Å}\) (lattice parameter of copper). Therefore, multiplication of the integers in column 3 by \(\lambda^2/4a^2 = 0.0455\) gives the values of \(\sin^2 \theta\) listed in column 4. In this and similar calculations, three-figure accuracy is ample.

Column 6: Needed to determine the Lorentz-polarization factor and \((\sin \theta)/\lambda\).

Column 7: Obtained from Appendix 11. Needed to determine \(f_{Cu}\).

Column 8: Obtained from Appendix 12.

Column 9: Obtained from the relation \(F^2 = 16f_{Cu}\).

Column 10: Obtained from Appendix 13.

Column 11: Obtained from Appendix 14.

Column 12: These values are the product of the values in columns 9, 10, and 11, according to Eq. (4-19).

Column 13: Values from column 12 recalculated to give the first line an arbitrary intensity of 10, i.e., “normalized” to 10 for the first line.

Column 14: These entries give the observed intensities, visually estimated according to the following simple scale, from the original film for copper in Fig. 3-13 (\(v = \text{very strong, } s = \text{strong, } m = \text{medium, } w = \text{weak}\).
### Applications to Structure Factor Calculations To Polycrystals

**Sample Intensity Calculations**

<table>
<thead>
<tr>
<th>Multiplicity Factors for the Powder Method</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Cubic:</strong></td>
</tr>
<tr>
<td><strong>Hexagonal and Rhombohedral:</strong></td>
</tr>
<tr>
<td><strong>Tetragonal:</strong></td>
</tr>
<tr>
<td><strong>Orthorhombic:</strong></td>
</tr>
<tr>
<td><strong>Monoclinic:</strong></td>
</tr>
<tr>
<td><strong>Triclinic:</strong></td>
</tr>
</tbody>
</table>

**Planes**

- **001 or 002**
- **010 or 020**
- **100 or 200**
- **00-1 or 00-2**
- **0-10 or 0-20**
- **-100 or -200**

Note that, in cubic crystals, for example, \( hhl \) stands for such indices as \( 112 \) (or \( 211 \)), \( 0kl \) for such indices as \( 012 \) (or \( 210 \)), \( 0kk \) for such indices as \( 011 \) (or \( 110 \), etc.

These are the usual multiplicity factors. In some crystals, planes having these indices comprising two forms with the same spacing but different structure factor, and the multiplicity factor for each form is half the value given above. In the cubic system, for example, there are some crystals in which permutations of the indices \( hhl \) produce planes which are not structurally equivalent in such crystals (AuBe, discussed in Sec. 2-7, is an example), the plane \( 123 \), for example, belongs to one form and has a certain structure factor, while the plane \( 321 \) belongs to another form and has a different structure factor. There are 24 planes in the first form and 24 planes in the second. This question is discussed more fully by Henry, Lipson, and Wooster [G.8].
Appendix 12

Atomic Scattering Factors (f)

Form Factor …… we need sin $\theta/\lambda$

<table>
<thead>
<tr>
<th>$\frac{\sin \theta}{\lambda}$ (Å$^{-1}$)</th>
<th>0.0</th>
<th>0.1</th>
<th>0.2</th>
<th>0.3</th>
<th>0.4</th>
<th>0.5</th>
<th>0.6</th>
<th>0.7</th>
<th>0.8</th>
<th>0.9</th>
<th>1.0</th>
<th>1.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1.0</td>
<td>0.81</td>
<td>0.48</td>
<td>0.25</td>
<td>0.13</td>
<td>0.07</td>
<td>0.04</td>
<td>0.03</td>
<td>0.02</td>
<td>0.01</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>He</td>
<td>2.0</td>
<td>1.88</td>
<td>1.46</td>
<td>1.05</td>
<td>0.75</td>
<td>0.52</td>
<td>0.35</td>
<td>0.24</td>
<td>0.18</td>
<td>0.14</td>
<td>0.11</td>
<td>0.09</td>
</tr>
<tr>
<td>Li$^+$</td>
<td>2.0</td>
<td>1.96</td>
<td>1.8</td>
<td>1.5</td>
<td>1.3</td>
<td>1.0</td>
<td>0.8</td>
<td>0.6</td>
<td>0.5</td>
<td>0.4</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>Li</td>
<td>3.0</td>
<td>2.2</td>
<td>1.8</td>
<td>1.5</td>
<td>1.3</td>
<td>1.0</td>
<td>0.8</td>
<td>0.6</td>
<td>0.5</td>
<td>0.4</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>Be$^{2+}$</td>
<td>2.0</td>
<td>2.0</td>
<td>1.9</td>
<td>1.7</td>
<td>1.6</td>
<td>1.4</td>
<td>1.2</td>
<td>1.0</td>
<td>0.9</td>
<td>0.7</td>
<td>0.6</td>
<td>0.5</td>
</tr>
<tr>
<td>Be</td>
<td>4.0</td>
<td>2.9</td>
<td>1.9</td>
<td>1.7</td>
<td>1.6</td>
<td>1.4</td>
<td>1.2</td>
<td>1.0</td>
<td>0.9</td>
<td>0.7</td>
<td>0.6</td>
<td>0.5</td>
</tr>
<tr>
<td>B$^+$</td>
<td>2.0</td>
<td>1.99</td>
<td>1.9</td>
<td>1.8</td>
<td>1.7</td>
<td>1.6</td>
<td>1.4</td>
<td>1.3</td>
<td>1.2</td>
<td>1.0</td>
<td>0.9</td>
<td>0.7</td>
</tr>
<tr>
<td>B</td>
<td>5.0</td>
<td>3.5</td>
<td>2.4</td>
<td>1.9</td>
<td>1.7</td>
<td>1.5</td>
<td>1.4</td>
<td>1.2</td>
<td>1.2</td>
<td>1.0</td>
<td>0.9</td>
<td>0.7</td>
</tr>
<tr>
<td>C</td>
<td>6.0</td>
<td>4.6</td>
<td>3.0</td>
<td>2.2</td>
<td>1.9</td>
<td>1.7</td>
<td>1.6</td>
<td>1.4</td>
<td>1.3</td>
<td>1.16</td>
<td>1.0</td>
<td>0.9</td>
</tr>
<tr>
<td>N$^{5-}$</td>
<td>2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>1.9</td>
<td>1.9</td>
<td>1.8</td>
<td>1.7</td>
<td>1.6</td>
<td>1.5</td>
<td>1.4</td>
<td>1.3</td>
<td>1.16</td>
</tr>
<tr>
<td>N$^{3-}$</td>
<td>4.0</td>
<td>3.7</td>
<td>3.0</td>
<td>2.4</td>
<td>2.0</td>
<td>1.8</td>
<td>1.66</td>
<td>1.56</td>
<td>1.49</td>
<td>1.39</td>
<td>1.28</td>
<td>1.17</td>
</tr>
<tr>
<td>N$^{+}$</td>
<td>7.0</td>
<td>5.8</td>
<td>4.2</td>
<td>3.0</td>
<td>2.3</td>
<td>1.9</td>
<td>1.65</td>
<td>1.54</td>
<td>1.49</td>
<td>1.39</td>
<td>1.29</td>
<td>1.17</td>
</tr>
<tr>
<td>O$^{2-}$</td>
<td>8.0</td>
<td>7.1</td>
<td>5.3</td>
<td>3.9</td>
<td>2.9</td>
<td>2.2</td>
<td>1.8</td>
<td>1.6</td>
<td>1.5</td>
<td>1.4</td>
<td>1.35</td>
<td>1.24</td>
</tr>
<tr>
<td>F$^{-2}$</td>
<td>10.0</td>
<td>8.0</td>
<td>5.5</td>
<td>3.8</td>
<td>2.7</td>
<td>2.1</td>
<td>1.8</td>
<td>1.5</td>
<td>1.5</td>
<td>1.4</td>
<td>1.35</td>
<td>1.24</td>
</tr>
</tbody>
</table>

D. Chandra
### Atomic Scattering Factors (f) (Cont’d)

<table>
<thead>
<tr>
<th>Element</th>
<th>f_1</th>
<th>f_2</th>
<th>f_3</th>
<th>f_4</th>
<th>f_5</th>
<th>f_6</th>
<th>f_7</th>
</tr>
</thead>
<tbody>
<tr>
<td>F^-</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>6.7</td>
<td>4.8</td>
<td>3.5</td>
</tr>
<tr>
<td>Ne</td>
<td>9.3</td>
<td>7.5</td>
<td>5.8</td>
<td></td>
<td>4.4</td>
<td>3.4</td>
<td>2.6</td>
</tr>
<tr>
<td>Na^+</td>
<td>9.5</td>
<td>8.2</td>
<td>6.7</td>
<td></td>
<td>5.25</td>
<td>4.05</td>
<td>3.2</td>
</tr>
<tr>
<td>Na^-</td>
<td>9.65</td>
<td>8.2</td>
<td>6.7</td>
<td></td>
<td>5.25</td>
<td>4.05</td>
<td>3.2</td>
</tr>
<tr>
<td>Mg^2+</td>
<td>9.75</td>
<td>8.6</td>
<td>7.25</td>
<td></td>
<td>5.95</td>
<td>4.8</td>
<td>3.85</td>
</tr>
<tr>
<td>Mg</td>
<td>12</td>
<td>10.5</td>
<td>8.6</td>
<td>7.25</td>
<td>5.95</td>
<td>4.8</td>
<td>3.85</td>
</tr>
<tr>
<td>Al^3+</td>
<td>9.7</td>
<td>8.9</td>
<td>7.8</td>
<td></td>
<td>6.65</td>
<td>5.5</td>
<td>4.45</td>
</tr>
<tr>
<td>Si</td>
<td>14</td>
<td>11.35</td>
<td>9.4</td>
<td>8.2</td>
<td>7.15</td>
<td>6.1</td>
<td>5.1</td>
</tr>
<tr>
<td>Si^4+</td>
<td>13</td>
<td>11.75</td>
<td>9.15</td>
<td>8.25</td>
<td>7.15</td>
<td>6.05</td>
<td>5.05</td>
</tr>
<tr>
<td>P^-</td>
<td>10</td>
<td>9.8</td>
<td>9.25</td>
<td>8.45</td>
<td>7.5</td>
<td>6.55</td>
<td>5.65</td>
</tr>
<tr>
<td>P</td>
<td>15</td>
<td>12.4</td>
<td>10.0</td>
<td>8.45</td>
<td>7.45</td>
<td>6.5</td>
<td>5.65</td>
</tr>
<tr>
<td>P^3-</td>
<td>18</td>
<td>12.7</td>
<td>9.8</td>
<td>8.4</td>
<td>7.25</td>
<td>6.5</td>
<td>5.65</td>
</tr>
<tr>
<td>S^-</td>
<td>10</td>
<td>9.85</td>
<td>9.4</td>
<td>8.7</td>
<td>7.85</td>
<td>6.85</td>
<td>6.05</td>
</tr>
<tr>
<td>S</td>
<td>16</td>
<td>13.6</td>
<td>10.7</td>
<td>8.95</td>
<td>7.85</td>
<td>6.85</td>
<td>6.0</td>
</tr>
<tr>
<td>S^-2</td>
<td>18</td>
<td>14.3</td>
<td>10.7</td>
<td>8.9</td>
<td>7.85</td>
<td>6.85</td>
<td>6.0</td>
</tr>
<tr>
<td>Cl</td>
<td>17</td>
<td>14.6</td>
<td>11.3</td>
<td>9.25</td>
<td>8.05</td>
<td>7.25</td>
<td>6.5</td>
</tr>
<tr>
<td>Cl^-</td>
<td>18</td>
<td>15.2</td>
<td>11.5</td>
<td>9.3</td>
<td>8.05</td>
<td>7.25</td>
<td>6.5</td>
</tr>
<tr>
<td>A</td>
<td>18</td>
<td>15.9</td>
<td>12.6</td>
<td>10.4</td>
<td>8.7</td>
<td>7.8</td>
<td>7.0</td>
</tr>
<tr>
<td>K</td>
<td>18</td>
<td>16.5</td>
<td>13.3</td>
<td>10.8</td>
<td>8.85</td>
<td>7.75</td>
<td>7.05</td>
</tr>
<tr>
<td>K</td>
<td>19</td>
<td>16.5</td>
<td>13.3</td>
<td>10.8</td>
<td>8.9</td>
<td>7.9</td>
<td>6.7</td>
</tr>
<tr>
<td>Co^-2</td>
<td>18</td>
<td>16.8</td>
<td>14.0</td>
<td>11.5</td>
<td>9.3</td>
<td>8.1</td>
<td>7.35</td>
</tr>
<tr>
<td>Ca</td>
<td>20</td>
<td>17.5</td>
<td>14.1</td>
<td>11.4</td>
<td>9.7</td>
<td>8.4</td>
<td>7.3</td>
</tr>
<tr>
<td>Sc^-3</td>
<td>18</td>
<td>16.7</td>
<td>14.0</td>
<td>11.4</td>
<td>9.4</td>
<td>8.3</td>
<td>7.6</td>
</tr>
<tr>
<td>Sc</td>
<td>21</td>
<td>18.4</td>
<td>14.9</td>
<td>12.1</td>
<td>10.3</td>
<td>8.9</td>
<td>7.7</td>
</tr>
<tr>
<td>Ti^-4</td>
<td>18</td>
<td>17.0</td>
<td>14.4</td>
<td>11.9</td>
<td>9.9</td>
<td>8.5</td>
<td>7.85</td>
</tr>
<tr>
<td>Ti</td>
<td>22</td>
<td>19.3</td>
<td>15.7</td>
<td>12.8</td>
<td>10.9</td>
<td>9.5</td>
<td>8.2</td>
</tr>
<tr>
<td>V</td>
<td>23</td>
<td>20.2</td>
<td>16.6</td>
<td>13.5</td>
<td>11.5</td>
<td>10.1</td>
<td>8.7</td>
</tr>
<tr>
<td>Cr</td>
<td>24</td>
<td>21.1</td>
<td>17.4</td>
<td>14.2</td>
<td>12.1</td>
<td>10.6</td>
<td>9.2</td>
</tr>
<tr>
<td>Mn</td>
<td>25</td>
<td>22.1</td>
<td>18.2</td>
<td>14.9</td>
<td>12.7</td>
<td>11.1</td>
<td>9.7</td>
</tr>
</tbody>
</table>
### APPENDIX 14

**LORENTZ-POLARIZATION FACTOR** \[\left(\frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta}\right)\]

<table>
<thead>
<tr>
<th>(\theta^\circ)</th>
<th>.0</th>
<th>.1</th>
<th>.2</th>
<th>.3</th>
<th>.4</th>
<th>.5</th>
<th>.6</th>
<th>.7</th>
<th>.8</th>
<th>.9</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1639</td>
<td>1486</td>
<td>1354</td>
<td>1239</td>
<td>1138</td>
<td>1048</td>
<td>968.9</td>
<td>898.3</td>
<td>835.1</td>
<td>778.1</td>
</tr>
<tr>
<td>3</td>
<td>727.2</td>
<td>680.9</td>
<td>638.8</td>
<td>600.5</td>
<td>565.6</td>
<td>533.6</td>
<td>504.3</td>
<td>477.3</td>
<td>452.3</td>
<td>429.0</td>
</tr>
<tr>
<td>4</td>
<td>408.0</td>
<td>368.2</td>
<td>349.9</td>
<td>352.7</td>
<td>336.8</td>
<td>321.9</td>
<td>308.0</td>
<td>294.9</td>
<td>282.6</td>
<td>271.1</td>
</tr>
<tr>
<td>5</td>
<td>260.3</td>
<td>250.1</td>
<td>240.5</td>
<td>231.4</td>
<td>222.9</td>
<td>214.7</td>
<td>207.1</td>
<td>199.8</td>
<td>192.9</td>
<td>186.0</td>
</tr>
<tr>
<td>6</td>
<td>180.1</td>
<td>174.2</td>
<td>168.5</td>
<td>163.1</td>
<td>158.0</td>
<td>153.1</td>
<td>148.4</td>
<td>144.0</td>
<td>139.7</td>
<td>135.0</td>
</tr>
<tr>
<td>7</td>
<td>131.7</td>
<td>128.0</td>
<td>124.4</td>
<td>120.9</td>
<td>117.6</td>
<td>114.4</td>
<td>111.4</td>
<td>108.5</td>
<td>105.6</td>
<td>102.2</td>
</tr>
<tr>
<td>8</td>
<td>100.3</td>
<td>97.80</td>
<td>95.37</td>
<td>93.03</td>
<td>90.78</td>
<td>88.60</td>
<td>86.51</td>
<td>84.48</td>
<td>82.52</td>
<td>80.00</td>
</tr>
<tr>
<td>9</td>
<td>78.79</td>
<td>77.02</td>
<td>75.31</td>
<td>73.66</td>
<td>72.05</td>
<td>70.49</td>
<td>68.99</td>
<td>67.53</td>
<td>66.12</td>
<td>64.00</td>
</tr>
<tr>
<td>10</td>
<td>63.41</td>
<td>62.12</td>
<td>60.87</td>
<td>59.65</td>
<td>58.46</td>
<td>57.32</td>
<td>56.20</td>
<td>55.11</td>
<td>54.06</td>
<td>53.00</td>
</tr>
<tr>
<td>11</td>
<td>52.04</td>
<td>51.06</td>
<td>50.12</td>
<td>49.19</td>
<td>48.30</td>
<td>47.43</td>
<td>46.58</td>
<td>45.73</td>
<td>44.94</td>
<td>44.00</td>
</tr>
<tr>
<td>12</td>
<td>43.39</td>
<td>42.64</td>
<td>41.91</td>
<td>41.20</td>
<td>40.50</td>
<td>39.82</td>
<td>39.16</td>
<td>38.51</td>
<td>37.88</td>
<td>37.00</td>
</tr>
<tr>
<td>13</td>
<td>36.67</td>
<td>36.08</td>
<td>35.50</td>
<td>34.94</td>
<td>34.39</td>
<td>33.85</td>
<td>33.33</td>
<td>32.81</td>
<td>32.31</td>
<td>31.00</td>
</tr>
<tr>
<td>14</td>
<td>31.34</td>
<td>30.87</td>
<td>30.41</td>
<td>29.96</td>
<td>29.51</td>
<td>29.08</td>
<td>28.66</td>
<td>28.24</td>
<td>27.83</td>
<td>27.00</td>
</tr>
<tr>
<td>15</td>
<td>27.05</td>
<td>26.66</td>
<td>26.29</td>
<td>25.92</td>
<td>25.56</td>
<td>25.21</td>
<td>24.86</td>
<td>24.52</td>
<td>24.19</td>
<td>23.00</td>
</tr>
<tr>
<td>16</td>
<td>23.54</td>
<td>23.23</td>
<td>22.92</td>
<td>22.61</td>
<td>22.32</td>
<td>22.02</td>
<td>21.74</td>
<td>21.46</td>
<td>21.18</td>
<td>20.00</td>
</tr>
<tr>
<td>18</td>
<td>18.22</td>
<td>18.00</td>
<td>17.78</td>
<td>17.57</td>
<td>17.36</td>
<td>17.15</td>
<td>16.95</td>
<td>16.75</td>
<td>16.56</td>
<td>16.00</td>
</tr>
</tbody>
</table>
### Lorentz Polarization factor (Cont’d)

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>21</td>
<td>12.95</td>
<td>12.81</td>
<td>12.68</td>
<td>12.54</td>
<td>12.41</td>
</tr>
<tr>
<td>22</td>
<td>11.66</td>
<td>11.54</td>
<td>11.43</td>
<td>11.31</td>
<td>11.20</td>
</tr>
<tr>
<td>23</td>
<td>10.55</td>
<td>10.45</td>
<td>10.35</td>
<td>10.24</td>
<td>10.15</td>
</tr>
<tr>
<td>25</td>
<td>8.730</td>
<td>8.651</td>
<td>8.573</td>
<td>8.496</td>
<td>8.420</td>
</tr>
<tr>
<td>26</td>
<td>7.984</td>
<td>7.915</td>
<td>7.846</td>
<td>7.778</td>
<td>7.711</td>
</tr>
<tr>
<td>27</td>
<td>7.327</td>
<td>7.266</td>
<td>7.205</td>
<td>7.145</td>
<td>7.086</td>
</tr>
<tr>
<td>30</td>
<td>5.774</td>
<td>5.731</td>
<td>5.688</td>
<td>5.647</td>
<td>5.605</td>
</tr>
<tr>
<td>31</td>
<td>5.367</td>
<td>5.329</td>
<td>5.292</td>
<td>5.254</td>
<td>5.218</td>
</tr>
<tr>
<td>32</td>
<td>5.006</td>
<td>4.972</td>
<td>4.939</td>
<td>4.906</td>
<td>4.873</td>
</tr>
<tr>
<td>33</td>
<td>4.685</td>
<td>4.655</td>
<td>4.625</td>
<td>4.595</td>
<td>4.566</td>
</tr>
<tr>
<td>34</td>
<td>4.399</td>
<td>4.372</td>
<td>4.346</td>
<td>4.320</td>
<td>4.294</td>
</tr>
<tr>
<td>35</td>
<td>4.145</td>
<td>4.121</td>
<td>4.097</td>
<td>4.074</td>
<td>4.052</td>
</tr>
<tr>
<td>37</td>
<td>3.720</td>
<td>3.701</td>
<td>3.683</td>
<td>3.665</td>
<td>3.647</td>
</tr>
<tr>
<td>38</td>
<td>3.544</td>
<td>3.527</td>
<td>3.513</td>
<td>3.497</td>
<td>3.481</td>
</tr>
<tr>
<td>41</td>
<td>3.138</td>
<td>3.127</td>
<td>3.117</td>
<td>3.106</td>
<td>3.096</td>
</tr>
<tr>
<td>42</td>
<td>3.003</td>
<td>3.029</td>
<td>3.020</td>
<td>3.012</td>
<td>3.003</td>
</tr>
<tr>
<td>43</td>
<td>2.954</td>
<td>2.946</td>
<td>2.939</td>
<td>2.932</td>
<td>2.925</td>
</tr>
<tr>
<td>44</td>
<td>2.884</td>
<td>2.878</td>
<td>2.872</td>
<td>2.866</td>
<td>2.860</td>
</tr>
</tbody>
</table>

### Applications to of Structure Factor Calculations To Polycrystals

**Sample Intensity Calculations**
### Lorentz Polarization factor (Cont’d)

<table>
<thead>
<tr>
<th>θ°</th>
<th>.1</th>
<th>.2</th>
<th>.3</th>
<th>.4</th>
<th>.5</th>
<th>.6</th>
<th>.7</th>
<th>.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>45</td>
<td>2.824</td>
<td>2.819</td>
<td>2.814</td>
<td>2.810</td>
<td>2.805</td>
<td>2.801</td>
<td>2.797</td>
<td>2.793</td>
</tr>
<tr>
<td>46</td>
<td>2.782</td>
<td>2.778</td>
<td>2.775</td>
<td>2.772</td>
<td>2.769</td>
<td>2.766</td>
<td>2.763</td>
<td>2.760</td>
</tr>
<tr>
<td>47</td>
<td>2.752</td>
<td>2.750</td>
<td>2.748</td>
<td>2.746</td>
<td>2.744</td>
<td>2.742</td>
<td>2.740</td>
<td>2.738</td>
</tr>
<tr>
<td>48</td>
<td>2.735</td>
<td>2.733</td>
<td>2.732</td>
<td>2.731</td>
<td>2.730</td>
<td>2.730</td>
<td>2.729</td>
<td>2.729</td>
</tr>
<tr>
<td>49</td>
<td>2.728</td>
<td>2.728</td>
<td>2.728</td>
<td>2.728</td>
<td>2.728</td>
<td>2.728</td>
<td>2.729</td>
<td>2.730</td>
</tr>
<tr>
<td>50</td>
<td>2.732</td>
<td>2.733</td>
<td>2.734</td>
<td>2.735</td>
<td>2.737</td>
<td>2.738</td>
<td>2.740</td>
<td>2.741</td>
</tr>
<tr>
<td>51</td>
<td>2.747</td>
<td>2.749</td>
<td>2.751</td>
<td>2.753</td>
<td>2.755</td>
<td>2.758</td>
<td>2.760</td>
<td>2.763</td>
</tr>
<tr>
<td>52</td>
<td>2.772</td>
<td>2.775</td>
<td>2.778</td>
<td>2.782</td>
<td>2.785</td>
<td>2.788</td>
<td>2.792</td>
<td>2.795</td>
</tr>
<tr>
<td>53</td>
<td>2.807</td>
<td>2.811</td>
<td>2.815</td>
<td>2.820</td>
<td>2.824</td>
<td>2.828</td>
<td>2.833</td>
<td>2.838</td>
</tr>
<tr>
<td>54</td>
<td>2.853</td>
<td>2.858</td>
<td>2.863</td>
<td>2.868</td>
<td>2.874</td>
<td>2.879</td>
<td>2.885</td>
<td>2.890</td>
</tr>
<tr>
<td>55</td>
<td>2.908</td>
<td>2.914</td>
<td>2.921</td>
<td>2.927</td>
<td>2.933</td>
<td>2.940</td>
<td>2.946</td>
<td>2.953</td>
</tr>
<tr>
<td>56</td>
<td>2.974</td>
<td>2.981</td>
<td>2.988</td>
<td>2.996</td>
<td>3.004</td>
<td>3.011</td>
<td>3.019</td>
<td>3.026</td>
</tr>
</tbody>
</table>

Applications to of Structure Factor Calculations To Polycrystals

Sample Intensity Calculations
Lorentz Polarization factor (Cont’d)

Applications to of Structure Factor Calculations To Polycrystals

Sample Intensity Calculations

<p>| | | | | | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>65</td>
<td>4.071</td>
<td>4.090</td>
<td>4.108</td>
<td>4.127</td>
<td>4.147</td>
<td>4.166</td>
<td>4.185</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>69</td>
<td>4.970</td>
<td>4.997</td>
<td>5.024</td>
<td>5.052</td>
<td>5.080</td>
<td>5.109</td>
<td>5.137</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>70</td>
<td>5.254</td>
<td>5.284</td>
<td>5.315</td>
<td>5.345</td>
<td>5.376</td>
<td>5.408</td>
<td>5.440</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>71</td>
<td>5.569</td>
<td>5.602</td>
<td>5.636</td>
<td>5.670</td>
<td>5.705</td>
<td>5.740</td>
<td>5.775</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>72</td>
<td>5.919</td>
<td>5.956</td>
<td>5.994</td>
<td>6.032</td>
<td>6.071</td>
<td>6.109</td>
<td>6.149</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>76</td>
<td>7.813</td>
<td>7.874</td>
<td>7.936</td>
<td>7.999</td>
<td>8.063</td>
<td>8.128</td>
<td>8.193</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>79</td>
<td>10.12</td>
<td>10.21</td>
<td>10.31</td>
<td>10.41</td>
<td>10.52</td>
<td>10.62</td>
<td>10.73</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>80</td>
<td>11.18</td>
<td>11.30</td>
<td>11.42</td>
<td>11.54</td>
<td>11.67</td>
<td>11.80</td>
<td>11.93</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>82</td>
<td>14.10</td>
<td>14.28</td>
<td>14.47</td>
<td>14.66</td>
<td>14.86</td>
<td>15.07</td>
<td>15.28</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>83</td>
<td>16.17</td>
<td>16.41</td>
<td>16.66</td>
<td>16.91</td>
<td>17.17</td>
<td>17.44</td>
<td>17.72</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>85</td>
<td>22.77</td>
<td>23.24</td>
<td>23.73</td>
<td>24.24</td>
<td>24.78</td>
<td>25.34</td>
<td>25.92</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>86</td>
<td>28.53</td>
<td>29.27</td>
<td>30.04</td>
<td>30.86</td>
<td>31.73</td>
<td>32.64</td>
<td>33.60</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>87</td>
<td>38.11</td>
<td>39.43</td>
<td>40.84</td>
<td>42.36</td>
<td>44.00</td>
<td>45.76</td>
<td>47.68</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

From Henry, Lipson, and Wooster [G.8]
**Structure Factor Calculations Example of ZnS**  
*(with Two different Types of Atoms)*

<table>
<thead>
<tr>
<th>Line</th>
<th>hkl</th>
<th>$\theta$</th>
<th>$\frac{\sin \theta}{\lambda}$ (Å$^{-1}$)</th>
<th>$f_S$</th>
<th>$f_{Zn}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>111</td>
<td>14.3°</td>
<td>0.16</td>
<td>12.3</td>
<td>25.8</td>
</tr>
<tr>
<td>2</td>
<td>200</td>
<td>16.6</td>
<td>0.19</td>
<td>11.4</td>
<td>24.6</td>
</tr>
<tr>
<td>3</td>
<td>220</td>
<td>23.8</td>
<td>0.26</td>
<td>9.7</td>
<td>22.1</td>
</tr>
<tr>
<td>4</td>
<td>311</td>
<td>28.2</td>
<td>0.30</td>
<td>9.0</td>
<td>20.7</td>
</tr>
<tr>
<td>5</td>
<td>222</td>
<td>29.6</td>
<td>0.32</td>
<td>8.8</td>
<td>20.0</td>
</tr>
<tr>
<td>6</td>
<td>400</td>
<td>34.8</td>
<td>0.37</td>
<td>8.2</td>
<td>18.4</td>
</tr>
</tbody>
</table>

| Line | $|F|^2$ | $\rho$ | $\frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta}$ | Relative intensity |
|------|--------|--------|-------------------------------------------------|-------------------|
| 1    | 13070  | 8      | 30.0                                            | 10.0              |
| 2    | 2790   | 6      | 21.7                                            | 1.2               |
| 3    | 16180  | 12     | 9.76                                            | 6.1               |
| 4    | 8150   | 24     | 6.64                                            | 4.1               |
| 5    | 2010   | 8      | 5.95                                            | 0.3               |
| 6    | 11320  | 6      | 4.19                                            | 0.9               |

- **Applications to of Structure Factor Calculations To Polycrystals**
- **Sample Intensity Calculations**
We will end the Chapter here