X-Ray Diffraction
MSE 416 and Graduate Students

Chapter No. 10
Determination of Crystal Structure

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Chapter No. 10
Determination of Crystal Structure

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10-1 Introduction

- **Crystal Structure:**
  Structure determines the properties: such as “Plastic Deformation”, “Alloy Formation”, or “Phase Transformation”.

- **Complex crystal structures need complex methods to solve and take long time to determine (like Proteins).**

- **The simple crystal structures and polycrystalline (powder) diffraction patterns will be introduced here to determine the structure.**

- **The basic principles involved in structure determination have been introduced in Chapters 3 and 4.**

- **Crystal Structure determines the diffraction pattern:**
  1. Shape and size of unit cell ⇔ Peak Positions
  2. Arrangement of Atoms ⇔ Peak Intensities
10-1 Introduction

- **The procedures of structure determinations are trial and error:**
  On the basis of educated guess, make an assumption of a structure, calculate its diffraction pattern, and compare calculated pattern with the observed one.

- **The determination of an unknown structure procedures in three steps:**
  1. “Indexing the Patterns”: The shape and size of the unit cell are deduced from the angular positions of the diffractions. Choose the crystal structure from seven crystal systems and assign the correct Miller indices to each peak. (Determine the unit cell)
  2. Computed the number of atoms per unit cell
     Chemical composition of the specimen
     Measure the density
  3. Determine the atom positions by calculating the relative intensities of diffraction patterns
10-2 Preliminary Treatment of Data

- The first step in determining the crystal structure of polycrystalline (powder) sample is recording the diffraction pattern over as wide a range of $2\theta$ as possible.

- **Calculate the value of $\sin^2\theta$ for each diffraction peak – to determine the unit cell size and shape.** (or obtain d-spacing values)

- The ideal pattern contains peaks formed by x-ray of a single wavelength. If $K_\alpha$ and $K_\beta$ radiations both appear, the relationship between diffraction angles ($\theta$) and wavelengths ($\lambda$) is:

$$\left(\frac{\lambda_{K\alpha}^2}{\lambda_{K\beta}^2}\right)\sin^2\theta_\beta = \sin^2\theta_\alpha$$

$$\left(\frac{\lambda_{K\alpha}^2}{\lambda_{K\beta}^2}\right) \text{ value is near 1.2 for most radiations}$$

- **The example of a correction curve for $\sin^2\theta$ values is given below (Figure 10-1):**
10-3 Indexing Patterns of Cubic Crystals

- Equation 3-11, \( s = (h^2+k^2+l^2) \) is always integral and \( \frac{\lambda^2}{4a^2} \) is constant. To indexing the pattern of a cubic is to find a set of integers \( s \) which will yield a constant quotient when divided one by one into the observed \( \sin^2\theta \) values.

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

- The sequential \( s = (h^2+k^2+l^2) \) values for four common Cubic lattices:
  1. Simple Cubic: 1,2,3,4,5,6,8,9,10,11,12,13,14,16,…
  2. Body-Centered Cubic: 2,4,6,8,10,12,14,16,…
  3. Face-Centered Cubic: 3,4,8,11,12,16,…
  4. Diamond Cubic: 3,8,11,16,…

The more detail in Appendix 9.

(Note: Certain integers, such as 7,15,23,28,31, etc., are impossible because they cannot be formed by the sum of three squared integers)
## 10-3 Indexing Patterns of Cubic Crystals

### Example of indexing the pattern and finding the lattice parameter for the cubic structure: (Table 10.1)

<table>
<thead>
<tr>
<th>Line</th>
<th>sin^2 θ</th>
<th>s = (h^2 + k^2 + l^2)</th>
<th>FCC</th>
<th>SC</th>
<th>BCC</th>
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<tr>
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<td>0.0467</td>
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<td>3</td>
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<td>8</td>
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### Table 10.1

<table>
<thead>
<tr>
<th>Line</th>
<th>( \sin^2 \theta )</th>
<th>( \frac{s}{\sin^2 \theta} )</th>
<th>( \lambda^2 / 4a^2 )</th>
<th>( a(\text{Å}) )</th>
<th>( hkl )</th>
<th>( \frac{s}{\sin^2 \theta} )</th>
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<td>0.101</td>
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</table>
10-3 Indexing Patterns of Cubic Crystals

- Calculated diffraction patterns for various lattices
  \( s = (h^2 + k^2 + l^2) \) (Figure 10-2)
10-4 Indexing Patterns of Noncubic Crystals

- **Tetragonal System:**
  \[ \sin^2 \theta = A(h^2+k^2) + C \]
  where \( A = \lambda^2/4a^2 \) and \( C = \lambda^2/4c^2 \)
  To Obtain \( A \) value: \((hk0) \Rightarrow \sin^2 \theta = A(h^2+k^2)\)
  To Obtain \( C \) value: \( \Rightarrow \sin^2 \theta - A(h^2+k^2) = C \) (or use (00l))

- **Hexagonal System:**
  \[ \sin^2 \theta = A(h^2+hk+k^2) + C \]
  where \( A = \lambda^2/3a^2 \) and \( C = \lambda^2/4c^2 \)
  (See example of zinc in Table 10.2, Table 3 and Table 10.4)

- **Orthorhombic System:**
  \[ \sin^2 \theta = Ah^2 + Bk^2 + C \]

- **Monoclinic and Triclinic System:**
  These crystal systems involve four or six independent constants, respectively. The corresponding powder patterns are of great complexity and may contain more than a hundred peaks.
The Effect of Cell Distortion on the Powder Pattern

- Figure 10-3. Effects of Cell Distortion on Powder Patterns:
10-6 Determination of the Number of Atoms in a Unit Cell

- The number of atoms in a unit cell must be known before their positions can be determined.
- The volume of the unit cell can be calculated from lattice parameters by means of the equations given in Appendix 3.

Cubic: \( V = a^3 \)  
Tetragonal: \( V = a^2c \)  
Orthorhombic: \( V = abc \)

Hexagonal: \( V = \frac{\sqrt{3}a^2c}{2} = 0.866a^2c \)

- The Weight of all the atoms in the unit cell: (Eq. 3-14)

\[
\sum A = \frac{\rho V}{1.66042} \quad (\sum A \text{ is the sum of the atomic weights of the atoms in the unit cell})
\]

- In case of an element:

\[
\sum A = n_1A \quad (n_1 \text{ is the number of atoms per unit cell and } A \text{ is atomic weight})
\]

- In case of the chemical compound or intermediate phase (simple chemical formula)

\[
\sum A = n_2M \quad (n_2 \text{ is the number of "molecules" per unit cell and } M \text{ the molecular weight})
\]
10-7 Determination of Atom Positions

- To find the position of a known number of atoms in a unit cell of known shape and size, the observed relative intensities of diffracted beam, are required.
- Equations 4-19 and 4-11 will be used.

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

\[ F = \sum_{1}^{N} f_n e^{2\pi i (h u_n + k v_n + l w_n)} \]  
(Give the value of the structure factor \( F \))

Atomic Scattering Factor (\( f \)): Appendix 10
Multiplicty Factor (\( p \)): Appendix 11
Lorentz-Polarization (L-P) Factor: Appendix 12
10-8 Example of Structure Determination

- Consider an intermediate phase of cadmium (Cd) and tellurium (Te) system:

  - Step 1: Chemical Analyses:
    - Composition: Cd: 46.6wt% Te: 53.4wt%
    - 49.8 atomic% 50.2 atomic%
    - Chemical Formula: CdTe

  - Step 2: Run X-ray pattern and obtain the values of \( \sin^2 \theta \) for each peak

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<th>Intensity</th>
<th>( \theta )</th>
<th>( \sin \theta )</th>
<th>( \sin^2 \theta )</th>
<th>hkl</th>
<th>( s = h^2 + k^2 + l^2 )</th>
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<td>0.8331</td>
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</table>
10-8 Example of Structure Determination

- Step 3: Indexing the Pattern
  First trial and error: Choose cubic system

Simple cubic, BCC, FCC, and Diamond

$$\frac{\sin^2 \theta}{s} = \frac{\sin^2 \theta}{h^2 + k^2 + l^2} = \frac{\lambda^2}{4a^2} = \text{constant}$$

<table>
<thead>
<tr>
<th>Peak</th>
<th>$\sin^2 \theta$</th>
<th>hkl</th>
<th>$s = h^2 + k^2 + l^2$</th>
<th>$\sin^2 \theta / s$</th>
<th>Simple Cubic</th>
<th>BCC</th>
<th>FCC</th>
<th>Diamond</th>
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<td>440</td>
<td>440</td>
<td>731</td>
</tr>
</tbody>
</table>
10-8 Example of Structure Determination

- Step 4: Calculate the lattice parameter, a:
  FCC: Using the first peak at $2\theta = 23.78^\circ$, $(hkl) = (111)$
  Obtain the lattice parameter $a = 6.482\text{Å}$

- Step 5: Measure density of the CdTe powder: $\rho = 5.82$ g/cm³

- Step 6: Calculate the Weight of all the atoms in the unit cell:
  Use Eq. 3-14
  $$\sum A = \frac{\rho V}{1.66042} = \frac{5.82 \times (6.482)^3}{1.66042} = 954.6$$

- Step 7: Calculate the number of atoms per unit cell

  “Molecular” weight of CdTe (Cd=112.41 & Te=127.60) is $M = 240.01$

  The “Molecules” per unit cell is: $954.6/240.02 = 3.977 \sim 4$.
  Unit cell of CdTe cubic contains 4 “molecules” of CdTe
  (4 Cd & 4 Te)
10-8 Example of Structure Determination

- **Step 8: Possible Structures:**
  - (a) Ionic Bonding \( \Rightarrow \) CsCl, NaCl
  - (b) Covalent Bonding \( \Rightarrow \) ZnS

Possible Structures: NaCl or ZnS
10-8 Example of Structure Determination

- **Step 9: Determine the structure factor:**  
  (Based on NaCl and ZnS Structures)

If CdTe is NaCl structure:

\[
F^2 = 16(f_{Cd} + f_{Te})^2, \quad \text{if } (h+k+l) \text{ is even.}
\]

\[
F^2 = 16(f_{Cd} - f_{Te})^2, \quad \text{if } (h+k+l) \text{ is odd.}
\]

If CdTe is ZnS structure:

\[
F^2 = 16(f_{Cd}^2 + f_{Te}^2), \quad \text{if } (h+k+l) \text{ is odd.}
\]

\[
F^2 = 16(f_{Cd} - f_{Te})^2, \quad \text{if } (h+k+l) \text{ is an odd multiple of 2.}
\]

\[
F^2 = 16(f_{Cd} + f_{Te})^2, \quad \text{if } (h+k+l) \text{ is an even multiple of 2.}
\]

Atomic Scattering Factor for \(f_{Cd}\) and \(f_{Te}\): Appendix 10

Multiplicity Factor \((p)\): Appendix 11

Lorentz-Polarization (L-P) Factor: Appendix 12
10-8 Example of Structure Determination

- **Step 10: Calculated relative intensities of NaCl and ZnS structures:**

<table>
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<tr>
<th>Peak</th>
<th>$hkl$</th>
<th>Observed</th>
<th>Calculated</th>
<th>Intensity</th>
</tr>
</thead>
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<td></td>
<td></td>
<td>NaCl Structure</td>
<td>ZnS Structure</td>
</tr>
<tr>
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<td>0</td>
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<td>100</td>
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<td>17</td>
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Calculated intensities have been adjusted so that the 220 peak has a relative intensity of 100 for both structures.

- **The structure of CdTe can be determined as ZnS type structure.**
10-8 Example of Structure Determination

Structure Determination by Using Computation Search Method:

Step I: Run X-ray pattern
10-8 Example of Structure Determination

- Step II: Open X-ray pattern under MDI Jade Program:
Step III: Find the possible Cd-Te systems in MDI Jade Program database:
10-8 Example of Structure Determination

- Step IV: 4 possible CdTe were found from database. PDF#15-0770 is matched the X-ray pattern.
Step V: X-ray Pattern is identified as cubic structure with lattice parameter $a = 6.481\ \text{Å}$ and space group F-43m (216).
10-8 Example of Structure Determination

- $2\theta$, Relative Intensities, and (hkl) are given:

![X-ray diffraction pattern of CdTe, Cadmium Telluride](image-url)

- $2\theta = 23.780/100.0\% (111)$
- $2\theta = 39.330/54.3\% (220)$
- $2\theta = 46.450/25.6\% (311)$
- $2\theta = 56.860/4.9\% (400)$
- $2\theta = 62.360/7.9\% (331)$
- $2\theta = 71.230/7.3\% (422)$
- $2\theta = 76.321/2.8\% (511)$
- $2\theta = 84.440/1.3\% (440)$
- $2\theta = 89.429/2.7\% (531)$
- $2\theta = 97.421/12.5\% (620)$
- $2\theta = 102.331/1.2\% (633)$
- $2\theta = 110.820/6.7\% (444)$
- $2\theta = 116.099/1.0\% (551)$
- $2\theta = 125.540/1.7\% (642)$
- $2\theta = 131.772/1.3\% (731)$