Chapter #2:
X-Ray Diffraction and the Reciprocal Lattice

Lecture 5: Structure Factor and Systematic Absences (BCC & FCC)

This lecture completes the diffraction theory by introducing the ***Structure Factor*** and explaining systematic absences (extinction rules) in BCC and FCC lattices.

1. Why Do We Need the Structure Factor?

- From previous lectures, the diffraction condition is:
  Δk = G
  This determines when diffraction is geometrically allowed. However, even when a reciprocal lattice vector exists, the intensity may be zero. This occurs due to destructive interference between atoms inside the unit cell.
- In our discussion, we assume there is only a single atom at each lattice point, whereas a crystal may have more than one atom per lattice point (a basis with two or more atoms).

2. From Electron Density to Structure Factor

The scattered amplitude from the entire crystal is given by:

$$F(\vec{G}) = \int \rho(r)\, e^{-\vec{G}.\vec{r}} d^3r$$

This equation represents the total amplitude of the scattered wave that is proportional to the integral over the crystal of $\rho(r)\ d^3r$ times the phase factor $e^{-\vec{G}.\vec{r}}$.
Rember that: ρ(r)represent the electron density at position **r**

Because the lattice is periodic: ρ(r) = ρ(r + R)

We can separate the crystal into:

- Bravais lattice
- Basis (atoms inside unit cell)

The amplitude can be separated into Bravais lattice and basis contributions:

$$F(\vec{G}) = \sum_{R} e^{-\vec{G}.\vec{R}} \sum_{j} f_j e^{-\vec{G}.\vec{r}_j}$$

The first summation is nonzero only when **G** is a reciprocal lattice vector.

$\sum_R e^{-\vec{G}.\vec{R}} \neq 0$ only if $\vec{G}$is reciprocal lattice vector.

The second summation is defined as the Structure Factor.

3. Definition of Structure Factor

$$S(\vec{G}) = \sum_j f_j e^{-\vec{G}.\vec{r}_j}$$

Where:

f_j = atomic form factor

r_j = atomic position inside the unit cell

Notes that:

Intensity is proportional to $|S(G)|^2$. $\left(I(\vec{G}) \propto \left|S(\overrightarrow{G})\right|^2\right)$

If **S(G) = 0**, the reflection is forbidden (systematic absence).

The Structure Factor is independent of the shape and size of the unit cell but depends on the positions of the atoms within the cell.

4. Structure Factor for Cubic Lattices

4.1 Simple Cubic (SC)

Basis: one atom at (0,0,0)

S = f

All (hkl) reflections are allowed. No extinction.

4.2 Body-Centered Cubic (BCC)

Basis: 2 atoms

(0,0,0)

(1/2, 1/2, 1/2)

$$S(\vec{G}) = f[1 + e^{-i\vec{G}.\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)}]$$

Evaluate the phase term:

$$\vec{G} = \frac{2\pi}{a}(h, k, l)$$

So,

$$\vec{G}.\vec{r} = \frac{2\pi}{a}\left(h\frac{a}{2} + k\frac{a}{2} + l\frac{a}{2}\right) = \pi(h + k + l)$$

Therefore:

$$S(\vec{G}) = f[1 + e^{-i\pi(h+k+l)}]$$

But: $e^{-i\pi n} = (-1)^n$

Remember that:

$$e^{-i\pi n} = \cos \pi n - i \sin \pi n$$

$$\sin \pi n = 0$$

$$\cos \pi n = (-1)^n$$

Thus:

$$S(\vec{G}) = f[1 + (-1)^{h+k+l}]$$

BCC Extinction Rule:

If $h + k + l$ is even → reflection allowed (S = 2f)
If $h + k + l$ is odd → reflection forbidden (S = 0)

Examples:

Plane	***h+k+l***	**Allowed?**
(100)	1	No
(110)	2	Yes
(111)	3	No
(200)	2	Yes

4.3 Face-Centered Cubic (FCC)

Basis:
(0,0,0)
(0,1/2,1/2)
(1/2,0,1/2)
(1/2,1/2,0)

$$S(\vec{G}) = f[1 + (-1)^{k+l} + (-1)^{h+l} + (-1)^{h+k}]$$

FCC Extinction Rule:
Reflections allowed only if *h, k, l* are all even OR all odd.
Otherwise forbidden.

Examples:
(100): forbidden
(110): forbidden
(111): allowed
(200): allowed
(210): forbidden

5. Physical Meaning of Extinction Rules

Extinction occurs because atoms inside the unit cell scatter out of phase.
In BCC, the body-center atom cancels corner atoms when $h+k+l$ is odd.
In FCC, face atoms cancel corner atoms unless parity conditions are satisfied.

- Forbidden reflection does NOT mean the plane does not exist.
  It means the scattered waves cancel due to phase differences inside the unit cell.

6. Relation to Reciprocal Lattice

The reciprocal of BCC is FCC, and the reciprocal of FCC is BCC.
This explains why the first diffraction peak in BCC is (110),
and in FCC is (111).

Exercise-1:

Try to find the structure factor for the diamond structure.

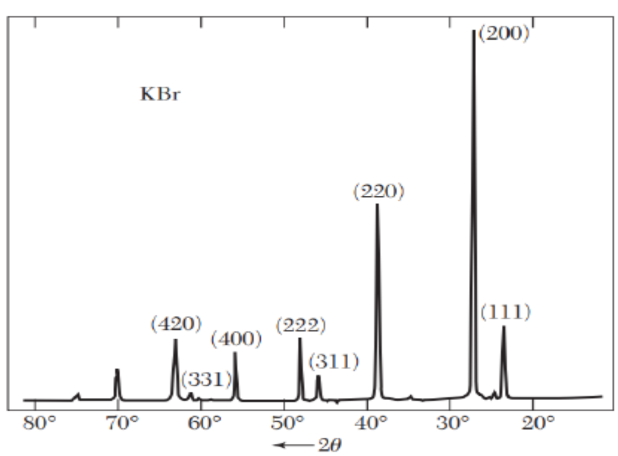
Exercise-2:

The figure shows the XRD spectrum of KBr. Based on the data presented in the spectrum, answer the following:

a) What is the lattice type of this compound?

b) Explain in detail how you determined the lattice type.

c) Is it possible to have a diffraction peak for the plane (101)? Why or why not?



Solution

1) One-Dimensional Crystal Lattice and Reciprocal Lattice

A one-dimensional crystal lattice consists of equally spaced lattice points along a line with lattice parameter a. The lattice points are located at positions:

$R_n = n\,a \quad (n = 0, \pm1, \pm2, ...)$

The reciprocal lattice of a 1D lattice is also one-dimensional. The reciprocal lattice vector G is defined as:

$G_m = m\,(2\pi / a) \quad (m = 0, \pm1, \pm2, ...)$

Thus, the reciprocal lattice spacing is $2\pi/a$, and the reciprocal lattice is also periodic.

2) Determination of the Lattice Type of KBr

From the XRD pattern, the observed reflections include planes such as:

(111), (200), (220), (311), (222), (400), (420), etc.

Notice that reflections such as (100) or (110) are absent.

For a Face-Centered Cubic (FCC) lattice, the extinction rule is:

Reflections are allowed only when h, k, l are either all even or all odd.

The observed reflections satisfy this condition:

(111) → all odd → allowed

(200) → all even → allowed

(220) → all even → allowed

(311) → all odd → allowed

Therefore, the lattice type of KBr is Face-Centered Cubic (FCC).

KBr crystallizes in the NaCl-type structure, which consists of an FCC Bravais lattice with a two-atom basis (K and Br).

3) Is (101) Reflection Possible?

For the plane (101):

h = 1 (odd), k = 0 (even), l = 1 (odd)

This is a mixed set of indices (not all even or all odd).

For an FCC lattice, mixed indices lead to complete destructive interference in the structure factor.

Therefore, the structure factor $F = 0$, and the intensity $I \propto |F|^2 = 0$.

Conclusion: A diffraction peak for the plane (101) is not allowed in an FCC lattice. Hence, it will not appear in the XRD spectrum of KBr.