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

Lecture 2: Scattering from Electrons and Diffraction Theory

1. Origin of X-ray Diffraction and Scattering from electrons

A solid consists of atoms and electrons. The atoms behave as ions, and the charged particles (electrons and ions) are responsible for X-ray scattering.

Why does the atom cause X-ray diffraction?

As we know, any atom is surrounded by electrons that accelerate under the influence of the electric field accompanying the X-ray beam. Since an accelerating charge emits electromagnetic X-rays, the electrons inside the atom re-radiate.

As a result, the electrons absorb energy from the incident beam and scatter it in all directions. However, electrons form a charge cloud surrounding the atom. Therefore, when considering diffraction from the entire atom, we must take into account the phase differences between waves scattered from different regions of the charge cloud.

Thus, we will now study how the path difference produces different diffraction patterns, how to calculate the intensity of the reflected radiation, and the conditions for constructive interference.

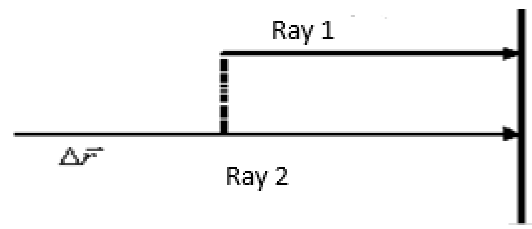
2. The General Equation for Determining Reflected X-Rays

Superposition of Two Waves

Suppose we have two rays, ray 1 and ray 2, and the difference between them is: $\Delta\vec{r}$

Ray 1:

$$\psi_1 = Ae^{i\vec{k}.\vec{r}} \quad (1)$$



Ray 2:

$$\psi_2 = Ae^{i\vec{k}.(\vec{r}+\Delta\vec{r})} \quad (2)$$

Where:

k: wave vector

A: wave amplitude

Total wave:

$$\psi = \psi_1 + \psi_2 \quad (3)$$

As we know, that Intensity is proportional to the square of the amplitude:

$$I \propto |\psi|^2 \quad (4)$$

One can rewrite (3) as follows:

$$\psi = e^{i\vec{k}.\vec{r}}(1 + e^{i\vec{k}.\Delta\vec{r}})$$

$\vec{k}.\Delta\vec{r}$ represents the phase difference caused by the path difference between waves scattered from two atoms.

Then, the intensity can be written as:

$$I = \psi\psi^* = A^2[e^{i\vec{k}.\vec{r}}(1 + e^{i\vec{k}.\Delta\vec{r}})][e^{i\vec{k}.\vec{r}}(1 + e^{i\vec{k}.\Delta\vec{r}})]^*$$
$$= A^2[e^{i\vec{k}.\vec{r}}(1 + e^{i\vec{k}.\Delta\vec{r}})][e^{-i\vec{k}.\vec{r}}(1 + e^{-i\vec{k}.\Delta\vec{r}})]$$
$$= A^2[1 + e^{i\vec{k}.\Delta\vec{r}} + e^{-i\vec{k}.\Delta\vec{r}} + 1] = A^2[2 + 2\,cos_{\vec{k}.\Delta\vec{r}}] \quad (5)$$

Remember that:

$$cos_\alpha = \frac{e^{i\alpha} + e^{-i\alpha}}{2}$$

By investigating eq. (5):

$$I = A^2[2 + 2\,cos_{\vec{k}.\Delta\vec{r}}]$$

- **Constructive interference condition:**

$cos_{\vec{k}.\Delta\vec{r}} = 1$ i.e, $\vec{k}.\Delta\vec{r} = 2\pi n$ (6)

- ✓ When the phase difference equals an integer multiple of 2π, the waves are **in phase**.

- **Destructive interference condition (I=0):**

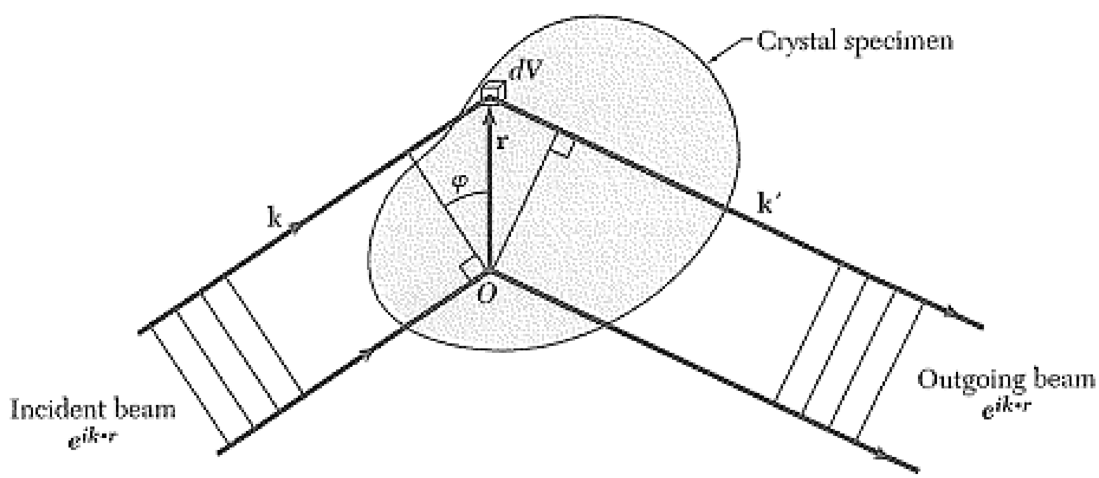
  $cos_{\vec{k}.\Delta\vec{r}} = -1$ 1 i.e, $\vec{k}.\Delta\vec{r} = (2n + 1)\pi$ (7)

- ✓ The waves are out of phase by π.

$where,$ (n = 0,1,2,...)

Diffraction is fundamentally a phase-matching condition. Only when the phase difference equals an integer multiple of 2π, does the crystal produce a measurable diffraction peak.

3. Electron Density Description and diffraction condition



From the figure, we observe that the electron density may be maximum in one region and zero in another. Therefore, diffraction depends on the chosen element.

We choose element **A** located at position $\vec{r}$.
We denote the incident wave vector by **k**, and the scattered wave vector by **k′** (in an arbitrary direction).

The reflected intensity from element A is proportional to the number of charges at A. Therefore:

$$\Delta I \; \alpha \; \text{number of electronc at A}$$

Let ρ(r) represent the electron density at position **r**. The number of electrons in a small volume element **dV** is:

$$number\ of\ electrons = \rho(\vec{r})\ \ dV$$

$$\Delta I \propto \rho(\vec{r})\ \ dV$$

Let us examine the path difference and phase difference at element **A**:

Incident Wave

$$\Psi_{incident} = Ae^{i\,\vec{k}.\vec{r}}$$

Scattered Wave

$$\Psi_{scattered} = Ae^{i\,\vec{k}`.\vec{r}}$$

Total path difference:

$$\vec{k}.\vec{r} - \vec{k}'.\vec{r} = -(\vec{k}' - \vec{k}).\vec{r} = -\Delta\vec{k}.\vec{r}$$

Phase factor: $e^{-i\Delta\vec{k}.\vec{r}}$

Therefore: $$I = \int_{The\ whole\ solid} \rho(\vec{r})\ \ dV\ e^{-i\Delta\vec{k}.\vec{r}} \qquad \textbf{(7)}$$

Where: $\Delta\vec{k} = \vec{k}' - \vec{k}$

It is called the scattering vector and measures the change in wave vector.

We note that if $\vec{k}$ is given, then the intensity I depends on $\vec{k}'$.

4. Condition for Constructive Interference in Crystals

For constructive interference from a periodic lattice:

$$\rho(\vec{r}) = \rho(\vec{r} + \vec{R})$$

Where R is a lattice translation vector and given by:

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

$$I(k') = \int \rho(\vec{r})\; d^3\vec{r}\; e^{-i\Delta\vec{k}.\vec{r}}$$

$$= \int \rho(\vec{r} + \vec{R})\; d^3\vec{r}\; e^{-i\Delta\vec{k}.\vec{r}}$$

$$let\ \vec{r} + \vec{R} = \vec{r}\,'$$

$$= \int \rho(\vec{r}\,')\; d^3\vec{r}\; e^{-i\Delta\vec{k}.(\vec{r}\,' - \vec{R})}$$

$$= e^{i\Delta\vec{k}.\vec{R}} \int \rho(\vec{r}\,')\;\; e^{-i\Delta\vec{k}.\vec{r}\,'}\; d^3\vec{r}\; = e^{i\Delta\vec{k}.\vec{R}}\; I(k')$$

$$I(k')\; (1 - e^{i\Delta\vec{k}.\vec{R}}) = 0$$

To satisfy this equation, there are two possibilities:

1- $I(k') = 0$ $===>$ This is **destructive** interference.

2- $(1 - e^{i\Delta\vec{k}.\vec{R}}) = 0$ This can be when: $e^{i\Delta\vec{k}.\vec{R}} = 1$ =➔ $\Delta\vec{k}.\vec{R} = 2\pi n$
   Where n=0,1,2….

Exercise

A cubic lattice with lattice parameter **a**.
Assume incident X-rays with a wave vector $\vec{k} = \frac{\pi}{a}\hat{\imath}$ are scattered by a crystal.

Determine whether the resulting pattern is **constructive or destructive** in the following directions:

1- $\vec{k}' = -\frac{\pi}{a}\hat{\imath}$

2- $\vec{k}' = -\frac{\pi}{a}\hat{\jmath}$

Solution:

The condition for constructive interference is $\Delta\vec{k}.\vec{R} = 2\pi n$

$$\left|\Delta\vec{k}.\vec{R}\right| = 2\pi n$$

$$\left|(\vec{k}' - \vec{k}).(n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3)\right|$$

$$= \left|(-\frac{\pi}{a}\hat{\jmath} - \frac{\pi}{a}\hat{\imath}).(n_1 a\,\hat{\imath} + n_2 a\,\hat{\jmath} + n_3 a\hat{k})\right|$$

$$= \left|-\frac{\pi}{a}(n_1 a + n_2 a)\right| = \pi(n_1 + n_2) = 2\pi n$$

$$\therefore (n_1 + n_2) = 2n$$

Since **n** is already defined as an integer (note that it is multiplied by 2, so the result is always an even number), the condition for **constructive interference** is that the sum (n_1+n_2) must be an even number.

If the sum is an odd number, then the interference is **destructive**.