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

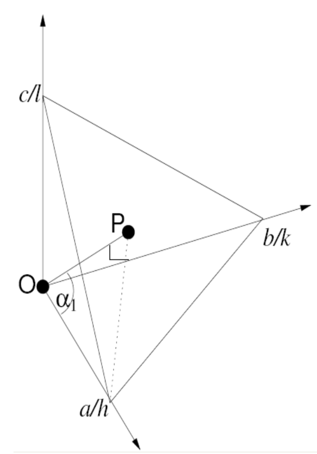
Lecture 4: Reciprocal Diffraction Condition, Bragg Law in Reciprocal Space, and Brillouin Zone

1. Diffraction Condition and Reciprocal Lattice

Now we will show how the reciprocal lattice vectors are related to the crystal planes of the direct lattice.

Consider a set of crystal planes with Miller indices (*hkl*). The associated reciprocal lattice vector is defined as:

$G_{hkl} = h\, b_1 + k\, b_2 + l\, b_3$



Two important properties follow:

1. The vector G_{hkl} is perpendicular to the (*hkl*) planes.
   See the proof below.
2. The interplanar spacing d_{hkl} is related to **G** by:

   $|G_{hkl}| = 2\pi / d_{hkl}$

   See the proof below.

Thus, reciprocal lattice vectors represent the normal directions to crystal planes in real space.

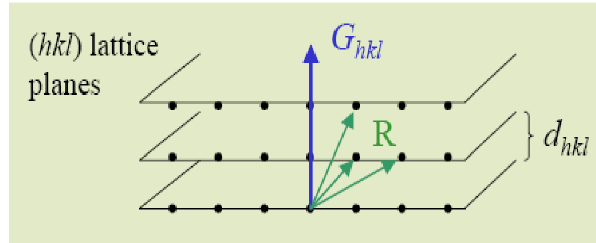
2. Diffraction Condition and Bragg's Law

From the general diffraction condition and what was discussed in the last lectures:

$$\Delta\vec{k} = \vec{G}$$
$$\vec{k}' - \vec{k} = \vec{G}$$
$$\vec{k}' = \vec{G} + \vec{k}$$

Squaring both sides:

$$(\vec{k}')^2 = (\vec{G}+\vec{k})^2$$
$$\vec{k}'^2 = \vec{G}^2 + 2\vec{k}.\vec{G} + \vec{k}^2$$



Since:

1- $\left|\vec{k}'\right| = \left|\vec{k}\right|$

2- If $\vec{G}$ is a reciprocal lattice vector, so is $-\vec{G}$.

=➔ $2\vec{k}.\vec{G} = \vec{G}^2$

This equation is used as the condition for diffraction.

$\vec{k}.\vec{G} = \frac{1}{2}\vec{G}^2$, where $\hat{n} = \frac{\vec{G}_{hkl}}{|\vec{G}_{hkl}|}$

$$\vec{k}.\vec{G} = |\vec{k}||\vec{G}|\cos\varphi = |\vec{k}||\vec{G}|\cos(\frac{\pi}{2} - \theta) = |\vec{k}||\vec{G}|\sin\theta$$

From the figure, we can also write:

$$sin_\theta = \frac{\frac{1}{2}G}{k}$$

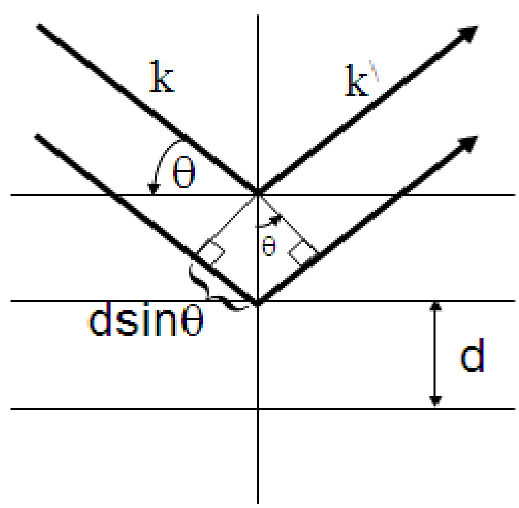
Then, we can get:

$$2k\, sin_\theta = G$$

$\because \quad d_{hkl} = \frac{2\pi}{|G|} \quad k = \frac{2\pi}{\lambda}$and =➔

$$2\frac{2\pi}{\lambda} sin_\theta = \frac{2\pi}{d_{hkl}}$$

$$2d\, sin_\theta = \lambda$$



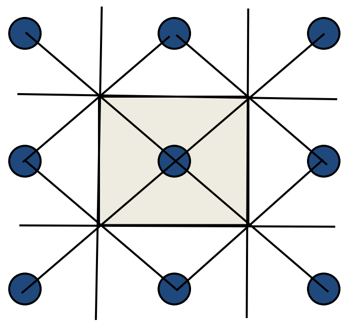
Here, θ is the angle between the incident beam and the crystal plane

This is exactly the form of Bragg's law that we obtained from the general description of diffraction theory. Therefore, physically, using the Bragg model has real meaning when we discuss reflection arising from atomic planes.

For each (*hkl*) family, x-rays will "diffract" at only one angle θ.

3. Brillouin Zones

The Brillouin zones are defined as the Wigner–Seitz cell in reciprocal space. They provide a natural description of diffraction and are fundamental in solid-state physics for describing electronic band structures and lattice vibrations.



The first Brillouin zone is the region in reciprocal space closer to the origin than to any other reciprocal lattice point.

=➔ Boundaries are Bragg planes.

Why do we need the Brillouin zone?

- ☑ Show the symmetry of allowed wave vectors $\vec{k}$.
- ☑ Define boundaries where diffraction conditions change
- ☑ Form the basis for electron band structure

You can visualize different Brillouin zone for SC, BCC, and FCC by visiting the following page: https://www.doitpoms.ac.uk/tlplib/brillouin_zones/printall.php

4. Laue's Condition

Bragg's law treats diffraction as reflection from planes, but crystals are 3D periodic objects.

Laue condition states that:

The phase difference between waves scattered from all lattice points must be an integer multiple of $\boldsymbol{2\pi}$.

Laue's diffraction condition is written as:

$$\Delta\vec{k}.\vec{a}_1 = 2\pi h$$
$$\Delta\vec{k}.\vec{a}_2 = 2\pi k$$
$$\Delta\vec{k}.\vec{a}_3 = 2\pi l$$

We can prove the 1st qu. As follows:

$$\Delta\vec{k}.\vec{a}_1 = (h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3).\vec{a}_1$$

We used $\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$ and $\Delta\vec{k} = \vec{G}$

We know that: $a_i.b_j = 2\pi\delta_{ij}$

This gives us:

$$\Delta\vec{k}.\vec{a}_1 = 2\pi h$$

This condition is equivalent to the reciprocal lattice condition and ensures constructive interference from all lattice points.

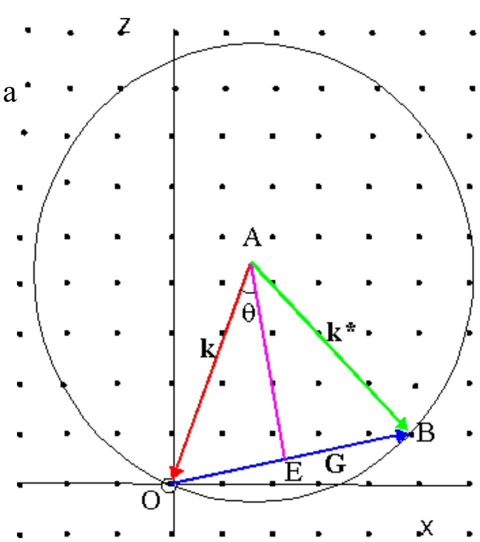
Laue's Condition

- ✔ Express diffraction as a **periodicity condition**
- ✔ Work for any crystal symmetry
- ✔ Naturally lead to: $\Delta\vec{k} = \vec{G}$

This is the **true fundamental diffraction condition**.

5. Ewald Construction

Ewald's construction provides a geometric interpretation of the diffraction condition in reciprocal space. Diffraction occurs when a reciprocal lattice point lies on the surface of the Ewald sphere of radius |k|.



- **Radius:**

$$|\vec{k}| = \frac{2\pi}{\lambda}$$

- Diffraction when the reciprocal point lies on a sphere.
- The Ewald construction is simply a graphical representation of the equation:

$$(\vec{k}^{\backslash} - \vec{k}) = \vec{G}$$

Exercise:

Consider a plane (*hkl*) in a crystal lattice.

(a) Prove that the reciprocal lattice vector G = *h* b_1 + *k* b_2 + *l* b_3 is perpendicular to this plane.

(b) Prove that the distance between two adjacent parallel planes of the lattice is given by:

d(*hkl*) = 2π / |G|

(c) Show that for a simple cubic lattice, the interplanar spacing satisfies:

$d^2 = a^2 / (h^2 + k^2 + l^2)$

Solution:

(A) We have learned that any vector $\vec{G}$ in the reciprocal lattice and any vector $\vec{R}$ in the real lattice are given by:

$$\vec{G} = h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3$$

$$\vec{R} = \frac{1}{h}\vec{a}_1 + \frac{1}{k}\vec{a}_2 + \frac{1}{l}\vec{a}_3$$

Choosing $\vec{A}_1$, $\vec{A}_2$, and $\vec{A}_3$ to be extended from the origin to the plan (*hkl*) and given by:

$$\vec{A}_1 = \frac{1}{h}\vec{a}_1$$

$$\vec{A}_2 = \frac{1}{k}\vec{a}_2$$

$$\vec{A}_3 = \frac{1}{l}\vec{a}_3$$

Now, we will choose other vectors that are in the plane and given by:

$$\vec{A}_{12} = \frac{1}{h}\vec{a}_1 - \frac{1}{k}\vec{a}_2$$

$$\vec{A}_{13} = \frac{1}{h}\vec{a}_1 - \frac{1}{l}\vec{a}_3$$

$$\vec{A}_{23} = \frac{1}{k}\vec{a}_2 - \frac{1}{l}\vec{a}_3$$

If the vector $\vec{G}$ is perpendicular to the plane (*hkl*); then

$$\vec{G} \cdot \vec{A}_{12} = 0$$
$$\vec{G} \cdot \vec{A}_{13} = 0$$
$$\vec{G} \cdot \vec{A}_{23} = 0$$

We introduced that $a_i \cdot b_j = 2\pi\delta_{ij}$

Then,

$$\vec{G} \cdot \vec{A}_{12} = (h\vec{b}_1 + k\vec{b}_2 + l\vec{b}_3) \cdot (\frac{1}{h}\vec{a}_1 - \frac{1}{k}\vec{a}_2) = (2\pi - 2\pi) = 0$$

This can be extended to the other two vectors $\vec{A}_{13}$ and $\vec{A}_{23}$.

(b)

Let's assume the distance between the origin and the plane (*hkl*) is **d** and given by:

$$d = \vec{R}.\hat{n}$$

Where $\hat{n}$ is the normal vector on the plane.

$$\hat{n} = \frac{\vec{G}}{|\vec{G}|}$$

From reciprocal lattice conditions: $\vec{G}.\vec{R} = 2\pi$

That will give us: $d = \vec{R}.\frac{\vec{G}}{|\vec{G}|} = \frac{2\pi}{|\vec{G}|}$

Where we used $a_i \cdot b_j = 2\pi\delta_{ij}$