RECIPROCAL LATTICE (KISI RESIPROK)

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Problem

Interplanar separation.(Problem 2.1 in Kittel.) Consider a plane hkl in a crystal lattice.

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

(b). Prove that the distance between two adjacent parallel planes of the lattice is $d(hkl) = 2\pi/|\boldsymbol{G}|$.

(c). Show for a simple cubic lattice that $d^2 = a^2/(h^2 + k^2 + l^2)$.

Problem #4

Hexagonal space lattice.(Problem 2.2 in Kittel.) The primitive translation vectors of the hexagonal space lattice may be taken as:

$$\boldsymbol{a}_1 = \frac{\sqrt{3}a}{2}\boldsymbol{x} + \frac{a}{2}\boldsymbol{y}, \quad \boldsymbol{a}_2 = -\frac{\sqrt{3}a}{2}\boldsymbol{x} + \frac{a}{2}\boldsymbol{y}, \quad \boldsymbol{a}_3 = c\boldsymbol{z} \tag{20}$$

(a). Show that the volume of the primitive cell is $\sqrt{3}a^2c/2$.

(b). Show that the primitive translations of the reciprocal lattice are:

$$\boldsymbol{b}_1 = \frac{2\pi}{\sqrt{3}a}\boldsymbol{x} + \frac{2\pi}{a}\boldsymbol{y}, \quad \boldsymbol{b}_2 = -\frac{2\pi}{\sqrt{3}a}\boldsymbol{x} + \frac{2\pi}{a}\boldsymbol{y}, \quad \boldsymbol{b}_3 = \frac{2\pi}{c}\boldsymbol{z} \tag{21}$$

so that the lattice is its own reciprocal, but with a rotation of axes.

(c). Describe and sketch the first Brillouin zone of the hexagonal space lattice.

Reciprocal lattice:

Diffraction pattern of the crystal lattice

Diffraction data:

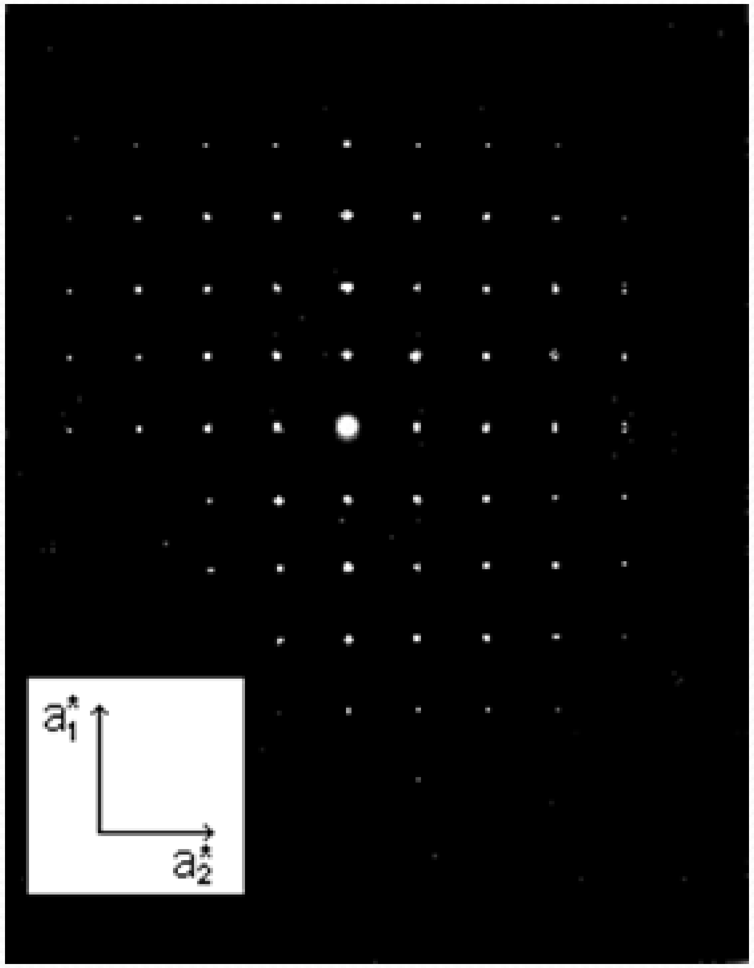
Reciprocal lattice X diffraction pattern of the unit cell content

The reciprocal lattice

- A diffraction pattern is not a direct representation of the crystal lattice
- The diffraction pattern is a representation of the ***reciprocal lattice***

We have already considered some reciprocal features -

Miller indices were derived as the reciprocal (or inverse) of unit cell intercepts.



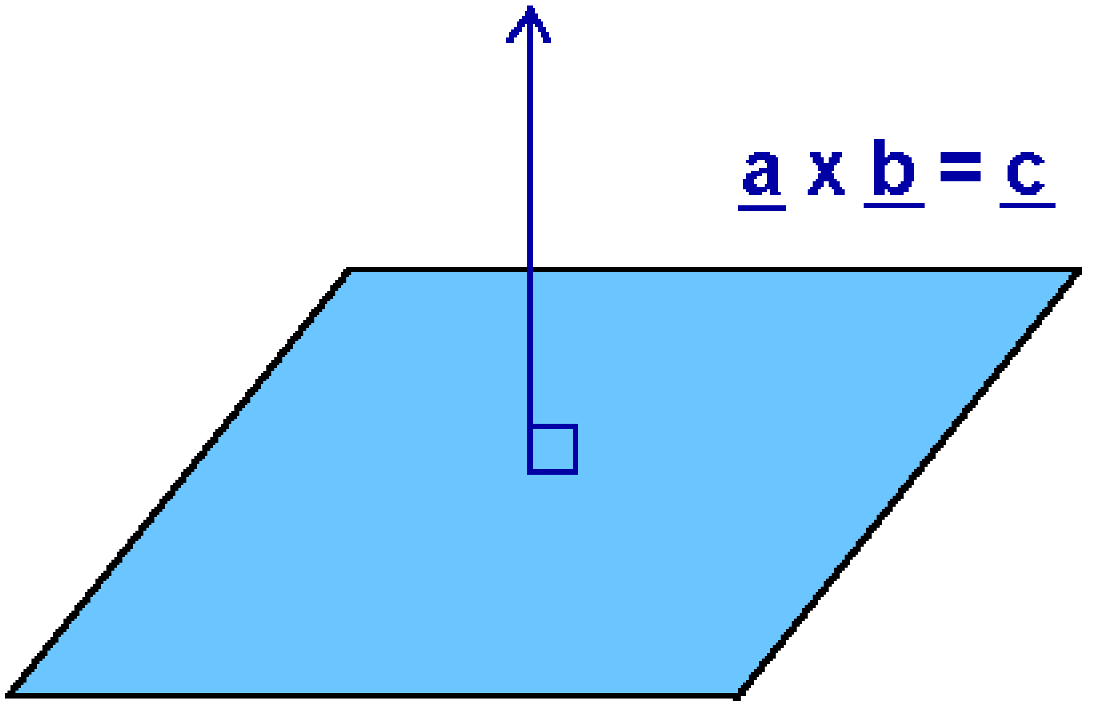
Reciprocal Lattice vectors

Any set of planes can be defined by:

(1) their orientation in the crystal (hkl)

(2) their d-spacing

The orientation of a plane is defined by the direction of a normal (vector product)



Defining the reciprocal

Take two sets of planes:

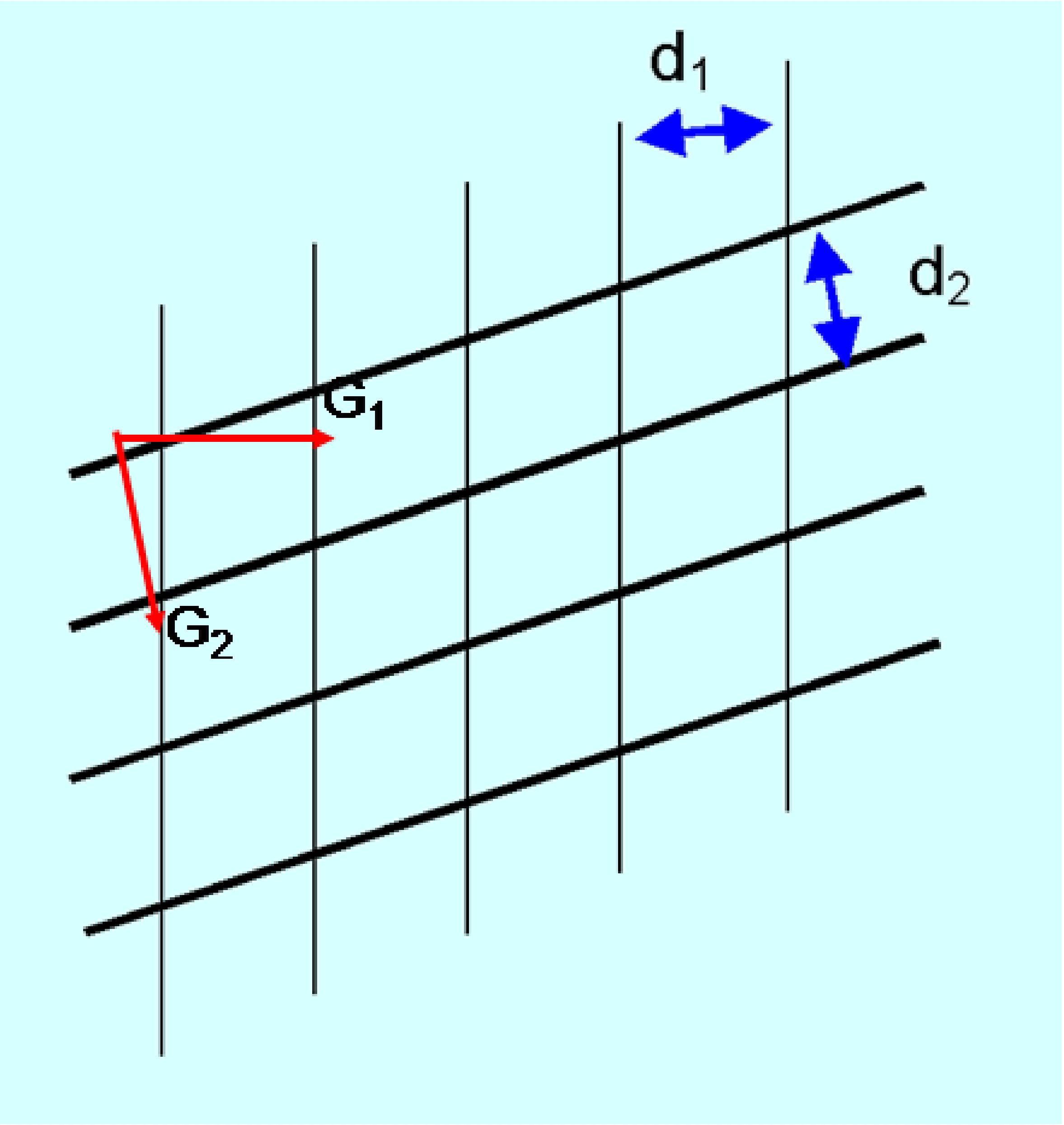
Draw directions normal:

These lines define the orientation but not the length

We use $\frac{1}{d}$ to define the lengths

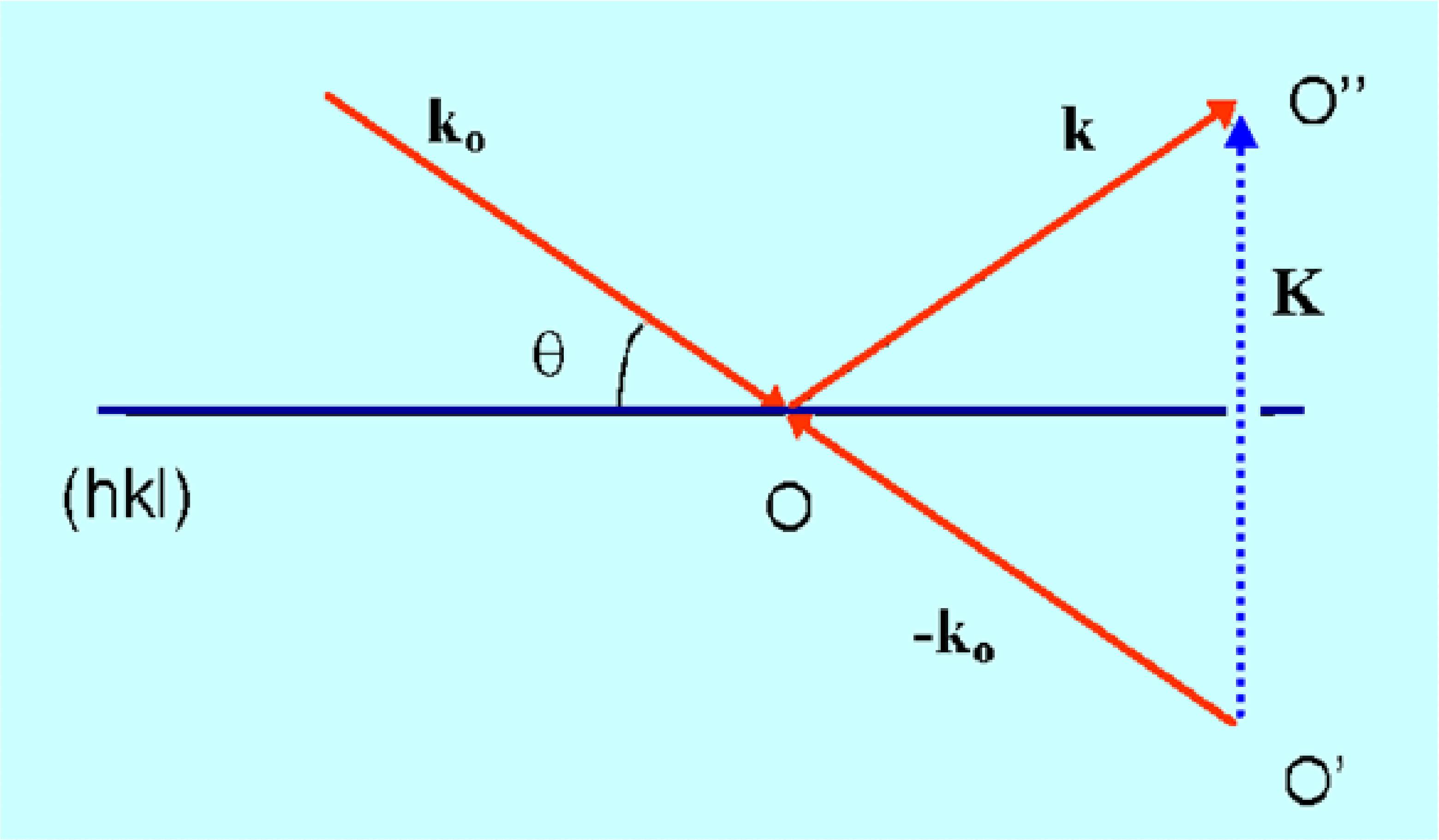
These are called reciprocal lattice vectors G_1 and G_2

Dimensions = 1/length



The K vector

We define incident and reflected X-rays as k_o and k respectively, with moduli $1/\lambda$



Then we define vector $\mathbf{K} = \mathbf{k} - \mathbf{k}_o$

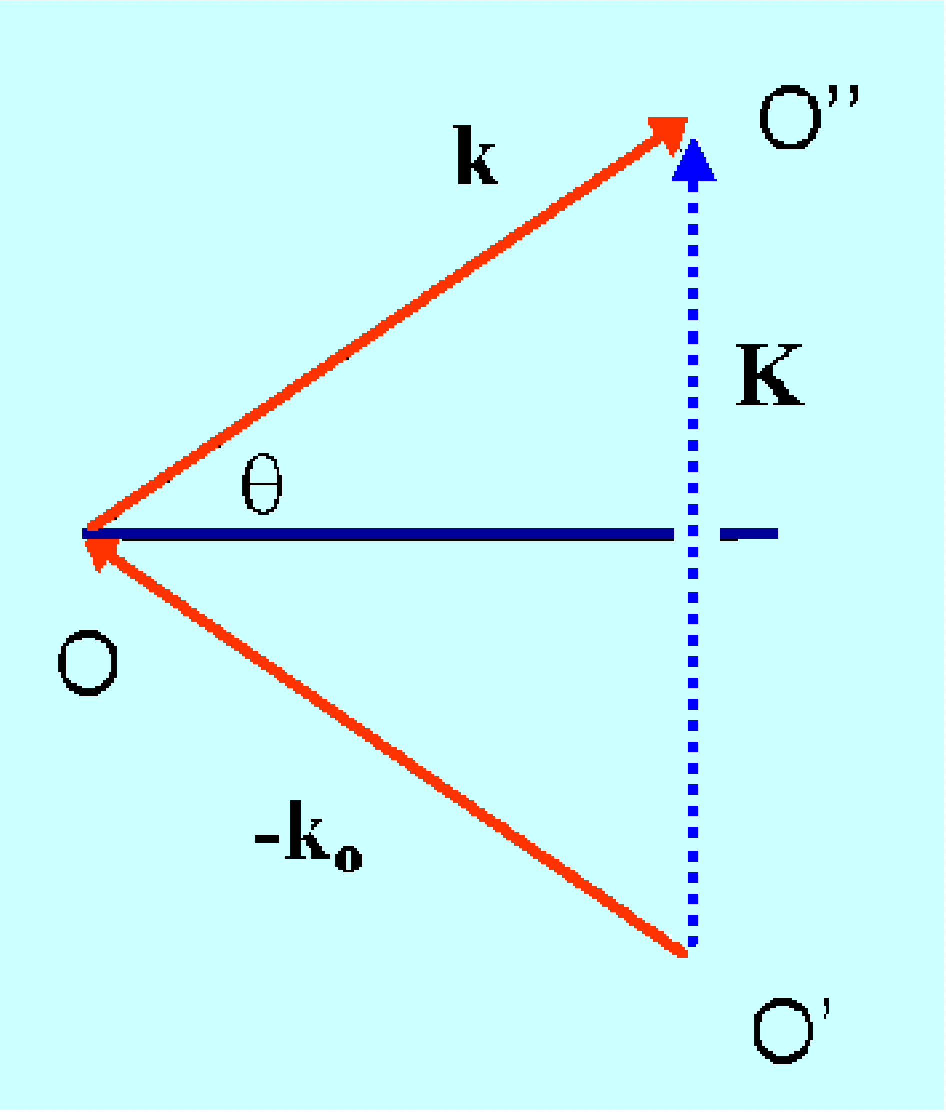
K vector

As **k** and **k**$_o$ are of equal length, $1/\lambda$, the triangle O, O', O'' is isosceles.

The angle between k and -k$_o$ is $2\theta_{hkl}$ and the hkl plane bisects it.

The length of K is given by:

$$|K| = 2|k|\sin\theta_{hkl} = \frac{2\sin\theta_{hkl}}{\lambda}$$



The Laue condition

K is perpendicular to the (hkl) plane, so can be defined as:

$$K = \left[\frac{2\sin\theta_{hkl}}{\lambda}\right]\hat{n}$$

where $\hat{n}$ is a vector of unit length

G is also perpendicular to (hkl) so

$$\hat{n} = \frac{G_{hkl}}{|G_{hkl}|}$$

$$\Rightarrow \quad K = \frac{2}{\lambda|G_{hkl}|}\sin\theta_{hkl}G_{hkl}$$

and $|G_{hkl}| = \frac{1}{d_{hkl}}$ from previous

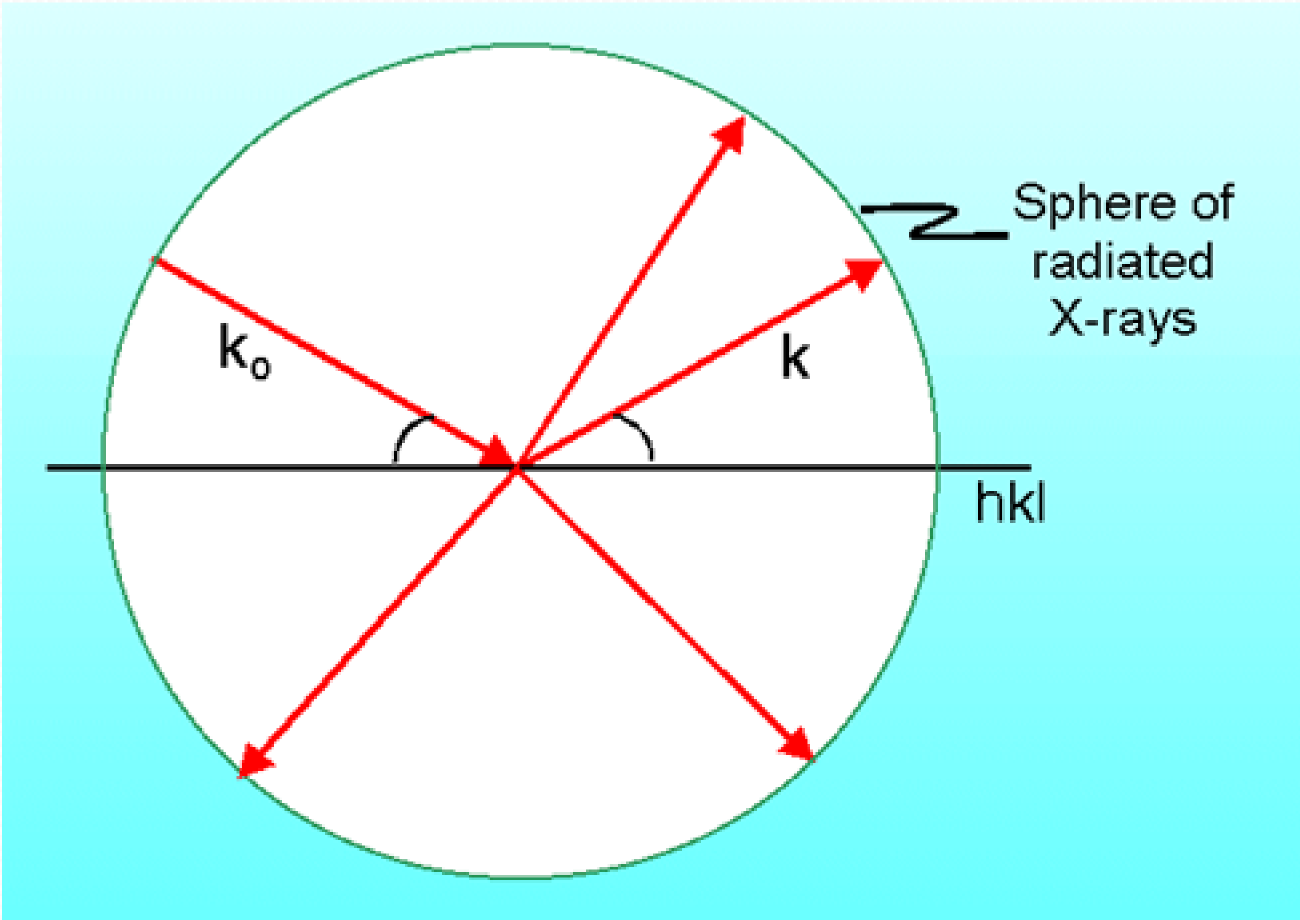
$$\Rightarrow K = \frac{2d_{hkl}\sin\theta_{hkl}}{\lambda}G_{hkl}$$

But Bragg: $2d\sin\theta = \lambda$

So **$K = G_{hkl}$ the Laue condition**

What does this mean?!

Laue assumed that each set of atoms could radiate the incident radiation in all directions



Constructive interference only occurs when the scattering vector, K, coincides with a reciprocal lattice vector, G

This naturally leads to the <u>Ewald Sphere</u> construction