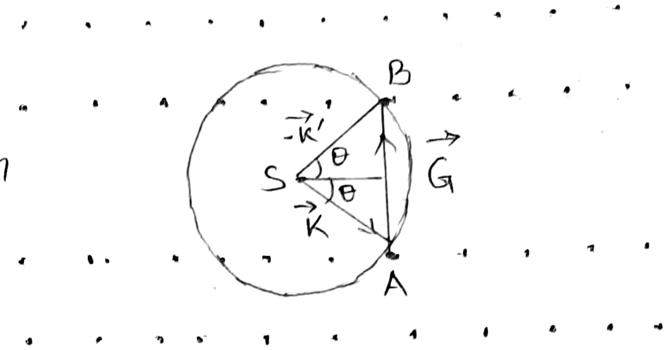
Ewald's construction

In order to obtain a relation between wave vector $\vec{k}$ and the direction of incident X-ray beam Ewald gave geometrical construction.

Considering figure,



let us draw a vector $\vec{SA} = \vec{k} = \frac{2\pi}{\lambda}$ in the direction of the incident X-ray beam and terminating at the origin of the reciprocal lattice. Now draw a sphere of radius $k = \frac{2\pi}{\lambda}$ about the point S as centre. Assume this sphere intersects some point B of the reciprocal lattice whose indices are (h', k', l'). The vector AB then represents the reciprocal lattice vector $\vec{G}$ and is normal to some set of direct lattice plane e.g. SC.

$$AB = |\vec{G}| = 2\pi\left(\frac{n}{d}\right) \qquad \text{--- (1)}$$

where n is the largest integral factor common to three integers (h', k', l') and d is the interplaner spacing for the set of direct lattice planes.

Bragg's diffraction condition:

If $\vec{SA} = \vec{k}$ = incident wave vector and $\vec{SB} = \vec{k'}$ = diffracted (or reflected) wave-vector,

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

It is clear from above result that the scattering changes only the direction of $\vec{k}$ and the scattered wave vector differs from incident wave vector by a reciprocal lattice vector $\vec{G}$.

Hence $\vec{k'} = \vec{k} + \vec{G}$

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

$$\therefore k'^2 = \vec{k}^2 + 2\vec{k}\cdot\vec{G} + \vec{G}\cdot\vec{G} \qquad \text{--- (2)}$$

Since the magnitude of $\vec{k'}$ = magnitude of $\vec{k}$, (2)

Hence $k'^2 = k^2$ —— (3)

Using (3) in (2), we get

$$2\vec{k}\cdot\vec{G} + \vec{G}\cdot\vec{G} = 0$$

or, $(2\vec{k} + \vec{G})\cdot\vec{G} = 0$

$$\therefore \left(\vec{k} + \frac{\vec{G}}{2}\right)\cdot G = 0 \quad —— (4)$$

The Eq. (3) is the vector form of Bragg's law and represents the Bragg's diffraction condition in terms of reciprocal lattice vector $\vec{G}$.

<u>Bragg's law in usual form:</u>

It is clear from Eq. (3) that

$\vec{k} + \frac{\vec{G}}{2} = \vec{SA} + \vec{AC} = \vec{SC}$ is $\perp$ $AB(\vec{G})$.

If $\angle ASC = \theta$,

$$\sin\theta = \frac{AC}{SA} \quad \therefore AC = SA\sin\theta$$

Hence $AB = 2AC = 2SA\sin\theta = 2k\sin\theta$

$$AB = 2\frac{2\pi}{\lambda}\sin\theta \quad —— (5)$$

From (1), $AB = |\vec{G}| = 2\pi\left(\frac{n}{d}\right)$ —— (6)

Comparing (5) and (6),

$$2\pi\left(\frac{n}{d}\right) = 2\frac{2\pi}{\lambda}\sin\theta$$

or, $2d\sin\theta = n\lambda$ —— (7)

This is Bragg's law.

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