Experimental geometries suggested by the Laue condition

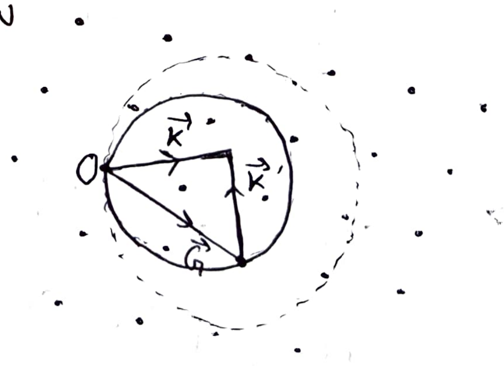
An incident wave vector $\vec{K}$ will lead to a Bragg peak if and only if the tip of the wave vector lies on ~~the~~ a K-space (G-space) Bragg plane. Now, the set of all Bragg planes is a discrete family of planes. These are the planes found by bisecting the $\vec{G}$ vectors w.r.t. an origin in the G-space with a perpendicular plane. So, the Bragg planes will not fill up the 3D K-space, and in general the tip of $\vec{K}$ will not lie on a Bragg plane. Thus, for a fixed incident wave vector — that is, for a fixed X-ray wavelength and fixed incident direction relative to the crystal axes, there will be no Bragg peak at all in general.

If one wishes to search experimentally for the Bragg peaks, one must relax the condition of fixed $\vec{K}$, either by varying the magnitude of $\vec{K}$ (changing the wavelength) or by varying it's direction, which in practice is obtained by varying the orientation of the crystal with respect to the incident direction.

The Ewald construction

Ewald construction is a simple geometric construction that is of great ~~half~~ help in visualizing various methods ~~and~~ to observe the Bragg peaks and in deducing the crystal structure from the observed peaks.

~~We draw~~ Consider the Laue condition. We have the incident wave-vector $\vec{k}$ originating from a point O and scattered wave vector $\vec{k}'$. Also, $\vec{G} = \vec{k} - \vec{k}'$ which also, say originate at O. Now, $\vec{G}$ must be a reciprocal lattice vector, meaning a vector in the reciprocal space. We draw a sphere in k-space centered on the tip of the incident wave-vector $\vec{k}$ of radius



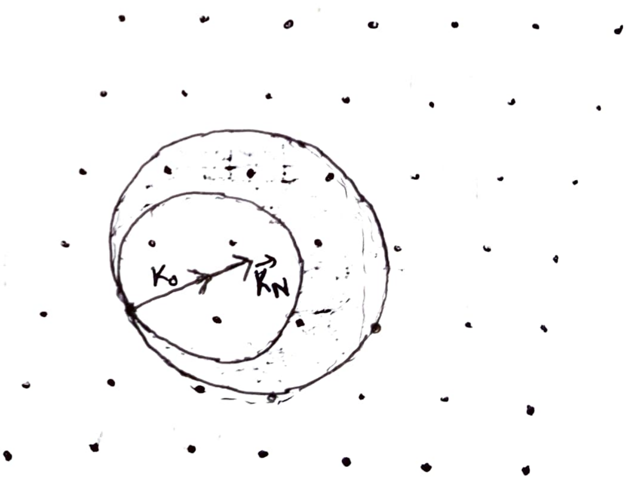
$k = \frac{2\pi}{\lambda}$, which means the point O will be on the surface of the sphere. This ~~is~~ is the

Ewald sphere. Now, since $\vec{K}$ and $\vec{K}'$ has the same magnitude, K' must also be the radius of the Ewald sphere, and so it's tail must be on the surface of the sphere. What it means is that, the scattered wave vector $\vec{K}'$ will satisfy the Laue condition if and only if the reciprocal lattice vector $\vec{G}$ ends on the surface of the Ewald sphere, meaning, if and only if the reciprocal lattice point is on the surface of the Ewald sphere. In that case, there will be a Bragg reflection from the family of direct lattice planes perpendicular to $\vec{G}$.

In general, a sphere in k-space with the origin of k-space on it's surface might have no other reciprocal lattice points on it's surface, and for a general incident wave-vector there will be no Bragg peak. One can, however, ensure that some Bragg peaks will be produced by several techniques, some of which are described here.

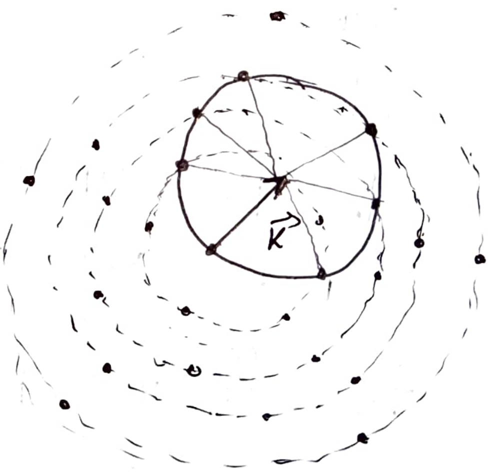
1. The Laue method: One can continue to scatter from a single crystal of fixed orientation from a fixed incident direction $\hat{n}$, but can search for Bragg peaks by not using a monochromatic X-ray beam, but a beam containing wavelengths from λ_N to λ_0, corresponding to wave-vectors $\vec{K}_N = \frac{2\pi}{\lambda_N}\hat{n}$ and $\vec{K}_0 = \frac{2\pi}{\lambda_0}\hat{n}$.

We will be now able to form many Ewald spher, and to be specific, the Ewald sphere will now expand into the region contained between the two spheres determined by $\vec{K}_0$ and $\vec{K}_N$. The Bragg peaks will then be observed if a reciprocal lattice vector lies in this region. Of course we are talking about a continuous range of wave-lengths from λ_N (min) to λ_0 (max).



Then, by making the spread in wavelength sufficiently large, one can be sure of finding some reciprocal lattice points within this region. Also, the spread shouldn't be very large, because then there will be too many Bragg peaks, and the picture ~~won't be~~ will get congested.

2. <u>The rotating crystal method:</u> This method uses a monochromatic X-ray, but allows the angle of incidence to vary. This is done by not changing the direction of the ~~X~~ X-ray, but the orientation of the X-ray is varied instead. In the rotating crystal method the crystal is rotated about a fixed axis, and the Bragg peaks that occurs during the rotation ~~is~~ are recorded on a ~~screen~~ film. As the crystal rotates, the reciprocal lattice that the direct lattice determines will rotate about the same axis as well. Thus, the Ewald sphere is fixed in the k-space (since it is determined by the incident wave-vector $\vec{k}$, that is not changing), while the whole crystal rotates

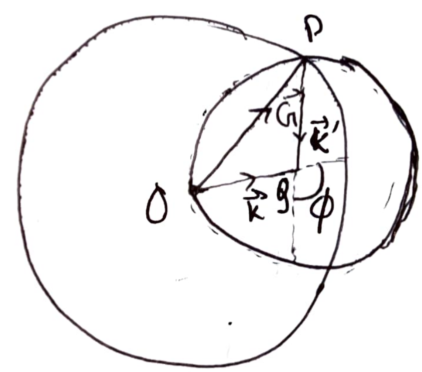


about the axis of rotation of the crystal. During the rotation process, each reciprocal lattice point traverses a circle in the reciprocal space about the rotation axis, and a Bragg peak occurs whenever the circle intersects the Ewald sphere (meaning the reciprocal lattice point lies on the surface of the sphere at that time).

3. The powder or Debye - Scherrer method: This is equivalent to the rotating crystal method, except the axis of rotation is varied over all possible orientations. For this it is not necessary to rotate the crystal itself. Rather, this is achieved by taking the ~~powed~~ powder of a crystal sample, grains of which are still enormous on the atomic scale and therefore capable of diffracting X-rays. Because the crystal axes of individual grains is randomly oriented the diffraction patteren produced by such a powder is what one would expect to be produced by combining the diffraction pattern of all possible orientations in a single crystal.

The Bragg peaks are now determined by fixing the incident wave-vector $\vec{k}$, and with it the

Ewald sphere as well, and then allowing the reciprocal lattice to rotate through all possible angles about the origin, so that ~~the~~ each reciprocal lattice vector $\vec{G}$ generates a sphere of radius G about the origin. ~~The vector joining~~ Such a sphere will intersect the Ewald sphere in a circle, provided that G is less than $2K$ (if $G > 2K$, the sphere with radius G will just enclose the Ewald sphere with radius k, without intersecting). The vector joining any point on the circle to the tip of $\vec{k}$ will be a scattered wave-vector $\vec{k}'$ for which Bragg peaks will be observed. The figure here shows a plane section of the two intersecting spheres. Each reciprocal lattice vector ~~with~~ ~~make~~ less than $2K$ will make a cone of scattered radiation at an angle ϕ in the forward direction (see the figure in Ashcroft and Mermin in page 103).



Since $\triangle OPQ$ is isoscele,

$$\angle POQ = \angle OPQ = \frac{180^\circ - \phi}{2} = \frac{\pi - \phi}{2}$$

Now, using the sine rule,

$$\frac{K}{\sin\left(\frac{\pi}{2}-\frac{\phi}{2}\right)} = \frac{G}{\sin\phi} \Rightarrow \frac{K}{\cos\frac{\phi}{2}} = \frac{G}{\sin\phi}$$

$$\Rightarrow G = \frac{K \times \sin\phi}{\cos\phi/2} = \frac{K \times 2\sin\frac{\phi}{2}\cos\phi/2}{\cos\phi/2}$$

$$\boxed{\therefore\ G = 2K\sin\frac{\phi}{2}}$$

By measuring the angles ϕ at which the Bragg peaks ~~occurs~~ are observed, one ~~theo~~ therefore learns about the length of all reciprocal vectors shorter than $2K$. Armed with this information, along with knowing some facts about the crystal symmetry, and the fact that reciprocal lattice is a Bravais lattice, one can usually construct the reciprocal lattice itself.