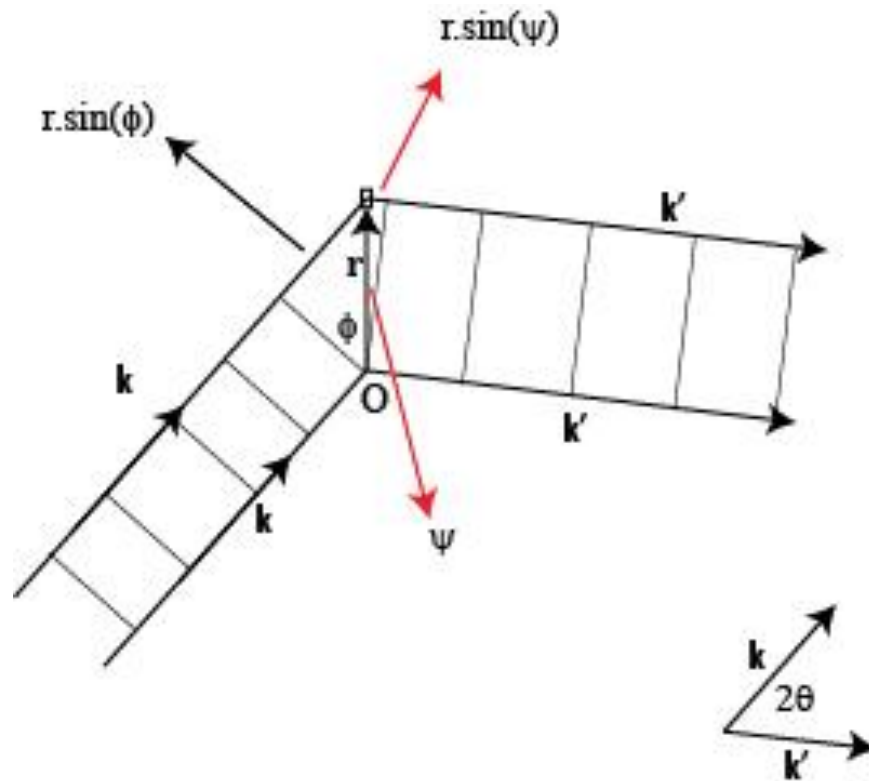


The explanation of the diffraction condition in Kittel is abstract, but I would like everybody to understand the physics of it.

I redrew Fig. 6 on page 30 below. The little cube is the volume segment of the crystal that we consider. It is a fraction of the unit cell. I have an incident plane wave indicated by \mathbf{k} , and a diffracted plane wave indicated by \mathbf{k}' . Both are wave vectors. Their directions indicate the direction of the incident and diffracted wave. Their magnitude is $2\pi/\lambda$. Since we only consider elastic scattering, both the \mathbf{k} and \mathbf{k}' vector have the same length. I redrew the \mathbf{k} and \mathbf{k}' vector on the lower right. The angle between them is of course the 2θ from the x-ray graphs of Fig. 17. So somewhere near the tail of the \mathbf{k} -vector is the X-ray source and somewhere near the head of the \mathbf{k}' vector is the X-ray detector. The location of the little cube is \mathbf{r} .



The incident and diffracted beam are plain waves. It is clear that the incident wave at the origin has another phase than the incident wave at the cube. For the cube the traveled length is longer, i.e. the wave needs to travel a longer length which will result in the incident plane wave having a different phase at the cube than at the origin:

$$r \sin(\phi) \rightarrow 2\pi \frac{r \sin(\phi)}{\lambda} \quad [1]$$

Note that $2\pi/\lambda$ is equal to the magnitude of \mathbf{k} and note that is equal to the magnitude of \mathbf{k}' . Furthermore note that the dot product of \mathbf{k} and \mathbf{r} is equal to:

$$\vec{k} \cdot \vec{r} = |\vec{k}| |\vec{r}| \cos(90 - \phi) = \frac{2\pi}{\lambda} r \sin(\phi) \quad [2]$$

Note that this is exactly equal to the phase difference given in equation (1) above. Similarly the diffracted waves from the origin and cube are out of phase as the diffracted wave from the cube has to travel a longer distance:

$$r \sin(\psi) \rightarrow 2\pi \frac{r \sin(\psi)}{\lambda} \quad [3]$$

The dot product of \mathbf{r} and \mathbf{k}' is given by:

$$\vec{k}' \cdot \vec{r} = |\vec{k}'| |\vec{r}| \cos(90 + \psi) = -|\vec{k}'| |\vec{r}| \cos(90 - \psi) = -\frac{2\pi}{\lambda} r \sin(\psi) \quad [4]$$

So equal to the phase difference between a wave coming from the cube and a wave coming from the origin. So the total phase difference for a ray diffracted from the origin and a ray diffracted from the cube is equal to:

$$\vec{k} \cdot \vec{r} - \vec{k}' \cdot \vec{r} \quad [5]$$

To find the scattering amplitude we will assume that the scattering is linear proportional to the local charge density $n(\mathbf{r})$. So summing up the contributions of all cubes gives:

$$F = \int dV n(\vec{r}) e^{i(\vec{k} \cdot \vec{r} - \vec{k}' \cdot \vec{r})} \quad [6]$$

Now substitute in the Fourier series we developed for $n(\mathbf{r})$:

$$F = \sum_{\vec{G}} \int dV n_{\vec{G}} e^{i(\vec{G} + \vec{k} - \vec{k}') \cdot \vec{r}} \quad [7]$$

Note that because of the phase factor which is different for each dV , normally the scattering amplitude will be zero. So only if the phase factor is constant, we expect a strong scattering amplitude. Note that each dV has its own \mathbf{r} , so the only constant phase factor occurs if $\mathbf{G} + \mathbf{k} - \mathbf{k}' = 0$ or if $\mathbf{G} + \mathbf{k} = \mathbf{k}'$. So notice that only when $\mathbf{k} - \mathbf{k}'$ is equal to a reciprocal lattice vector we expect strong constructive interference of the scattered x-ray and thus a diffracted beam. So the diffraction pattern tells us the reciprocal lattice. Of course once we know the reciprocal lattice we can determine the normal crystal structure. Taking the magnitude square on both sides and using the fact that the magnitude of \mathbf{k} and \mathbf{k}' are the same we find the diffraction condition:

$$2\vec{k} \cdot \vec{G} + G^2 = 0 \Leftrightarrow 2\vec{k} \cdot \vec{G} = G^2 \quad [8]$$