Solid State Physics
Lecture 7
Diffraction Condition

Hello, we were discussing reciprocal lattice vectors and while discussing reciprocal lattice vectors. We defined $\overrightarrow{b_1}$,$\overrightarrow{b_2}$ and $\overrightarrow{b_3}$ the axis vectors in reciprocal lattice. (Refer Slide Time: 00:40)

And we have also mentioned the condition that $\overrightarrow{b_i} \cdot \overrightarrow{a_j}$ where $\overrightarrow{a_j}$ are the real lattice axis vectors this must be $2\pi\delta_{ij}$. So, Kronecker δ_{ij} as you already know equals 1 if $i = j$ and this is 0 sorry it is 1 if $i = j$, it this is 0 if $i \neq j$. So, we must see why this condition is necessary for the reciprocal lattice vectors. For our arbitrary function $n(\overrightarrow{r})$ that we have considered in three-dimension, we represented this as a Fourier series and that was $\Sigma_{\overrightarrow{G}}$, these are the equivalent of translation vectors in reciprocal lattice. Thus so called reciprocal lattice vectors $n_{\overrightarrow{G}}$, the Fourier coefficients $\exp{(i\overrightarrow{G} \cdot \overrightarrow{r})}$. Now, if we consider a translation in real space $\overrightarrow{T} = u_1\overrightarrow{a_1} + u_2\overrightarrow{a_2} + u_3\overrightarrow{a_3}$. If we considered this kind of a translation, then subject to this translation our function $n(\overrightarrow{r})$ must remain invariant that means, $n(\overrightarrow{r} + \overrightarrow{T})$ must be equals $n(\overrightarrow{r})$. Now, let us see what this quantity is according to this definition of the translation vector. This quantity can be given in terms of the Fourier series as $\Sigma_{\overrightarrow{G}} n_{\overrightarrow{G}} \exp{(i\overrightarrow{G} \cdot (\overrightarrow{r} + \overrightarrow{T}))}$ which essentially becomes $\Sigma_{\overrightarrow{G}} n_{\overrightarrow{G}} \exp{(i\overrightarrow{G} \cdot \overrightarrow{r})} \exp{(i\overrightarrow{G} \cdot \overrightarrow{T})}$this. And if this quantity has to be $n(\overrightarrow{r})$ that is given like this expression here that is basically this part, then this part has to be 1 in other words, in order to satisfy the conditions that we have laid down, $\exp{(i\overrightarrow{G} \cdot \overrightarrow{T})}$, this has to be 1 and in order to this be 1, we require $\overrightarrow{G} \cdot \overrightarrow{T}$, this quantity to be $2\pi m$ where m is an integer so, this is the condition we have. (Refer Slide Time: 05:15)

How can we satisfy this condition? So, how do we represent $\overrightarrow{G}$in the reciprocal lattice? Just like $\overrightarrow{T}$ in the real lattice, we represent $\overrightarrow{G}$ in the reciprocal lattice as $v_1\overrightarrow{b_1} + v_2\overrightarrow{b_2} + v_3\overrightarrow{b_3}$. So, with this definition of $\overrightarrow{G}$ in order to satisfy $\overrightarrow{G} \cdot \overrightarrow{T} = 2\pi m$. This is the condition that we found to be necessary to have the periodicity in the crystal we require that $\overrightarrow{b_i} \cdot \overrightarrow{a_j} = 2\pi\delta_{ij}$. If we have this condition satisfied, then we will have the boxed condition here implied from that ok. After discussing this much, we should now see how the diffraction takes place in a lattice. Earlier, we have derived Bragg's law, the way Bragg did it earlier considering reflection from crystallographic planes, but in reality, it is not reflection it is diffraction. So, we must see how the diffraction takes place and how we can understand the physics by working out the mathematics related to the diffraction. (Refer Slide Time: 06:52)

So, we consider a crystal specimen here looking something like this of any arbitrary shape and we consider some incident wave coming and falling here, it gets scattered, maybe goes along this direction, incident wave comes like this, get scattered here sorry I could not draw it parallel, I want to make it parallel something like this. So, this is the incident wave of the wave vector $\overrightarrow{k}$ and this is the scattered wave of wave vector $\overrightarrow{k'}$. Let us say, here is the origin and from this origin, this point of diffraction is placed at a position vector $\overrightarrow{r}$. We consider a volume element here like this and we draw a perpendicular wavefront like this so, this angle must be $90°$. Similarly here, we draw a perpendicular wavefront where this angle must be $90°$. This volume element we call dV and this is our crystal specimen. The incident beam maybe represented with the waveform $e^{(i\overrightarrow{k} \cdot \overrightarrow{r})}$ and the outgoing beam here that may be represented with $e^{(i\overrightarrow{k'} \cdot \overrightarrow{r})}$ and here, the difference between $\overrightarrow{k}$ and $\overrightarrow{k'}$. So, $\overrightarrow{k}$ is somewhere along this direction, $\overrightarrow{k'}$ is somewhere along this direction, this vector is $\Delta\overrightarrow{k}$. So, $\overrightarrow{k'} - \overrightarrow{k} = \Delta\overrightarrow{k}$. So, we consider diffraction of wave in this crystal specimen as we can see in this figure and the difference in the phase factors of the incident and the diffracted wave, scattered wave that can be represented as $\exp{[i(\overrightarrow{k} - \overrightarrow{k'}) \cdot \overrightarrow{r}]}$. This is the difference in phase factor ok and this is for the beams hitting at a distance r apart separated by a vector $\overrightarrow{r}$. Now, the wave vectors of the incoming and outgoing beams as we have marked here k and k prime so, we assume that the amplitude of the waves scattered from the volume element here dV is proportional to the local electron concentration in the specimen. So, if we have n as the electron concentration it is of course a function of $\overrightarrow{r}$, it is the local electron concentration. It is no longer the arbitrary function that we have considered in case of Fourier transform. So, this is the local electron concentration and when some photon gets reflected sorry scattered, it depends its scattered amplitude depends on the local electron concentration in there so, $n(\overrightarrow{r})$ is going to be important. The total amplitude of the scattered wave in the direction of $\overrightarrow{k'}$ that is proportional to the integral of $n(\overrightarrow{r})$ that is the local electron concentration times this phase factor that we have considered. So, the amplitude of the electric or magnetic field wave vector in this scattered electromagnetic wave is proportional to the integral of $n(\overrightarrow{r})$ times the phase factor so, that thing we can calls scattering amplitude. (Refer Slide Time: 13:32)

Let us go to a new page, let us define this term scattering amplitude, it is called F. So, F can be given as $\int dV$, the volume element $n(\overrightarrow{r})$ that is local electron concentration times $\exp[i(\overrightarrow{k} - \overrightarrow{k'}) \cdot \overrightarrow{r}]$; this quantity which if we write $\Delta\overrightarrow{k}$ for this $(\overrightarrow{k} - \overrightarrow{k'})$ can be written as this. So, $\Delta\overrightarrow{k}$ measures the change in wave vectors so, $\Delta\overrightarrow{k}$ is called the scattering vector. Now, we introduced the Fourier components of $n(\overrightarrow{r})$. So, $n(\overrightarrow{r})$ is here the local electron density, but in a periodic crystal, it is also a periodic function therefore, the same kind of Fourier transform, Fourier series that we have discussed earlier is applicable for $n(\overrightarrow{r})$ as well. Now, if we write $n(\overrightarrow{r})$ in terms of the Fourier series, we can write $F = \Sigma_{\overrightarrow{G}} \int dV n_{\overrightarrow{G}} \exp[i(\overrightarrow{G} - \Delta\overrightarrow{k}) \cdot \overrightarrow{r}]$. Let us discuss two situations, 1st $\overrightarrow{G} = \Delta\overrightarrow{k}$. If we have this kind of a situation, what do we get? You can clearly see that the argument of this exponential goes to 0 in this condition and if the argument of the exponential goes to 0, the exponential gives us 1 so, in this condition, F will be nothing but $Vn_{\overrightarrow{G}}$, this would be F. And the 2nd condition is certainly $\overrightarrow{G} \neq \Delta\overrightarrow{k}$. If $\overrightarrow{G} \neq \Delta\overrightarrow{k}$ that is if $\Delta\overrightarrow{k}$ differs significantly from any reciprocal lattice vector, then F becomes negligibly small, F is nearly 0 in this condition and it is a homework for you to show this. (Refer Slide Time: 17:34)

Now, in case of elastic scattering of a photon, its energy is conserved so, its energy is $\hbar\omega$ that quantity is conserved and the diffracted beam let us say has a frequency ω' which is c that is the velocity of the photon times the $|\overrightarrow{k'}|$ and that must be ω because the energy is conserved and this ω' times $\hbar$ is the same as ω. So, conservation of energy requires the $|\overrightarrow{k}| = |\overrightarrow{k'}|$ although, they may be at different directions that is allowed in other words, $\overrightarrow{k}^2 = \overrightarrow{k'}^2$. And we have earlier seen that for a diffraction pattern a bright spot we need $\Delta\overrightarrow{k} = \overrightarrow{G}$ for non-vanishing scattering amplitude. And if $\Delta\overrightarrow{k} = \overrightarrow{G}$, we can write $(\overrightarrow{k} + \overrightarrow{G})^2 = \overrightarrow{k}^2$. Remember $\Delta\overrightarrow{k}$ is nothing but $\overrightarrow{k} - \overrightarrow{k'}$ and we can also recast this equation in the following form $2\overrightarrow{k} \cdot \overrightarrow{G} + \overrightarrow{G}^2 = 0$. Now, if $\overrightarrow{G}$ is a reciprocal lattice vector, $-\overrightarrow{G}$ is also a reciprocal lattice vector, negative of $\overrightarrow{G}$ is also a reciprocal lattice vector and we can as well call it $\overrightarrow{G}$, there is no difference. Therefore, we can also write $2\overrightarrow{k} \cdot \overrightarrow{G} = \overrightarrow{G}^2$ by putting $\overrightarrow{G} = -\overrightarrow{G}$ and this expression is often used as the diffraction condition. Although, every statement that we have here, starting from here, all these are diffraction conditions, this is particularly useful in many cases ok. In fact, from this diffraction condition, we can find out Bragg's law. So, your homework would be to show to prove Bragg's law from the diffraction condition.