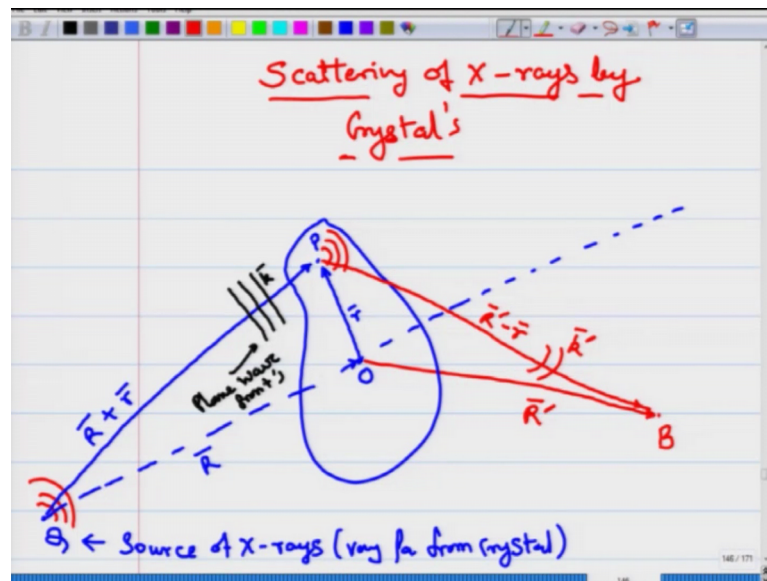


Introduction to Solid State Physics
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Lecture – 35
Scattering of X-rays from crystals Part-II

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In the last lecture, we came across the concept that X-rays can be scattered by an atomic lattice. And X-rays are nothing else, but electromagnetic waves. The reason that you use X-rays to study the crystals is that the wavelength is very small and they are comparable to the spacing between the atoms inside the crystal and that is why you use X-rays these electromagnetic waves to study the scattering from a crystal.

So, let us investigate the behaviour of this scattering, and some of the principles associated with this scattering. So, let us describe how the X-rays are falling on a crystal and diffracting from the crystal or getting scattered from the crystal. And for that let us set up some directions. So, we have a crystal which we are showing here. And very far from the crystal, we have the source of X-rays, this is the source of X-rays which is very far from the crystal. So, for all practical purposes, you can consider it at infinity.

So, from this source, of course, at the source it is generating spherical wave fronts, and therefore, the light is going all across. Let us first set up a line of sight, it intersects with

the crystal at point O and let point P be some point on the crystal with respect to point O it is located with r and this is capital R. Now, this is $R + r$.

And now because the queue is very far away from the crystal the wave fronts which are reaching the point P are nothing else but plane wave fronts. Because by the time they reach the crystal these wave fronts have become, so large that you can consider them as part of very large spheres which you can take as plane wave fronts. So, these are plane wave fronts. And these wave fronts have a wave vector k , the wave vector of these wave fronts is k .

Once they strike the point P, now the point P starts acting as the scatterers which are present at point P start generating secondary waves which will diffract the light. And the light will reach your point of observation which is B. And now these could be spherical waves which will reach the point B. So, plane waves actually reach point P, and from there they generate secondary waves which are spherical waves which cause the scattering of light and then your light reaches point B.

So, you can describe this point with respect to O as R' ; the light which is getting scattered this is $R' - r$, and the spherical waves which are reaching this have a wave vector k' . So, you have plane waves which strike point P generate spherical waves or secondary waves which scatter the light with a wave vector k' . This is the wave vector of the wave fronts which are reaching point P and they reach point B. Now we will analyse this picture as we go along next.

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Plane wave which reaches point P

Electric field → Amplitude $A_p = A_0 e^{i \vec{k} \cdot (\vec{R} + \vec{r})}$ just e

A_0 : amplitude roughly at the source

From pt. P → spherical waves which are generated.

We to write the Amplitude of the waves reaching point B

So, I can write the plane wave which reaches at point P the plane wave which reaches point P has an amplitude which is basically the electric field by amplitude I mean the electric field A_p the electric field is A_p which is basically the amplitude of the electric field is $A_0 e^{i \vec{k} \cdot (\vec{R} + \vec{r})}$.

If you recall the figure that the plane waves are these plane waves \vec{k} is the wave vector, and $\vec{R} + \vec{r}$ is the location of this point P. So, the plane wave which reaches at this point has is located at $\vec{R} + \vec{r}$, and it has an amplitude A_p is where A_0 is the amplitude roughly at the source. And there is $e^{i \omega t}$ or $e^{-i \omega t}$ is the frequency of the wave. I am not writing that part; I am just considering this part of the term. It is a monochromatic X-rays, so there will be $e^{i \omega t}$ which is the time dependent part of the wave.

So, this is the amplitude of the wave which is reaching point P. Now, from point P there are spherical waves which are generated. So, you have spherical waves which are generated from point P, but what is important is that the intensity or the net amplitude of the waves which reach point B we would like to find out what is the amplitude of the waves which are reaching point B. When I speak of amplitude of the X-ray or the electromagnetic wave in the course in this part of the lecture, then I mean by amplitude I mean the electric field vector. By amplitude I it will be synonymous with the electric field vector.

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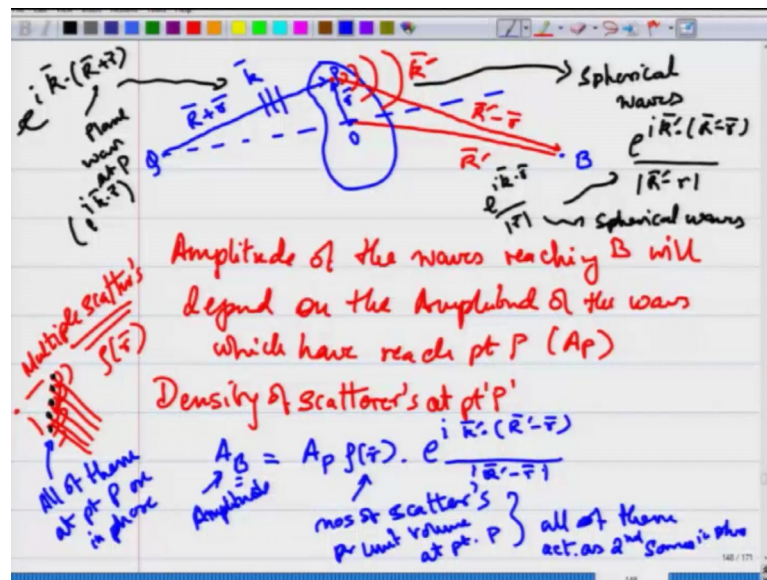
The image shows a digital whiteboard with handwritten notes in red ink. At the top, the equation $A(\mathbf{r}, t) = A_0 e^{i\mathbf{k} \cdot \mathbf{r} - i\omega_0 t}$ is written. Below it, ω_0 is defined as the frequency of the wave, and \mathbf{k} is defined as the wave vector of the wave. The equation is then rewritten as $A(\mathbf{r}, t) = A(\mathbf{r}) (e^{-i\omega_0 t})$. An arrow points from $A(\mathbf{r})$ to the text "Spatial of the Amplitude" and another arrow points from $(e^{-i\omega_0 t})$ to the text "Always Electric field vector".

So, when I write my amplitude of the electric field vector A of r, t I basically mean by electric field vector if I write it as $A r, t$ I basically mean the electric field vector as a function of position and time. If it is a plane wave, it will be e raise to i some initial amplitude A naught or the amplitude of the electric field vector e raise to $i k \cdot r$ bar minus $i \omega$ naught t , where ω naught is the frequency of the wave, and k is the wave vector of the wave.

So, I will use this notation to denote the electric field vector which I will be calling as also as amplitude, it has a special part and it has a time dependent part. And during the course of the derivation, I will assume that this is always present namely A of r, t will be written as A of r the spatial part e raise to minus $i \omega$ naught t , this is always present. And so therefore, I will not be writing it often, but it is assumed to be always present whenever I write the amplitude the time dependent part is implicitly present, I will not write it out explicitly, I will be writing essentially the spatial part of the amplitude or which is also the electric field vector of the electromagnetic wave which in our case is the X-ray which is falling on the crystal.

So, the next part of the calculation is we want to find out or write we want to write we want to write the amplitude of the waves reaching point B which is your point of observation ok.

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So, your point Q and you had your crystal at point P, this is point O. This is r ; this is R plus r . And you have plane wave fronts which are reaching and these have a wave vector k . And you have a point B which is not very far away from the crystal. And there are secondary waves which are emitted from this point P. There are secondary wave fronts which are emitted which are spherical waves. This is R bar prime, this is r bar prime minus r , and the spherical wave fronts have k prime as their wave vector. Incoming wave vector is k ; outgoing vector is k prime; its direction has changed, and it is coming in this direction.

Now, the amplitude of the waves reaching point B will depend on the amplitude of the waves which have reached point P that is they will depend on A . So, the amplitude of the wave which has reached point B will depend on A_P which is the amplitude of the wave at point P. Larger the amplitude or stronger the electric field of electromagnetic wave which has reached point P will generate much more intense scattered light which will reach or scattered electromagnetic waves which will reach point B. So, it will be clearly proportional to the intensity or the amplitude of the waves which have reached point P.

But apart from that it will also depend on the density of scatterers which are present at point P at point P. Because at point P, if you have 10 such points, each of them is considered to be generating spherical waves. So, you have a wave with strikes point P, but you have multiple points there are large number of scatter as if you have more

number of scatterers, each of them will generate a spherical wave and so you will get a scatter intensity which will get multiplied by the number of points which are present at point P.

So, at point P you might have multiple scatterers, you might have multiple scatterers. And so therefore, your amplitude of your outgoing wave will get multiplied by the number of points which are present at point P. The number of scatterers which are present at point P, they will multiply your amplitude because each of them acts like a scatterer. So, at point P if you have more number of scatterers, then the amplitude of the scattered wave will get multiplied by the number of scatterers that you have. So, you actually multiplied by the density. And furthermore most since these are spherical waves, whereas plane waves have a form, the plane waves have a form $e^{i\mathbf{k} \cdot \mathbf{R} + r}$ or $e^{i\mathbf{k} \cdot \mathbf{r}}$ this is the point P of course, this is the plane wave which reaches point P plane wave at point P.

The spherical waves which are reaching point B have a form $e^{i\mathbf{k}' \cdot \mathbf{r}}$ divided by $R - r$. They have the form $e^{i\mathbf{k} \cdot \mathbf{r}}$ divided by magnitude of r these are spherical waves. You would have studied this in electromagnetism as well as and quantum mechanics that when you have spherical waves, they had a form $e^{i\mathbf{k} \cdot \mathbf{r}}$ divided by the magnitude of r . And when you have the incident plane wave, they have the form $e^{i\mathbf{k} \cdot \mathbf{r}}$ plane waves have the former $e^{i\mathbf{k} \cdot \mathbf{r}}$.

So, the amplitude at point B, the amplitude of the electromagnetic wave which reaches point B will be determined by the amplitude of the electromagnetic wave which reaches point P into the density of scatterers which is present at point B more the number of scatterers, more will be the density. It will just get multiplied, I will consider all of them is in phase all of them at point P are in phase namely they are scattering in phase they are not out of phase.

So, I will assume that in the small point P if there are large number of scatterers all of them roughly in phase. And so my intensity at point B or my amplitude at point B is determined by the amplitude which is reaching at point P into the number of scatterers which are present at point P which is multiplied by the density, it is given by the density. This is the number of scatterers per unit volume at point P, because each of them is in

phase all of them are in phase all of them act as secondary sources in phase into the spherical wave front which is of the form $e^{i k' \cdot r' - r}$ divided by magnitude of $r' - r$.

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Handwritten notes on a whiteboard showing the derivation of the Fraunhofer diffraction formula. The notes include a diagram of a crystal with points S, P, and B, and vectors \vec{R} , \vec{R}' , and \vec{r} . The equations are:

$$A_B = A_P \rho(\vec{r}) \frac{e^{i \vec{k}' \cdot (\vec{R}' - \vec{r})}}{|\vec{R}' - \vec{r}|}$$

We consider $\vec{R}' \gg \vec{r} \Rightarrow |\vec{R}' - \vec{r}| \sim |\vec{R}'| = R'$

$$A_B \approx A_0 \frac{e^{i \vec{k} \cdot (\vec{R} + \vec{r})}}{R'} \cdot e^{i \vec{k}' \cdot (\vec{R}' - \vec{r})} \rho(\vec{r})$$

$$A_B = A_0 \frac{e^{i(\vec{k} \cdot \vec{R} + \vec{k}' \cdot \vec{R})}}{R'} \cdot e^{i(\vec{k}' - \vec{k}) \cdot \vec{r}} \rho(\vec{r})$$

$I(\theta) \propto \left| \int_{\text{Volume of crystal}} A_B(\vec{r}) d^3 r \right|^2$

So, the amplitude at point B is the amplitude at point P into the density at point P $e^{i k' \cdot R' - r}$ divided by magnitude of $R' - r$, magnitude of this vector. And for all practical purposes, we consider that R' is much much larger than r ok. Namely If this is Q, this is point P, this is R, and this is point B, this is r . Then this distance is much larger than this distance. This is anyway your crystal, this is your crystal which is much smaller. You take a point of observation such that it is much larger than these distances.

And so, a b you can write it as now I will substitute for A P, the wave fronts this wave fronts which are reaching point P this is $R + r$ with an incident wave, wave vector k . It is $e^{i k \cdot R + r}$ divided by R' the magnitude I will replace this will give $R' - r$. If you work it out a little you can show it has equal to roughly the magnitude of R' which is R' . So, I approximate it as I replace this by R' into $e^{i k' \cdot R' - r}$.

And now let me simplify this A_B is $A_0 e^{i k \cdot R + k' \cdot R}$ divided by R' into a term and there is a ρ of r . There is a term which is ρ of $r e^{i k' \cdot r - r}$.

And this is your expression for amplitude of the scattered light which is reaching point B from some set of scatterers which are present at point P. The amplitude of that which is reaching B is given by this. Now, we can find the intensity this is nothing else, but the electric field of the outgoing wave the intensity at point B is proportional to A B square ok. And of course, we do not want to look at just this intensity we would like to find out the net intensity from all such points like P on the crystal ok.

So, my net intensity will be proportional to the net intensity at point P will be proportional to the net A B, I would like to find out what is the net this is the net amplitude which is coming at point P, point B because of all points which are present on the crystal ok. This is the total amplitude which is reaching from different points like point P distributed all across the crystal. So, I will take an integral of it, integrated over the volume of the crystal, this is the volume of the crystal. And square of that will give me my intensity. This is the amplitude and square of that will give me my intensity. So, my intensity at point B is now related to this.

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The image shows a whiteboard with handwritten mathematical derivations. At the top, it says "Constant" with an arrow pointing to the expression for the amplitude A_B . The expression is $A_B = A_0 \frac{e^{i(\vec{k} \cdot \vec{R} + \vec{k}' \cdot \vec{R}')}}{R'} e^{i(\vec{k} - \vec{k}') \cdot \vec{r}} \rho(\vec{r})$. To the left of this, there is a small diagram of a crystal volume with a point P and a vector \vec{r} pointing from P to a point B . Below the amplitude expression, the intensity I_B is given as $I_B \propto \left| \int_V A_B(\vec{r}) d^3r \right|^2$. This is followed by a boxed equation: $I_B \propto \frac{A_0^2}{R'^2} \left| \int_{Vol.} \rho(\vec{r}) e^{i(\vec{k} - \vec{k}') \cdot \vec{r}} d^3r \right|^2$. At the bottom, two simplified expressions are shown: $I_B \propto \frac{1}{R'^2}$ and $I_B \propto \left| \int_{Vol.} \rho(\vec{r}) e^{i(\vec{k} - \vec{k}') \cdot \vec{r}} d^3r \right|^2$.

So, let me find out the intensity at point B. If you recall A P, A B was A naught e raise to i k dot R plus k prime dot R divided by R prime e raise to i k minus k prime dot r. This is of course, a constant; the variable is this ok. You have different points which are located on the crystal. This is r which is locating the point P, but if I want to find out intensity because all different points on the crystal this is my variable r. So, my intensity at point

B, because of scattering from all such points like P is proportional to A_0 which is the function of r d^3r integrated over the volume of the crystal. The intensity at point B this is anyway of constant this will be proportional to A_0^2 by R' square and this is multiplied by ρ of r . So, this will be integral over the volume of the crystal ρ of r $e^{i\mathbf{k} \cdot \mathbf{r}}$ minus $\mathbf{k}' \cdot \mathbf{r}$ d^3r the whole square.

So, the intensity of the scattered light which is reaching a point B because of the entire crystal the intensity of the scattered light which is reaching the point B because of scattering from all points on the crystal is of course going down inversely as the distance from R' it goes as inversely square of the distance which is expected as you take the point B further the intensity is going to go down has $1/R'^2$. So, the intensity of B is going down has $1/R'^2$ the distance from this crystal which is expected inverse square law of intensity.

But the intensity is now importantly proportional to a quantity which is integrated over the volume of the crystal; ρ of r is the density of the crystal at a point r $e^{i\mathbf{k} \cdot \mathbf{r}}$ minus $\mathbf{k}' \cdot \mathbf{r}$ d^3r the whole square.

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$$I_B \propto \frac{A_0^2}{R'^2} \left| \int_v \rho(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}} d^3r \right|^2$$

where $\mathbf{K} = \text{scattering vector} = \mathbf{k}' - \mathbf{k}$

The intensity at point B is proportional to A_0^2 divided by R'^2 the whole square integral of integrated over the volume ρ of r $e^{i\mathbf{k} \cdot \mathbf{r}}$ minus $\mathbf{k}' \cdot \mathbf{r}$ d^3r the whole square, where \mathbf{K} is the scattering vector \mathbf{L} is the scattering vector, and it

is equal to $k' - k$. The scattered wave vector k' minus the incident wave vector k .

We will look at the consequences of this in the next lecture.