Symmetry and Structure in the Solid State
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Lecture – 34
Solid State and Structural Chemistry Unit

So, we just saw that the 2 equations which are very crucial to our structure determination or these the structure factor expression and the electron density expression.

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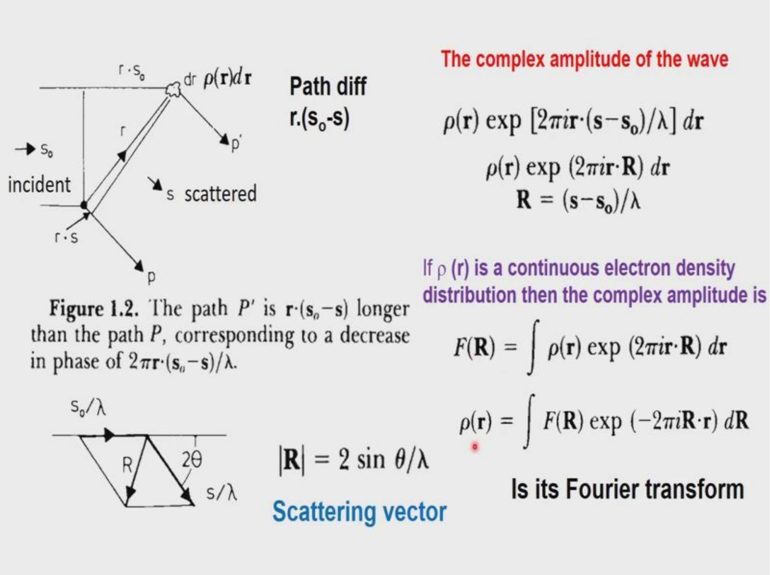

Path diff
$r.(s_0\text{-}s)$

Figure 1.2. The path P' is $\mathbf{r}\cdot(\mathbf{s}_0-\mathbf{s})$ longer than the path P, corresponding to a decrease in phase of $2\pi\mathbf{r}\cdot(\mathbf{s}_0-\mathbf{s})/\lambda$.

$|\mathbf{R}| = 2\sin\theta/\lambda$

Scattering vector

The complex amplitude of the wave

$$\rho(\mathbf{r})\exp\left[2\pi i\mathbf{r}\cdot(\mathbf{s}-\mathbf{s}_0)/\lambda\right]d\mathbf{r}$$

$$\rho(\mathbf{r})\exp(2\pi i\mathbf{r}\cdot\mathbf{R})\,d\mathbf{r}$$

$$\mathbf{R} = (\mathbf{s}-\mathbf{s}_0)/\lambda$$

If ρ (r) is a continuous electron density distribution then the complex amplitude is

$$F(\mathbf{R}) = \int \rho(\mathbf{r})\exp(2\pi i\mathbf{r}\cdot\mathbf{R})\,d\mathbf{r}$$

$$\rho(\mathbf{r}) = \int F(\mathbf{R})\exp(-2\pi i\mathbf{R}\cdot\mathbf{r})\,d\mathbf{R}$$

Is its Fourier transform

Now we will see what is the relation that comes in the geometry point of view because the relation that comes from the electron density we now know because the more the electron density the more is the scattering. Suppose you have a very big atom and a small atom the contribution from the big atom is more to the scattering compared to that of a small atom.

So, X rays therefore, now if one used whenever we use them; we will have the intensities depending upon the strength of the electron density that is associated with the unit cell. Now let us see what happens in terms of the geometries let us look at this figure; this figure is essentially showing this that we have the incoming incident radiation. The unit vector is associated with this is s_0 we now normalize it with respect to λ; so, it becomes independent of λ. So, we can use any λ remember that we are talking about atom sizes of the order of 1 Å.

So, the wavelength can be anywhere between 0.4 to 2.5 Å; if we use that wavelength we will be in a position to see the details associated with atoms and molecules and so on. So, therefore, we prefer to use X rays in that range about 0.5 Å to 2.5 Å is the range of X rays we like to use. It is recommended that since with the λ is coming up as a normalization factor; it is recommended that we use a single wavelength.

So, at this particular stage I can introduce the way in which we generate X rays; there is no slide or a diagram for that because I thought it is probably not necessary. Instead I will just give a narration and that narration should be sufficient for our understanding of how we generate X rays. You have all seen an X ray tube I suppose and you have used; in fact, you have gone to whenever you broke a hand or a leg which most of you do you go to a doctor and the doctors puts you through the X rays.

So, X rays are generated in a vacuum tube and these X rays are generated in such a way that they come up from what is known as thermionic emission. That is you take an element a filament in fact, a tungsten filament and that tungsten filament is heated with a certain small current. As the tungsten filament is heated that is just like the light source we have in olden days we had those incandescent lamps which still some people use, but now we have replaced everything by LEDs.

But this incandescent lamp are used to have a filament and when once you put on the switch when the power goes in the power is actually heating the element. The heated element now generates luminescence and that is how you get the light. So, the light becomes now on and as a consequence the filament glows and filament glows because we have heated the element. So, the same heating we do and now we have the there is an vacuum tube which encloses the filament.

Now, what really happens is in this case of the filament heated there is a certain region around that where we generate electrons. So, electrons get emitted there is of course, the usual heat the joule heat will be there. So, that is why if you put the light for about half an hour the incandescent light and go and touch it your hand will burn; the reason is we have generated a lot of Joule heat. Apart from that we have also use the concept of luminescence which occurred in the tungsten filament.

Now, the process is now essentially generating electrons. So, these generated electrons now are put in a large electric field. So, we put what is known as a cathode and this becomes now the anode. So, the cathode is now made up of an element ok, So, that particular element maybe I will have to write some picture for that. So, instead what I will do is I will explain and tell you now in very simple terms that the electrons now get accelerated, when we apply a very large field and these field could be 30 to 40 kV that is the X ray generator you will see.

So, in the case of a typical medical X ray it is about 60 to 80 kV of power which now accelerates these electrons. There is also a certain current which is involved in it we want the electrons to be generated faster rate than we increase the current. In a typical laboratory experiment where we expose the crystals that current is in mA; on the other hand in a medical X ray the current is in A. So, it is about 60 A; so 60 A and something like 60 to 80 kV is what is applied in a medical X ray situation.

In a when we want to expose the crystals as you know it is very small; the size of the crystal one uses it is about 0.3 mm^3; it is a very small crystal and therefore, the power is not very high it is not required. In fact, we can calculate the power. So, if you multiply 40 by 20; it is about 800 right; so this is 800 W. So, the power that is generated will be 800 W.

So, depending on 800 to 1200 W is the power which we use in the case of when we expose the crystals to X rays. On the other hand in the medical X ray it will be now 60 times 80 or something; so that is 4800 W its a very you know almost half a kW.

So, the X rays now what happens is that these electrons now hit the cathode which is an element. Now this element has a certain characteristic X ray maybe we will discuss that in a later class, when we actually see the experimental setup; when we actually see how we set up the experiment to measure the diffraction, how do we use the detector, how do we generate X rays at that time we will consider that.

But at this moment these X rays are accelerated to the cathode; the cathode is a particular element. Now this element has some what we call as characteristic behaviour depending upon where the *k* shell electrons are there with respect to these element we get the intensity going up in X rays. Otherwise generally we get X rays normal X ray which is known as the white radiation, like any other radiation you get you get a white radiation; along with that white radiation there is a characteristic radiation corresponding to the elimination of the k_α elimination of the *k* shell electrons.

When the *k* shell electron goes out *l* shell electrons drop in and therefore, we generate the X rays and those X rays in case of medical X rays are very strong. So, they pass through our body there is no harm. But the X rays which we use in the laboratory is so low in the power that we should not get ourselves exposed to X rays. Anyway let us say that we have generated X rays now for our discussion; we will go to the experimental detail later.

So, we have the generated X rays; so this is the X rays which are generated with a certain wavelength λ. So, we all these discussion came up because since we using this λ as the normalization factor, it is better that we in most of these experiments we try to get the λ to be a single value. In earlier experiments which Laue and others did which we are going to discuss now they used white radiation.

However, it is now recommended that we use what we call as the monochromatic X rays. So, there is a single wave length X ray. So, the incoming incident beam is normalized with respect to that. So, this is the way in which it comes and falls on these electron density $\rho(r)dr$ let us say it is up here. So, if the there was no electron density this would pass through and therefore, this is now called the incident direction; s_0/ λ is known in this particular direction it goes out into the system.

In fact, depending upon the amount of electron densities present since the energy that is associated with the incoming radiation is so large most of the radiation will go through except a little bit which now we will go in the direction s/λ because of the presence of the electron density it depends upon how much of electron density is there.

So, the amount of electron density decides how much of scattering intensity should come; so this goes in this particular direction. Now you see that if you calculate this angle if you call these angle as 2θ or now the vector R which is $(s - s_0)/ \lambda$ is the bisector of these two. So, there is s_0/λ, s/λ this is the bisector; the vector R therefore, is the bisector of s_0/λ, s/λ. You can calculate what should be the value of R; a little bit of trigonometry you have to do yourself. So, I will leave the choice to you how to get to this expression.

So, we get $|R| = 2\sin\theta /\lambda$**.** So, we therefore, get the actual value of R depends upon now the so called scattering angle; the more the scattering angle you see that the value of R it depends upon the value of λ. So, for a given λ the value of the scattering vector depends upon the value of θ; that means, the direction in which it goes the scattering direction in which it goes, is not really indicative in this expression which only giving us the $|2\sin\theta/\lambda|$. So, the direction in which it goes is following the s_0/λ, s/λ because that is the bisector of that.

So, depending upon different values of 2θ this vector s/λ can go anywhere between this to that; this can go from 0 to nearly 180^0. Now what how does s/λ vary with respect s_0/λ; we can consider that detail by considering the possibility of having atoms put here which we will discuss later.

So, at this moment $|R| = 2\sin\theta/\lambda$; what you notice immediately is therefore, this quantity R as we have been telling already is inversely proportional to length. And therefore this scattering vectors represent the vectors in reciprocal space. So; obviously, we have to now define a reciprocal space which we will do in an little while from now. So, the essentially the idea is now to see that we can get the value of the magnitude of R; the phase angle anyway has to be determined and therefore, we still have the phase determination remaining, but we can get the magnitude of R.

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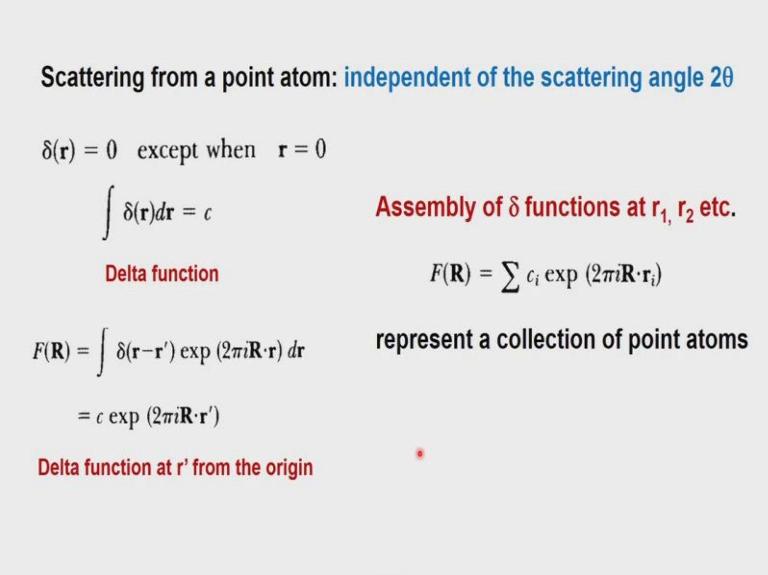

Scattering from a point atom: independent of the scattering angle 2θ

$\delta(\mathbf{r}) = 0$ except when $\mathbf{r} = 0$

$$\int \delta(\mathbf{r})d\mathbf{r} = c$$

Delta function

$$F(\mathbf{R}) = \int \delta(\mathbf{r}-\mathbf{r}')\exp(2\pi i\mathbf{R}\cdot\mathbf{r})\,d\mathbf{r}$$

$$= c\exp(2\pi i\mathbf{R}\cdot\mathbf{r}')$$

Delta function at r' from the origin

Assembly of δ functions at r_1, r_2 etc.

$$F(\mathbf{R}) = \sum c_i \exp(2\pi i\mathbf{R}\cdot\mathbf{r}_i)$$

represent a collection of point atoms

Now, we will go into the realistic situation until now we generally discuss scattering we generally discuss scattering with respect to some electron density which is lying in some space $\rho(r)dr$; now we will say that the electron density is associated with an atom. And more so we will make this atom a point atom; that means, suppose you consider a carbon atom, there are 6 electrons associated with the carbon and of course, there is nucleus core and valence electrons and so on.

Now, the whole thing we will condensate as though it has 6 electrons and say it is belonging to a point x y z. Then what happens is that any scattering that will occur if we go back here then is scattering that will occur; now we will become independent of 2θ. Because this is now a simple point if you now have a certain volume associated with this particular point like here small elemental volume we said; then we will have the scattering angle changing, otherwise if it is a point atom you will just see the point atom and the scattering will go; so it is independent of θ.

So, this is an very serious approximation, but it will allow us to imagine a situation where we can calculate what is the quantity of what is the total information we can get from this. In this particular case you see that the we define now because of the fact that there is a scattering from a point atom; the point has all the electrons in it. So, therefore, if we now calculate this quantity called $\delta(r)$ which is referred to as a delta function which is written here this delta function will be equal to 0 everywhere else because atom is only at one point; a single point atom we have taken the atom is at one point and let us say this atom is located at $r = 0$.

So, if the atom is located at $r = 0$; the expression of here which we have written here $\rho(r) \exp(2\pi i r \cdot R)$, there is no dependence on the phase. So, it will be $\rho(r)dr$. So, that will be $\int \rho(r)dr$. So, what happens therefore, is it becomes $\int \rho(r)$ will be now written as $\delta(r)dr$; this δ will be the total number of electrons. The total number of electrons present in this quantity $\int\delta(r)dr$ therefore, equals to c; c is a number which represents the total number of electrons and in case of carbon it will be 6 nitrogen it will be 7 and so on.

So, this allows us to identify the atom as a single atom single point atom and then prove the delta function. So, it has certain special properties that it is equal to the $\int\delta(r)dr = c$ at $r = 0$, but everywhere else surround the surroundings; it is not actually a measurable quantity it equals to 0. Now what happens if there is an atom which is situated not at $r = 0$, but away from $r = 0$.

So, we now see that $F(R)$ can be written as $\int\delta(r - r')$ now the phase factor comes in; how does it come in? It comes in because of the fact now the atom is not the point atom is not at the origin; it is removed by a quantity r'. It is located distance r' from the origin and therefore, we get this expression away from the origin by r' distance. Then we have the phase factor coming in and the delta function is at r' from the origin and then we will get these express c which is still the total number of electrons multiplied by the phase factor which is exp ($2\pi i$ r . R').

So, this therefore, now gives us the expression for the structure factor. So, if we consider a delta function which is at the origin; we get this expression, delta function is a special case of F(R) essentially and therefore, we now define F(R) in the following fashion. So, this happens if you have a point atom; now suppose we have a large number of point atoms which is essentially the crystal. In a crystal we have let us say 100 atoms let us consider all and each and every atom as a point atom if we consider each and every atom as a point atom; they are located at r_1, r_2, r_3 from the origin.

So, we sit at an origin consider r_1, r_2, r_3, r_4 etcetera the positions of the atoms then now corresponding to each one of these points we have to add it up; the total F(R) therefore, will be a summation and this summation will be your all the r_1, r_2, r_i. So, therefore, it represents c(i); so c(i) therefore, is the total count of the electron density. So, if there are let us say $C_{10}N_2O_5H_{13}$; that kind of a molecule and that are there are 4 molecules in the unit cell.

Then c(i) is the total number of electrons of the entire unit cell and therefore, we see that the summation is over the entire unit cell, but then the summation is overall only the atom positions because these are point atoms. And these summation will now give us the total number of electrons inside the crystal. And every one of them now as a phase factor depending upon where they are sitting, if they are sitting at r_1 there is a phase factor, r_2 there is a phase factor, r_3 there is a phase factor and therefore, this now represents the structure factor for a collection of point atoms.

So, what we have done here is we have considered all the atoms to have only all the electrons and everything associated with the atom to be with a point. And this approximation is a very very valid approximation from the point of view of calculating the structure factors. In fact, this is what we are going to use when we determine the structure by what are known as direct methods. So, we will assume that of course, this is an impossible situation atoms cannot be associated with one point; they have their own diameter in which they distribute the nucleus and the electron density around it and so on.

For practical purposes to get the evaluation of the structure factor this therefore, is a good and convenient method. So, we say that there are collection of point atoms, but what is the reality? The reality is the following.

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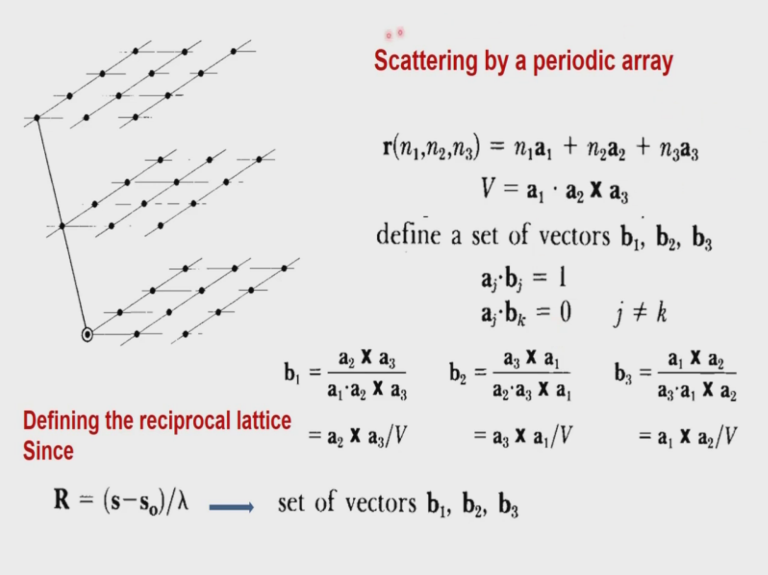

Scattering by a periodic array

$$\mathbf{r}(n_1,n_2,n_3) = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$$

$$V = \mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3$$

define a set of vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$

$$\mathbf{a}_j \cdot \mathbf{b}_j = 1$$
$$\mathbf{a}_j \cdot \mathbf{b}_k = 0 \qquad j \neq k$$

$$\mathbf{b}_1 = \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3} = \mathbf{a}_2 \times \mathbf{a}_3 / V \qquad \mathbf{b}_2 = \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot \mathbf{a}_3 \times \mathbf{a}_1} = \mathbf{a}_3 \times \mathbf{a}_1 / V \qquad \mathbf{b}_3 = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot \mathbf{a}_1 \times \mathbf{a}_2} = \mathbf{a}_1 \times \mathbf{a}_2 / V$$

Defining the reciprocal lattice

Since

$$\mathbf{R} = (\mathbf{s} - \mathbf{s}_o)/\lambda \longrightarrow \text{set of vectors } \mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$$

The reality is that there is a scattering coming from a periodic array. So, when the scattering comes from a periodic array we have a 3 dimensional lattice; we have the *a* axis, we have the *b* axis, we have the *c* axis.

Suppose we now consider the atoms to be associated with lattice points; it is not necessary, but let us say each atom is now associated with the lattice point; then we can generate this diagram. Now if we generate this diagram then we have to be able to calculate what is happening with respect to the scattering.

So, any vector in this unit cell; let us say we start from the origin and let us say I take this lattice point where let us say we have an atom in that lattice point because of the periodicity it repeats itself. So, from this point to that point let us call this vector as r; the little vector r a little vector r is in real space this is the actually the position vector the position vector corresponding to that atom let us say. So, this now is r which is now represented by (n_1, n_2, n_3); 3 integers in the representing the 3 directions the *a* direction the *b* direction and the *c* direction.

So, let us say if it is one unit cell you have the *a, b* and *c* values coming up here. So, these are therefore, the integral values or rational values more appropriate. So, any vector r therefore, can be expressed in terms of these rational numbers are integral values $n_1a_1 + n_2a_2 + n_3a_3$.

So, we have therefore, a lattice a lattice of points instead of point atoms being randomly distributed as we discuss before; the point atoms are now associated with a lattice point. When we do that we get the vector r to be $n_1a_1 + n_2a_2 + n_3a_3$. The volume of the unit cell is given by $a_1 . a_2 \times a_3$; this provides the volume of the unit cell.

At this stage we now define a set of vectors b_1, b_2, b_3 with very special properties; the properties are that if we take a_j and take the dot product with b_j that is equal to 1. And $a_j . b_k = 0$ whenever $j \neq k$ so; that means, when we have $a_1 . b_1$; the value = 1, $a_1 . b_2$; the value goes to 0. Now such set of vectors when we define using this expression these vectors are supposed to be reciprocal of a_1, a_2, a_3.

Now, it becomes; obvious to you why we are doing this? We are doing this in order to get the representation of R which is our scattering vector and we also know it has dimensions of reciprocal length. So, we are now trying to get how to express R given the r in the in a 3 dimensional lattice. So, if when you have a periodic array we consider the r and we now want to define the R. So, when we do this operation we can show that $b_1 = (a_2 \times a_3)/(a_1 . a_2 \times a_3)$; $a_1 . a_2 \times a_3$ by definition is volume.

So, this now becomes $a_2 \times a_3$ divided by the volume similarly b_2 and b_3. So, when we have these 3 vectors b_1 ,b_2 ,b_3 following these vector expressions $(a_2 \times a_3)/V$, $(a_3 \times a_1)/ V$ and $(a_1 \times a_2)/V$; defining the values of b_1 ,b_2 ,b_3; then these set of vectors b_1 ,b_2 ,b_3 will be able to quantify or will be able to represent these are called scattering vector R because it defines now a lattice of vectors b_1 ,b_2 ,b_3 just like this lattice.

Suppose we now set at an origin and now these are b_1 b_2 b_3 we can define the values of b_1 ,b_2 ,b_3. I am not telling a_1 ,a_2 ,a_3 = b_1 ,b_2 ,b_3. The b_1 ,b_2 ,b_3 is inverse of b_1 ,b_2 ,b_3 or inverse of a_1 ,a_2 ,a_3 or the reciprocals of a_1 ,a_2 ,a_3. So, if there are 3 vectors a_1 ,a_2 ,a_3; the reciprocal vectors that is $1/a_1$,$1/a_2$, $1/a_3$ will be b_1 ,b_2 ,b_3.

And therefore, these b_1 ,b_2 ,b_3 in principle should describe our vector R which is (s - s_0)/λ. So, we therefore, define what is known as a reciprocal lattice which is built up of the 3 vectors b_1 ,b_2 ,b_3. So, a_1 ,a_2 ,a_3 are the real space vectors; b_1 ,b_2 ,b_3 are the reciprocal space vectors.

So, what we have done so far and this part of the discussion is to consider the atoms to be point atoms. And then we have consider the collection of point atoms and then we have distributed this collection of point atoms to various lattice points in real space. And then we have defined the quantities which define now the reciprocal space such that b_1,b_2,b_3 are reciprocal vectors of a_1,a_2,a_3. This will allow us to describe with the r which is in direct space and the R which is in the reciprocal space.

So, r and R have dimensions of reciprocal length with respect to each other r is the position vector in real space R in principle is the position vector in the reciprocal space. So, if we have this knowledge we will see what happens when we have a realistic crystal ok?

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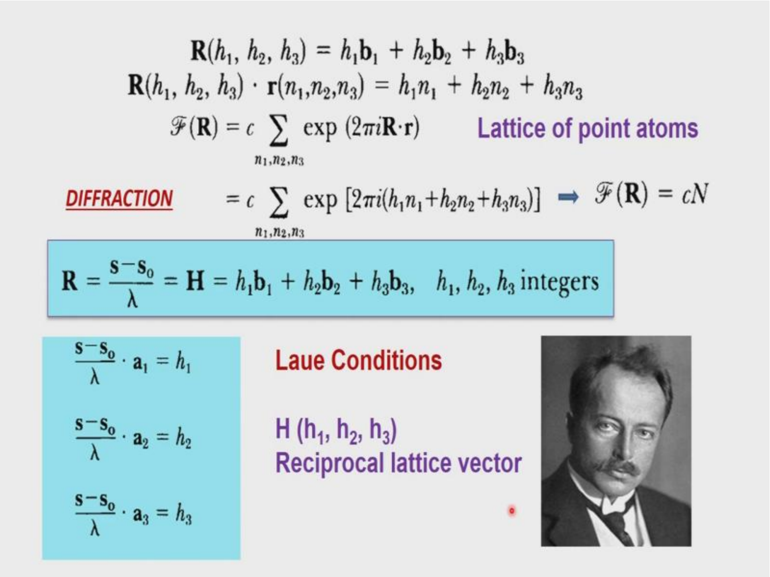

$$\mathbf{R}(h_1, h_2, h_3) = h_1\mathbf{b}_1 + h_2\mathbf{b}_2 + h_3\mathbf{b}_3$$

$$\mathbf{R}(h_1, h_2, h_3) \cdot \mathbf{r}(n_1,n_2,n_3) = h_1n_1 + h_2n_2 + h_3n_3$$

$$\mathscr{F}(\mathbf{R}) = c \sum_{n_1,n_2,n_3} \exp(2\pi i\mathbf{R}\cdot\mathbf{r})$$

Lattice of point atoms

DIFFRACTION

$$= c \sum_{n_1,n_2,n_3} \exp[2\pi i(h_1n_1+h_2n_2+h_3n_3)] \Rightarrow \mathscr{F}(\mathbf{R}) = cN$$

$$\mathbf{R} = \frac{\mathbf{s}-\mathbf{s}_0}{\lambda} = \mathbf{H} = h_1\mathbf{b}_1 + h_2\mathbf{b}_2 + h_3\mathbf{b}_3, \quad h_1, h_2, h_3 \text{ integers}$$

$$\frac{\mathbf{s}-\mathbf{s}_0}{\lambda} \cdot \mathbf{a}_1 = h_1$$

$$\frac{\mathbf{s}-\mathbf{s}_0}{\lambda} \cdot \mathbf{a}_2 = h_2$$

$$\frac{\mathbf{s}-\mathbf{s}_0}{\lambda} \cdot \mathbf{a}_3 = h_3$$

Laue Conditions

H (h_1, h_2, h_3)
Reciprocal lattice vector

Now, let us go further this is what was done by Laue that is why I put his picture here which you already saw in the earlier class because this is his contribution. Now, what is it that is going to happen if we have a crystal, we have a lattice, we have a_1,a_2,a_3 defining the vector r and b_1,b_2,b_3 defining the reciprocal lattice vector. So, just like we describe the r; n_1,,n_2, n_3 as n_1a_2 + n_2a_2 + n_3a_3 where n_1,n_2,n_3 are integers. Now we can describe the vector R in terms of h_1,h_2,h_3; these are again 3 integers which will define $h_1b_1 + h_2b_2 + h_3b_3$.

So, effectively from the real space you have gone on to a reciprocal space where you are able to express vectors in the reciprocal space. Now what we will do? We will do a little small little mathematical operation that is to take the dot product of r . R. Now you might worry why we are doing this r . R dot product we need this r . R dot product because you see here you have in this expression r . R the calculation of the structure factor will be accomplished if we get this quantity r . R ok?

So, we need to have this dot product between the real space vector and the reciprocal lattice vector. What happens when we do this is that r . R will become $h_1n_1+ h_2n_2 + h_3 n_3$ n_1,n_2,n_3 are integers h_1,h_2,h_3 are integers. So, sum of 3 sets of integers will be an integer; so this will be an integral number. So, the structure factor F(R) which can be now expressed see now we will take the total electrons in the unit cell outside; total number of electrons which equals the total count of the number of electrons associated with all the atoms in the structure total count is see.

Then summit over n_1,n_2,n_3 sum over all values of n_1,n_2,n_3; we then write the exp (2π i R . r). So, this exp(2π i R . r), now is the expression which will now allow us to determine the phase. This is the amplitude and this is the phase you notice that the amplitude is now directly proportional to the total number of electrons. So, that why we are in a very comfortable position; so, we now substitute R . r at this expression.

So, when we do this R . r substitution we will get exp(2π i ($h_1n_1 + h_2n_2 + h_3n_3$)) and this now represents every time a point in 3 dimensional space and that 3 dimensional space is the reciprocal space. And therefore, we get c N, c is the total number of electrons N is the total number of reciprocal lattice points and therefore, we get F(R) = c N.

Now, what is happening here? If in terms of light what is happening? So, the incoming radiation is X ray. So, the X rays now come and fall on the crystal; the crystal now acts as a periodic array and because it acts as a periodic array, it generates the vector the every position vector $\bar{r}$ generates the $\bar{R}$ and therefore, the product R . r will be an integer value. So, whenever the product R . r is an integer value you get light coming out whenever the R . r is not an integer value; we will not get a light coming out.

So, what was continues scattering you know we talked about scattering occurring from an object; it scatters in all possible directions now these directions get in sometimes in a very loose term quantized. So, these therefore, now will occur in such a way that these atoms therefore, will now become these sorry, these points will now become organized. And they get organized in such a way that they have to satisfy these expression c $\exp(2\pi i (h_1n_1 + h_2 n_2 + h_3 n_3))$ this now being an integer.

And therefore, only when these integral values are there you will get the light out and whenever the integral values are not there you will not get the light and this process is the so called process of diffraction. And this has been done by some experiments in your college days which you might recollect; you would have done it with light. You would have done the light diffraction experiment and you were given a diffraction grating.

So, this is essentially a glass piece where there were grating marks; they were marked with equal distances, this is essentially likely the discussion we had on the 2 slit experiment. So, as we put more and more slits it is equivalent of putting more and more gratings and therefore, the moment you put gratings; the light which is coming in we will now get into go through the grating. And the diffraction grating will give the specific directions in which light can pass through and therefore, you get a diffraction data.

This is a essentially coming because of the lattice because of the fact that we have a 3 dimensional unit cell which now repeats itself in all 3 directions we get this information. So, it can happen only in crystals or crystalline materials. So, therefore, we get the diffraction and this is what was discovered by Von Laue for which he was given the Nobel Prize.

So, what did he do? How did he explain this? He explained it in this fashion if you take R; R is now $(s - s_0)/\lambda$; we know this is the scattering vector. This is the direction of the scattering vector it its magnitude is $2\sin\theta/\lambda$ we have just calculated that. Now, this now becomes vector h and these vector h will not be all over the place; it is not a continuous function now; it will happen only if this value is satisfied when it is $h_1b_1 + h_2b_2 + h_3b_3$; h_1,h_2,h_3 being integers.

That means, these 3 conditions which are written down here $(s - s_0)/\lambda$ is in fact, you can write it as H. H a_1; this is your unit cell dimension a. So, $H . a_1 = h_1$, $H . a_2 = h_2$, $H . a_3 = h_3$. You can replace h_1,h_2,h_3 by h, k, l which is normally used in many text books which you read and these are the so called Miller indices; $a_{1,}a_{2,}a_3$ you can replace by a,b,c therefore, this is the expression which Laue derived.

So, the $H(h_{1,}\ h_{2,}\ h_3)$ represents what we call as a reciprocal lattice vector; the dimensions of the reciprocal lattice vector is proportional to $2\sin\theta/\lambda$. And therefore, the diffraction will occur only when these Laue conditions are satisfied. So; that means, when you send in the X ray beam on to the crystal only when all these conditions are simultaneously satisfied then only you will get the diffraction; that means, when you have a 3 dimensional crystal the diffraction will occur only in certain given directions and those directions now will generate a point.

And therefore, we get a reciprocal lattice point; how does it generate a point is still a question which we will answer as we go along.