Solid State Physics
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Lecture – 31
Intensity of Bragg Diffraction (Contd.)

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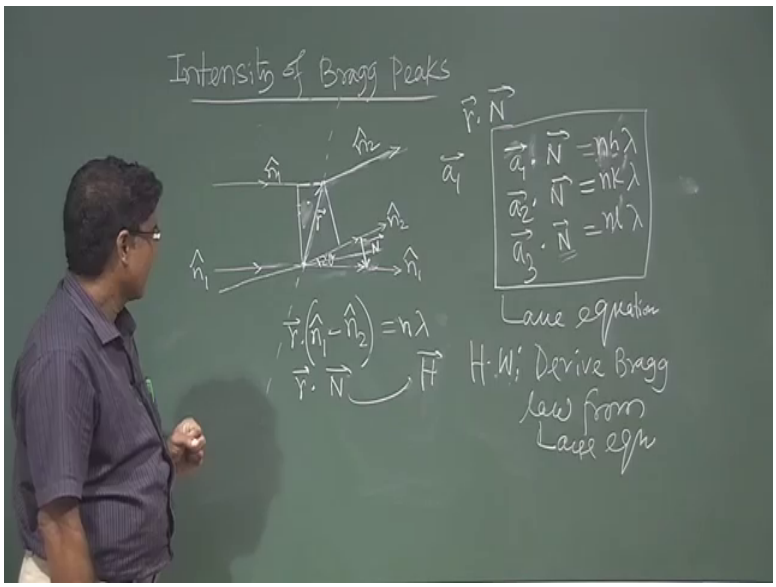

So, we will continue about the intensity of Bragg Peak. In last class I use this picture and here what I was telling that if you have scattering centers X-ray will fall and scattered in all directions scattered in all direction.

So, this on this row if other scatters are there if their distance are say same. So, then if a for a particular direction I will get the scattered equivalent to reflected X-ray and they will interfere and this interfere this effect will see. So, here they are just condition we have put here there is for constructive interference, if it is constructive interference then this condition are satisfied. So, it is equivalent to Bragg condition not equivalent similar to Bragg condition, but this another treatment ways process. So, this Laue treatment and one can get from this from this concept one can get Laue equation.

So, but I do not need this to know to know about the intensity of the Bragg Peak , but what I need I need this concept this scattering from an charge particle from an electron. So, when X-ray scattered from these 2 center scattering center if they are electron if they are electron.

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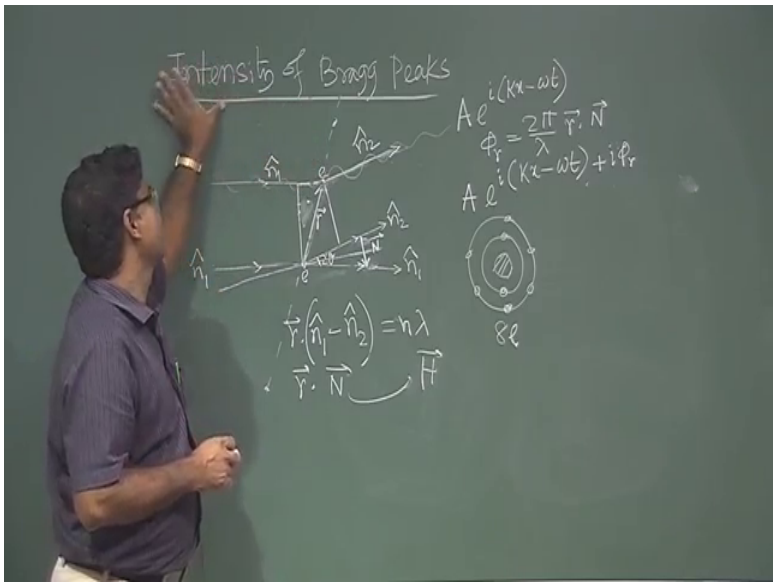

Now, it is so for 1 for 1 it can be for 1 this incident x rays falling with wavelength and reflected 1 or diffracted 1 it is diffracted with the same wavelength, but in different direction.

So, this incident 1 that it is say A is wave equation I can write in which we write some amplitude and e to the power i omega t minus k x or k x minus omega t whatever, k x minus omega t. So, that is the wave equation wave equation like this. So, it represent the say it is incident wave incident wave, now if I consider the another one another one if I consider. So, in both cases incident one is this now that is after reflection whatever this into direction we are taking now this so these 2 will have; these 2 will have some phase difference. So, that because of this path difference so equivalent phase difference is will be say for this scatter at r distance so for this distance; for this distance so there will be path difference this one and this corresponding phase difference one can write 2 pi by lambda 2 pi by lambda to r dot N, that will be that will be path difference.

Now so this your then this your resultant wave is basically resultant wave is basically now after diffraction. So, it will be A e to the power i k x minus omega t and now additional this phase difference will be as i i phi r I phi r. Now this because of periodicity this other will have this same similar will be yes it will have the same phase phase difference between these to this these or it will have the integral multiple right.

So, what did this telling that X-ray is scattered by the electron now if it is scattered by more than electron so resultant effect scattering after scattering resultant intensity or amplitude. So, that will be that will depend on their separation, position or their distribution. So, that is the point if this electron from single electron whatever if another electron is there. So, then interference effect will be there and that interference will depend on this difference or phase difference. So, when X-ray scattered by atom X-ray scattered by atom and atom is having more than one electron different atoms have different number of electron and their distribution are different they are distributing different cell so if it is nucleolus surrounding right.

So, they are distributed in different way now x ray is falling; x ray is falling on it is it cannot be equivalent it is scattered by a single electron, it can be single electron it has say here I have taken 8 electron 8 electron I have taken. So, from one electron whatever the scattering strength, it has 8 electron so for so if that total scattering strength or total amplitude it cannot be right times of e right from single electron whatever the amplitude I am getting, when it is it will scatter from 8 electron. So, it cannot be 8 times of this single.

Because of this there will be phase difference and there will be interference effect and the resultant amplitude or interest will be different. So, that is the point about this because this extra intensity after diffraction from the crystal. So, crystal have will identify that that crystal has a in terms of unit cell. So, now, in unit cell so as I mentioned earlier that it is enough to consider only 1 unit cell, because others are just replacement of reputation of that one. So, that is why in unit cell the atoms or lattice points are distributed right and now in each lattice point or Atom. So, they are electrons are distributed. So, x ray is scattered by electron not by Atom. Now, in Atom so when we will tell this scattered by atom basically it is scattered by the by the all electrons.

So, here that for one electron whatever the scattering strength it cannot be multiple of number of electrons in that this atom it will be different from that. So, that means, this that amplitude square of that amplitude is basically intensity right. So, it will depend on the atom right how many electrons are there, how they are distributed there. So, that is called atomic form factor that is called atomic form factor.

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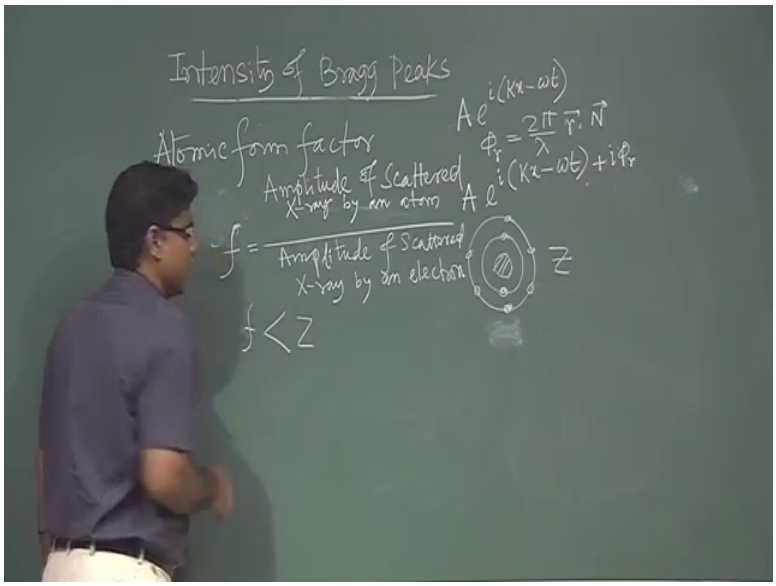

Atomic form factor right f atomic form factor f is defined that Amplitude of Scattered X-ray or o f amplitude of scattered X-ray by an atom divide by amplitude of scattered X-ray or of if by an electron by an electron. So, that is called form factor.

If it is just multiple of this one if so one atom is atomic number whatever. So, that many number of electrons are their Z so this atomic number Z. So, this is not simple just it is Z right Z times of this amplitude. So, it is different why it is different that will discuss and that one has to consider. So, it will be, these f these f will be always; these f will be always less than Z except in (Refer Time: 13:23) direction if they are scattered in (Refer Time: 13:25) direction. Then it can be Z for any other angle scattered in other angle it is always less than Z and this is it is less than Z because of this interference effect and that interference effect is coming from for because of the different position of electrons in atom.

So, that is the this that factor will has to be multiplied with the so this factor has to be multiplied with the amplitude of n electron and from each electron it is just scattered and thereafter there is no interference. So, whatever the total so that is basically Z time of this one and with that this factor has to be multiplied. So, then you will get the basically the what is called this actual amplitude of the scattered x ray form an atom.

So, this is one factor is controlling the intensity of Bragg Peaks; obviously, because so here is that it depends on the basis which type of basis right, which type of basis how many number of electrons are there. So, it will depend on the type of atom, this is clear.

Second is the now this atoms how they are distributed in unit cell. So, that is second important second part and this very important so; that means, it will depends on the structure of the crystal right because distribution of the atoms in crystal it say it will follow the lattice point.

Now, the each basis is attached with the lattice point right. So, which type of basis that will be controlled by this atomic form factor and then second it will depend on the type of the it will depend of the type of the lattice Bravais lattice right and so as I earlier I discussed that for body centered orthorhombic and base centered orthorhombic. So, this distribution number of lattice point are same as distribution are different so the distributions are important why they are important how it is contributing controlling the intensity, that would like to discuss. So, that is also it will depend the structure of the material structure of the lattice. So, that is why it is called structure factor.

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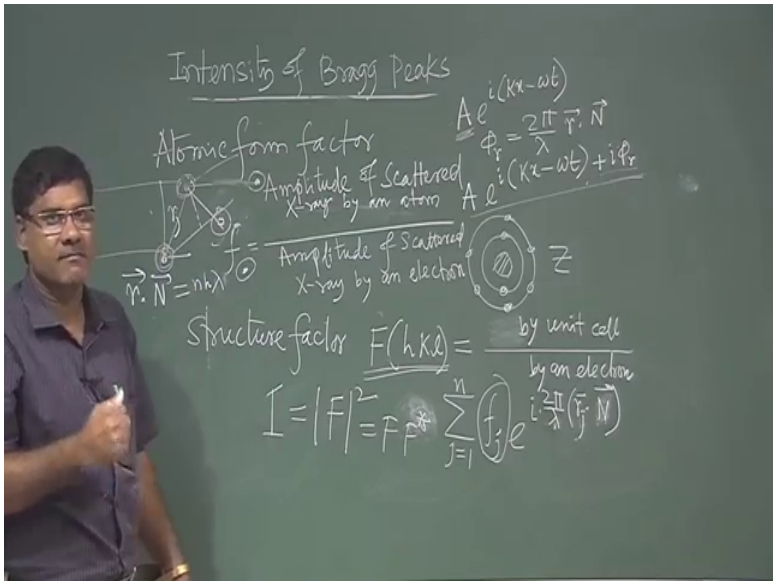

So, one can find the expression basically this f equal to one can calculate, but I will not do so just here mainly I am giving you the concept just qualitative concept. So, quantity that I will not derive that is not tough it is very easy. So, if you wish we can just try to try yourself as we are given reference. So, from there you can try so, but probably if you do

not try also this is fine, but this concept will be if for we for this undergraduate course. So, this structure factor so it depends on the structure. So, that is written as F and for a particular it is for a particular plane if I consider.

So, for different plane intensity will be different that is obvious for a same plane what are the factors what are how it is intensity is called. So, h k l plane right one a one should take a particular plane and then see what are the factors control the defect the structure factor depends on what are the factors right. So, this h k l, this now here also this same that is scattering center now we think this the atom X-ray are falling on atom diffracted right. So, your this of difference, they will interact their of difference that whatever we got it is not there.

So, what we got r dot N right there is the path difference and that I wrote this one can write this n h say n h n h lambda right or just n h just lambda whatever. So, here this is atom now so for each atom what is the scatter scattering strength that I know from factor for each I know right, now again they will interfere and depending on this on this path difference will get the resultant amplitude.

So, this structure factor so it is similar to this say definition also this similar amplitude of scattered wave by an, by an unit cell, by an unit cell. So, here by an unit cell right amplitude of scattered X-ray by an unit cell by unit cell divide by amplitude of scattered X-ray by an electron. So, what about the one electron with a compare to that so from one unit cell has a whole unit cell what are the scattered amplitude so you by an electron. So, by an electron now from that is because for other cases some interference effect will be there and amplitude will be modified there are the amplitude will be modified that one has to find out.

It is obvious that this again because of this your phase difference will be this will be this now if here we have retrained r. So, now, this similar things for atom, but amplitude is modified basically this is the amplitude will be modified by factor f right. So, here one can right, you have many atoms you have many atoms. So, if you take this 2 not between this 2 what will happen? So, this amplitude it is similar you know this now this you can take this as for this one atom and then from other atom separated by r, what is happening so this same thing. So, same thing you can use so it will be like this resultant one will be like this.

So, your scattering amplitude one will get, from each atom if it is F j some say in unit cell n number of atoms are there at different position. So, one can so one has to take summation one has to take summation. So, f j for each f j of each from jth so j equal to j equal to 1 to n number, whatever the number you have in unit cell. Now it is from one one now it is modified right modified with this amplitude e to the power it is modified with this amplitude with this phase factors so e to the power i phi r right.

So, e to the power i phi r, this i phi r so 2 pi by lambda i 2 pi by lambda, 2 pi by lambda r dot l. Now if it is in the unit cell so this difference. So, here as I mentioned that. So, this n can be written in terms of reciprocal vector. So, one can write reciprocal vector, but here I cannot write just reciprocal vector keeping this factor so one as to use appropriate. So, it also depend on this H when you define, whether you are taking 2 pi there or not if you do not take 2 pi. So, then you have to consider 2 pi here if you one take 2 pi there in b 1 b 2 b 3 whatever we have define. So, then we do not need this 2 pi, this things are there so better you just give it like N.

So, now, this r it is for a for a particular lattice this r will be, this will depend on the for it will depend on the distribution of this distribution of this atoms in the crystal, now if same types of atoms so this factor f j this will be same for all. If different types of atoms are there, so for different atom f will be different, but for same type of atom. So, here I am varying this j here so this the position with respect to one has to take origin with respect to with respect to this what all the distance asked.

Now, you have different position so and for first atom, second atom, third atom jth atom. So, it is one has to write r j. So, one has to write r j right. So, r j will vary so for each atom. So, if it is f 1 so for that say it is position is r 1 f 2 r 2 f 3 r 3 etcetera. If this atoms are same atoms this is are same then f 1 will be equal to f 2 will be equal to f 3 and f of course, has come from here one has to get this f. So, ultimately you will get this so this structure factor and this structure factor depends on the distribution of this from this factor if here you can see distribution of the atoms in lattice in crystal in itself as well as this factor is telling that it depends on the type of atom and their this value this will be different.

So, this one contains about the information it depends on the type of atoms as well as it depends on the distribution of atoms in itself. So, this intensity that is a intensity of X-ray it is basically just it is the amplitude right this is the amplitude of scattered 1.

So, 1 has to take F F star then it will 5 intensity and; obviously, intensity will depend on the type of atoms which is in this f and distribution of atoms which is in this path. So, now, we know this if so one can just monitor experimental monitor is if atoms is shifting from it is position original position it will be shifted. So, intensity changes intensity changes. So, thus from intensity one can study stress right due to stress (Refer Time: 29:29) it is either contacted or expanded.

So, intensity will vary it is there will be shifting in this if lattice parameter changes shifting will be the angle also.

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So, different type of different type of information one can get from these intensity of Bragg Peak one information is type of atoms type of basis second information is how the basis are distributed in the unit cell.

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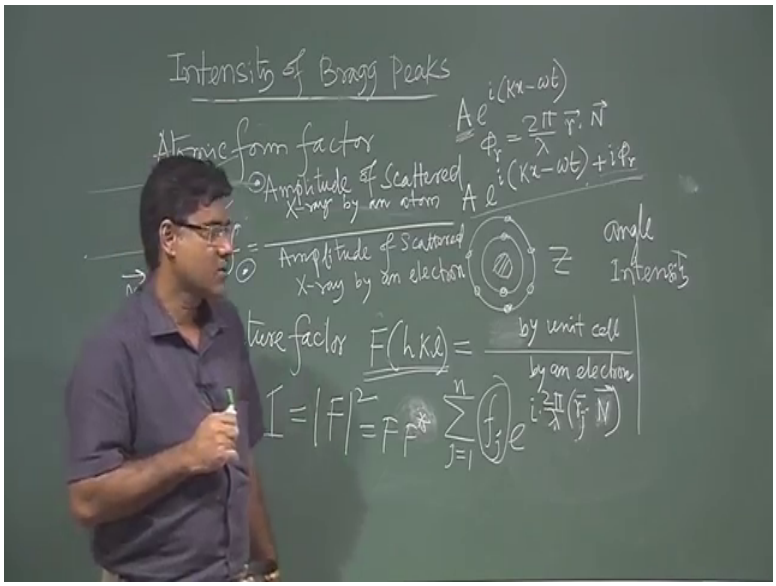

So, from Bragg Peak angle as well as intensity; angle as well as intensity angle as well as intensity both we need both we need to know the completes detailed structure of the crystal because not only lattice parameter we would like to know what are the atoms are

there and how the atoms are distributed whether they are sitting at original position or whether they are shifted. So, all kinds of information one can get as I told this vast subject and this just I try to give you this preliminary concept, but in details it is out of out of this course basically. So, one has to wait for the next for higher class, but these are good enough just if you will understand whatever I try to tell you for your course. So, I will stop here.

Thank you for your attention