Solid State Physics
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Lecture – 30
Intensity of Bragg Diffraction

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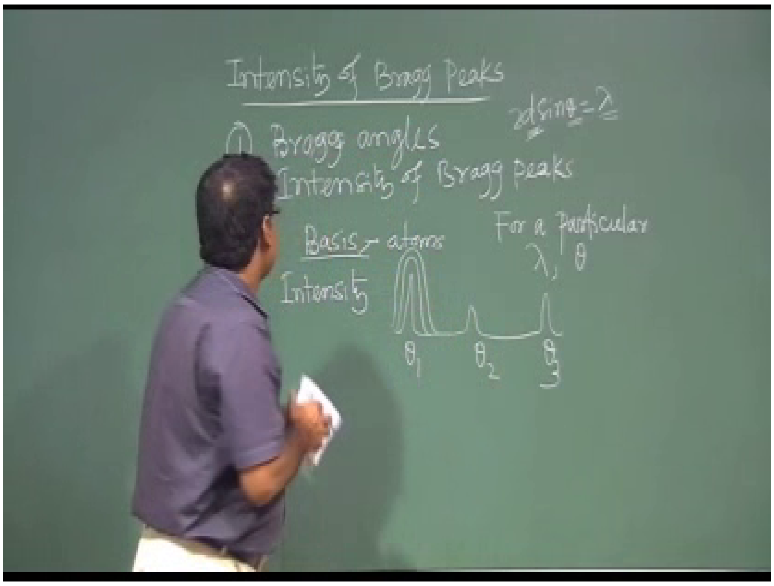

Now, we are discussing about intensity of Bragg diffraction or Bragg peaks. So, it has importance as I mentioned that when x-ray diffracted from the crystal, so one factor is the Bragg angle and another factor is the intensity of the Bragg peaks. So, I have shown you the sodium chloride, this x-ray pattern, where there are few diffraction peaks having different intensity. So, these peaks are from different planes Bragg planes, crystal planes and so different planes are different density aerial density of lattice points. So, one may think that intensity because of that intensity are different, but it is not only the reason. So, that is one factor, but another factor is the basis means atoms a group of atoms how they are arranged in Bravais lattice.

So, for a particular lambda and theta, so we will get so that means, we have fixed a particular angle and for a particular x-ray, so we will get intensity different intensity at different angle. So, here one Bragg peak, here one Bragg peak like this we will get. So, what else left to the sin theta equal to n say lambda equal to say lambda. So, 2 d sin theta equal to lambda or n lambda. So, for a particular lambda and particular theta, so d, so d is left. So, for a particular d, so for a particular theta means d is defined, because this theta is decided by the lattice parameter of lattice spacing. So, this is also for a particular plane theta 1.

Now, as I mentioned that this for a particular lambda and theta that means for a particular plane now intensity varies; it is increase for some cases, decrease for other cases. Sometimes these peaks are missing, so missing means intensity is 0. So, why so, so that as I mentioned that depends on basis or depends on the distribution of atoms or even lattice points in the crystal.

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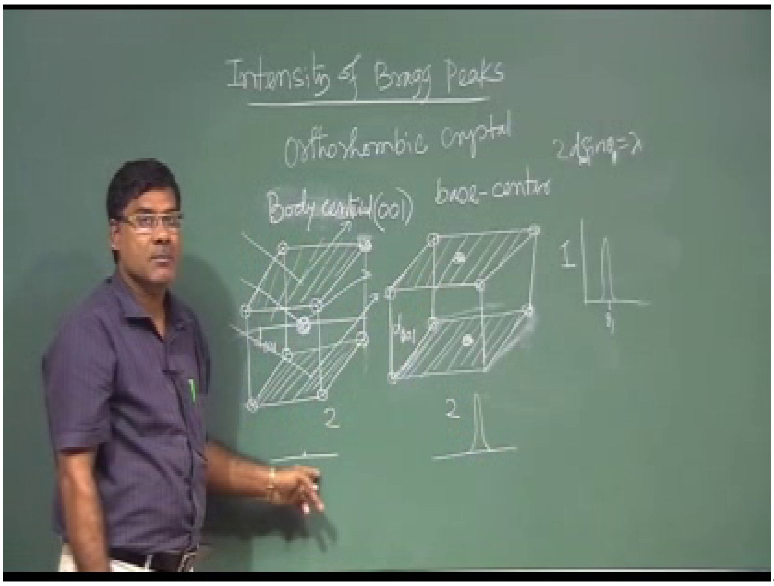

So, I will give you one example. If you take that is orthorhombic crystal, so it has 4 Bravais lattice. One is simple cubic, another is presented not simple cubic simple orthorhombic, body centered orthorhombic, face centered orthorhombic and base centered orthorhombic. See, if I consider the simple of orthorhombic and base centered orthorhombic, so basically so four atoms or four lattice point in a not 4, 8, 8 corner, 8 lattice point or atoms in it 8 corner, so that is simple orthorhombic. And for base centered orthorhombic for base centered orthorhombic, so eight are there at eight corners, and one additional new base.

Now, if you considered the 001 plane 001 plane. So, this is the 001 plane right if the z-axis. So, this plane is 00 plane right and here also 00 plane right. So, separation this also 001 plane. So, separation between these two plane is d 001, and here separation is also same d 001. So, reflection or diffraction from these 001 plane, so we will get the peak at 00 for this 001 plane whatever the theta one can calculate 2 d sin theta equal to lambda, this is 001 right. So, at the theta we will get diffraction peak.

Now, what about the intensity of that that peak. So, these are basically in these two cases its lattice spacing are same, and we suppose to get the peak at a at a particular angle one can calculate and then what about the intensity at that. Say if I tell theta also, theta 1 say at theta 1, so this is the angle at theta 1, so we will get this is the intensity. So, we will get peak. Now, in both cases, so we suppose to get this Bragg peak at same angle for both cases for simple as well as space centered, but for this case, no I am doing mistake. So, actually I have to not simple one, I want to take not simple one, I want to take body centered that means, in body there is a I think here I can at a the body is there is atom or this lattice point and yes.

So, here this what do we want to mention that this in both cases the number of lattice point per unit cell are same; it is 2 per unit cell; number of lattice point per unit cell here is 2 and here also 2. So, what about the intensity, angle we will get at same angle because this spacing are same, this spacing are same, this is the lattice spacing. So, at this angle, what happens about the intensity, all though both are having these two atoms or two lattice point. See interestingly we will see that is in one case, you will get Bragg peak with the high intensity and other case for this body centered the intensity zero there. So, for body centered, here intensity 0 means practically we will not get no peak; and in this case, you will get a peak with the high intensity.

What is the reason, reason is that from this plane here also you will get one plane, you will get one plane. From this plane, there will be reflection or diffraction; and from this plane, there is no diffraction. So, they will interfere and give the Bragg peak. Now, here since this is the periodicity this is the periodicity, so x a reflecting x a, this one and this one, they are in phase right, so that was on that condition we have derived this one. Now, this is exactly this in middle this plane. Now, the x-ray diffracted from this plane or this reflected one, so it will be it is if they these two are Bragg differences lambda or phase the phase difference is to pi by. So, this will be exactly out of phase; its Bragg difference will be half or phase difference will be half. So, they will cancel each other.

Now, this and this next plane, so there are many numbers of planes. So, they will be cancel with each other, they will be cancel with each other. So, we will not get any peak at this angle where you supposed to get. So, all the time it is not 0, this case it is 0, but on the time their intensity are not zero. So, intensity varies, so it does not depend, intensity does not depend on this of course, not on these this lattice spacing; it depends on plane, but for same plane it depends on plane because it has different aerial density, so that is fine. But for a same plane intensity also varies because of the distribution of because of the distribution of lattice points or atoms in itself. So, here and here the difference is the distribution of lattice points. So, these in terms of basis I was talking that if atoms are exactly sitting on the lattice point or a group of atoms is sitting around these. So, then two factors, so one is type of atoms, and another factor is distribution of atoms.

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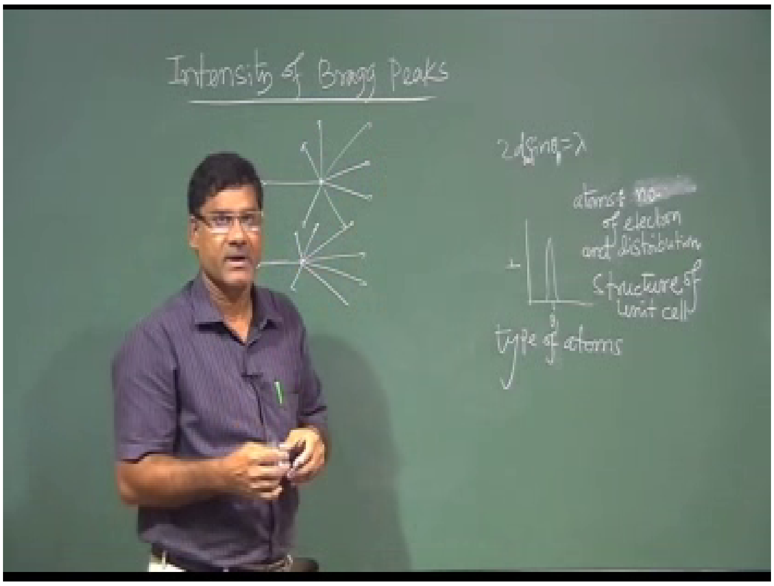

So, it will depend on the atom in the atoms what is there, atoms to atom, this number of electrons are different. So, intensity will depend on basically the distribution of electrons in that atom. So, this is one factor - distribution of electron or I should say yeah number of electrons and distribution in the atoms. So, different type of basis means here their atoms are different, so number of electrons and distribution of electrons in that atom are in different atoms are different. So, intensity will vary because of this.

Second is those atoms how they are distributed in these unit itself. So, basically the structure of unit cell is another factor, structure of unit cell structure of unit cell that is the another factor to decide the intensity of the drag peak. So, why they are important? So, to understand that one, so we have to slightly discuss from the route it is how x-ray are defected from materials. So, materials having particular structure and their electrons are distributed in atoms, and these atoms are sitting in the unit cell or in the lattice or in the materials. So, when x-ray falls on these material, x-ray falls on this material actually interaction of x-ray with the electrons so that means, so if I tell these then x-ray is scattered by the electrons, so in general if I talk about the scattering center it can be electron it can be atom it can be charge density whatever.

So, now x-ray is falling on it and then so these electron will oscillate with the same frequency of this x-ray, and then charge it is a oscillating means accelerating, de-accelerating that is happening and because of that it will emit radiation of the same frequency of length we have, but in all directions, it will emit in all directions. So, this x-ray is scattered in all directions by a scattering center it. And if I consider another scattering center here, so this x-ray is falling on it and again this things this same way it will scatter in all directions. So, now, this scattered x-ray, now they will interfere. So, if I look at a particular angle, the interference effect, so then what we do?

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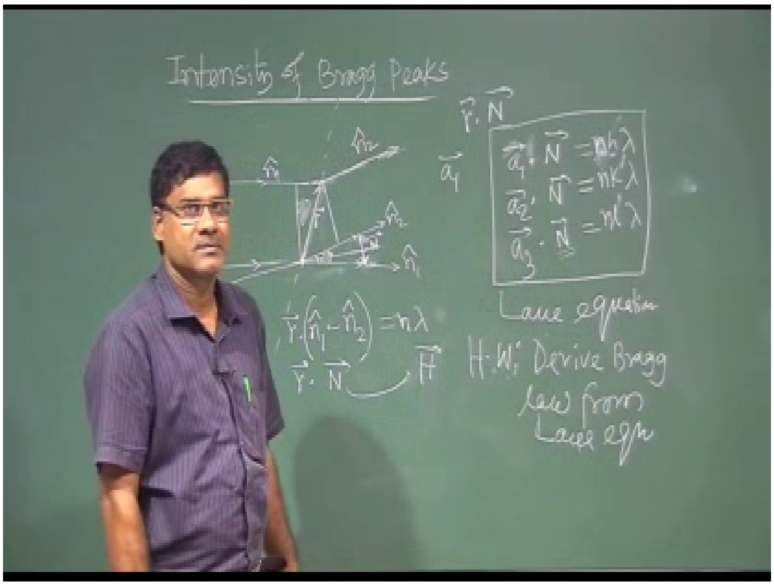

Just take, so this just at this angle. So, it is say like see if we take this from each, so at one direction, so these two will be parallel scattered at a particular direction, it will take them and if we see the interference between these two then we will get the as whether we will see constructive interference or destructive interference. So, if we if we expect the constructive interference then we will set the condition for that. So, they have to be in phase. So, in this case, if this distance between these two scatterer, if it is r, if it is the incident direction unit vector in n 1 and this is the n 2.

So, now they will interfere and I will get the constructive interference setting the condition. Now, what will be the condition? So, for difference has to be integral multiple of lambda, so to calculate first difference what we can do, just you have to yeah, so these two are parallel. So, this side path are same, this side path are same, this is not right one, second one I think I should draw this way between this to this side I think this is ok yeah. So, path difference between these two, this is a here this extra path and here is extra path. So, in these two, in these two ways, so path difference will be say this minus this or this minus this, so that will be the net path difference.

So, if it is the unit vectors in this direction, it is a vector. So, if it r, so if you take the r dot n 1, so you will get this one projection of these two on this direction. So, if we seen it random as we discuss about this earlier. So, this minus r dot n 2 r dot n 2, so that will be the path difference and it has to be integral multiple of lambda. So, this into some integral, so this I can so some integral multiple, so I think I can put n I can put n yeah. So, this I can write r dot capital N say, capital N is n 1 minus n 2. So, what is the n vectors what is that N capital N, so that will be. So, this is the n 2 direction and this is the n 1 direction, n 1 direction n 2 direction.

So, you know this when it is scattered or this has if you construct the diffracted and interfere at constitutively. So, this angle between this incident and reflected one or diffracted one is two theta right say if it is two theta. So, what do you what will be the n 1 n 2. So, this will be, so this is both are unit vectors, so take unit value. So, let me so this is the say unit value magnitude has to be 1, but their direction are different. So, this will be it is in this direction or other direction whatever just depending on n 1 minus n 2 or a n 2 minus n 1. So, this will be N right because n 1 plus N equal to n 2, n 1 plus N, so direction will be opposite basically. This direction will be this means n 2 plus N will be equal to n 1 as we have written say if it is n 2 minus n 1 then direction will be other direction.

So, this is incident and this is reflected. So, from which plane, so this plane must be passing through right. So, this will be the reflecting plane, these will be the reflecting plane. So, crystal plane basically from there the x-ray is falling and it is reflected here. So, now we can see that this N capital N is nothing but the it is the so these crystal plane this one, so this one crystal plane is the basically perpendicular bisector of this one. So, that we have seen earlier, this crystal plane showing all sphere you have seen that crystal plane and that is we attach this origin of the of the reciprocal lattice and it is connected with the another point on the sphere or on the circle. So that we told that is the normal bisector of this, this is the normal or perpendicular bisector of this crystal plane. So, this is, but N is the significant of N is nothing but it is the it is the reciprocal vector h, it is nothing but the reciprocal vector. So, direction wise it is reciprocal vector magnitude wise, it can be different.

So, reciprocal vectors h direction wise same magnitude wise it may be different because here it is in vector. So, one has to multiply with appropriate factor right 2 pi or lambda. So, this is very important one and these gives this is this is the path differencing and this will give the phase difference between this scattered x-ray phase difference how to write phase. So, I will discuss this one. So, let me just so this r dot N. Now, if I think about the crystal, these are the periodic in crystal if I think this is the scattering center means this lattice point or atoms are same sitting there. So, on this array all this array whatever the lattice points are there. So, all will be all are will be in phase. So, along the x-axis along the x-axis not x-axis along the a 1, along the a 2, along a 3 axis if I consider, so this is giving along a along a row right along a row.

So, if I consider along a 1 axis, so what will be r distance between these two; if it is along the a axis distance between these two will be a 1; and direction will be i right dot or just I can write a 1, so it will be a 1 N. There has to be integral multiple of lambda right to get the constructive interference. So, here n, I am putting another constant h, n h I am writing. Why I am writing I will tell you then a 2 dot N, so these two together is a constant yes it will give integral value. So, I can write. So, or I can write just like h dash a dash and a 3 l dash right that I can write, and this I am writing because this is valid along a row.

Now, I have taken this one along a row. So, in which direction a 1 direction, so it will work a 2 direction individually it will work a 3 direction it will work. Now, this for a three dimension, I will get constructive diffraction or Bragg peak when these three together will satisfy. If it is two dimensions, so these tool has to satisfy; if it is one dimension, this only one can will satisfy I will get when three dimension, these three condition has to be satisfied. So, this is just something similar to the Bragg condition right this is the condition for the diffraction. So, this is called basically lave treatment I did not discussed earlier. So, these three equation for lave equation, these are lave equation.

And now it is easy to understand for you, when I will tell about the h, k, l, now this seems this one you see N as a related with the h as a related with the h - reciprocal vector. So, this h this coordinate be the h, k, l. So, here I have whatever h, k, l here I have written h dash k dash l dash. And now in reciprocal let us I mention that this common factor in miller indices we remove common factor, but in reciprocal let us common factor is important. So, that is why in h dash I can write with factor n h, n k right n, h, k, l is basically miller indices. So, this is the lave equation. And since we know now the reciprocal lattice. So, this N as a as I mentioned that one can replace with the reciprocal vector h, but as I mentioned it is the different between unit. So, h is magnitude will be different, but direction wise they are same. So, this homework for you just show that Bragg law can be derived from this is very easy, just you try to do itself. So, derive Bragg law from lave equation. So, I will stop here I will continue in next class.

Thank you.