Solid State Physics
Prof. Amal Kumar Das
Department of Physics
Indian Institute of Technology, Kharagpur

Lecture - 24
X-ray Diffraction from Crystal (Contd.)

So, we are discussing about the powder method right. And I mentioned that using photography, plate or X-ray plate basically X-ray plate. So, we get this pattern diffraction pattern on the film. So, that I have shown you, right.

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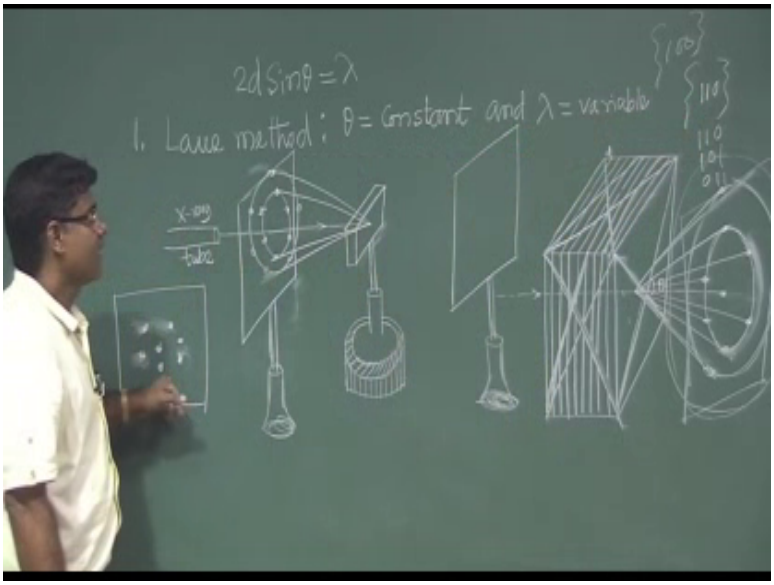

If this is the film, so this way I will continue. So, one place, we will get this almost straight line. Say any way. So, from here as I discuss that one can find out theta and from that theta. So, sin theta d lambda is known one can find out d right.

So, this nowadays in laboratory we are not using this film, but we are using another geometry. As I told this so what we are getting. So, we are getting as from this method, we have seen that we will get concentric cones. And this on surface of the cone basically all lines you can say continuously if you draw lines. So, all are because this whole surface are diffracted rays, but so is it has difference, you know this lave method this in lave method this whatever cone formed it was also form cone concentric cones, but they are on the surface this not all and not the diffracted rays. So, only few are on it will be

there will be on the cone surface, but there are few, but here it is not few. It is the whole on a whole surface if you draw any lines.

So, that will be different way. So, basically you will get in in laves in case of lave this. So this on cone on cone if you just cut it that cone. Then basically there you see this some spot. So but in powder method, we are not seeing spot it is a continuous. It is a continuous if you will get each point and that diffracted intensity and each point. So, it is basically then it is circle. Now here in this case it is circle not spot on a circle. So, that is the difference. So, it is a depends on the geometry. How angles are varying etcetera. So, you will get concentric cones means concentric circle right.

Now, if I take detecting system that, with respect to sample. So, you have you have you have sample here. So, let me draw this a. So, here say we have sample. So, this is the initial direction of the X-ray. Now if you if it is at the taking the center at the position of sample, if you if you have arrangement to rotate a detector to rotate a detector to rotate a detector. So, and this say point detector it is a point detector. So, initially this angle will be taken as a 0 right. This angle will be taken as a 0 incident direction. Now this detector is moving right.

So, what I will see. So, detector started moving. So, angle is 0. Now it is moving. So, angle this so basically I will see, when detector here it will not see any intensity, but when here it will see intensity. So, I will get; so intensity 0 or very some background intensity. So, I will get intensity. So, this called peak Bragg, peak generally we call. So, at which angle will see basically, this is the cone I told this incident and this are diffracted. So, angle is 2 theta angle is 2 theta basically this angle is 2 theta right. So, basically detector also is moving when 2 theta. So, that then I will get (Refer Time: 07:08). So, that is why here generally if we see in all cases we plot not theta it is 2 theta when detector is moving it is 2 theta.

So, again next I will not get any intensity I will get another right another right. So, this is for this point right. So, then moving low intensity here I will get intensity; so this way if we continue. Now, I know the angle directly, I know the angle of this peak because detector is moving with known angle because I have arrangement there is a scale; so how much starting from 0, how much it is moving that. So, I will get peaks. So, these are Bragg peaks and from this measurement directly I will know the angle directly I will

know the angle. I can find out angle and from there 2 d sin theta equal to n lambda 2 d sin theta equal to n lambda. So, n take first order then.

So, this for this say this is theta 1 can find out theta 1 theta 2 theta 3 right; so half of it. So, here this theta will be half of it, because this 2 theta will be half of it. So, this is say d 1 for d 1 for d 2 for d 3. So, angle is theta 1 by 2 angle is theta 2 by 2 angle is theta 3 by 2 right. So, lambda is constant for all the cases. So, I can find out basically and d again, if it is cubic d again, what is this d, d how it is related with the cubic lattice. So, I think this is a by I can not a by a h square h square plus k square plus l square right and this to the power half right.

So, d I can replace with this right. Now here again unknown h k l is unknown right. And for this for different plane it will be it will have different value, but one can notice that one can find out take this h square plus k square plus l square as a 1 2 3 4 etcetera right, because you see based to this value 0 0 1 0 1 0 0 plane. So, what is that this value? It is it will give 1 h square plus k square plus l square, it will be one then for all others 1 0 1 etcetera. So, next is say 1 1 0 what will be the value one square plus 1 square 2 right. So, it will be 2. So, this way you can show that, this h k l square.

So, all sorts of planes, if we consider it will give h square plus k square plus l square it will give value; so 1 2 3 4 5. So, from here what we do a will be considered right a has to be constant, right. So basically here, if I put this relation in place of d; so what I am getting 2 a then divided by h square h square plus k square plus l square plus l square right, to the power half right then sin theta sin theta equal to lambda right. So here we see a is constant for this lattice lambda is constant for this experiment right. So, sin theta. So, for this sin theta, I will get from this experiment right. So, I will put. So, for here I have taken 3 planes 3 peaks; so for 3 peaks.

So, from here basically, if I find out that basically theta is varying and theta is varying for different peaks means for different planes and h k l also will vary for different plane right, but they have they will if you see here I will just interesting themes is that, if we take lambda by 2 a equal to lambda by 2 a will be equal to will be equal to sin theta, by h square plus k square plus l square right. So, now, this is constant. Whatever sample I have taken this for this a is constant right. If that is not depend on this peaks plane are

different, but lattice constant are same; so for this experimental lambda also constant. So, this part is constant.

So, here I will consider one peak, I will find out this sin theta 1 by 2 value sin theta 1 by 2 value right. And then what I will do? I will divided by 1. What I mean sin theta 1 by 2, because this is the angle for this. So I do not know this, so it will have some value and I do not know this one right, but I know this h square plus k square plus l square it can take value only 1 2 3 4. So, I will divide I will divide by 1. Then I will get some value. Then I will divide sin theta 1 by 2, it is not 2 square root of 2. Then I will some value. So, this way I will get some value.

So, this way I will get different value. Again I will take another peak, theta 2 by 2 I will put theta 2 by 2 right and I will choose this is 1 2 3. And find out the value for this peak also I will find out the value. Now as I told this has to be constant. So, from this chart data you will find this is whatever this value for other set I am getting for. So, same value I am, I will get from this 3 sets. And then from there I will see for which h k l value. This I am getting this same value right. So, I will get h k l value. Immediately I can I did not say this just arbitrarily I am writing.

So, when h square, k square, l square, this is 1 and in this case this is 2, and this other cases it is 3. For this value I am getting same value. So, then I will know the indices. So, I will use that constant. That constant will be equal to lambda by 2 a, I know lambda I will find out a. So, in this method I can find out lattice constant for this crystal. And also I can index this Bragg peak, whether it is from which plane these are. So, this is the method. So, here just I will quickly show you one experiment. This way just X-ray data is taken x, ray data is taken on salt sodium chloride salt right. So, I showed you this it is in powder form.

Now, this using the detector we scanned as a function of theta varying the theta. So, then that detector noted down the noted down the intensity as a function of angle. So, that is the experimental result and using the copper k alpha, you see using the copper k alpha. So, lambda is fixed. So, that is basically, what is lambda; 1.54 angstrom right. So, we are getting these different peaks. So, here just we have identified this. So this generally software is identify, but we do not need we can identify as I mentioned this one. And this

value of lattice constant is known. It is reported that 5.64. So, let us let us that way if I calculate, I have calculated.

So, I have calculated whatever I told just I have taken this 2 plane. I have taken this 2 plane this and this. So I have taken this taking these indices. So, just here you see this. For these indices only it will show this constant value for both this constant value you know. Now, lambda by 2 a this this constant value it will take. So, this in it this indices are not given if this indices are not given. So, as I mentioned that, then you have to take all sorts of combination; so all sorts of value of h k l right. Means h square plus k square plus l square starting from 1 2 3; then you have to make chart. For each peak you have to make chart and you have to find out that in all cases, for all peaks which value are common. So, that value will pick up.

So, for that value which h k l value we have used. So, that will be the indices of that of that peak. So, here just I have calculated. So, I got this value 5.5 say 8. So, it is post the reported here just roughly I have taken this 32 degree, but accurately it will take accurately. So, I have just not chosen decimal point. So, it is 32 I have taken this other way in this 46, but it is not a exactly 46, I 46 point something or 45 point something. So, if you take exactly this angle. So, this roughly I have calculated find out this it is 5.58 and reported value 5.6. So, 5.58 and 5.6 is very close, but this discernments is because of that is roughly I have taken the angle.

So, this is the very nice experiment on our known sample sodium chloride salt and salt just taken in a tube and put in X-ray. So, you will get this type of X-ray spectra. So, one can analyze and one can get a lattice parameter of the crystal sodium crystal our salt whatever we are getting. So, another geometry is there. So, just let me mention quickly. That is very nowadays it is used very useful. So, that one is it is similar to the powder crystal; so instead of powder crystal. So, this one thing you will admit that this a very convenient method, powder method and using that detector is very convenient to find out the lattice parameter or also the 2 index the planes right.

So now, if takes single crystal and you do not want to destroy it means you do not want to make it powder. So, on their single crystal itself you want to do experiment. So that is that also can be done using this geometry by except this instead of powder, what will take that single crystal sample. So, then we will rotate. So, this call theta 2 theta just I

think I should. So, basically it is called it is called theta, 2 theta scanned. So, X-ray diffractometer. See it is geometry is similar to the powder method. So, but here we tell generally theta 2 theta scan.

So, basically what happened this you have sample. So, instead of powder we have sample. So, X-ray is falling on it, X-ray is falling on it X-ray is falling on it monochromatic X-ray is falling on it. Now this angle is theta varying this angle is theta it is reflecting theta. So, now, there is a arrangement to rotate to just change this angle theta. So, grazing it is a angle you can change; so using goniometer basically and simultaneously with respect to this same axis. So, we use the detector and the detector also rotate with angle 2 theta. So, these 2 rotate simultaneously.

So, starting from the 0 angle say X-ray is in this way. Now starting from the 0 0 angle, now it is, now we are changing the angle. We are changing the angle by theta. Then if when we reflection is there. So, that will reflected one will change with respect to the with respect to the incident one with respect to the incident one initially 0 angle. So, now, if I change this that crystal by angle theta; so reflected one will change by angle 2 theta right. So, that is the middle principle reflection principle right. So 2 ways you can change the angle incident angle either you can change this X-ray itself right. This reflection wall will follow the same angle, but now X-ray is fixed right now. So, X-ray direction is this.

So, now if you change this crystal angle rotate the crystal. So, by 5; so your whatever the incident earlier incident on there. So, instead of one and corresponding the reflected one was there. Now for changing this middle by angle 5; so this reflected one will change by 2 5 from the earlier reflected one. So basically you will get for any change of theta here if anything happen. So, that will happen at angle 2 theta. So, simultaneously starting from 0, that sample will rotate by theta and detector will be rotate by 2 theta. So, that way it is scanned so that way it is scanned and basically if you if you plot with respect to detector angle. So, that is 2 theta. So, then you will get again it is a different Bragg peak.

So, that is a for single crystal in a without making powder one can do experiment and get this similar as in powder method whatever the in powder method angle already is in all direction, but here we are changing the direction instead and getting the particular position angle of this diffracted rays or Bragg peaks. And then similar way you can analyze and find out the crystal lattice parameter. So, I think that is what I wanted to

mention. So I think this is the all about this different method of crystal diffraction, X-ray diffraction from the crystal. And we can find out the symmetry we can find out the just Bravais lattice of the crystal we can find out the lattice parameter.

So, one thing if you notice that, if you see the lave spot. So, each lave spot is representing a plane; so in crystal whatever the plane. Now after diffraction what you are getting we are getting some spot and each spot is a plane. Now all this spot we are we are taking on a photographic plate X-ray plate is say flat plate. So, on flat plate what you will see you will see many spots right and these assembly of this spot is nothing but the assembly of the planes right crystal planes. Now, in real in crystal to follow the orientation of the crystal planes it is slightly difficult, but if we have some alternative, if I think that whatever the on plate whatever this. Now we can represent the planes by a point.

Now, if I set a axis system on this on this plate, now I can find out the distance of each point and that is nothing but distance with respect to that origin if we choose. So, whatever the distance of this points is nothing but that distance of the planes and this orientation of the different spots it will be the angle between that between the 2 planes respective plane. So, that each point is basically give us the planer distance. And the angle between the 2 spot with respect to this origin will get the angle between these 2 planes. Now it is a diffraction pattern lave spot is giving us advantage that it is directly. It is telling us the planer distance and orientation of that crystal orientation of the planes in terms of some points.

So, that in crystal we cannot in crystal lattice point the way we have identify lattice point or generated the lattice point. So, lattice point are basically it has coordinate right. It has coordinate lattice point has coordinate, but lattice planes had do not have coordinate. So, lattice planes are different taking that coordinate, but reciprocal of that and simplification etcetera after that we have getting plane, but if it. So, locating the lattice point in space lattice using the coordinate is easier than the locating the planes in the crystal. So, point representation is easier than the plane representation. So, in diffraction after diffraction whatever spot you are getting that is nothing but it is representing the symmetry of the crystal. So, it is representing the crystal. So, if we can do alternative way to identify these points.

So, it will be just like the coordinate system for the crystal whatever this convenient way we have seen; and in this case to locate the planes and their orientation etcetera. So, in terms of coordinate will be able to see. So, people think about another way to explain to describe the crystals. And that is basically the concept of reciprocal crystal reciprocal lattice that we will discuss in next class.

Thank you very much for your attention.