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Lecture - 23 X-ray Diffraction from Crystal (Contd.)

Today we will discuss another method, X-ray diffraction method.

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That is powder method or it is called also Debye Scherer method. So, earlier we have discussed about lave method, where theta is constant, but lambda is variable. Then we have discussed about the rotating crystal method, where lambda is constant monochromatic X-ray, but theta is variable. Now in this powder method, here also this lambda is constant. In this method lambda is constant and theta is variable, but there is a difference between this 2 method this powder method and the other one rotating crystal method. In both cases this theta is variable lambda is monochromatic X-ray.

So, what is the difference and what information we will get from this method, so this information mainly the same. We want to know the crystal structure. We want to determine the crystal lattice parameter right. We and which type of lattice it is so, but different method has different advantage. So, lave method it is it is basically use to know the symmetry of the crystal. So, it is easy way to know that one and this rotating crystal method is very helpful to know the unknown crystal even. So, which type of crystal it is

without knowing the details of lattice constant etcetera. So, we can we can tell them about the bravais lattice of this crystal; so but here this method. So, let us see what we can know from this. So, here it is very convenient to get the lattice constant value. It is easily we can determine the lattice constant.

But that is not easy from the lave method. Lave from lave method it may not be that accurate determination of this lattice constant and it is not also easy way to determine, but that is very convenient to know the symmetry of the crystal, whereas, this method is not suitable for knowing the symmetry of the crystal, but very suitable for determining the lattice constant. So, different method whatever 3 method we discussed. So, they have own advantage. So, here experimental geometry we have to take in such a way the theta has to be variable. And lambda constant that we can choose from X-ray source we can choose using filter we can choose a particular lambda generally copper or molybdenum k alpha is chosen because it has high intensity incident X-ray will have the high intensity if we choose k alpha X-ray.

So, that is that is easy to choose. And now this again this crystal we have to that X-ray will fall on the crystal right. Now here crystal in other 2 cases this we have used single crystal of small dimension, it is in millimeter dimension. So, in this case here the crystal we used in powder form. And I showed you that powder form means if you take salt we eat salt right. So, whatever the form of salt is very small particles, it is we tell this powder form of the crystal. So, even if it is single crystal this bigger piece. So, one can break it and make it this powder form. And then this crystal in powder form we take in the in a say tube.

So, here we have our single crystal in powder form right. So, now, it is in powder form then whatever X-ray is falling here. So, what is the angle, what will be the angle of say 1 1 1 plane. So, crystal it is in parallel form, but it has planes so each, so here if I just want particle if I just draw in bigger form. So, it will be say this 1 1 particle right. So, here it has plane it has all sorts of plane right, it has all sorts of planes. So, each particle have all planes right. Because a small particle, but it is in say it is size is in micrometer size. So, in micrometer size how many unit cell will be there. So, one can what is the dimension of unit cell? Dimension of unit cell is few angstrom say even it is 5 angstrom right even it is 10 angstrom say biggest one.

So, in one micrometer how many unit cell will be there? One micrometer means 10 to the power 4, 10 to the power 4 angstrom right. 1 micrometer is equal to 10 to the power or 1000 nanometer and 1 nanometer is 10 angstrom. So, it will be 10,000 angstrom right. So, 1 unit cell if it is 10 angstrom. So, you will have thousand unit cell in this small particle if it is one micro size. So, it is each particle is a single crystal again. So what I try to find out say if I consider that is 1 1 plane. So, in this particle these planes are there. So, now, this planes this particle will form this X-ray will form angle with this 1 1 1 plane right. What is this angle? That I do not know because this particle here in which orientation, it is sitting I do not know.

So, but here thousands and thousands particles are there right. So, with this for in this plane in this particle, 1 1 1 plane form a particular angle say 70 degree. So, in another plane another particle so that 1 1 plane. So, it will form different angle, same plane it will form different angle. So, you can imagine that thousands and thousands particles are here and each particle have 1 1 1 planes right. So, they are they are randomly oriented here. So, you can expect that, is angle between this X-ray and 1 1 1 plane here have all values all values starting from 0 to 180 or 360 degree. It will have all angle.

So, it has continuous angle with 1 1 1 plane. Similarly, for any planes this will happen, because here this 1 1 1 plane with respect to that 1 0 0 plane. So, there is the relative orientation. So, they will they are oriented as a whole. So, if this angle varies this plane with this plane angle varies with this. So, it will happen for all planes. So, this is the technique used to vary the angle incident angle of X-ray with different plane. So, angle is varying basically continuously it has all sorts of angle, and not it is not is in in orientation in one plane it will have orientation all sorts of plane all sorts of direction right all sorts of direction it will have. So, this plane will have angle continuous variation of angle not only in a in a plane right. It will have in all direction theta variation will have all direction.

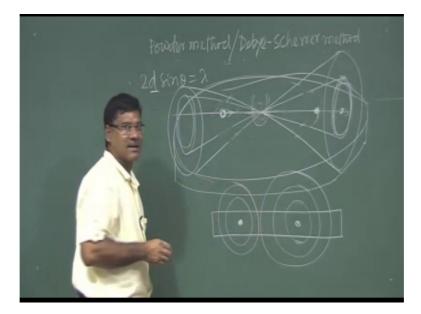
So, that is very important, because in rotating crystal method there we have seen this this variation this angle variation was it depends on the orientation. So, it is orientation was only with respect to this one axis right. So, it was rotating it was rotating; so whatever the angle variation was there. So, that is say with respect in this plane right in this plane so, but automatically this other plane which was inclined with this this plane. So, automatically that is will that will varies in the same way, but for this plane also it will

vary on this in this horizontal plane. So, here all the in that case all the because of this rotation all the angle variation was horizontal on horizontal plane, but in different level for different axis. So, here it is not. So, that way; so here it is this angle variation with respect to this it is not varying only this way it is varying in all direction in all direction.

So, whatever you can imagine as if this in sphere if you take it is sphere of center; so this angle variation in all direction. So, that is important. So, that will tell us this basically pattern of the diffraction; so that we will discuss. So, now, what will happen? So, here this X-ray falling. So, all sorts of angles are available for each plane. Now I have to. So, diffraction will be on all direction you know. And now this pattern will depend how you are placing your screen, how you are placing your detector how you are placing your X-ray plate. So, whatever the detecting system you are using people used to different system. So, I will discuss in terms of photographic plate.

So, here photographic plate is placed again it is in cylindrical form, but with small it is small width. So, this type of photographic plate is placed I think let me. So, what I want to say it is not cylindrical form. It is a circular form. It is in on a circle, it is on a circle, but this film has some width. So, film has some width.

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So, that is what I want to mean. So, I think I have to I think if I represent this way. So, it has it is in circular form, but it has small width. So, X-ray is falling. So, here on this film

we generally key fall. So, that X-ray can enter and the falling on the sample. Now direct X-ray is going.

So, here we can tell that this is the direct X-ray and this the or forward X-ray and it is backward X-ray is back side reflecting backward and reflecting forward or incident direction. So, you will get this here one point. So, here basically we keep one hole here also we keep one hole. So, X-ray can go out for the X-ray is falling on the sample it can go out. Now what will happen? If, so now, think that. So, here X-ray is falling say if you consider the 1 1 1 plane. So, it is. So, 1 1 1 plane are in all directions, on all directions is oriented in all directions right. So, that a experimental geometry. Now 2 d sin theta equal to n lambda. So, n we take first order. So, it is 1. So, here. So, 1 1 1 plane, if I am considering 1 1 1 plane.

So, now this angle is variable lambda is constant. So, angle I will get. Because angle are available all sorts of angle are available with this 1 1 1 plane. So, I will get easily one angle will which will satisfy this condition; so will get reflection in that direction. Reflection will be in many directions, but we will consider those reflections will which will give us the constructive interference, will give the highest intensity right. So, now, if that is the reflected one if say that is the reflected one from 1 1 1 plane right. So, what will happen. So this is the incident X-ray right. Now I have plane. So this way or if I with some plane what will happen. So, this say 1 1 1 plane. So, it will satisfy this condition for angle theta. So, I will get reflected one right. Now these planes have all sorts of orientation right.

So, keeping this angle theta I will have different orientation of this plane. So, I will have different orientation of this planes right, keeping this angle theta. So, basically that forms cone. So, here because this this angle is continuously variable right for this same plane. So, I will get this diffraction or reflection this all the along the surface of this it is not discontinues continuously on the surface all lines will be the reflected lines which will give this constructive interference this all direction on a cone; so here along the cone. So, this is a solid cone. This is a cone these surfaces on the surface of these cones, all are allowed, all reflections are allowed.

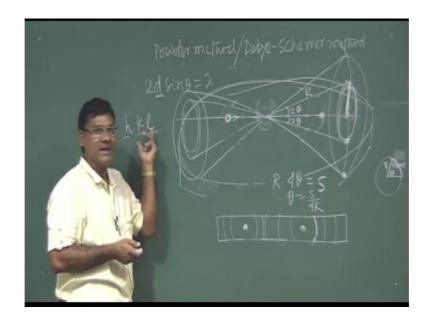
It will form diffraction it will give diffraction constructive diffraction. And so if I put a screen here; so what I will see? I will see a circle. So, this circle will represent if I put a

put a screen here, plate here. I will see a circle this circle is basically for 1 1 1 plane right. Similarly, for other say 1 0 0 plane. So, it will have the same way it has all sorts of angle. So, it will give another circle. So, it will form another cone. So, this each cone will have a for a it will represent a particular planes right. So, on the screen whatever I will get says if I put the screen this way I will get concentric circle. So, each circle for each scale similarly backwards also we will get similar as for lave spot I have shown you.

So, here also it will form cone right, so this also for same plane. So, now, if I put photographic plate this way, if I put photographic plate say here I can extend it. So how I have put photographic plate? So, here what will happen? It has some width right. So this photographic plate on this basically what I will get? So, I will get this see. So, if it is bigger 1, I will get circle on this, but if it is with the smaller; so I will get just with respect to this both side some r. So, basically on photographic plate, if I just this; now it was in circular form, now if I make it straight.

So here, basically one hole and one photographical here; basically, another hole this; so here with respect to holes; so these are circles are there. So, these circles are there. So, basically on photographic plate, what we will see because here photographic plate is not there X-ray plate is not there. So, basically what we will see. So, this type of pattern you will see on the photographic plate. So, if you know. So, from here one can easily find out this this d. So, to find out this one has to know angle theta right. One has to know angle theta.

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So, here imagine that this is the incident direction and this is for this, this circle. So, this is the reflected direction right.

So, angle between these 2 if incident angle grazing incident angle is theta. So, angle between the incident and reflected rays it is 2 theta. So, it is 2 theta right. So, this also will be 2 theta. So, this total is 4 theta right; so this 4 theta. Now this one here whatever part we are getting. So, from this center here from this center. So, this will basically here whatever is this arc right arc. So these will be the radius, this this arc. So, now, if it is theta and these if this is arc. Because it is circle and these distance. So, I think I this radius of circle is, to find out the arc what you do. So, you have a circle, I can see circle right.

So, from center if it is angle theta if it is radius r, what is this arc? Arc is basically r theta. Arc is basically r theta right; r theta I think here. I can write r theta right. So, this equal to if I write s. So, this arc if it is s and this radius if it is r; so from here this whatever this you can find out the relation that r 4 theta r into 4 theta it will be s. So, this r and this a you will find out this form. From geometry basically one has to find out because what is the distance of your film that we have to know and radius you can measure from here. So, from here you will get the theta value. So, that is basically s by 4 r, s by 4 r. So, you will find out from this explain theta if you find out theta then you can lambda is known to you. So, you will find out d.

So, if d is known you know the lattice constant if it is cubic crystal one can find out lattice constant a. So, this way, this method is quite simple. And very useful and it is frequently used in laboratory. So, here in terms of film I told, but nowadays film is not used. It is we are using different geometry; we are using detector to detect this intensity. So, detector now, here detector is moved in this direction. Detector is move in this direction. So, it is not we are. So, detector will not see the intensity as on the circle. So, detector will move in this direction. So, (Refer Time: 29:42) it will see diffraction spot here means intensity here. Then it will see here right. So, this is a half of this generally we do not scan full. So basically detector when move. So, this will give a.

So, on the circle it is same this all points are same for a one plane. So, these detectors will that intensity will find out. So, this for a it will represent a plane. So, we tell this. Generally, we tell this Bragg peak high intensity will see. Then for next one we will see this next (Refer Time: 30:20) Bragg peak. So, this will correspond for different planes and detector when it is moving. So, it will find will get this diffraction peak at different angle. So, that one has to note down one has to calculate and note down this angle variation. So, then what is that angle this peak has formed at which angle. So, experimentally we know. So, if you know then which plane, it is from here we can find out. So, we will get different peaks. And from there we will get that each peak corresponds to different planes.

But lattice constant is same whether planes are different their spacing are different, but for that crystal lattice constant are same right. So, taking different peaks one can find out the lattice constant as I mentioned earlier, but one has to know h k l value also. One has to know h k l value also right. So, this h k l value, how to know for that we need more diffraction peaks.

So, from that diffraction peak, but as I told it will represent this it is for a particular crystal, and it has only particular lattice constant miller indices will be different. So, if we have few number of peaks and then for same lattice constant say if it is cubic a, then one can find out the miller indices of this each plane and ultimately we will find out the lattice constant.

So, we will stop here. We will continue in next class.

Thank you for your attention.