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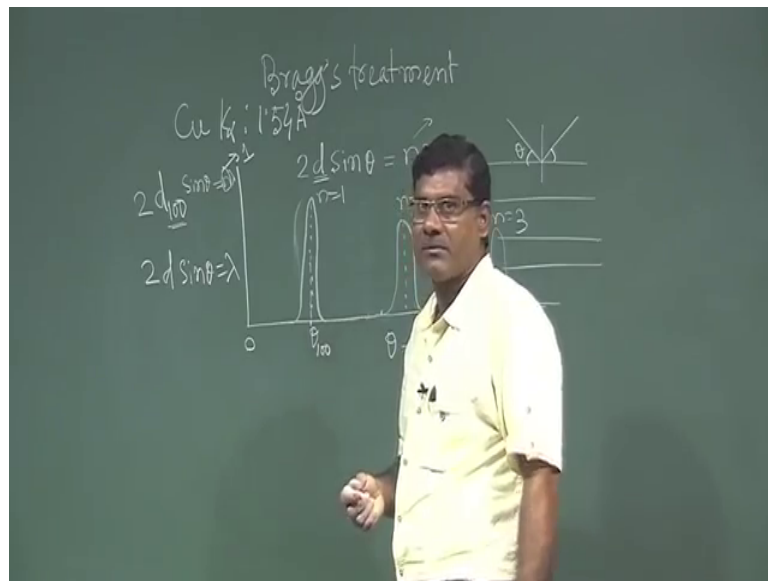**Prof. Amal Kumar Das**
Department of Physics
Indian Institute of Technology, Kharagpur

Lecture – 20
X-ray Diffraction from Crystal (Contd.)

So, we will continue discussion on crystal diffraction by x-ray.

(Refer Slide Time: 00:33)

So, in last class we have seen that Bragg, Bragg's treatment it is based on model, reflection model. So, Bragg considered that x-ray will fall on the crystal and crystal will diffract x-ray from the crystal. Now, it diffracts in different angles, that diffracted rays basically they interfere with each other and we get constructive interference, destructive interference, we get basically the fringe. So, this that fringe is we generally express in terms of peaks, that I have shown you in case of grating.

So, in Bragg treatment, considering the Bragg treatment what we derived, that condition for diffraction 2 d sin theta equal to n lambda. What is d? d is the basically lattice spacing. So, these are parallel planes, this is the lattice spacing and theta is the grazing incidence angle with the plane. So, this is diffracted, when x-ray falls on this planes on this crystal, then it will be diffracted in different angles. Then diffracted rays interfere and we get the interference effect when the variation of the intensity, deep interference.

These diffracted rays, is basically will get in different direction and we will get constructive, destructive interference ok.

So, here, Bragg select those diffractive rays, which follows the reflection rule and assume that those reflected rays will interfere constantly. They picked up the right set of diffracted rays which will interfere and give the constructive interference. Among many diffracted rays, they picked up those rays which are basically equivalent to reflected rays and they interfere constructively. So, that is the assumption and gives this relation; where d is the lattice spacing, theta is grazing incidence angle and lambda is the wave length of this x-ray, n is the order of the interference. You are familiar with the order first order second order third order interference maxima right.

So, from here what we will get, this we will get like just as for getting what we got, this some principal maxima, here is same. Here, if it is angle, say at different angle, I will not draw this one first. So, if it is, a instead of in middle let me, this is a 0 degree if I take, now, for a particular d and if x-ray wave length is also monochromatic and if we choose a particular lambda, say you are taking copper from copper target, copper k alpha, x-ray its wave length is 1.54 angstrom right and say you are taking a particular d. If it is 1, 0, 0 planes is h, k, l, 0, h, k, l, 1, 0, 0. So, then this planes ah will be d 1, 0, 0 then sin theta equal to n lambda.

So, lambda is constant, these also for a particular planes, these also constant, now when this equation this relation will be satisfied then we will get the peak, that is constructive interference that peak will get. So what we will do, this we will vary theta, will just change this angle, how to change the angle I will discuss, we have to change the angle and then for a particular angle, this relation will be satisfied. This relation will be satisfied for a first order for n equal to 1, say first order and then if we continue the change of angle, we will get the second peak, we will get the third peak right. So, this peak is for n equal to 1, n equal to 2, n equal to 3.

So, first order, second order, third order peak. And this angle, it depends on lambda, lambda we have fixed it, it will depend on this d value that also we have fixed, this corresponding will get theta. So, that theta basically for this plane, here, we will get for second order peak, third order peak, it is there. If I scan this whole angle, I will get for a particular plane; I will get the diffraction peak or interference peak at different angle.

Now you see this, if we consider n equal to 1, only if we consider the first order peak then, from the beginning we will put n equal to 1, 2 d sin theta equal to lambda. We will consider only first order peak because second third order peak is not giving me any additional information right.

We can consider any one peak and corresponding angle, we can put here, for that order. We can take any one order, generally we take first order, all the time we use this n equal to 1. But, one has to be careful, sometimes what happens, for second order peak also appear, that I will discuss. Here, it is not the only one plane in crystal, because I have a, this is a crystal and this is not only one plane. So, this is a one plane which is equivalent to a set of parallel planes, if it is 1, 0, 0 say 1, 0, 0 say then there other 1, 1, 0; 1, 1, 1; 2, 0, 3, there are 100 and 100, 1000 and 1000 planes are there. X-ray is falling, I am changing the angle, when it will reflect from a particular plane, it will reflect from a particular set of plane having a d, lattice spacing, satisfying this relation, for a particular angle I will get the peak.

(Refer Slide Time: 11:51)
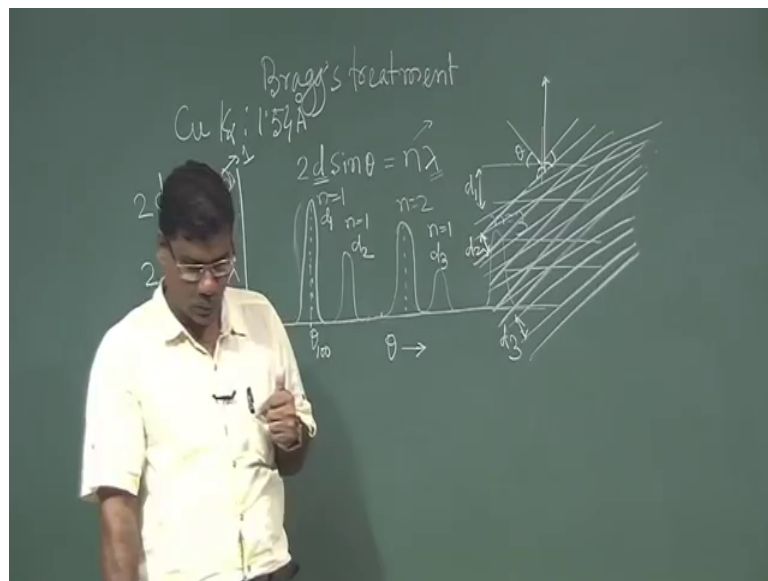
So, simultaneously, what happens here another set of planes are there already, this x-ray it is falling on all planes, all set of planes, having different h, k, l, this x-ray falling on this plane and getting reflected, this x-ray will fall on this plane also. And now we can see this for this plane, this angle is different. Earlier this angle, now for this plane angle is different. So, following the reflection rules it will be reflected having the same.

Similarly, from this sets of plane, we will get reflected rays, this spacing is a now this spacing is say this is d_1 1, d_1, this spacing is d_2 right. When I am changing the angle, it is this incident x-ray is changing angle with all planes right.

From this sets of plane for d_1 lattice constant, lattice spacing, from this plane I will get peak at a particular angle when it will satisfy this relation right. So, say this is the peak first order I am getting and from this sets of plane lattice spacing d_2, I will get the first order peak for this sets of plane at different angle which will satisfy this relation. So, say I am getting here I am getting here. We may a consider another sets of planes, this which way I can then we may another sets of plane. I think I have to, in between say another set. It is a this spacing is d_3, continuously we are changing the angle and then from all planes this x-ray are diffracted right.

So, depending on the d value. So, this relation will be satisfied because lambda is constant this relation will be satisfied at different theta, when at that theta will get peak for a particular d value right. This way we will get anonymous many number of peaks many number of peaks which will for first order which will basically the peak for a particular each peak for a particular plane. I will get the third plane, this third peak for d_3. This is for d_1, this is for d_2, n equal to 1, this is for d 3, n equal to 1. Here we will get many first order peaks, each peak will basically indicating a set of planes, a set of parallel planes h, k, l planes.

Here one has to be just careful; here just I have done different order. Generally, we consider the first order only, but one has to consider that at higher angle sometimes this n 2 second order may come second order peak may come. We should not confuse with the whether it has come from different plane or it has come from same plane, but it is second order, one has to be careful when analyze this x-ray data. Using this relation we can get peak and each peak will correspond to a particular plane. I am just considering that only first order peak. I will talk, I will not mention if necessary then I will mention for other order otherwise you may consider that only I am talking about the first order peak.

So, we will get different peaks, which correspond to different planes.

(Refer Slide Time: 17:56)
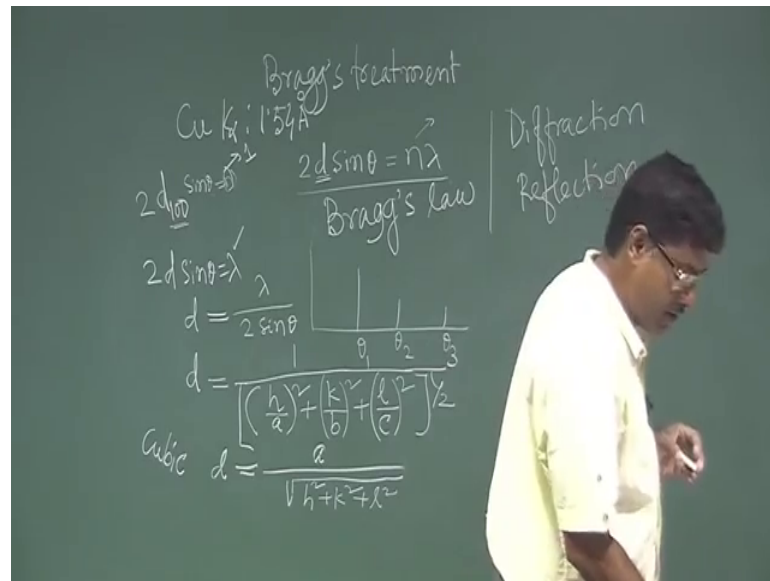
From that scan experimentally, what you are getting, you are getting different peak. Basically, experimentally we are measuring the angle, diffraction angle or reflection angle whatever we are measuring the angle and this lambda is known we are measuring the angle theta, from this relation then you will get d value, that is lambda by 2 sin theta right. I will get the lattice spacing d value now, d is related with the lattice constant. So, let us consider only simple cube, it is then it will be easy to understand.

So, we know the relation between the lattice parameter, lattice constant and the lattice spacing, what was that relation; it was basically 1 by h by a whole square, plus k by b whole square, plus l by c whole square, in this square root, it is under square root. That was a relation between the lattice parameters and this for cubic for system, d equal to say a equal to b equal to c, d equal to basically a by square root of h square plus k square plus l square. From this relation one can find out the lattice constant right a value for cubic system a value, for other system also orthorhombic or tetragonal, one can find a b c value.

For that, you need, you have to analyze the data properly to get because here you have to know the h, k, l value right. So, this d for, just here d I will get, but from which plane, that I do not know h, k, l also unknown to me, one has to get the lattice parameter, one has to know the h, k, l value, so that, there is a way to analyze and find out this lattice parameter. So, that I will discuss later on, now, just here I try to tell you that using the

simple relation that is called Braggs law, and in case of Braggs law diffraction and reflection, these 2 term are used, are frequently used, but both are having the same meaning.

So, they are interchangeable. In case of Braggs law, generally, we use the reflection term not diffraction term, but basically it is diffraction term. These both terms are used in same sense, so we tell this Bragg reflection instead in place of Bragg diffraction. Why it is diffraction basically, but it is a reflection, that as I mentioned this, they have considered the constructive interference only, where we will get the peaks and those diffracted rays which follow the reflection rule and they interfere constantly. So, that is why these 2 terms are equivalent in case of Bragg treatment and from there this simple this relations are there this d, one can find out experimentally measuring the angle theta, Bragg angle these are called Bragg angle and then this d is related with the lattice parameters.

So, one can find out the lattice parameter, for that, one has to know the Miller indices of this plane. We will have many planes, so this different planes have different Miller indices right. One has to analyze in proper way to get this a, doing this Miller indices. So, that will be discussed during analyze the data, I think I will discuss. Now, what happens, here just theoretically I told, this way theoretically I told that, this way one can find out the lattice parameter, but for that you need the experimental arrangement. There are basically, 3 experimental arrangement, for all experimental arrangement, this is the parent relation, Braggs law, based on this relation this law, there are 3 experimental arrangement. So, that I will mention.

(Refer Slide Time: 25:08)
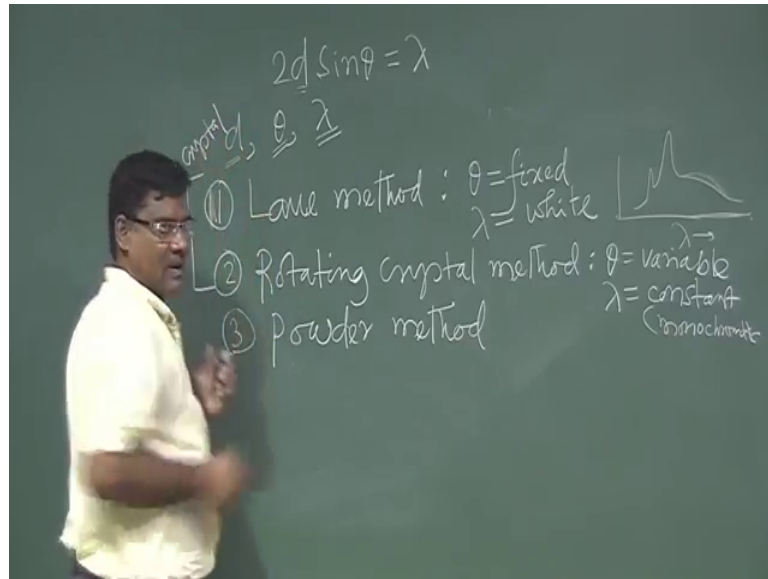
So, I have basically 2 d sin theta equal to lambda, this is the Bragg law, Bragg equation. Now, we will get whatever we will get that for that this relation has to be satisfied. We have 3 parameter basically here, one is d, one is theta, another is lambda. Our aim is to find out this d and d again related with the lattice constant like a, b, c etcetera. So, this variable mainly these 2 are one has to vary or one can be taken constant, other one can be varied. One variable is must, because this to satisfy this condition there has to be one variable minimum one variable right.

So, experimentally, this there are, I told there are 3 method experimental arrangement; one is called this Laue method, one is called Laue method. In case of Laue method, theta is fixed, but lambda varies, basically white x-ray is taken, where all lambdas are there. I have shown this type of x-ray spectra, this is the lambda; all sorts of wavelengths are there, white light. Lambda is variable here in this method, lambda is variable. Theta is fixed, now lambda is variable. So, d, depending on d, lambda is, lambda will vary to satisfy this relation, this sin theta is having a fixed value now for different d in crystal, what is there different d are there, different sets of planes are there, to satisfy this one for d_1, d_2, d_3, whatever for each set of planes, for each set of parallel planes, for a particular d value, it will, it have chance to pick up the right lambda to satisfy this one. For another sets of plane for d_2 say, it will pick up the another lambda to satisfy this relation, we will get peaks, will get peaks or constructive interference for all planes in crystal.

So, this is the Laue method and second method is called rotating crystal method. So, rotating crystal means x-ray is falling on the crystal, now crystal is rotating, its plane, angle with these planes are changing. In this case, theta is variable theta is variable, other one can be constant, lambda is constant, means monochromatic x-rays is used. So, this is monochromatic, this monochromatic x-ray.

So, generally this k alpha it has maximum intensity that is generally filtered from this white x-ray and use for this as a monochromatic x-ray. So, in this case, crystal this is rotating with respect to this incident x-ray. Now crystal is rotating this is the incident x-ray, angle with the planes will change, theta will vary, lambda is constant; now for different d, theta is available, it will pick up a particular theta for a particular planes. I will get again just due to the variation of this angle, it will at different angle for different planes, this relation will be satisfied, so I will get again many peaks.

So, third one is called powder method, third one is called powder method. Powder method means, a this both these 2 are for single crystal I think it is I will, it is for single crystal, whether I can show this. So, this is a silicon crystal, you tell this wafer, generally this 3 inch 4 inch diameter silicon wafer is available. This is a one piece of that silicon crystal. So, single crystal means this type of crystal, this type of crystal of different materials are used, this type of ah materials are used and these are the basically heart of electronics instrument you know, different materials are deposited on these crystal and (Refer Time: 32:28) IC's on different electronic circuit.

So, just here I want to just show that this crystal are this type this is silicon crystal; you have germanium crystal, gallium crystal, sodium chloride crystal. This is just one, this is single crystalline, now if I break this one and make very small piece in micrometer order, few of this each particle will be of few millimeter, few micrometer. So, then we tell this is a powder, its best example is a sodium chloride, is salt we take salt right in our with our food, this is just I have taken salt. So, this nothing, but is a its a sodium chloride crystal, it if you break it and make many pieces like this, then we tell this is a powder form of the crystal. So, what does it means; each particle or each piece is a single crystalline, now, we have many single crystalline particles together, now these single crystal particles have all sorts of plane right.

So, now if you consider 1, 0, 0 plane, in one particle this planes are there, in another particle this planes also there. In all particle this planes are there, now, in which direction they are oriented, in which direction they are oriented, so, that is the main importance factor for powder method. We can tell that if x-ray is falling on this, 1, 0, 0 plane for a particle it is making angles say some angle say 5 degree. So, the another particle that same planes will make angle 5.5, 5.9 etcetera. You can assume that, for this powder crystal x-ray will make angle from 0 to 180 for a particular plane. Each plane will have all 0 to 80, all angles continuous change of angles for this powder method.

So, this is the basically, what I want to tell that, this is the powder and in this method we are using basically this type of powder crystal, where angle, incident angle of x-ray for different planes are continuously variable. So, in this case, this angle is variable.

(Refer Slide Time: 35:51)
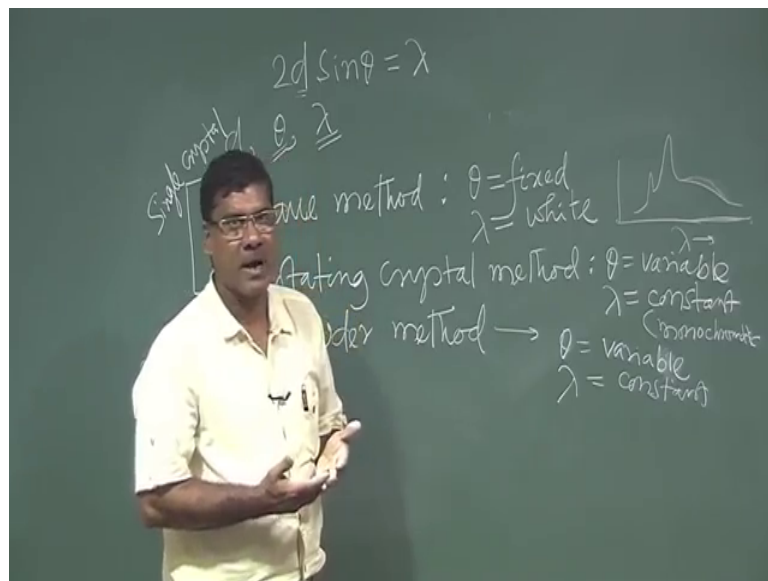
So, it is not, we are not rotating, but using the powder, we are getting this variation and lambda is fixed constant. This basically, this lambda, x-ray is monochromatic. Here, also we have theta variable, lambda is constant, usually these crystal, this relation will be satisfied for different planes at different angle. So, will get again many Bragg peaks and from that Bragg peaks we can basically get different d and then different d will be related with the lattice parameter and one can find out the lattice constant. We will continue discussion on this topic.

Thank you.