Experimental Physics - III
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Lecture - 59
X - Ray Diffraction and Crystal Structure (Contd.)

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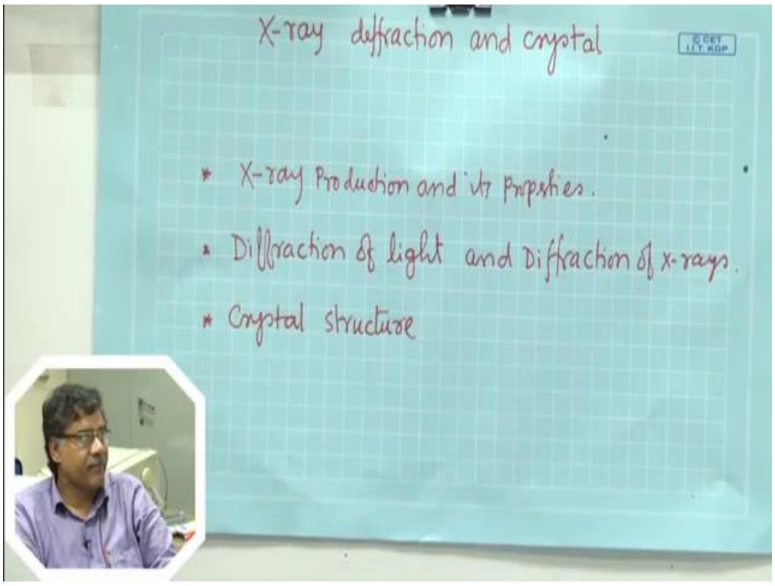

In last class I have discussed about the about the X-ray production and its properties. Now I will discuss about diffraction of light and diffraction of X- rays.

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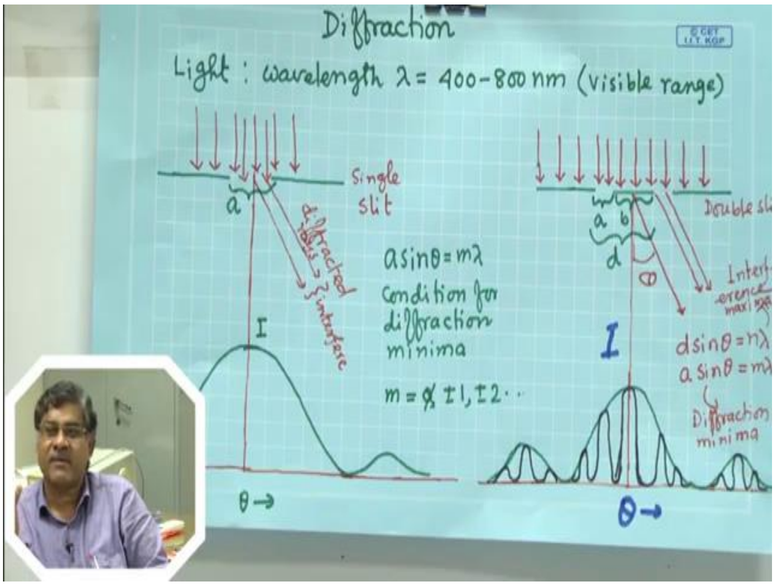

What is secondary wavelength? this this waves are coming falling on a slit falling on a slit say this is the single slit. Now when it get it is obstacle, this light when it is propagating and it obstacle by say screen having a small hole. It is a dimension is a, if this dimension of this hole is comparable to the wavelength of the light. Then we tell that this the light at this point it will diffracted in all sorts of direction; it will diffracted in all sorts of direction. There will be diffracted light; there will be diffracted light.

So this diffracted light when it will reach a screen when it will reach a screen at a distant say some distance one can see the variation of intensity of light on the screen like this; it is a like this. these are minima, these are diffraction maxima and these are diffraction minima. These diffraction minima, it depends on the angle; it depends on the angle wavelength as well as the slit width. this relation is a sin theta equal to m lambda.

For a particular wavelength lambda and for a particular slit width a, so at which angle one will get the one will get the diffraction minima that is that that is fixed. In addition, you will get diffraction minima of different order different order; so there that is the m is the order so first order second order.

It will be symmetrically from the central maxima from the central maxima. this is the first minima towards the left minus m equal to you can take minus 1 and here m equal to plus 1 plus 2 plus 3 minus 1 minus 2 minus 3. This type of intensity variation as a function of angle one can see and this is called single slit diffraction. this you know this all these things, but just I want to just want to discuss once more and want to correlate with the with the X rays.

Now when you take when you take the double slit that will two slits are there so that that a slit width and this b is the slit separation so a plus b equal to d. See in this case, also, there will be this diffracted light from this source and diffracted light from this slit and the diffraction light from the other slit. As if this two source two coherence source from there this light are coming they, those light will interfere. Therefore, one can expect that due to single slit effect, there will be diffraction pattern as well as there should there will be interference due to two coherence source. Two or more coherence source will give the interference apply from this all this coming from all these sources coherence sources. There will be superposition of interference pattern with the diffraction pattern single slit diffraction pattern.

here in case of double slit so one can see the intensity variation as a function of theta; intensity variation as a function of theta, it is a like this ok; it is a like this you can see this is the this is the so these are the principles; these are the diffraction pattern, diffraction pattern here to wherever the that is modulated with the sorry these are the interference pattern that is modulated with the single slit diffraction pattern.

All peaks you will see here diffraction peaks you will see here or interference peaks you will see here. the intensity all peaks will not be the same. It is a modulated; it is the module, but in case of interference this is the dark b, dark b it is a contrast we see that intensity of b lines are same. In this case, the intensity will not be the same since intensity is modulated with the diffraction pattern

These are this is the diffraction pattern of single slit and this peaks you are seeing these are the interference maxima. this condition, condition for this a sin theta equal to m lambda you have seen this is the condition for a single slit minima. In addition, this interference peaks this is the b fringe condition for constructive interference that is d sin theta equal to n lambda. You can see this n is the this interference fringe order and in this case m is the diffraction minima order of diffraction minima

This is the condition for diffraction maxima in to the interference maxima and diffraction minima. this due to diffraction this you can see this how nicely the intensity are distributed on the screen. This we are seeing the variation of intensity on the screen. it is a just b dark this contrast we are seeing that is nothing, but it will tell the fringe that is the fringe for a particular wave if wavelength dependent, then we tell this is the spectra.

spectra and fringe there is a difference one is wavelength dependent, another is another is wavelength for a particular wavelength how the intensity are distributed on the on the space so that we tell the fringe this is the diffraction from single slit and diffraction from double slit. now, similar way one can go for diffraction from multi slit, so that is called grating; diffraction from multi slit n number of slit then that is called that is called grating here; obviously, you can see this a plus b that is the d there are n number of n number of slits.

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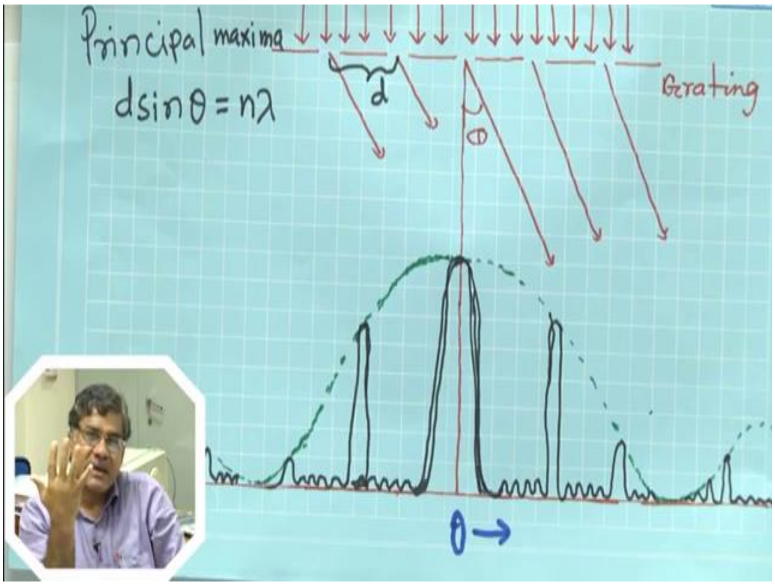

This d is called the grating element, grating element. So this is this slit width plus this separation. that is d is called grating element; so in this case also this diffracted ray from each source at a particular angle they will interfere. In addition, depending where on their depending on their path difference it will decide at that at that angle whether we will get constructive interference or destructive interference.

This theta is diffracted ray will get in all directions. So if we plot the intensity at different angle then we get the interference pattern; we get the pattern diffraction pattern where the interference and diffraction they are superimpose to with each other this type of pattern is observed ok, so this again this intensity here; so these black one is interference effect and this dotted one is this is the diffraction effect

Single slit diffraction so this envelope so mainly we just we see this envelope we do not see, just we see these kind of peaks. These peaks are call the principal maxima and between two peaks principal maxima, there are many there are many minima maxima minima maxima. these are called the secondary maxima. Intensity of the secondary maximum is so low compared to these principal maxima. Practically we cannot see this peak, so only we see the principal maxima.

Now, you see this principal maxima, so we are from grating if see the spectra not spectra if you see the fringe we will see these some b lines we will see some b lines. Each b lines is principal maxima. The condition of principal maxima is d sin theta equal to n lambda;

what is theta that is the diffraction angle. here for a particular d for a particular d for a particular grating element and a and for a particular wavelength at different theta, we will get different order n equal to 0, n equal to 1, 2, 3, minus 1, minus 2, minus 3; so this we are getting.

Now from here from here if you know the wavelength of light, then you can find out you can find out the grating element d. Now from here idea has come for X ray diffraction. This is the light diffraction from a grating. condition for diffraction is that the grating element has to be comparable to the wavelength of the electromagnetic radiation. For light the wavelength is in 500 say around 5 - 600 700 nanometer. this grating element generally it is in that order p 1 then nanometer.

Now if you replace light with X ray, light is electromagnetic wave X ray also is electromagnetic wave. Now only problem is this wavelength of light is few angstrom. That is nanometer few 100 nanometer, 5 600 nanometer and in case of X ray the wavelength is in angstrom 1 2 3 angstrom or less than 1 angstrom. Say let us see this consider this X ray, you are taking that is wavelength is 1 angstrom.

Now, if light diffracted from a grating, so X ray also can diffract from grating. Now, if grating element is few angstrom because it has to comparable to the wavelength of light. If that wavelength of light not light X ray; if it is 1 1 angstrom wavelength you need grating of grating of that having the grating element of around 1 2 3 angstrom. Now, it is impractically impossible to get this kind of grating.

People have somehow got idea that that if it would if we take a crystal in crystal planes are there, crystal planes are there. this crystal plane separation is 2 3 4 5 maximum 5 angstrom, so now this can be can be taken used as a grating. crystal planes you have crystal planes, so between two crystal plane this space is this this slit one can take this is the slit width and this plane that have the atoms plane of atoms .

X ray only see the electron density so on the plane the electron density high and between two planes, the electron density is very low. X ray will see that this is the this whole material is nothing, but the but the separation of the these are these are the discrete in nature. Some planes of high electron density and between these two planes, there will be low electron density. high low high low high low this type of contrast that X ray will see so the separation of these two planes is 3 4 angstrom 2 3 4 angstrom.

that separation is comparable to the wavelength of X ray this crystal can be used as a natural grating for X ray diffraction light diffraction now X ray diffraction light and X ray both are electromagnetic wave only wavelength difference are there condition for diffraction is that only diffraction it is possible to see the diffraction. When the width slit width is comparable to the to the wavelength of the electromagnetic radiation

From here, one can tell that this X ray diffraction is possible from a crystal so now so if it is same if it is same; if it is same diffraction in case of whatever light it is so it is expected that same kind of same kind of pattern diffraction pattern, one should see in X ray diffraction also. now, what will be the, what will be the condition for the for the this kind of peaks; whatever we are seeing what will be the condition here this in case of grating this condition is d sin theta equal to n lambda.

these are the for principal maxima, so what is d what is theta; here you can see, theta is the angle with the normal to this angle with the normal to this to the grating angle of the diffracted ray with the normal to the grating, so similar way this Bragg, one scientist William Bragg they if derived the condition of this interference maxima. that we generally tell Bragg peak, Bragg peak is nothing, but the principal maxima whatever in this case we are seeing, so this William Bragg derive such condition diffraction n condition for X ray.

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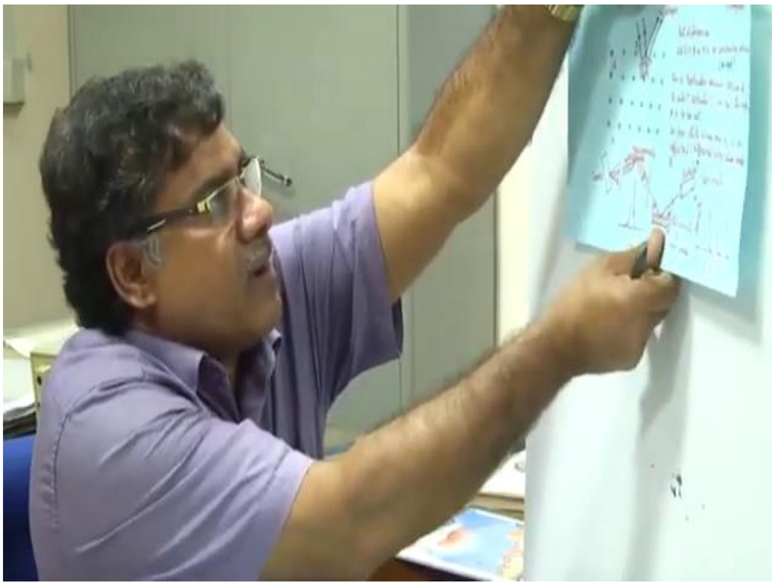

That you can see here that you can see here, so if this is a set of parallel planes one set of parallel planes. this the separation of this planes are d and if X ray is falling like this X ray is parallel X ray beam are falling like this so angle is this angle theta just look at here. This angle is with the crystal planes what is the angle of that with the crystal plane so that is theta. If this is, theta so now, this X ray is diffracted or reflected from this top atom and another one reflected from the bottom atom.

These two diffracted ray or reflected ray will interfere so what is the path difference of this two ray one can calculate at that, path difference is 2 d sin theta. Now if path difference is 2 d sin theta if it is equal to n lambda, so that is the condition for constructive interference. One should see the maxima, inference maxima, one should see. This condition 2 d sin theta equal to n lambda, this is the condition for principal maxima; it is slight different from this earlier case for grating whatever.

this relation in X ray diffraction the condition is 2 d sin theta equal to n lambda how this relation has come so that is that I have explained here, so other things live it for the time being. now here one thing I mentioned that let me clarify that I told that in this from source this white X ray will come from that white X ray we want to select k alpha.

for that we generally use filter, filter it can only it cannot remove the all wavelength it can only reduce the intensity of the intensity of the X rays at different wavelength that intensity the reduction in intensity is very high in all wavelength except this k alpha 1. So that means, that out coming X ray filtered X ray will have will have k alpha line intensity of which is very, very high compared to the intensity of the X rays of other wavelengths

It is not that way it is not a monochromatic light, but there is a way to there is a way to select X ray, which is nearly monochromatic. this is one practice, this is one practice; so it is called single crystal monochromator. Now you see here see Bragg condition is satisfied this condition is satisfied see if you know if you take a crystal thus crystal surface this one plane say one plane. one plane is parallel to the crystal surface if you know that plane; so if you know that plane; that means, d is d of that this d is known to you, so for a known d for a known d.

you can put that crystal we tell monochromator so now, X ray are falling up all wave it is coming. Now if these known these known then at which angle at which angle I will get maxima for that d. if I want to select k alpha wavelength is known to you’d known lambda known for that what will be the theta you can calculate and you can set you can set your monochromator at that angle with the X ray.

then as if this k alpha 1 will be k alpha is reflected from that surface, so this k alpha now it is a wavelength dependent selection in such case the X ray you are getting k alpha X ray is getting, so there is in that X ray only k alpha is there, no other X ray are there. That way it is the nearly monochromatic light it is the nearly monochromatic not light X ray ok, so using this single crystal as a monochromator as I explained people also select k alpha from the white X ray source.

So other things let me discuss later so now, you see these that X ray; X ray from the source X ray from the source is ready how to generate X ray and how k alpha X ray should be chosen from the white from the X ray coming from source. Then that k alpha X ray, we will use for to study our crystal to study our sample to study our crystal material that we are telling sample now monochromatic or k alpha X ray are coming so it will fall on your sample. Now when it will fall on your sample now this sample; obviously, it is made of atoms so this sample have different, so sample have so sample have particular crystal structure

So to get the diffraction to get the diffraction from this sample, we should have arrangement to satisfy the Bragg condition, we should have arrangement to satisfy the Bragg condition. What is the Bragg condition? This 2 d sin theta equal to lambda n forget. Generally n equal to 1 we take, so only first order diffraction we consider 2 d sin theta equal to lambda, so we have chosen a particular lambda k alpha wavelength is now known for copper source it is a 1.54 angstrom if you use the molybdenum source. K alpha that wavelength is 0.71 angstrom so now wavelength is known lambda is known

Now this this material depending on their depending on their structure, crystal structure that d value; d will depend on this crystal structure d is what is d is the in crystal how the planes a set of parallel planes how a set of parallel planes what is the separation of this of this set of parallel planes ok, so this is one it is not one plane. It is a set of parallel planes this is one set there will be there will be 1000 and 1000 numbers of other sets of parallel planes

There d will be different there d will be different, so in a in one crystal there are 1000 and 1000 set of parallel planes. there are 1000 and 1000 d now interestingly that all planes, so with respect to a setup parallel planes another set off parallel planes so they are fixed. If you know one plane and separation of the parallel planes then you can correlate there is a relation of this d planar separation with the with the lattice parameters.

What is the lattice parameters so that is in crystal there are axis a axis b axis c axis. there is the reference axis with respect to that x axis the planes how the plane cut those axis so depending on that we give the name of the planes so to study the crystal structure using the X ray diffraction X ray diffraction will give me back peaks or interference maxima. For first order different interference maxima, you will get for different, different d different set of parallel planes ok

Now, one has to one has to be has to analyse those data and from there one can find out the lattice parameters we should have some knowledge of crystal structure in next class I will discuss the crystal structure before showing you the experiment.

Thank you.