Solid State Physics
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Lecture – 18
X-ray Diffraction from Crystal

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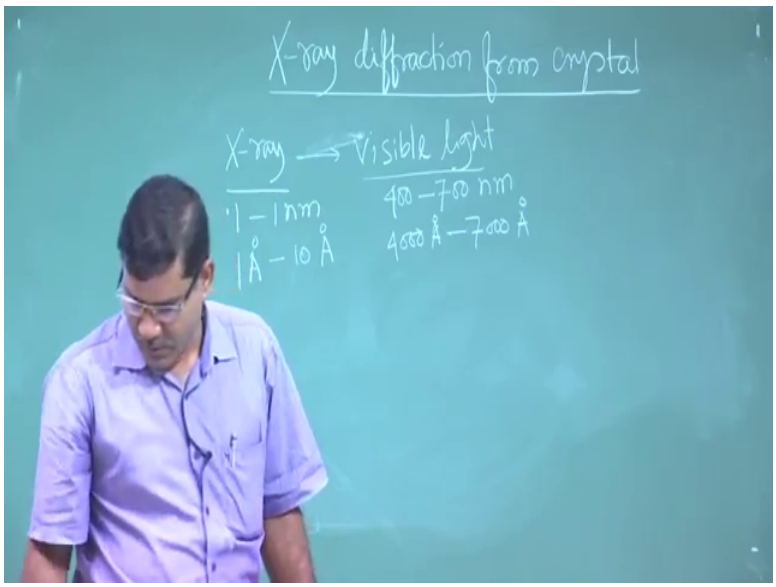

In this class we will we will study about the X ray diffraction from crystal X ray diffraction from crystal this very important in the sense that this is the only method which is used to determine the crystal structure experimentally. If we have a material unknown material and we want to know the structure of that material. So, one has to use this X ray diffraction from the crystal to then you can find out the structure of that material. In that sense is these are very important. It is a experimental aspect. Here X ray must you must we familiar with the X ray what is X ray? X ray is a electromagnetic wave just like visible light.

Visible light have sets the similar to visible light only difference is the wavelength of frequency. So, visible light you know this wave length is the range of 400 to 700 nanometer right and X ray, this wavelength is I think is in the range of 0.1 to say 1 nanometer. In this we close to this. So, 0.1 nanometer is basically 1 angstrom to 10 angstrom in angstrom units one can write 1 angstrom or 10 angstrom to 10 angstrom and this 4000 angstrom to 7000 angstrom right. It is very is very small wavelength compared

to this visible light and how X ray generated, that hopefully you know, but still I will just I will mention because, for this experiment we use X ray source and which type of source are used what are the wavelength is selected. So, that let me tell you.

This in X ray machine basically we have a X ray tube, it is X ray tube means, it is a vacuum it is a vacuum tube means, here is taken out from that tube right it is under vacuum and now at 1 end of the tube inside tube at 1 end is the cathode is there. So, basically this type of this the filament.

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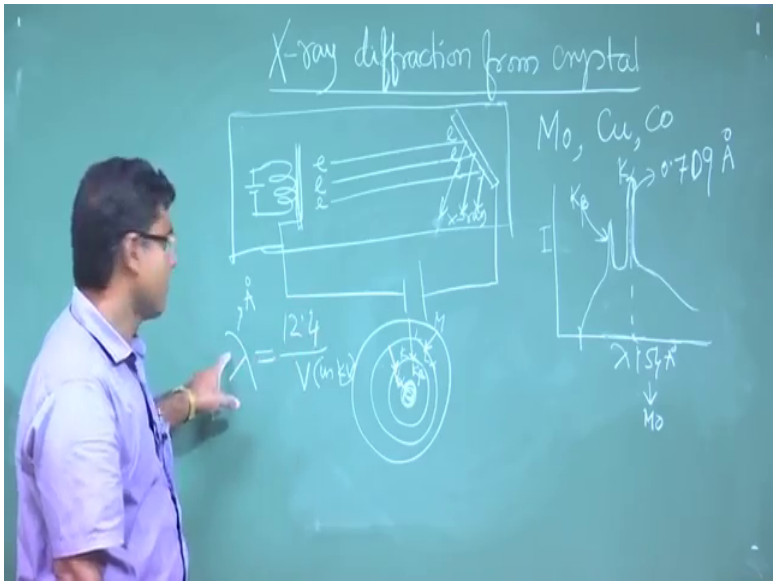

Current will flow through the filament and 1 material is here. It is it will cathode. Basically this filament is heats this cathode material which emits electrons which emits electron. From this cathode, electron will be emitted and now we have we have anode, we have anode means we have target. That the target is generally it is we use this molybdenum target copper target, molybdenum copper target, is used for this for this X ray generator. Now, this electron is emitted.

But we want this electron should be accelerated and heat this target. When it will heat this target then from this target anode from this anode X ray will come out. X ray will be generated there and it will come out. How it will generate I will tell you. This so; that means, to accelerate the electron. You have to apply we have to apply, voltage difference between these 2 right. This anode is connected with this positive terminal of battery and this other one is negative terminal. Electron will accelerate it and hit the. This whole

system is kept in a in a tube whole system is kept in a tube and this thing is under vacuum because, if it is not under vacuum. If here is there. So, it will collide with the air molecule. It will be scattered in different direction. So, that is that we do not want.

It should accelerate and directly hit this our target anode material. When it will it will be accelerated and hit this material? What will happen? 2 things will happen, these electrons these electrons will we paint will penetrate the material and it will be decelerated it will lose energy right. When any charged particle is accelerated or decelerated it emits electromagnetic wave right. There is the principle it emits electromagnetic wave. When this charged particle penetrating the target anode. It will be decelerated it will lose energy and that energy will come out as a electromagnetic radiation electromagnetic radiation. That is we are telling it is X ray.

Because it is wavelength generally become very small it cannot be in the range of visible light. This X ray is coming out this electromagnetic radiation is coming out. If I draw if I draw intensity of X ray whatever coming out the intensity of this X ray versus this wavelength versus this wave length of this X ray. It is these type of curve one can see, it is if [int/intensity] intensity is maximum at a particular wavelength, but simultaneously it has a minimum wavelength, it has a minimum wavelength and another things happens, when this X ray charged particles hits this target now this target are made of atoms. So, now, this is either it is made of molybdenum or copper some others other target can be also cobalt people use also cobalt. In conventionally these are the target we use in our laboratory X ray generator.

This target having the atoms and atom atomic structure you know, right atomic structure you know, it has L shell L shell M shell right. This electrons also knocks hits this ah hits this electrons of this core shell and it take out from that shell then again from higher shell higher shell electron jumps to the lower shell, then that energy difference comes out as a electromagnetic wave and that wavelength is generally in this in the range of for this material in the range of X ray. So, it is nomenclature is like this K alpha if electron jumps from L to K, it is k alpha K alpha X ray if it is jumps from M to K, it is called K beta right if it jumps from M to L, it is called L alpha right etcetera. You will get the K alpha K X ray L X ray. These are called this characteristics X ray these are called characteristics X ray ok.

Because it depends on the atom. It is energy difference are fixed, it is wavelength also fixed. So, apart from this X ray this is called continuous X ray these are called continuous X ray this is because, of deceleration of the of the of the accelerated electron in the in the metal when it is penetrate in through the material and. From there you will get this continuous X ray and also you will get this the X ray characteristic X ray. It will come as I told this only different it will come only difference. This energy difference yeah. It will come from different energy levels. It is wavelength is fixed. Here we will get say here you are getting this type of peak generally this type of peaks you will get then you will you are getting this type of peaks etcetera.

Overall what is it, so whatever the intensity will see that is the summation of this these 2 intensity and basically you will see at this position, it is at this position, at this wavelength, whatever the X ray spectra we will see overall X ray spectra we will see that we will see that we will see this type of variation of the X ray intensity as a function of wavelength as a function of wavelength. These are the characteristics X ray K beta it is K alpha. Why it is K beta K alpha? because for K beta this energy depends is higher. So, wavelength will be smaller. It is coming at lower energy side and K alpha is coming at a higher energy side. This you can see this characteristics X ray having the highest intensity highest intensity and K alpha is clearly have the highest intensity. If we if 1 want to choose a particular wavelength of X ray from this X ray spectra.

Generally we should prefer to choose this K alpha, if target is copper, we tell copper K alpha copper K beta right, copper K alpha again K alpha have 2 component K alpha 1 and K alpha 2. That is because of this is a shell these then again these a shell are subdivided right into sub shells. Because of that, this some minor change some minor change of energy, it is there K alpha 1, K alpha 2, but for the timing forget just take as a K alpha. Copper K alpha this wavelength of this copper K alpha is 1.54 angstrom, but if you take this molybdenum source, this copper K alpha this is for this is for molybdenum source and if you take cobalt source means target here cobalt target.

Then this yeah 0.7 yeah around 0.771 0.71, we write 7 0 9 accurately it is 7.709 angstrom, it is a angstrom, that is the molybdenum K alpha wavelength of molybdenum of k alpha. This just in our laboratory whatever the X ray we use what are the target we use and from that target when we choose a particular wavelength. We choose copper K alpha. So, that wavelength is fixed nobody can change it does not depend on does not

depend on anything if it is say it is the characteristics X ray and it is fixed for that particular target. This way X ray are generated. And ah here the voltage range you know it is in kilo electron kilovolt range that you know that relation probably this lambda equal to lambda equal to 12.4 by V.

When V will be in kilo volt in kilo volt then angstrom this lambda will be in angstrom. If we use 12.4 kilo volt voltage 12.4 kilo volt voltage then you will get wavelength that minimum wavelength you will get that is 1 angstrom. To get the minimum wavelength, 1 can estimate this how what is the voltage on depend, but this intensity since this wavelength does not depend on this voltage characteristics X wavelength it does not depends on the voltage, but what depends on the voltage depends it is intensity if I want to choose K alpha and with higher intensity. We have to, if we apply the higher voltage. Then what will happen? Accelerated energy will be higher, more electron will go and hit the target and you will get more and more X ray. So, intensity will be higher ok.

Here just I wanted to say that in X ray machine generally that voltage we apply between the cathode and anode. This voltage in the range of kilo volt and the target we use that is generally this type of target we use the for X ray diffraction generally we choose wavelength that is, generally this copper K alpha or molybdenum K alpha or cobalt K alpha. These are the practical aspect I told you apart from the principle of X ray spectra. These the about the X ray this the about the X ray now here another portion is there this sometimes for experiment we use we need all sorts of wavelength of X ray. Then there is no problem. So, from the target whatever the X ray is coming. So, that will have the all sorts of wavelength all sorts of wavelength.

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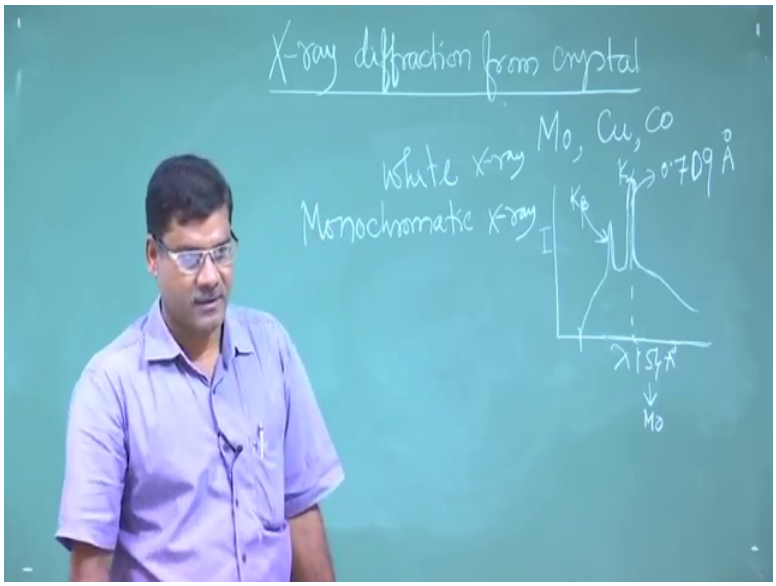

This we tell it is a white X ray, because it has all white light it has all wavelength white X ray it has all wavelength ok.

Sometimes for the experiment we need white X ray having all sorts of wavelength and another X ray we also use that is of white all wavelength. That is called monochromatic X ray monochromatic X ray monochromatic X ray. Monochromatic X ray. So, for monochromatic X ray then see X ray source always giving this type of spectra we have to choose one particulars wavelength. There are different ways to choose that one. So, we use sometime there is called filter absorb, the it basically absorbs all wavelengths except one except one wavelength. It gives then it is that that basically it just pass one wavelength absorbing all other wave length. That that the that type of filters are available and for different wavelength different filters are used this is 1 way others other ways I will tell you later on because generally if we take mirror reflection.

So, this called brag reflection that I will I will tell you later on now I cannot say because before that I have to I have to tell you something more. For X ray diffraction from the crystal we may need white X ray, we may need monochromatic X ray then diffraction. So, you are also familiar with the diffraction, you are also familiar with the diffraction right light electromagnetic wave ok.

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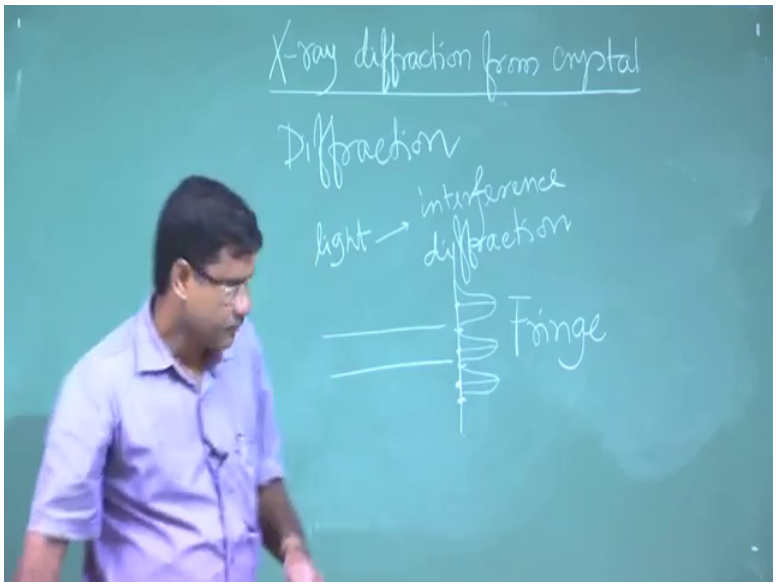

Electromagnetic wave light it is a wave; it shows the it shows the interference diffraction right interference diffraction that basically, what is interference? this 2 waves are coming 2 waves are coming, they overlap and then interestingly they show the they show the that resulted intensity are not the uniform, it is not the just summation of these 2, so it is shows the nicely variation of intensity right variation. it will bright dark bright dark bright dark ok.

When these 2 waves electromagnetic waves light visible light overlaps, they interfere with each other under some condition, it does that happen always. There are some condition you know this it has to be coherent this 2 this 2 coherent waves if they overlap then only you will see the interference. What is the coherent? Waves basically this between these 2 waves all the time they are phase difference between these 2 waves that that will remain constant with time. So, it will not change with time. Wave are moving whatever the initial phase difference between these 2. All the time this phase difference will remain same. So, then we will tell that they are coherent source. They will interfere they will overlap means they will interfere and you will see the nice distribution of light intensity distribution of the light. So, you will see bright dark bright dark.

These are called basically fringe right, these are called basically fringe interference fringe. This where this where this bright fringe you see where this dark fringe you see when if at this it depends on position you know. So, because this light are coming

interfere, they are from the source they are coming right. When depending on the position. There will be path difference between these 2 wave there will be path difference between these. Here whatever path difference here this path difference are different here path difference are different. When this path difference is multiple of lambda or phase difference is multiple of 2 pi then we tell this constructive interference there will be constructive interference and we will get the bright peak bright fringe and when path difference is multiple of lambda by 2 multiple of not multiple odd multiple of lambda by 2 1 can say or the odd multiple of phase difference is odd multiple of pi then you will see this.

This is they are out of phase we tell out of phase. They will distract each other. So, you will see destructive interference. These the interference and diffraction is basically, diffraction is basically, the interference among the secondary wave signal, what is secondary waves? basically waves are coming, waves are coming, we tell plane waves, plane waves are coming means, on this plane this phase are same on this plane is whatever if you draw plane here. So, phase are same.

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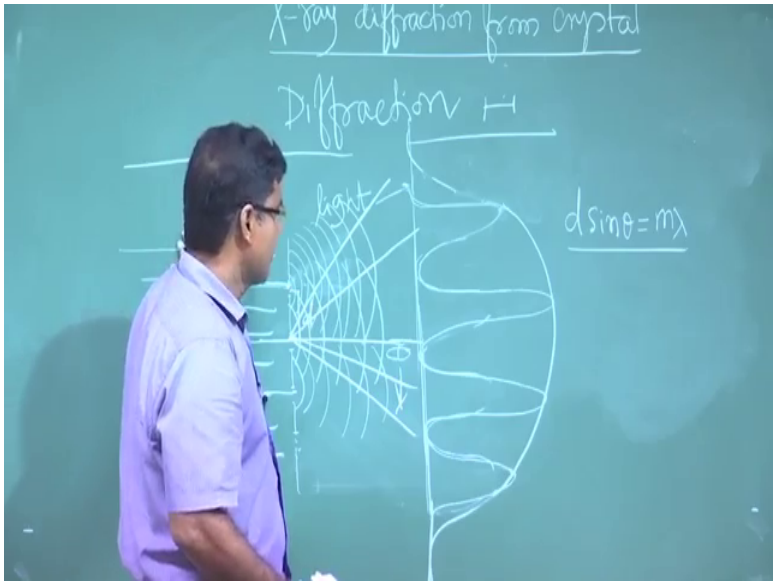

Then we tell it is a plane wave, plane wave is coming and falling on some obstacle you know falling on some obstacle. This obstacle have some hole these obstacle have some hole these obstacle have some hole ok.

When there is a hole on this obstacle, it pass through it pass through it pass through it yeah it pass through it. Then this holes are comparable with the wavelength of light. It is just not it is it does not pass like just as it is. Here it is feel some obstacle. We tell generally people tells this it bends. It bends from it is from this direction it bends to other direction, it bends to other directions, it bends to other direction. So, that generally we tell diffraction, but it is not the good way to define the diffraction. What we tell that, whenever wave comes here waves comes here that this a obstacle it is face some obstacle although hole is there, but wavelength is comparable to this hole off. Here we tell this is the source it acts as a source and it generates it generates it is generates waves similarly from each from each hole.

These we tell the secondary wave secondary wavelength. So, is the primary wave is coming and then getting obstacles. Then this each point this act as a source and they meets the waves. So, these waves are called the secondary waves so. Now, they overlap the secondary waves they are coming from different holes, they overlap this because of this the overlap that we are telling that is they interfere with each other. This basically interference among these secondary wavelengths is basically here whatever we will see there is the diffraction. If it is here basically I have drawn this grating right. It has some grating it has many holes. If you have if this obstacle has only one hole says the single slit diffraction if it has 2 holes then we tell double slit diffraction if it has many holes then we tell it is a grating and grating diffraction ok.

And their distance between these 2 middle to middle if we define by D, this we tell is getting element D. Now here we will get the basically interface among this among this secondary waves and here in case of getting, we will get we will get interference pattern you know this as we have seen for as I drawn earlier. So, the, but this intensity distribution will not be like this. So, it is a modulated with the diffraction pattern of the single slit interference diffraction. It is basically, let me here is basically, we will get intensity distribution is like this. So, all will not have the equal intensity as we have seen earlier for interference case. Here interference peak I am getting, but their intensity is varying their intensity of heading the intensity are varying ok.

This peaks are basically with a principal maxima we tell principal maxima. So, it is equivalent the interference right peaks they are eqvispaced and why do we get this are picture I have done that that this is the intensity the intensity versus this angle theta what

is the angle theta say is basically, with the incident 1. whatever this, it is from a different angle different position. We tell diffraction angle diffracted angle, this it satisfy this condition D sine theta equal to M lambda. So, D is the grating element theta is this basically this diffraction angle theta at different angles, at which angle we will get the maxima. So, if for a particular wavelength whatever going to satisfy this condition. So, we will get different maxima starting this value or m 1 2 3 4 ok.

We get many maxima depending on the first order second order this the order M is order of the interference or diffraction, this M equal to 1 first order, second order, third order etcetera. From grating and diffraction in grating diffraction of the waves visible light we get this type of change of the distribution of the intensity and that follows this expression. These are these are the very important relation where basically here this relation is basically one can get the information of the about the grating element also one can get information about the wavelength if theta is measured and one of them is known. Other one can be find out from this grating that getting experiment. I think I will stop here, I will continue in next class.

Thank you very much.