Experimental Physics - III
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Lecture – 58
X – Ray Diffraction and Crystal Structure

Today I will discuss about X-Ray Diffraction to study crystal. Crystal means if you have a material, now this material is made of atoms. Now how atoms are arranged in the material. So that we define in terms of crystal. Therefore, if atoms are ordered, atoms are arrange with some order then we tell it is the crystalline material.

If atoms are randomly arranged in the materials, then we tell it is an amorphous material. How X-ray diffraction is used to study the crystalline structure of a materials. that is what today I will discuss. X-ray diffraction and crystals.

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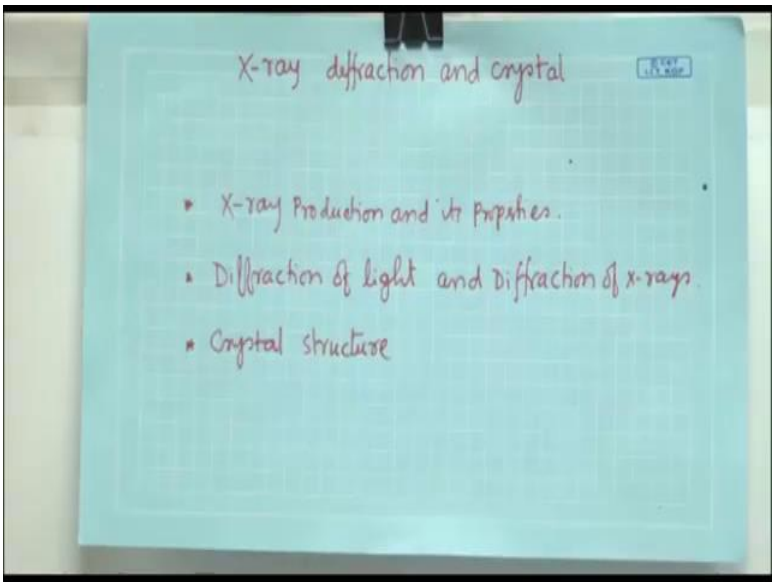

From here, you can see this one should know how X-ray is produced in laboratory and what its property? Then what is X-ray diffraction of light? Then what is the connection of diffraction of X-ray with diffraction of light? That also one has to understand. Then one should know the crystal structure of materials.

I will discuss in three steps: first, I will discuss how X-ray is produced and what is the property of X-ray? Then I will discuss diffraction of light and its connection with X-ray.

Next, I will discuss about the crystal structure and then finally, I will show how this X-ray diffraction is used to determine the structure of a crystal structure of a material,

First, let me discuss this X-ray and its property X-ray and its property. So X-ray; obviously, it is electromagnetic radiation.

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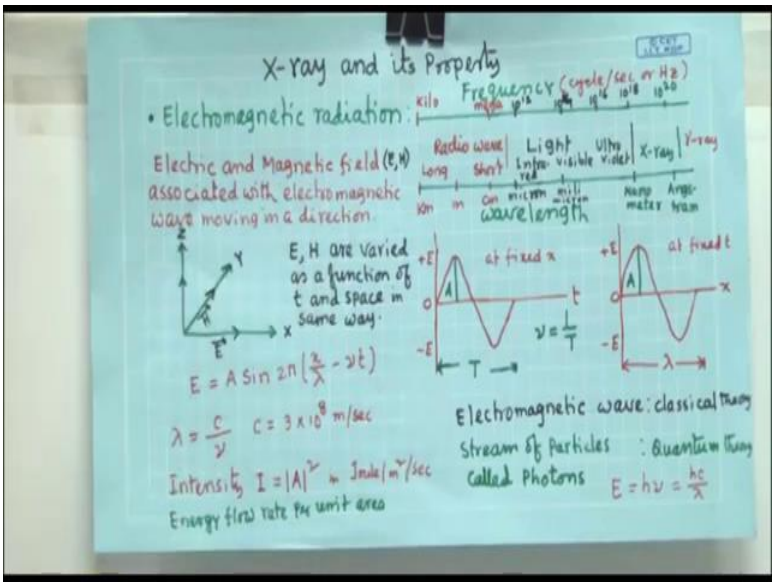

See it has electric and magnetic field component, Associated with electromagnetic wave moving in a direction. Electromagnetic wave it is moving in a direction. electric field and magnetic field is associated with this electromagnetic wave.

So, that means, in electromagnetic wave it is. It has it has electric component E and it has magnetic component H and the Z direction if it is direction of propagation of electromagnetic wave. These 3 E, H and the direction of propagation they are mutually perpendicular with each other,

E and H it's not just constant value, it varies with time and space. In same way, the way E varies, H also varies in same way as a function of time and the space. So that means that is so one can just one can deal with one of them E or H., we prefer to deal with E because E component is very stronger than the H component. Generally, that is why we deal with E, but we do not neglect H. the way H varies the same way the way E varies, the same way H varies. if you just study one, if you just consider one then other one is automatically associated with it.

We do not need to discuss the other component separately. E variation in time is if it is like this. This is the time period capital T then, we tell the frequency of this electromagnetic wave that is mu equal to 1 by T and this variation in space. this one period in space this is called wavelength lambda. This lambda and nu they are related they are related with the with this nu equal to c by lambda.

By electromagnetic wave, this wave concept is it is a classical concept. It's a we consider classical theory when we deal with the wave. electromagnetic wave when it is wave, then we treat it generally using the classical theory. However, in quantum theory, this electromagnetic wave is a beam of particles beam of particles. this particles or steam of particles. This particles are called the photons the called the photons.

It is now discrete. It is as a particle now in no longer it is a wave it is a particle nature. So of course, this in quantum mechanics, quantum particle, it behaves as a particle as well as it behaves like wave. the energy of this photons is written as E equal to h nu h nu equal to hc by lambda light is of electromagnetic is can be considered as a wave as well as it can be considered as a stream of particles, steam of photons,

energy in quantum mechanics mechanical energy E equal to h nu equal to hc by lambda where as in classical theory, the energy of an waves is its a amplitude square this is the amplitude, this is the amplitude, amplitude squares amplitude square is the not energy sorry, its the intensity. Intensity is the square of the amplitude is the intensity.

This intensity is not its nothing but the energy flow rate per unit area. This intensity is related with the energy. In classical mechanics, the intensity is the square of the amplitude and it is related with the energy. energy flow rate per unit area. Unit of intensity is Joule per meter square per second,

This is the classically this we considered the energy or intensity of a wave. Whereas in quantum mechanics, we deal with the energy is a like a discrete particle photons and that is its a energy of quantum E equal to h nu equal to hc by lambda, X-ray is an electromagnetic wave, like other electromagnetic wave. So this electromagnetic wave, their various names are there depending on their range of wavelength and range of frequency, as well as their origin of their of the electromagnetic wave, how it is produced.

This in kilometer meter range this wavelength is in kilometer in meter. That we tell this radio wave then from meter centimeter to micron, in micron range then it tell we tell this the infrared and then millimicron. That is a we tell a visible light visible light is in millimicron range.

Also ultraviolet light. infrared visible and ultraviolet. It has an it's the in micron millimicron range. Then from micron to a nanometer range, it is going then it is X-ray and if it is going to in angstrom in angstrom range 1 nanometer equal to 10 angstrom. Then less than 1 angstrom. then it is gamma ray.

Of course, all are electromagnetic wave their origin, how they are produced there that is different. That is why it has a name are different.

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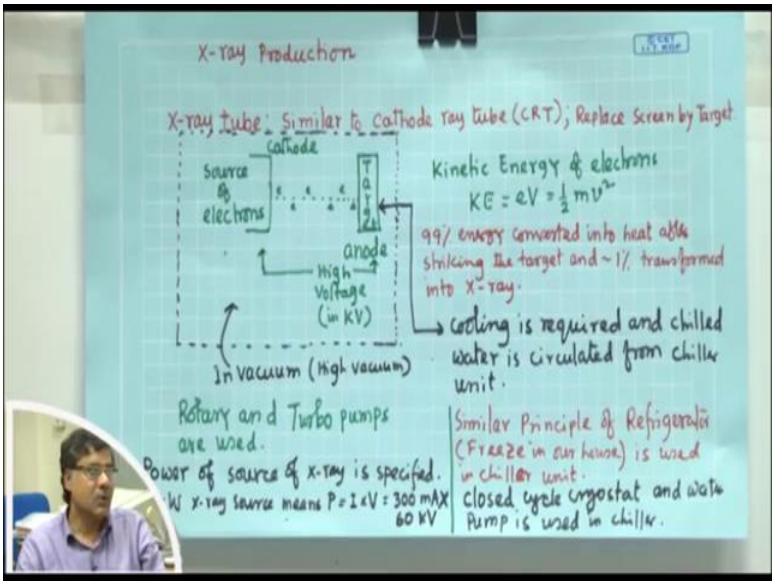

X-ray we use X-ray tube it is just similar to cathode ray tube, as I have discussed during the CRO: Cathode Ray Oscilloscope, their main part is cathode ray tube. In cathode ray tube this electrons are produced and then this electrons are accelerated and it hits the screen. Then we can see the position of the electron beam on the screen. X-ray tube also this similar to cathode ray tube, just if you replace the screen of CRT by a target. A target is a made of a material.

We tell the target. The electron will hit not the screen, it will hit the target it will hit a particular material these there is a source of electrons, cathode and between cathode and target one can tell anode.

There is a high voltage is applied in kilo volt range, high voltage is applied in kilo volt range. Now electrons will eject from this cathode and it will be accelerated due to this high voltage and it will move towards the anode and it will hit the target it will hit the target and when it will hit the target then from target X-ray is generated. X-ray comes out from the target how X-ray is generated from the target. That is what we will discuss.

This electron. this energy of this electron is ev v is the voltage between the anode and cathode and electrons will have the kinetic energy half mv square. With energy half mv square and that v is related with the eV energy of the energy of the electrons in the voltage difference v. when this electrons with this half mv square energy kinetic energy will come and hit this target. 99 percent energy will be converted into will be converted into heat after striking the target and only 1 percent will transform into the X-ray.

1 percent energy of the electron only will be transformed into X-ray, So now, you can imagine here. These highly energetic electrons are coming and hitting this target and 99 percent energy will be converted into heat. there will be tremendous temperature of this target. We need cooling arrangement; cooling arrangement. generally we use chilled water. Chiller unit. There is a unit it is called chiller unit it is just like refrigerator, just like fridge in your house. How this the chamber of the fridge is cooled using the closed cycle cryostat

Here also, same principle used to cool the water and there will be water pump. this it will pump the water, chilled water into the system say to towards the target. That arrangement one has to made has to make to cool this target otherwise; it will just melt after sometime.

To produce X-ray what arrangement we need. We need chilling arrangement cooled water we need. In addition, electrons you see this from cathode to anode, it is moving through the free space. That is that space should be free space, there should not be any air molecule then there will be scattering from the air molecule. that is why we need this whole system whole things in vacuum. We need vacuums its generally high vacuum 10

to the power minus 6 power or milli power vacuum we need. We need vacuum arrangement also

This turbo rotary and turbo pump are used to get the high vacuum. we need also this vacuum arrangement. We need vacuum arrangement, we need cooling arrangement to produce the X-ray also we need very high voltage. It is an in kilovolt range that arrangement also one need for generating X-ray. X-ray this source X-ray source generally commercially available. Now, it has different power you know. The power of the source of X-ray is specified like this say 18 kilo Watt X-ray source. What is the meaning of 18 kilo Watt X-ray source?

Power is I into V. if volt is 6, maximum volt you can apply this 60 kilovolt then and if the current, what is the current? Current in this free space you know, electron are moving this current this current is if 300 milli amperes. current naturally it will be very small current, its milliampere range whereas, voltage you need kilovolt range because it is in free space between this anode and cathode this space is free.

You need very high voltage to pass current through this free space and that current amount will be very small. That is that is a here you can see generally current in is in milliampere range. Why does voltage in kilo volt range? One should know what is the range of current and voltage in the source.

18 kilo Watt power X-ray source is very powerful X-ray source, but higher the power intensity of the X-ray will be higher. It will be convenient to study the material. that is why people try to have the higher power X-ray source in the laboratory.

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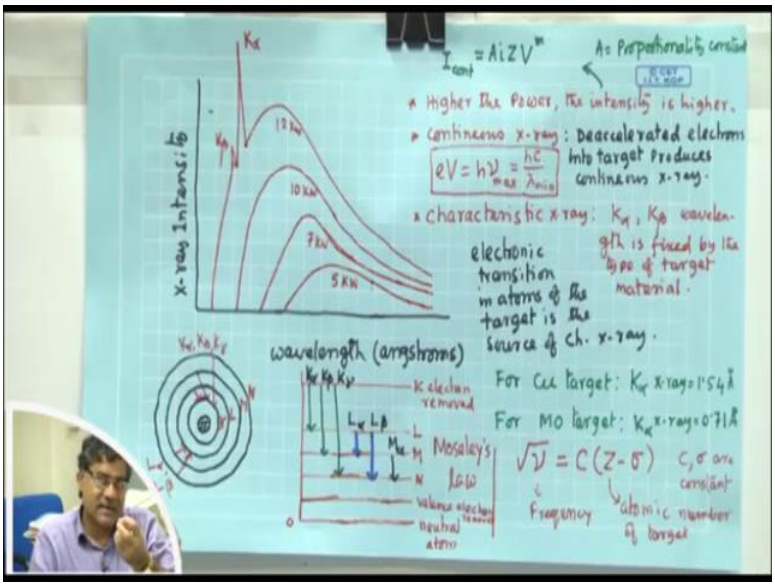

So now, as I told that electron accelerator electron will hit the source, hit the target will hit the target and from the target, X-ray will be generated, X-ray will come out. That then if you just catch this X-ray detect the X-ray and plot, if you plot the X-ray as a function of wavelength as a function of wavelength and the X-ray intensity as a function of wavelength. This depending on the power depending on the power of the X-ray source, what is the current and voltage we have chosen. It will vary like this it will vary like this,

When it is higher power then it have otherwise it is a continuous. You see this there is a minimum wavelength and then above that wavelength this all sorts of wavelengths are there and there is a peak intensity is highest at some particular wavelength, but this the X-ray will come out. So that is having the continuous wavelength all sorts of wavelengths are available. Now at higher power generally. These are continues this we tell the continuous X-ray continuous X-ray.

Apart from this continuous X-ray sometimes some peaks comes, as if here I have written K beta K alpha. this we tell the characteristics X-ray. All the time this continuous X-ray will come, source of continuous X-ray that is when the electron hit the material hit the target. Now, it will painted into the material and it will be deaccelerated.

Any charge particle when it is deaccelerated or accelerated. It emits electromagnetic radiation, due to deacceleration of the electrons into the material, into the target. There will be radiation and that radiation is it is that is an X-ray continuous X-ray.

That is the origin of continuous X-ray and with this continuum X-ray, some characteristics X-ray some peaks are superimposed. The origin of this peak is the characteristics of the target material. Therefore, that origin of this characteristic X-ray is the atomic transition of atomic transition in atoms. Electrons in the atoms or transform from one energy level to another energy level. that is the source of these characteristics X-ray.

Here you can see the nomenclature of this characteristics X-ray. It is a nucleus then there is a circular orbit. So now, when this energetic electron hit the target so the some electrons of atoms will excited in the higher energy level, then after sometime, they will come back to the original level.

Therefore, there will be; there will be radiation due to this kind of transition and when this transition you will get some radiation. That radiation is wavelength in the range of X-ray. When transition from higher energy level to the K level. those X-ray are called K alpha, K beta, K gamma, ok

In addition, when this transition from higher energy level to the L level, so then its called L alpha, L beta, L gamma. This way this there is a nomenclature of K alpha X-ray, K beta or L alpha L beta. naturally you know that to get this K X-ray. One has to knockout electron from these core energy levels. You need higher energy of the electrons, which will hit the target.

That is why you need higher power X-ray source. If it is lower power X-ray source, then this K X-ray will be absent you may get other X-ray L alpha, L beta, but their intensity are small we generally prefer K alpha X-ray for our experiment.

As I mentioned this, is the way we produce X-ray in the laboratory and what is the source of the X-ray? How it is produced? That is what I was trying to explain and this what will be there is a relation between the frequencies of the X-ray, characteristics X-ray with the atomic number with the atomic number. This square root of nu frequency equal to see a proportional constant Z minus sigma, sigma is the skin constant.

It is proportional to square root of nu is proportional to atomic number of the atom of the target. this is nothing, but Moseley law, this is Moseley law and as I told this this characteristic X-ray depend on the target material. If you take copper target ok, then this

K alpha X-ray this wavelength is 1.54 angstrom. If you take molybdenum target, then this K alpha X-ray this wavelength is 0.71 angstrom different target people use for in the laboratory produce the X-ray.

here this another thing say X-ray intensity X-ray intensity X-ray intensity is here you can see, it is proportional to the current voltage V to the power m is vary it depends on the this power is m. m may not be 1, it can be some other value, its a constant for a particular its a constant for a particular system and Z is the atomic number. Intensity depends on the atomic number of the atomic number of the target material.

if higher the power then intensity is higher; obviously, from here you can see its a intensity is a proportional to i and proportional to V to the power m. that is why higher power X-ray source we prefer because the then outcoming X-ray intensity will be higher and for studying the crystal structure using the X-ray diffraction. We need higher intensity of X-rays.

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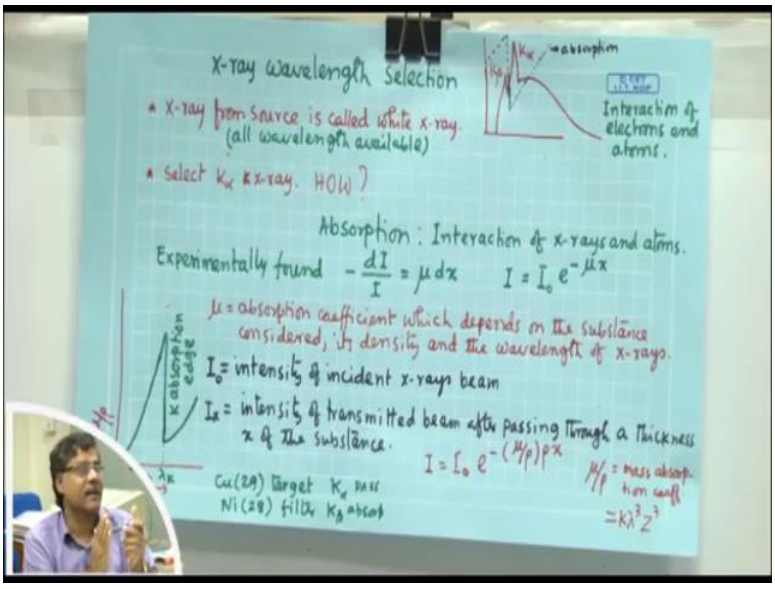

As I told, this from the source X-ray is coming like this, continuum X-ray with some peaks characteristics peaks. Now if I want to select this K alpha X-ray for our experiment I have to take out this K alpha X-ray and other X-ray should be stopped. how it is possible? For that, one has to know this absorption, absorption phenomena. that is nothing, but the interaction of X-ray and atoms.

Experimental it is found that I equal to I 0 e to the power minus mu x. What does it mean? I 0 is the incident X-ray when it is passing through a material, it is passing through a material when it will covers the x distance. at x distance its intensity will change exponentially.

So it depends on mu, mu is the linear absorption co-efficient linear absorption co-efficient which depends on the substance considered. Its density and wavelength of the X-ray. It depends on the mu it depends on the wavelength and the material the density of the material,

We prefer to express this in terms of mass density. Mass density is mu by rho mu by rho is the mass absorption co-efficient mass absorption co-efficient and this mass absorption co-efficient is proportional to the lambda cube and Z cube. If higher Z absorption will be higher, here Z to the power cube and it is a lambda dependent what people do? People use filter we tell the filter absorption filter we used to absorb all wavelength except a particular wavelength.

Say here we want to select K alpha. This K alpha this we have used the source here say copper source we have used. if we use copper source if Z is 29, atomic number is 29. So now, people use the nickel filter nickel material, a sheet of nickel material. If we use; if we use the just a material whose atomic number is slightly less than the material of which is producing this K alpha. Nickel it is an atomic number is 28,

What happens? This absorption this absorption we tell the absorb K absorption edge absorption edge means this K absorption edge means when the energy to knockout you see, this K energy level. To extract K electron from this from the atom we have to supply energy. If it gets sufficient energy, to come out from this K from the K shell. At that point if energy is close to the energy of this binding energy of this K electrons. There will be huge absorption at that energy, at the frequency, at that wavelength,

That is why if we use the nickel whose atomic number is 28 which is close to the copper, copper we have used as a target and this K alpha K alpha how it was generated. from higher energy level to the K level, the when this electron jumps so corresponding that energy difference come out as a K alpha X-ray. this K alpha, the energy of this K alpha will be close to the absorption edge of the K absorption edge of the filter material the that

filter material, if filter material have the atomic number slightly less than the target material,

This is the absorption curve. there is sharp absorption at this place. there will be absorption like this here at this just at this level absorption is less, absorption is minimum, So this is the position at the minimum position this is the position higher this K alpha position, so this curve here if you put here, so it varies just like the absorption varies like this. Absorption is very high now here very low, low minimum and then again very high.

All will be absorbed except this K alpha line. this K alpha X-ray we can select using the nickel filter if it is copper target, So using the filter, absorption filter we generally select 1 wavelength generally, K alpha X-rays from the white X-ray. Whatever all the time we get white X-ray from the X-ray source, now from that X-ray source we can select we can select particular X-ray, generally we prefer K alpha because its intensity is higher and it is also easy to find out the suitable filter absorption filter for that,

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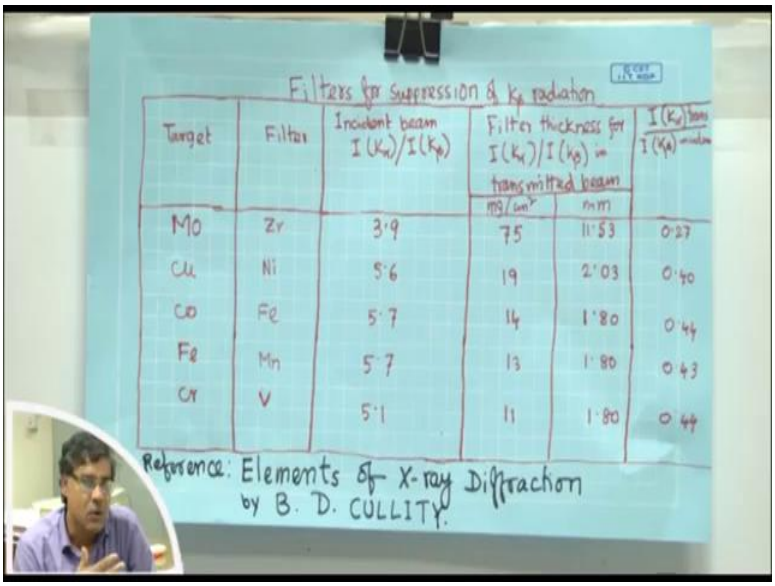

Therefore, this is. Here there is a data here there is a data that this filter for suppression of K beta radiation. K alpha and K beta generally this in X-ray, characteristics X-ray their intensity is very high compared to the continuous X-ray. Mainly one can see this K alpha and K beta that is the higher highest intensity compared to other intensity of continuum X-ray. when you will use filter when target is this that filter is used just less

than 1, you know the copper, nickel, cobalt, iron just 1 atomic number less this for filter then the target 1.

If you use this is the data experimental data. I have taken this elements of X-ray diffraction by B D CULLITY. This is the very fantastic book of on X-ray diffraction. If you have chance, you can read this book from where I have taken data and this data is showing if you use filter.

You will get so your that intensity of K alpha and intensity of K beta. this ratio it depends on the thickness if you take it will depend on the thickness of the filter. One has to choose proper filter as well as there will be drastic you see, here you can see this that K alpha and K beta this is the height highest intensity.

If you want to if, you want to select K alpha, K alpha. this K beta we have to; we have to drastically reduced this K beta. this K this intensity of K alpha with respect to intensity of K beta it has to be; it has to be reasonable so that it can may not be the perfectly monochromatic, but its a its close to the monochromatic light. Other it is not monochromatic at all so but intensity of other wavelength will be very small compared to the intensity of K alpha.

That way we use filter although it cannot give very good monochromatic light, but it give a light of very high intensity of a particular wavelength. That is K alpha compared to other intensity of other wavelength this is about the about the X-ray, there are more things on X-ray.

I think in next class I will continue this discussion.

Thank you.