X-Ray Crystallography
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Lecture – 08
Basics of X-Rays

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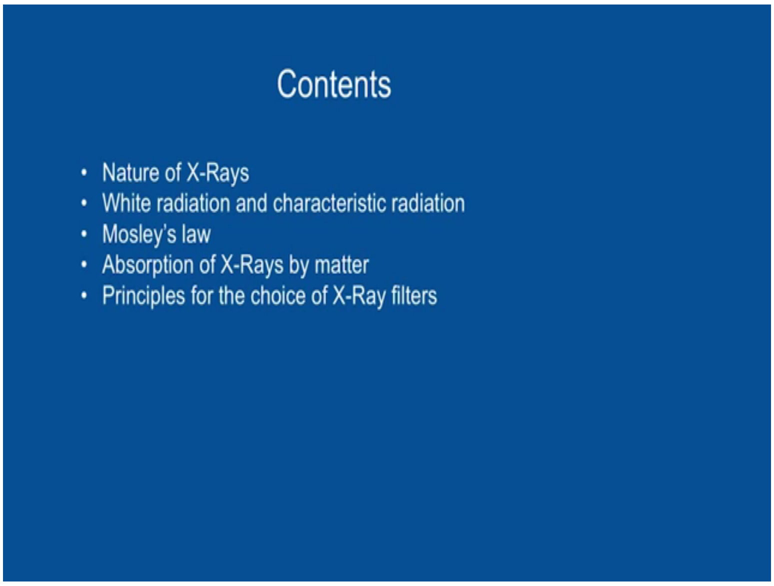

Up till now I have been discussing about crystals; what crystals are, how atoms are arranged in a regular and periodic fashion in 3 dimensions in crystals, what is meant by the crystal systems, unit cells lattice parameters etcetera. Then I discussed about the way atoms are arranged at the lattice positions and also how atomic groups are arranged throughout the 3 dimensional crystals. Now the thing is with a naked eye it is not possible to figure out the locations of atoms in the unit cells of crystals, but it is very important to know the structure or actual crystals, you know what kind of crystal system they have, what kind of lattice parameters they have, what is the units alike, etcetera, etcetera.

So, how we are going to do that? Why this is so important to know about the structure of crystals? Because the structure of crystals will dictate what kind of property the material is going to have. And since we cannot see through the crystal with our naked eye, we need to send some kind of an agent through the crystal so that that agent will bring in all the information from within the crystal. So, this we normally do by using what are known as X-rays.

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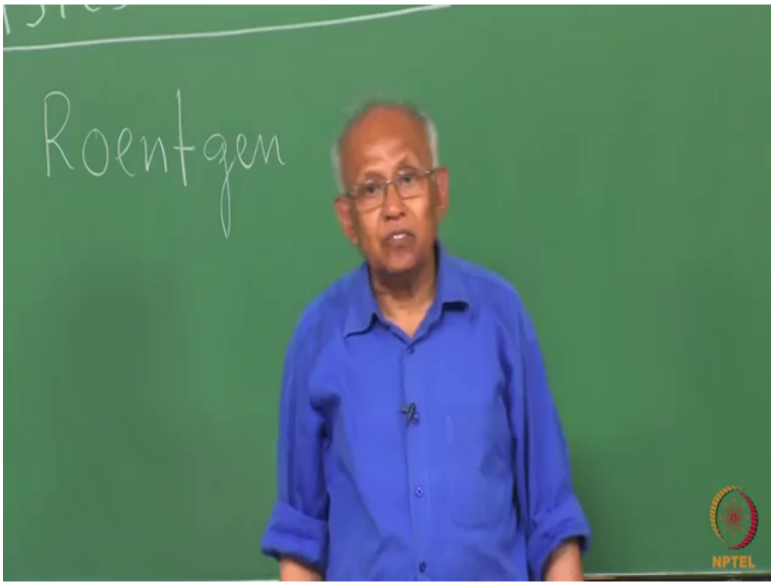

So, in this lecture, I will deal with the basics of X-rays. Now X-rays were discovered by the German physicist Roentgen discover it 1895 by the German physicist Roentgen he found this new kind of rays of experiments which have lot of similarities with ordinary light in the sense that this X-rays they are electromagnetic radiations as is ordinary light. Now X-rays an affect photographic films in the same manner as ordinary light X-rays can travel in straight lines like ordinary light, but there are some basic differences also. X-rays are much more than ordinary light and the X-rays waves are much shorter than light rays.

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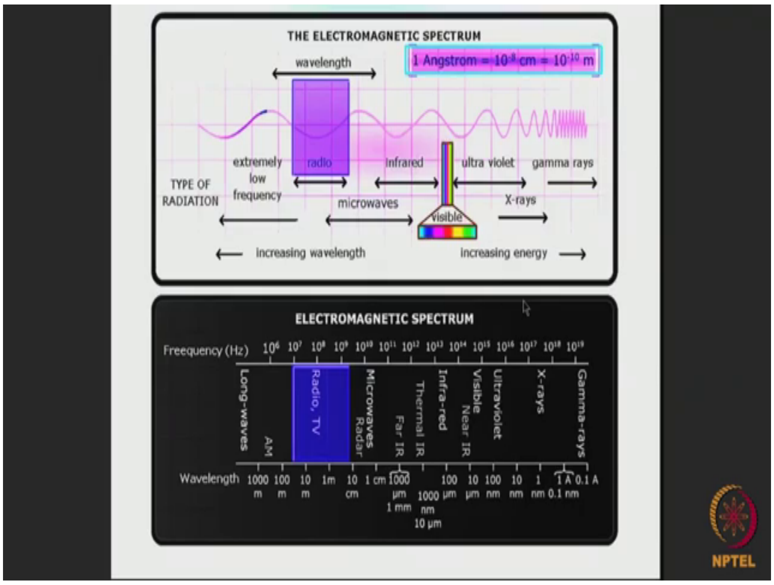

Now, here is the electromagnetic spectrum. It shows the different types of radiation with their frequencies and this is the range for visible light and this is where the X-rays come. Normally the wavelength of X-rays we use in the study of crystals is about 0.5 to 2.5 angstrom wavelength.

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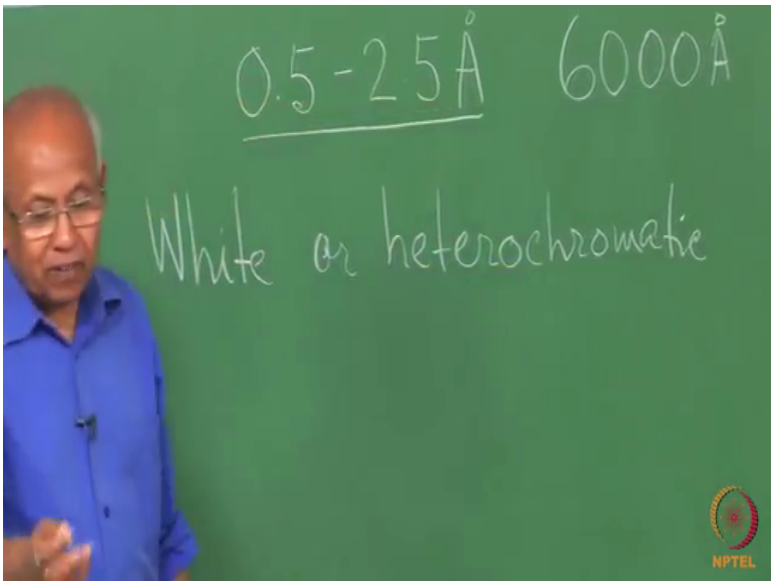

So, this is normally the wavelength of X-rays which we use to study crystals. On the other hand the average wavelength of visible light is of the order of say about 6000 angstrom. So, you can say that X-rays are much more penetrative than ordinary light. So, this has got certain advantages which we normally utilize to study crystals with.

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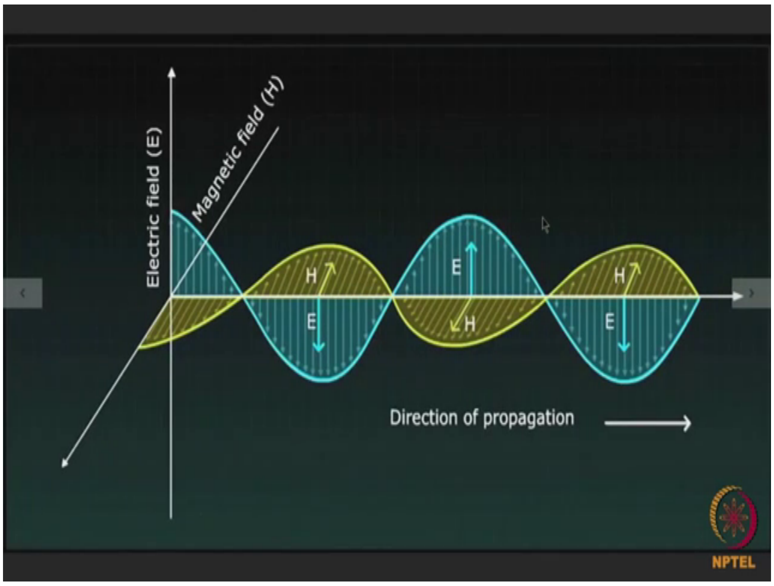

Now, as we have already mentioned that X-rays are electromagnetic waves. So, what is an electromagnetic wave? That means X-rays are associated with both an electrical field and a magnetic field. So, if this is the direction of propagation of X-rays say in the X direction then in the Y direction you can find an electric field associated with the wave and in the Z direction you can find a magnetic field associated with it.

Since the magnetic field is of no concern to ask in this study we are not going to mention it at all. So, it is the electric field that we will talk about. Now the electric field and the magnetic field you know which they can assume any direction in the Y Z plane. So, if you consider the Y Z plane in the Y Z plane the electric field and the magnetic fields which are perpendicular to each other they can assume any position in the X Y plane. If that is the case we say that the radiation is un-polarized.

On the other hand if for you know we could have the electric field lying in the X Y plane in that case we will say that that the wave is polarized. Now the electric field is a function of both time and space.

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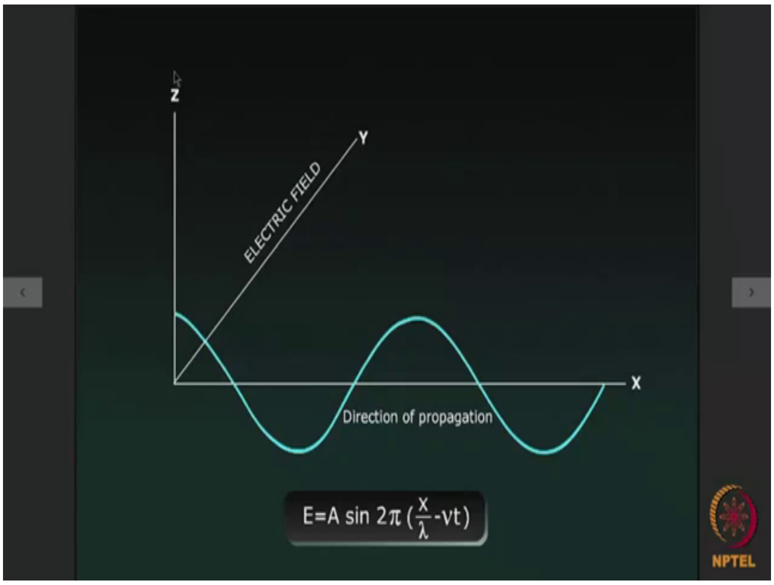

And this is how the electric field varies with respect to these terms and with respect to time both. Now how X-rays are produced? Now X-rays are normally produced by allowing a beam of highly energetic electrons to strike a metal target.

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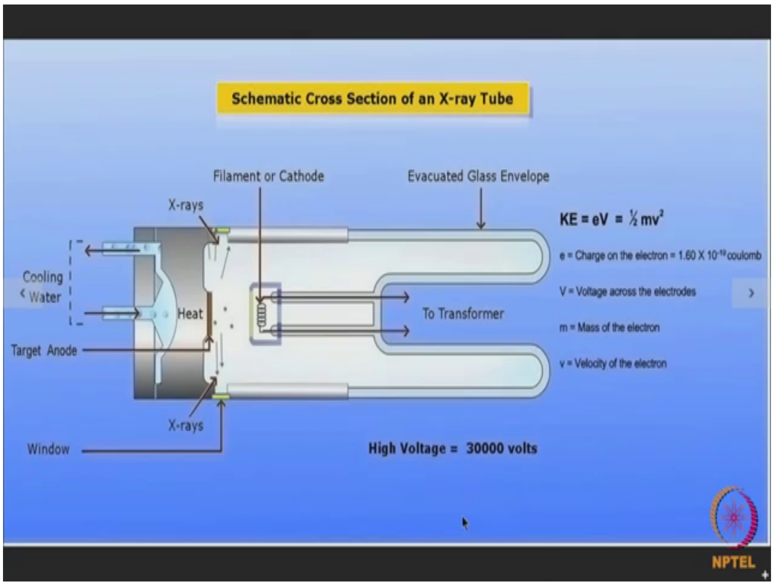

now this is a typical schematic cross section of an X-ray tube and here we have a filament or a cathode made up of say tungsten and when a current is passed through this filament there will be thermionic emission of electrons and if we have a anode or a target made up of a metallic material or an alloy and if a high potential is maintained between the anode and the cathode and the high potential maybe of the order of say 30000 volts or even more.

Then what will happen the negatively charged electrons will be drawn towards this anode of the target and due to the impact of this electrons some X radiation is produced which is invisible to the naked eye and you know in the tube which is a highly evacuated one you provide some windows made up of very thin low absorbing material like beryllium and you can take the X-rays out of the tube and you can utilize that X-rays for all crystallographic purpose now due to the impact of the electrons with the target the target becomes heated to a great extent.

And that is why you know the target must be kept cooled by passing cooling water otherwise the temperature of the target will become very high and the material may melt. So, the kinetic energy of an electron of charge e passing through a potential difference of V will be equal to e V and that can be equal to half m V square where e is the charge on the electron V is the voltage across the electrodes m is the mass of the electron and small V is the velocity of the electrons.

Now, let us suppose that we have a target made up of molybdenum say we have in the X-ray tube a target made up of molybdenum and we start with a potential difference of 5 K V between the anode and the cathode. So, what we observe who we observe from the tube the X-ray that comes out is made up of a large number of wavelengths.

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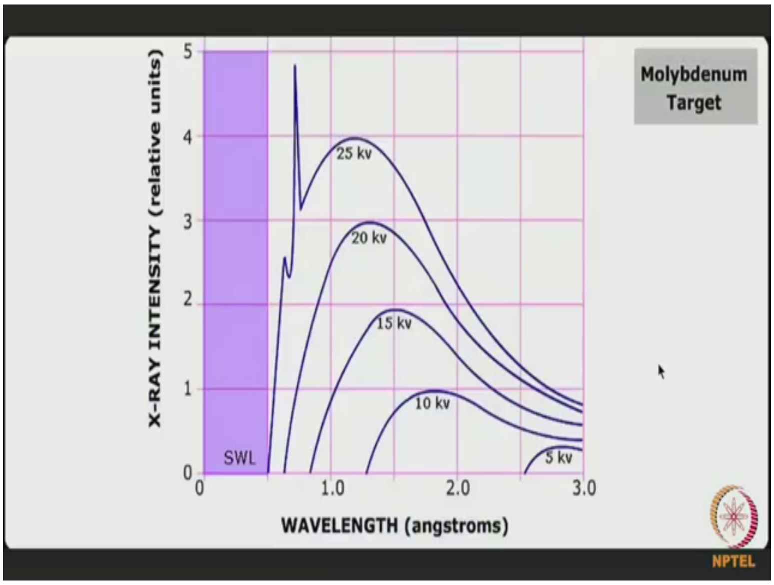

So, those wavelengths are. So, close that we can plot the intensity of individual waves and their wavelength by a smooth line of this type say we have maintained a potential difference between the anode and the cathode which is of the 5 K V. So, we produce quite a few you know the radiation that is coming out of the tube is made up of a number of you know wavelengths and the wavelengths are very close to one another so much so that the wavelengths that are produced you know if you plot their intensity and a wavelength we can draw it by a smooth line of this kind well you should know very well a smooth line you know you know the meaning is the wavelengths that are produced discrete, but still they are very close together we can denote them by a smooth line of this type.

Now, let us say increase the potential to the 10 kilo volt and then again if we measure the wavelengths if X-rays coming out of the tube and the intensity of each and every wavelength and if we plot the intensity versus wavelength we get a curve of this type then if we go for say 15 kilo volt potential difference then you know it goes in this fashion with 20 kilo volt this fashion and for the molybdenum target when we apply a potential difference of 25 kilo volt then over and above a host of wavelengths that we get we get 2 very sharp wavelengths as shown by these 2 lines over here and these wavelengths over here these wavelengths this and this are known as the characteristic radiation.

So, to begin with before we go up to 25 kilo volt whatever voltage we apply across the anode and the cathode we get a host of radiation different wavelengths. So, that host of radiations of different wavelengths is known as the white radiation or heterochromatic white or heterochromatic radiation many wavelengths, but what happens when we raise the potential to 25 K V over and above the white radiation we get 2 very sharp wavelengths very high intensity compared to the rest and these are known as the characteristic radiations. So, these are known as the characteristic radiation.

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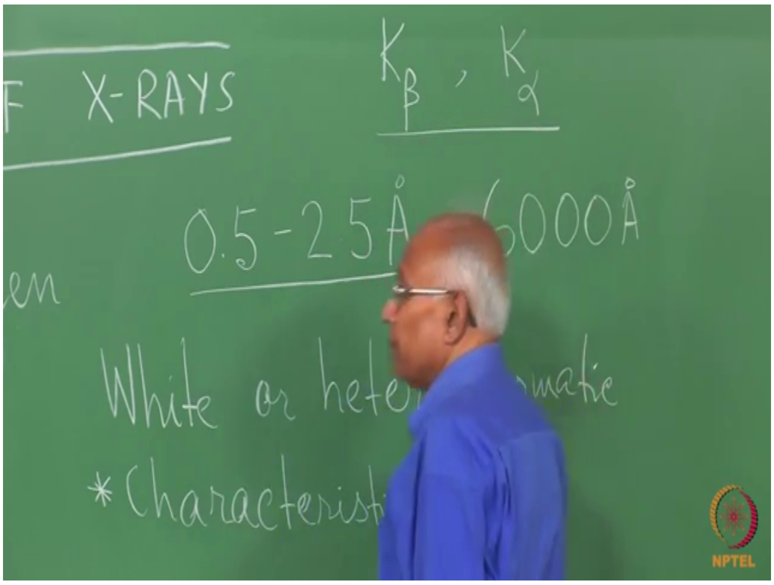

So, why it is called characteristic why and what it is characteristic of it is characteristic of the target that has been used if you use a molybdenum target the characteristic radiation starts coming at say 25 K V and more for some other target the characteristic radiation will appear at a different voltage. So, that is why the characteristic radiation is very much dependent on the target materials it is a characteristic of the target material now this wavelength here is known as the K beta wavelength this wavelength is K beta the shorter one and the more intense characteristic radiation of the larger wavelength is known as the K alpha radiation.

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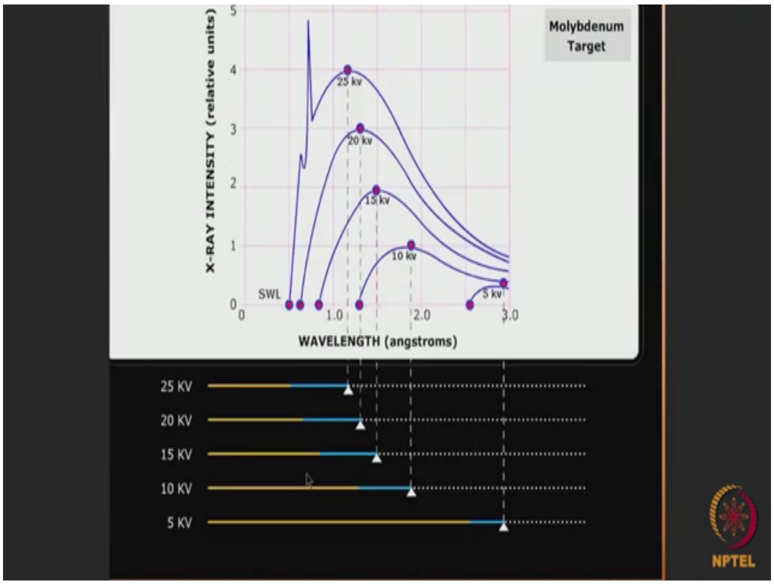

When we study the intensity versus wavelength plots at different potential potentials across the anode and the cathode we realize 2 things; 1 is at any particular voltage used there is a minimum wavelength radiation that is obtained for example, when the potential is 5 kilo volt we find that this is the minimum value of the wavelength that we get in the white radiation now when we increase the potentials with 10 K V then what we find we find that this limit of wavelength which we got in case of 5 K V now it becomes even shorter. So, for 10 K V this minimum wavelength that we can get is shorter in case of what we got at K V. So, this limit is known as the short wavelength limit or SWL.

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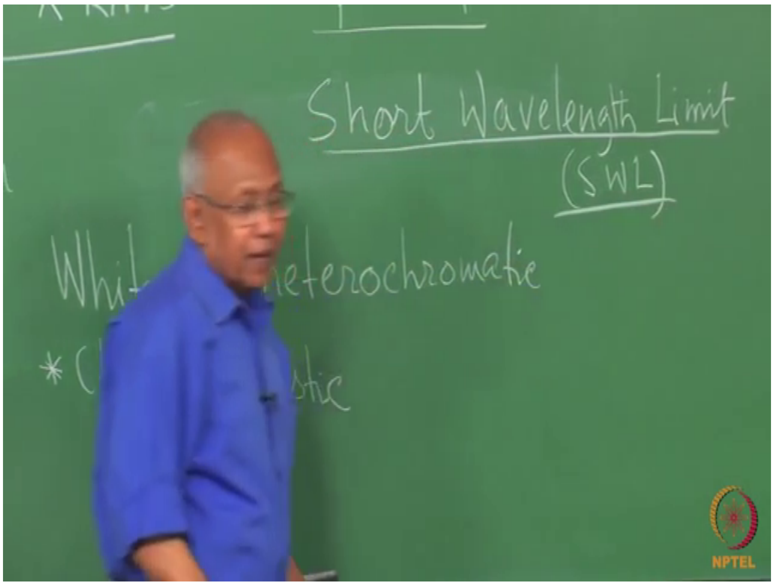

So, this limit is known as is known as the short wavelength limit or SWL.

Now, as we increase the potential even further say 15 K V again we find that the short wavelength limit goes to even shorter value. So, 2 things we notice 1, the maxima in the plot you know it shifts towards you know it improves the maxima the value of the maxima goes up as we increase the potential not only that it shifts towards the left and at the same time the short wavelength limit also goes to shorter values. So, this is after 15 K V potential between the anode and the cathode and then we apply a potential of 20 K V this is the kind of plot we get the short wavelength limit is then even shorter and a 25 K V we find it is even shorter now if we increase the voltage to more than 25 K V in case of molybdenum target the entire plot entire plot you know shifts in a manner similar to the other ones and these characteristic radiations also become more sharp. So, as I mentioned this characteristic radiation is called the K beta radiation and this characteristic radiation is known as the K alpha radiation K beta radiation wavelength is shorter than that of K alpha.

Now, if we use as I already said another kind of material as a target material say nickel or iron we will find beyond a certain voltage corresponding to that metal you will again get the characteristic radiation over and above the white radiation, but the threshold voltage might be will be different. So, it depends on the target material at which threshold voltage the characteristic radiations will appear.

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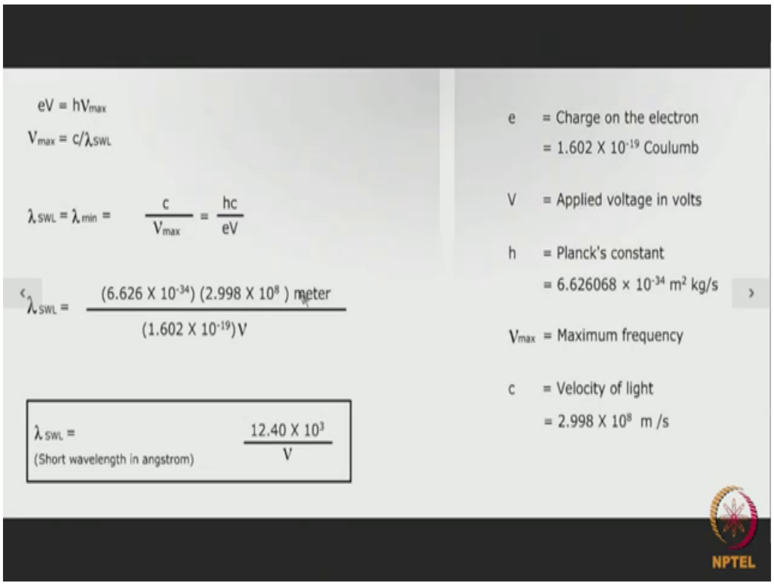

Now if we look at a single electron when it of charge e after going through a potential field of magnitude V now we can write e V is equal to h nu max after all nu max is the maximum wavelength for the electrons. So, nu max we can write is equal to c by lambda SWL you see what happens when the beam of electrons from the filament strikes the target you see after striking the target it may. So, happen that one of the electrons it will lose the entire amount of energy it has in 1 impact and the X-ray photon coming out of that impact will have the highest amount of energy and smallest wavelength maybe another electron which strikes the target looses only a part of its energy.

So, the corresponding extra photon that is produced will have low energy and it will be having a high wavelength. So, since we are dealing with a large number of electrons coming from the cathode and striking the target. So, what will happen we will have a number of cases in 1 case some of the electrons will lose all the energy in 1 impact and the total energy is converted into energy of an X-ray photon?

So, those X-ray photons will be the ones having the highest amount of energy associated with them and therefore, the lowest wavelength value associated with them the other electrons may not be losing the entire energy in 1 impact and there can be so many variations. So, due to the impact of thousands and thousands of electrons we will get a host of X-ray photons of varying energy you know you know which are quite different one from the other. So, we will get a host of electrons you know host of X-ray photons coming out due to the impact of the electrons with the target material and these host of X-ray photons that are coming out they will have all kinds of energy all kinds of energy and therefore, all kinds of wavelengths and that explains why from and when we have an X-ray tube from the X-ray tube we get a large number of X-ray wavelengths or we get the white radiation.

So, when we look at the lambda short wavelength limit which is associated with the electron having the highest energy we can simply write as lambda SWL is the lambda minimum it will be c by nu max from these 2 equations is equal to h c by e V and. So, if we put the value of Plank's constant value of the velocity of the electrons charge of the electron and the voltage we use you know we can find out lambda SWL in angstrom will be equal to 12.4 into 10 to the power 3 divided by V where V is the voltage applied voltage in volts. So, you see that for any particular applied voltage you can find out what should be the lambda SWL of the short wavelength limit.

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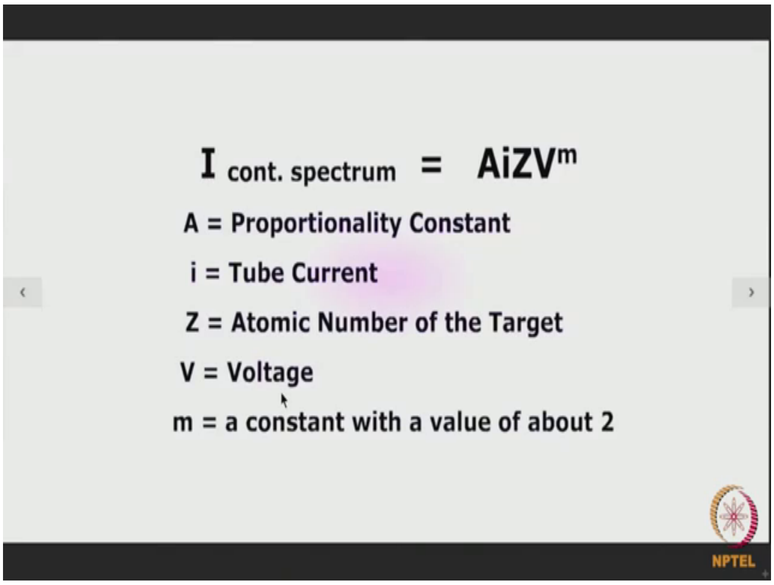

Now if we look at the white radiation which is also called the continuous spectrum the intensity of the white radiation of the continuous spectrum is equal to A i Z V to the power m where a is the proportionality constant I is the tube current Z is the atomic number of the target V the voltage m is a constant with a value of about 2 you see sometimes it is necessary as we say later on to have a white radiation of sufficiently high intensity you know for some particular crystallographic word. So, how to get a high enough intensity of the white radiation of the continuous spectrum?

Now, as we can see here there are several possibilities one of the possibilities is you know the value of Z say if you increase you know a target of a sufficiently high atomic number that will immediately give you a high value of i of the white radiation for example, you know in many cases we use a heavy metal target say for example, tungsten or molybdenum in order to get a high enough intensity of the white radiation now if we look at the characteristic of radiations that are obtained you know due to the impact of the electrons in the target we produce as I already mentioned 2 characteristic radiations like K beta and K alpha.

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Element	Z	K_α	K_β
Cr	24	2.29092	2.08480
Fe	26	1.93728	1.75653
Co	27	1.79021	1.62075
Cu	29	1.54178	1.39217
Mo	42	0.71069	0.632253

Now, this table gives us an idea of the wavelength of the K alpha and K beta radiations for different target material for example, you know if you have a molybdenum target with an atomic number 42 this is the wavelength of the K alpha radiation in angstrom and this is the K beta in angstrom. So, for copper 1.54178 angstrom is a wavelength of K alpha and 1.39217 the wavelength of the K beta radiation. So, in this way you know you can have different values of the wavelengths of K alpha and K beta from the different targets and as we go through this course we will find that how we are going to use them for crystallographic purpose.

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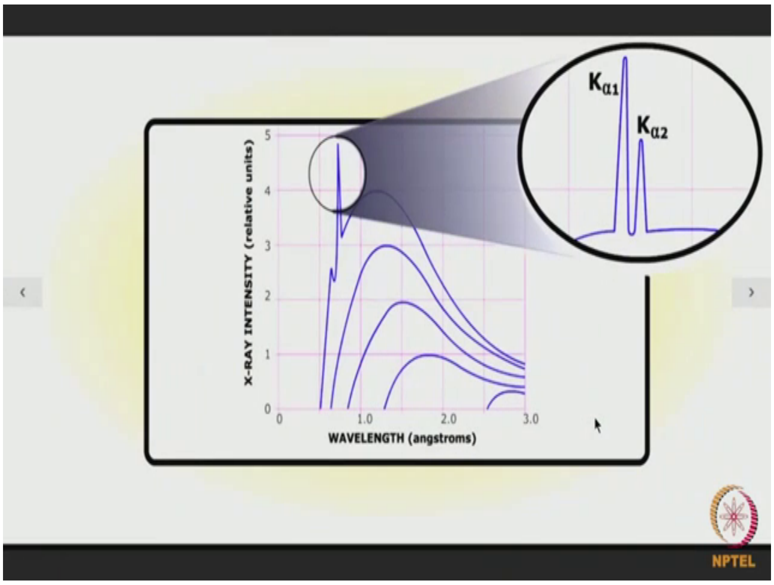

Now if we look at the K alpha radiation it appears to be single wavelength, but. In fact, it is made up of 2 wavelengths very very close by. So, it is a doublet of K alpha 1 and K alpha 2.

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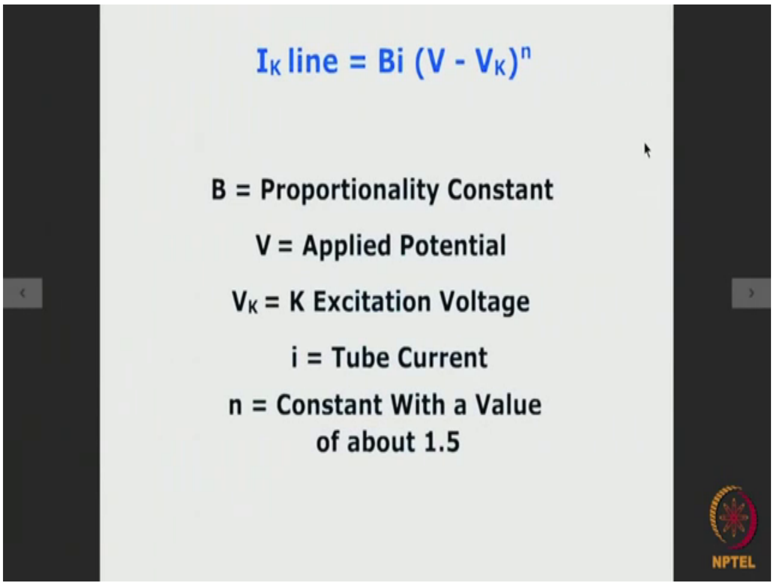

Now, when we look at the intensity of the characteristic lines intensity of the characteristic line can be given by an expression of this type B i V minus V K to the power n here b is a proportionality constant V is the applied potential and V K is what is known as the K excitation voltage or its the threshold voltage beyond which the characteristic radiations will appear. So, it is that voltage below which there will not be any characteristic radiation produced and above which the characteristic radiation will be produced. So, V K is K excitation voltage for that particular target it is not the same for all targets. So, V K will differ from target to target i is a tube current the current passing through the filament and small n is a constant with a value of about 1.5.

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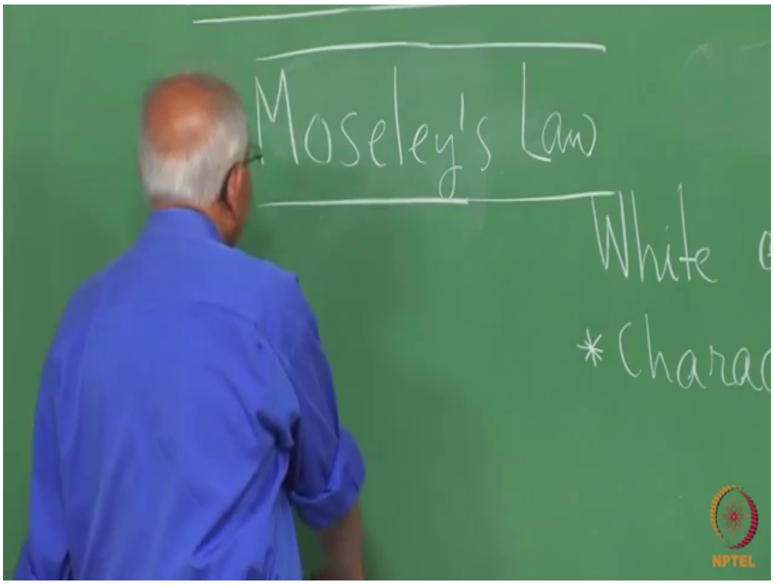

Now it was Moseley who found out a relationship it was Moseley who found out a relationship between the wavelengths of X-rays.

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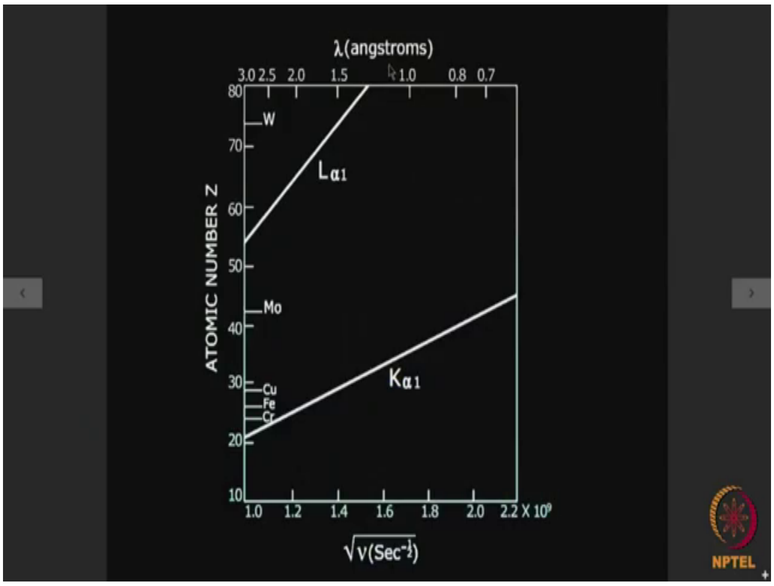

And root over nu the frequency of the waves for different characteristic radiations say for example, the K alpha 1 radiation. So, if you plot atomic number versus root nu they found out that there is a straight line relationship now on this axis the lambda is given the wavelength of the X-rays. So, you see that there is a straight line relationship existing between the atomic number and root nu and this relationship was found by Moseley and is known as Moseley's law.

Now, before we come to discuss the interaction of X-rays with matter I would like to tell you about how white and characteristic radiations are produced from an X-ray tube.

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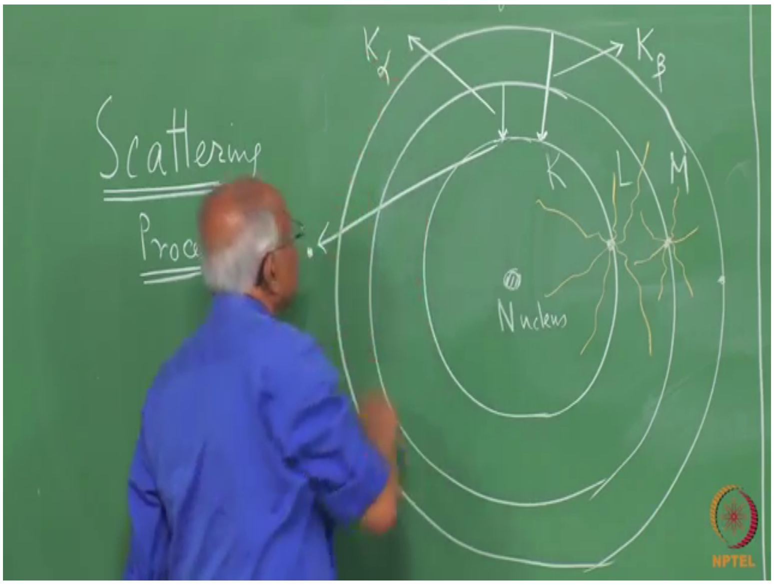

So, as you have seen when a high energy when high energy electron beam falls on the target X-rays are produced now what is the mechanism say here we have got 1 atom of the target material. So, this atom will have a heavy nucleus this centre and the electrons will be arranged in K shell L shell m shell etcetera, etcetera. So, when high energy electrons are incident on this atom in the target material if suppose there is an electron here in the K shell or an electron in the L shell or an electron in the m shell the moment high energy electrons are impacted when the strike against these electrons then these electrons momentarily will take away quite a bit of energy from the striking electrons.

So, momentarily they will be accelerated and according to theory of electron dynamics any accelerated charge will give out energy. So, what happens when this things happens when there is an impact then this electron here in the K shell of the target material it will start to give away the extra energy it got due to the impact in the form of radiation in all directions similar thing will happen you know to the other electrons also they will give up the extra; extra energy got from the striking electrons and it will given out in the form of X-rays in all possible directions.

So, these electrons in the atom of the target material actually what they do they scatter. So, to say the incident energy obtained from the striking electrons. So, the process is called the scattering process their process is called the scattering process. So, when a beam of electrons strikes the atom of a target material the electrons in the atoms of the target material which are impacted start acting as scattering centers and they scatter that radiation that X-ray in all possible directions.

So, this is the origin of the white radiation and you know the amount of energy which a particular electron in the atom of the target can have from the striking electrons will vary a lot and as a result the wavelength that will be produced will also vary a lot and the total totality of all the wavelengths coming or X-ray wavelengths coming out of the target material you know it will constitute what is known as the white radiation or the continuous spectrum.

Now suppose if a situation arises such that the electrons are having energy sufficient to knock out an electron from the K shell say for example, he striking high energy electrons are so strong energetically that they can knock out an electron from the K shell of an atom. So, this is a K shell atom say this is knocked out of the atom by the striking electrons then what will happen in order to you know minimize the energy of the system as a whole in order there will be electrons coming from say the L shell or the m shell to occupy the vacancy over here. So, you know when this electron is you know struck out knocked out from the shell K shell it comes out. So, this vacancy will be filled up by either an electron from the L shell or the m shell.

Now, we know that the energy of a K shell electron is a minimum. So, in order to make the energy the system as a whole minimum what will happen there may be a transition of electron from the L shell to the K shell or there is also a possibility that an m shell electron will come and occupy the vacancy in the K shell now when this kind of behavior happens then what will happen this electron from the m shell which has got a much higher energy than the electron of a K shell if it wants to come from the L shell to occupy the vacancy in L shell it has to give out its extra energy.

So, that extra energy when it gives out it comes out in the form of an X-ray photon and we call it the K beta radiation on the other hand when an L shell electron comes and occupy the vacancy in the K shell then the extra energy which it has to share because L shell electron has a higher energy than K shell electron it has to give up that extra energy in order to come to this position. So, that extra energy comes out as a characteristic radiation which is known as the K alpha radiation.

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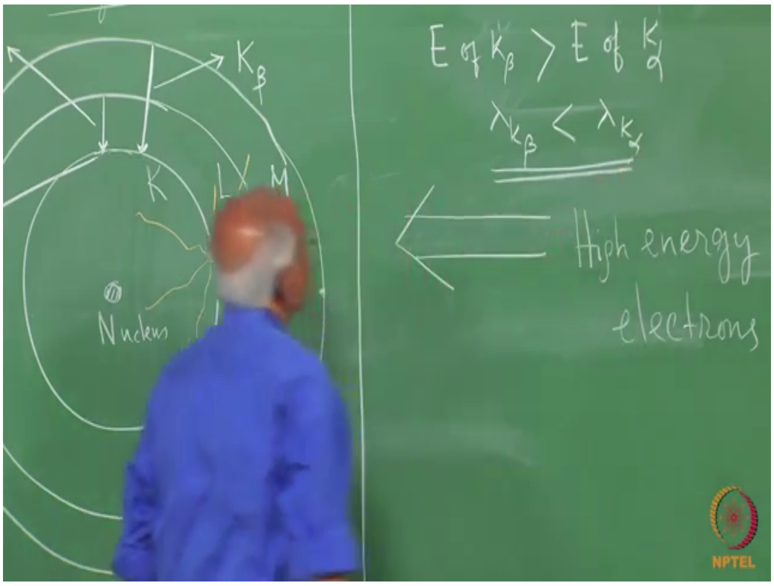

So, what will happen? So, the energy of K beta energy of K beta radiation as you can see over here is much higher than the energy of K alpha radiation because in this case the amount of energy the m shell electron has to geek away is much larger because then energy difference is much larger than over in this region.

So, as a result the wavelength of the K beta radiation is much less than the wavelength of the K alpha radiation. So, this is important energy of K beta X-ray photon is higher than the energy of the K alpha X-ray photon and as a result the wavelength of the K beta X-ray photon is less than that of the K alpha X-ray photon.

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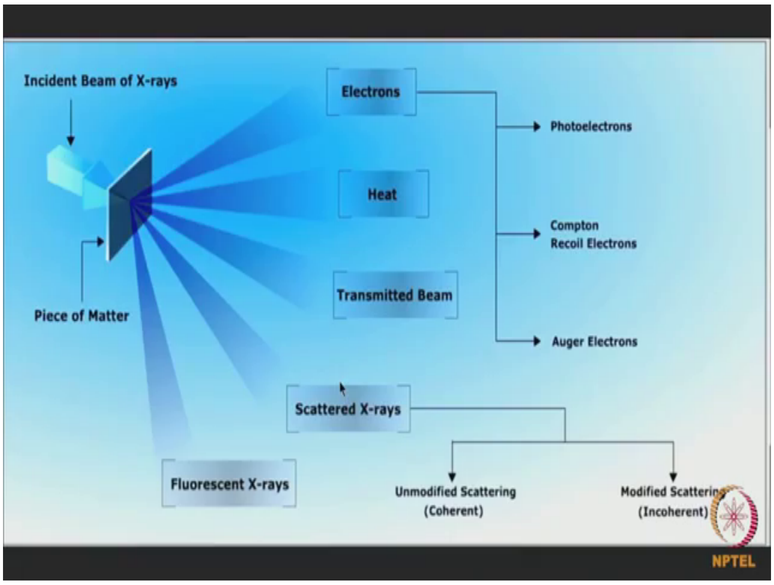

Which we really found out as we have already seen that as we have already seen that the you see the wavelength of K beta is less than that of the wavelength of K alpha, but what about the intensity of K alpha and K beta we find that K alpha has a much higher intensity here as you can see than the K beta why this is. So, well this is due to probability you see when there is a vacancy in the K shell electron then who will have the maximum chance of occupying the vacancy naturally the electrons which are in the nearby shell.

So, the L shell electrons will have a much higher probability to come and occupy the special vacancy as a result you know the K alpha radiation will be much more intense because of probability of such a reaction taking place is much higher than the probability of this reaction to occur. So, you see that although the wavelength of the K beta radiation is much shorter than that of the K alpha radiation the intensity of the K alpha is much higher than that of K beta.

So, now we know what is the origin of the white radiation and continuous and the characteristic radiation now let us talk about the interaction between the X-ray and X-ray beam and a piece of matter you see ultimately we are going to use X-rays into unto the mystery that lies inside a crystal. So, we must know what are how the X-ray how an X-ray beam interacts with a piece of matter say for example, if you have an X-ray beam and if this is a piece of matter then we will see that first of all it produces heat lot of heat will be generated and along with that you will produce a strong transmitted beam. So, the major part of the incident beam will pass through the matter. So, it will give you a transmitted beam lot of heat will be generated and lot of a few electrons will be produced quite a bit of scattered X-rays will be produced and fluorescent X-rays will be produced you see just as a beam of electrons when it strikes a target it produces X-rays in a similar manner.

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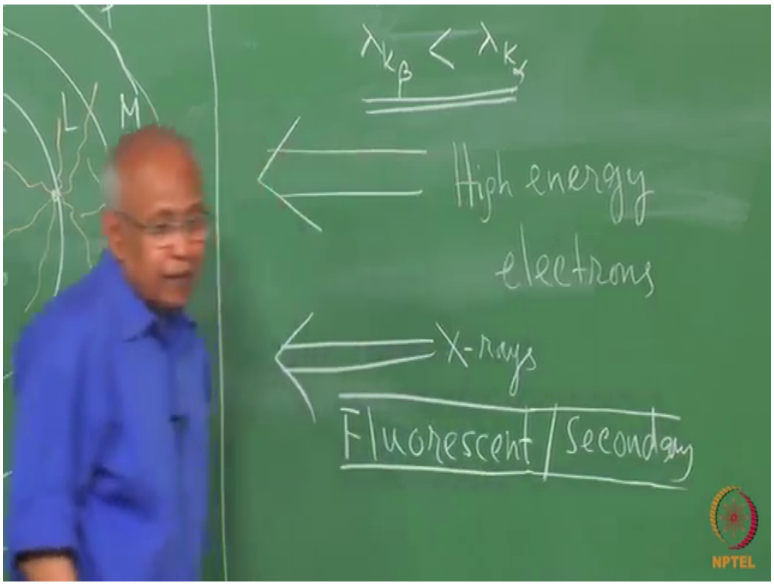

If we have a beam of X-rays if we have a beam of X-rays X-ray photons striking a metal piece then also X-rays will be produced.

And those X-rays are known as fluorescent X-rays now fluorescent X-rays have quite a bit of application in chemical analysis of material as we will see later on. So, we can produce X-rays by bombarding a target material with high energy electrons X-rays can also be produced by bombarding a target with X-rays and the X-ray that is produced thereby is known as fluorescent X-rays or secondary X-rays. So, this is known as fluorescent X-rays or secondary X-rays.

So, you see that by interaction we know you can produce a transmitted beam heat fluorescent X-rays and then there will be scattered radiation as we have already shown here the scattering process and the scattered radiation can be a 2 times what is a coherent and the incoherent type and here the radiation that is scattered is having the same wavelength as the as the incident wavelength and in the other case it has a slightly larger wavelength now this particular type of scattering we will use for what is known as X-ray diffraction and this is a very important phenomenon using which we can find out the structure of crystals easily.

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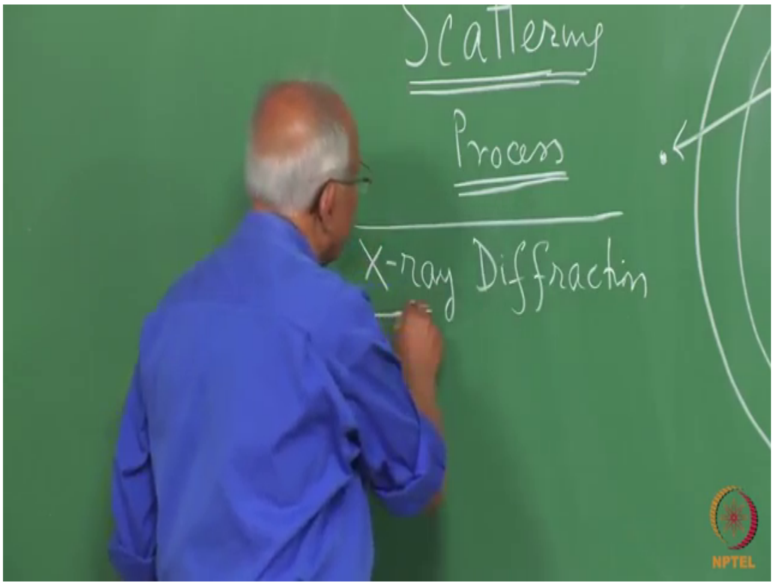

So, using the coherent radiation we can find out you know we can have what is known as a diffraction and that is very useful now different kinds of electrons are also produced for example, there will be photoelectrons what are photoelectrons when X-rays strike against a material it will produce secondary X-rays. So, whenever it knocks out an electron you know from the target material that is what is known as a photoelectron similarly there will be another kind of electrons called the Compton recoil electrons these are produced by the tightly bound electrons in matter and the auger electrons which are produced by the loosely bound electrons in the atoms of the target material.

So, this is the in totality the different kinds of effects that are produced when X-rays interact with matter now I am going to tell you about how matter absorbs X-rays as we are all aware when you pass X-ray through a material part of it gets absorbed and only a part gets transmitted.

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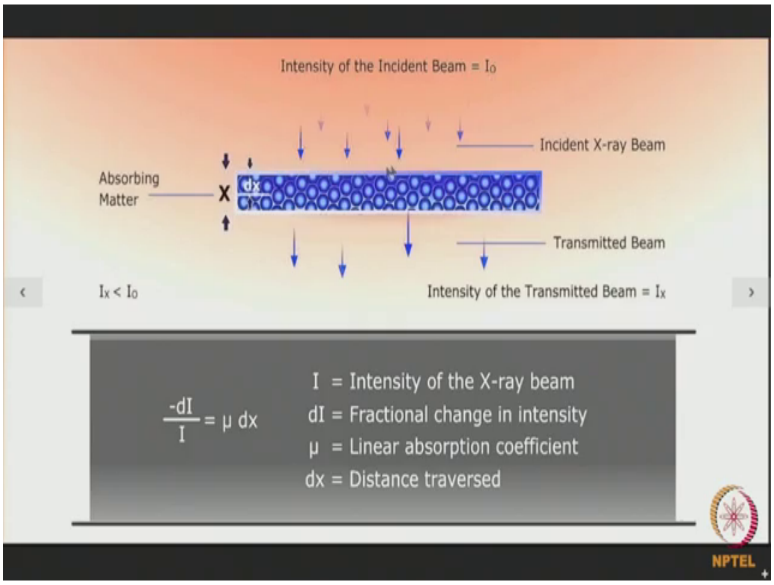

Say for example, say this is a material absorbing material of thickness x. So, this is an absorbing material of thickness X we have got an incident X-ray beam which has got an intensity I 0 and we have got a transmitted beam through this matter and say the intensity of the transmitted beam is I x naturally I x is less than I 0 now the fractional change in intensity when X-rays pass through this matter can be written as minus d I by I; I stands for intensity and it is proportional to the thickness of material it penetrates. So, if we take a very you know small thickness d x to the material and we consider how much is the fractional change in intensity then minus d I by I.

Because you know intensity decreases that s where the minus sign comes it is proportional to d x the proportionality constant is written as mu. So, we can write minus d I by I is equal to mu by d x where mu is known as the linear absorption coefficient of this material.

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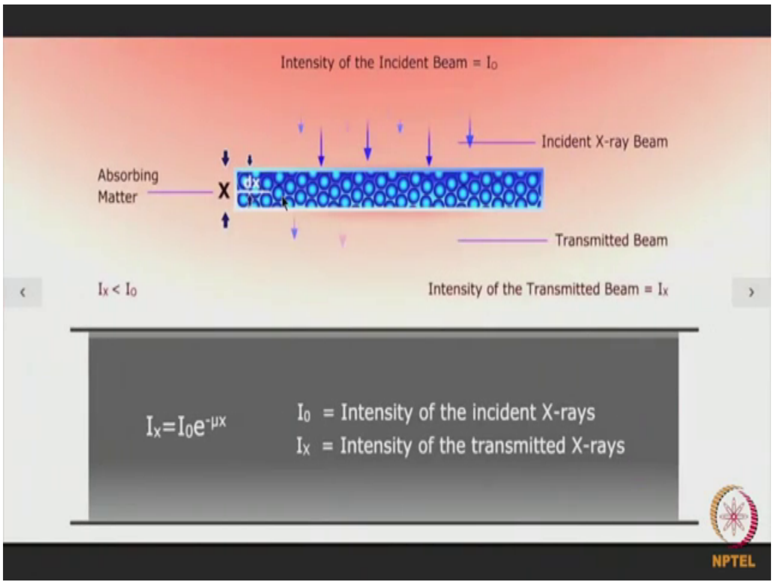

Now if we integrate you know the above equation within the limits we find that I x the transmitted beam is equal to I 0 the incident beam into e to the power minus mu X. So, the transmitted beam and the incident beam are related by this type of an equation.

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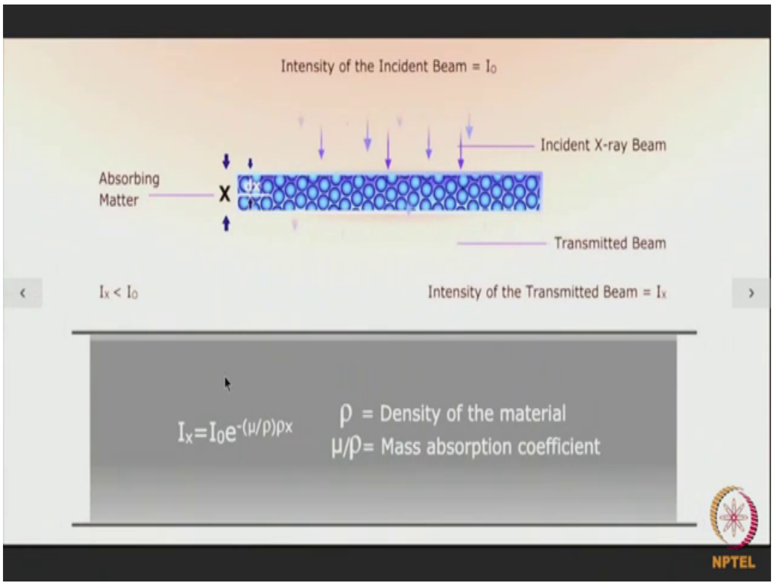

Now instead of writing e to the power mu X we can also write it as e to the power rho into rho X why we do that rho is a density of the material and mu by rho is known as the mass absorption coefficient of the material where as mu is known as the linear absorption coefficient of a material. So, you see that he constant of proportionality mu is known as the linear absorption coefficient of the material where as mu by rho is the mass absorption coefficient of the material.

Now, mu by rho is a constant for any material regardless of in what form it may exist a solid a gas or a liquid sometimes.

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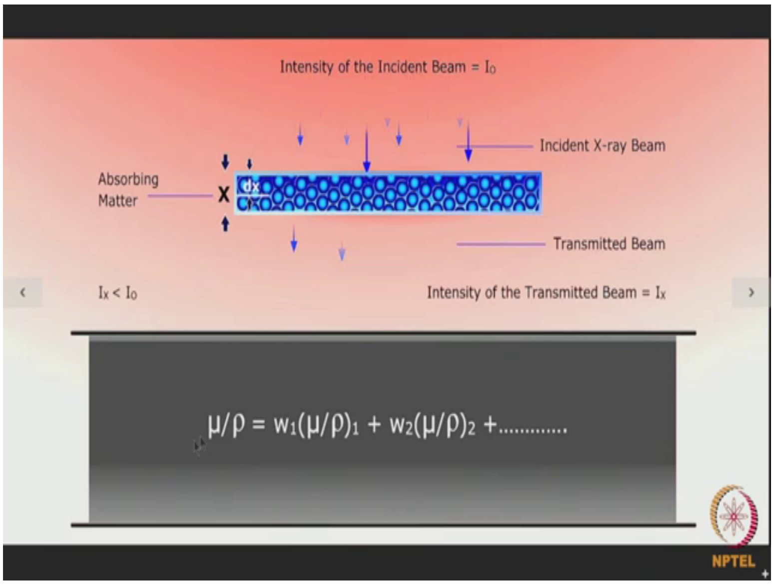

We have a composite material through which X-ray passes through. So, for a composite material how much will be the mu by rho mu by rho say we have a composite 1 and 2 and suppose the mu by rho of the substance 1 is mu by rho 1 mu by rho of substance 2 is mu by rho 2 and say weight fractions of 1 is w 1 weight fraction of substance 2 is w 2. So, in the composite material the total mu by rho if the composite material will be w 1 mu by rho 1 plus w 2 mu by rho 2 now if there are more than 2 components 3 4 5 you can easily find out what is the mu by rho of the entire composite material when we have an interaction of X-rays with matter.

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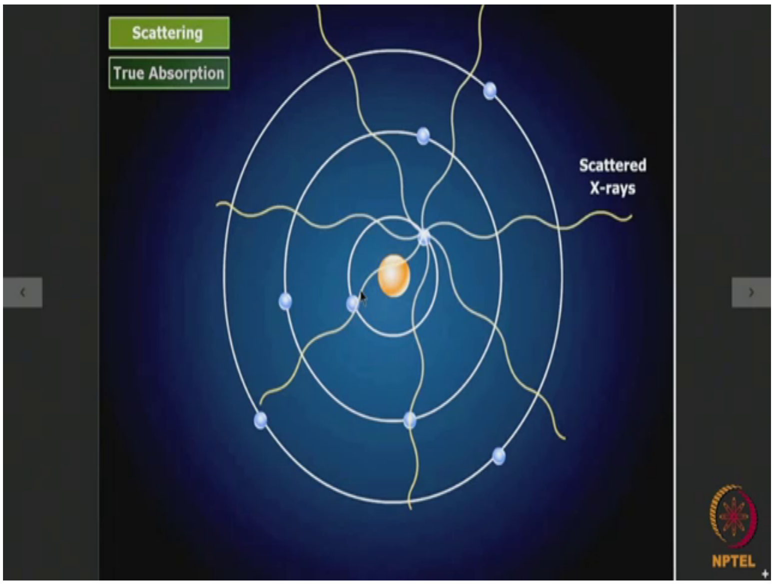

Now, we have realized; what are the things that are possible some of the X-rays will be simply scattered away in all possible directions.

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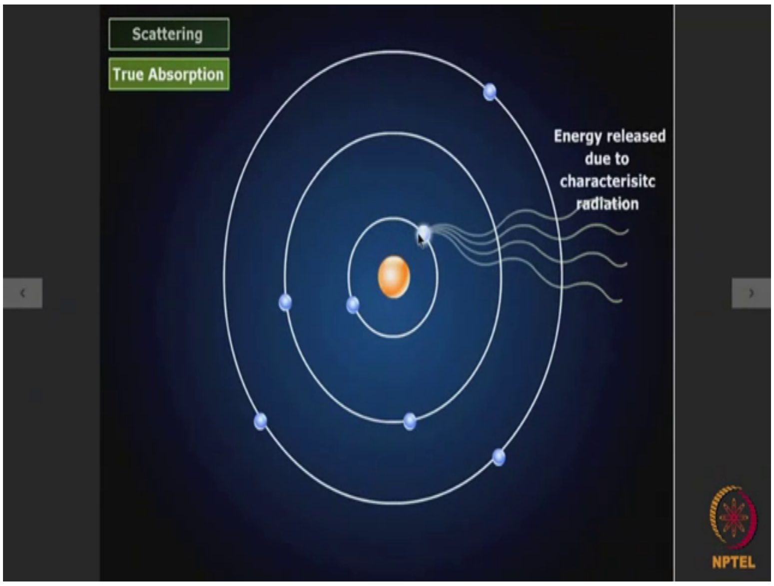

And in addition to that some of the energy will also be lost when a characteristic radiation is produced when an electron will be knocked out of the K shell. So, these are the 2 rays you know by which energy will be lost and so far as we are concerned we can say that the material absorbs some amount of energy while giving away some. So, the scattering and process and energy released due to the formation of characteristic radiation of the 2 waves by which absorption takes place in the material.