X-Ray Crystallography
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Lecture - 09
Production and detection of X-Rays

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In many applications of X-rays in crystallography, we need to use an X-ray beam of a single wavelength or a monochromatic beam of X-rays. Now how to get a monochromatic beam of X-rays from the x radiation that comes out of an X-ray tube as we all know from the X-ray tube we get a host of X-ray wavelengths which constitute the white radiation and also when the X-ray tube is operator above a threshold voltage, we get what are known as the characteristic radiations K alpha and K beta. Out of all these wavelengths K alpha has the highest intensity. So, when we want to use a monochromatic or single wavelength X-ray beam what we do is we filter out the K alpha wavelength from the total x radiation coming from the tube made up of the white radiation, and the characteristic radiations.

So, now I will describe the principle behind this procedure of filtering out the wanted K alpha radiation from the unwanted white and K beta radiations. Now let us suppose we have a metal nickel.

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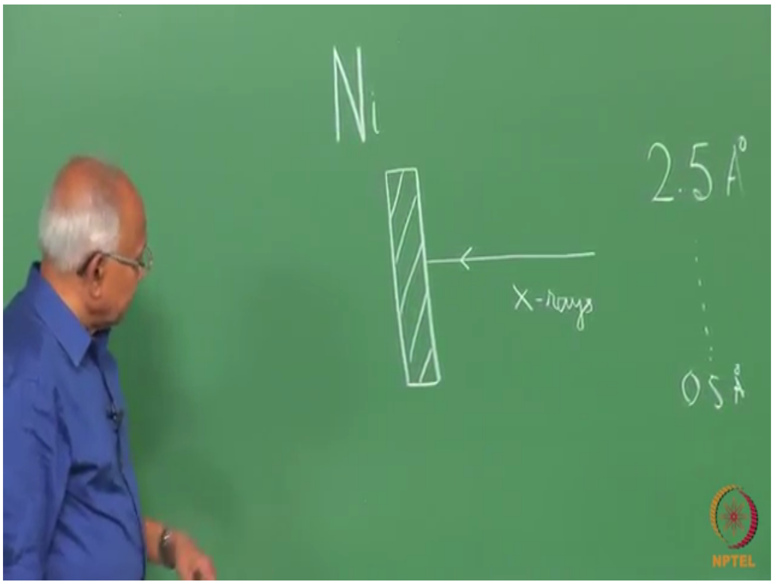

Let us take a metal nickel say if we have a thin sheet of nickel and we do an experiment say in which we bombard this thin nickel sheet by X-rays of different wavelengths. Say we do a hypothetical experiment where we have a piece of nickel a thin sheet of nickel and we bombard it by X-rays of different wavelengths starting from a high wavelength of say 2.5 angstrom and weighing up to say about 0.5 angstrom. So, the experiment is we are bombarding a thin foil of nickel by X-rays of varying wavelengths.

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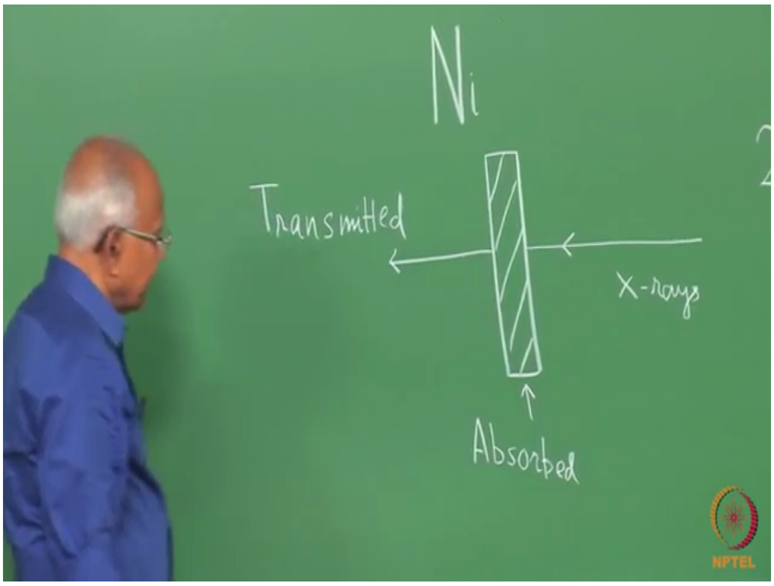

Now, if we do that and if after every bombardment we find out how much of the beam is transmitted. If we find out how much of the incident beam is transmitted we can find out how much is absorbed also. So, the total beam the transmitted beam part of the beam will be so to say absorbed by the nickel piece.

So, we start with say 2.5 angstrom wavelength X-rays, and find out how much of it is transmitted so that we can find out how much is not transmitted or rather how much is absorbed by the material.

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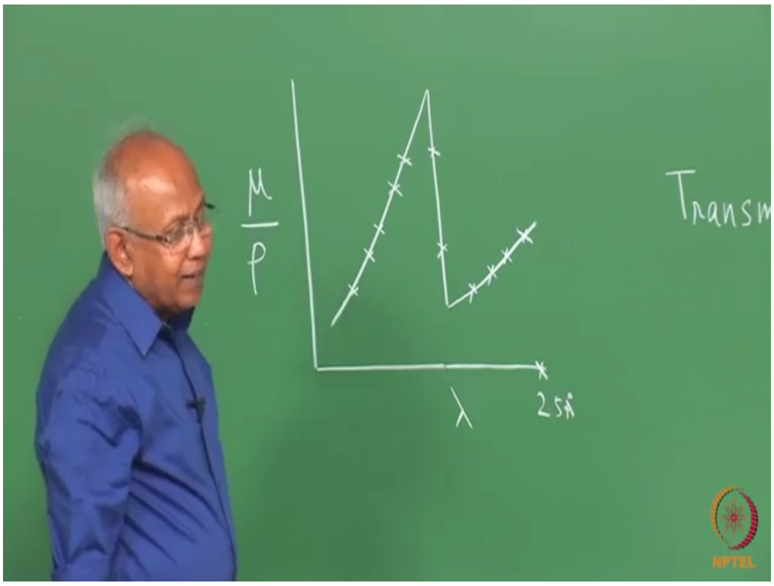

Now, if we plot mu by rho of the material that is nickel here versus the wavelength then we see that there are the plot shows a behavior similar to this. So, we start with say 2.5 angstrom wavelength of X-rays, in the second experiment say it is 2 angstrom X-rays then 1.5 say 1.3 1.2 1.1 in this 0.5. And at each after each experiment from the transmitted intensity we find out how much is mu by rho and then plot those mu by rho values in this manner join them by a smooth curve.

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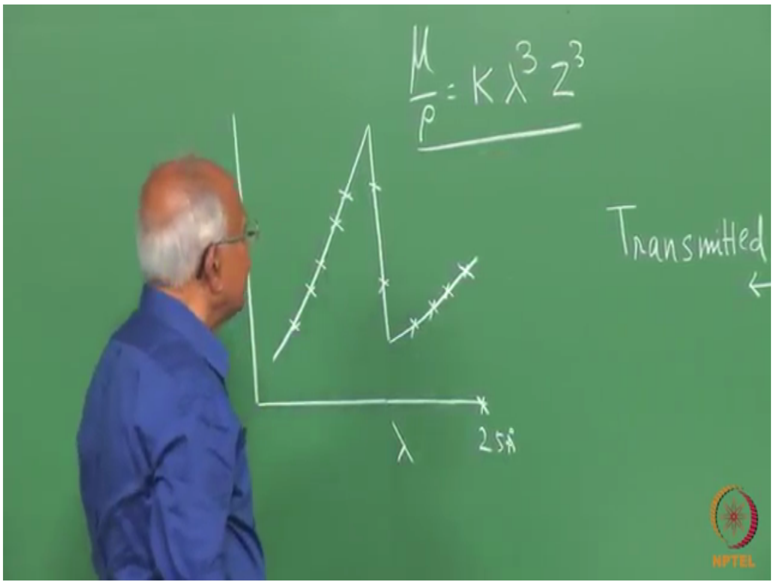

Now, if we look at this we find that mu by rho essentially can be written as K lambda cube Z cube where Z is a atomic number of the absorbing element K is a constant, whose values differ for the two different parts of the curve and lambda is the radiation with which the nickel is bombarded in this case.

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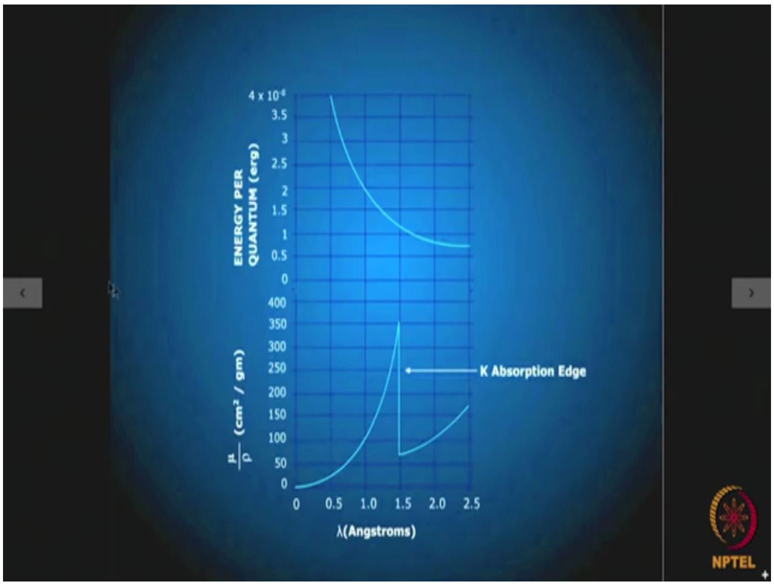

Now, corresponding to each and every wavelength with which we bombarded the nickel piece, we can find out; how much is the corresponding value of the energy of the X-ray quantum.

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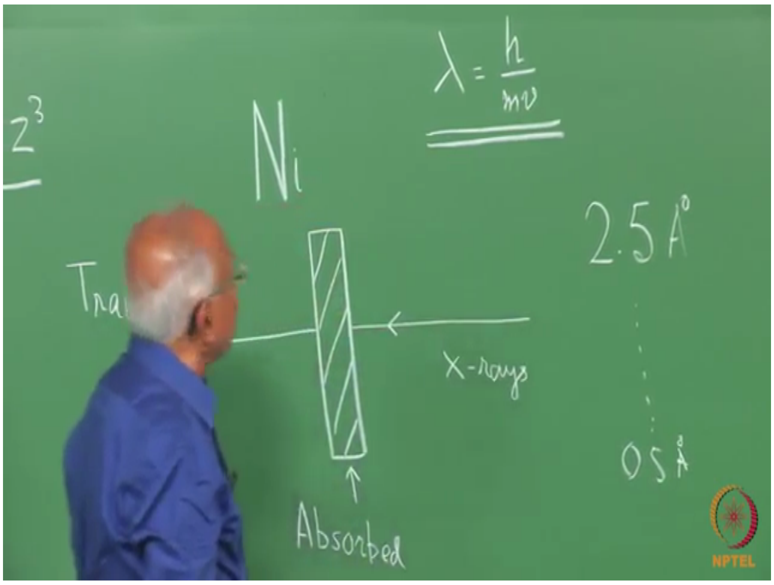

And this we can easily find out from the well known relationship lambda is equal to h by m v. So, if we know the lambda value the wavelength of the radiation then using this relationship h is plans constant, m is the mass of the photon, v is the velocity of the photon we can find out how much is the corresponding energy per quantum and that has been plotted here. So, this plot shows the energy per quantum of x radiation having different wavelengths as shown by this (Refer Time: 07:30).

So, what if I what s the behavior of this plots, you see as we start bombarding the nickel piece which say a wavelength of X-rays say 2.5 angstrom and from the transmitted beam, we calculate then this is the value of the mu by rho of this specimen for this particular wavelength. Then say we take a wavelength of x radiation just two angstrom and use it to bombard the piece of nickel and the mu by rho is given by this point here. However, as we come down to every wavelength slightly less than 1.5 angstrom wavelength, we find the value of mu by rho suddenly jumps you know to a high value.

So, for this particular wavelength the mu by rho is as gone up to 350 centimeter square per gram. Beyond that again the same kind of behavior is followed. So, when it is one angstrom wavelength you know this is the mu by rho when it is 5 angstrom wavelength this is the mu by rho etcetera, etcetera. Now, what essentially happens when the nickel piece is bombarded by x radiation having a wavelength slightly less than 1.5 angstrom?

You see if you look at the top clock over here this particular wavelength corresponds to a value of energy given by these points.

So, you can find out the energy corresponding to this particular wavelength. So, essentially what happens is as we are bombarding the piece of nickel by x radiation of different wavelengths, naturally lower the wavelength more is the penetration power of the X-rays. And therefore, less will be the value of mu by rho. So, this is exactly what happens here now when we have come to a wavelength as given by this point as over here the X-ray quantum corresponding to that particular wavelength its energy is such that that X-ray quantum is capable of knocking out a an electron from the K shell of nickel.

So, what will happen there, will be a fluorescent radiation? That means, X-ray will be produced from this material and it will be going out of the system. So, for all practical purposes it will appear as if the material has absorbed quite a bit of energy which was incident on it. So, that is the reason why the mu by rho value becomes so high at this point; that means, any X-ray quantum having this much of energy or this much of wavelength is capable enough to knock out an inner shell electron from one of the atoms of the piece of nickel. So, when this happens there will be production of X-rays. So, there will be production of the characteristic radiation from nickel which goes out into space. So, as a result when we look at the transmitted beam we automatically notice that the intensity of the transmitted beam is much much lower, as if that extra energy has been absorbed by the material that is the reason why we find that mu by rho suddenly shoots up.

Now this particular wavelength here is known as the K absorption edge wavelength of nickel. So, this particular wavelength here is known as the K absorption edge wavelength of nickel.

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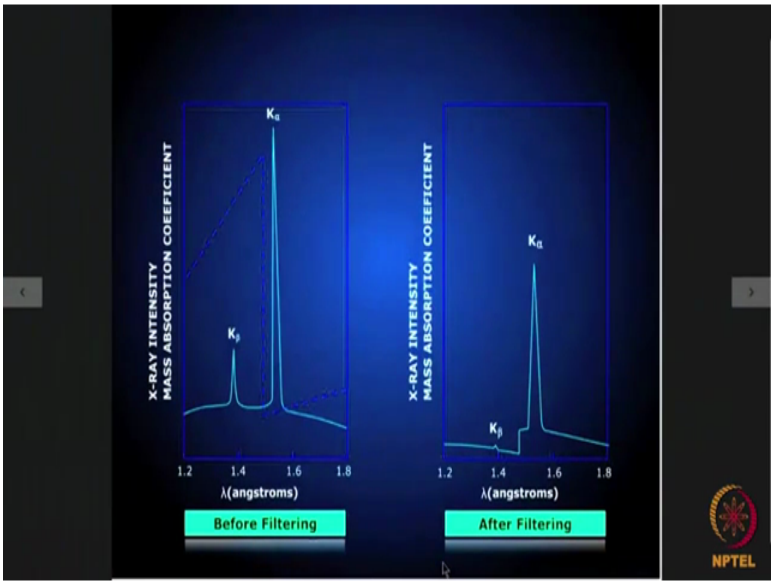

Now, in this diagram we have plotted part of the white radiation along with the K beta and K alpha wavelengths as we observe from coming out of a copper tube. So, this left hand side diagram shows part of the white radiation along with the K beta and K alpha from an X-ray tube with copper as a target material. So, this particular K alpha is copper K alpha this particular K beta is copper K beta, now copper K alpha has got a wavelength given by say 1.542 angstrom. Now if we superimpose on this diagram if you superimpose on this diagram the previous diagram for example, this particular diagram here see if we superimpose this particular diagram onto this particular diagram. So, you see that the mu by rho versus lambda plot is this one. So, here we have superimposed the mu by rho versus lambda plot for nickel on top of the radiation coming out from a copper target.

Now, what we find here, we find that mu by rho; that means, the mass absorption coefficient of nickel is very high for any wavelength less than the K alpha wavelength you see at every point the mass absorption coefficient is very very high. On the other hand when it comes to the K alpha radiation the mu by rho value is very low and again for other wavelengths on the right hand side the mu by rho value increases what does that mean? That if we use a nickel in front of the radiation coming out of a copper target in an X-ray machine, most of the radiations other than K alpha will be absorbed to a much higher degree than the K alpha radiation itself.

So, in other words the output of the X-ray machine when it goes through a nickel filter will be containing mostly the K alpha radiation along with lower intensities of K beta and other white radiation components. So, nickel can be used as a filter. In case of a X-ray machine having copper as a target material, in this way we can figure out what kind of filter material we can use to have the K alpha radiation from different kinds of targets.

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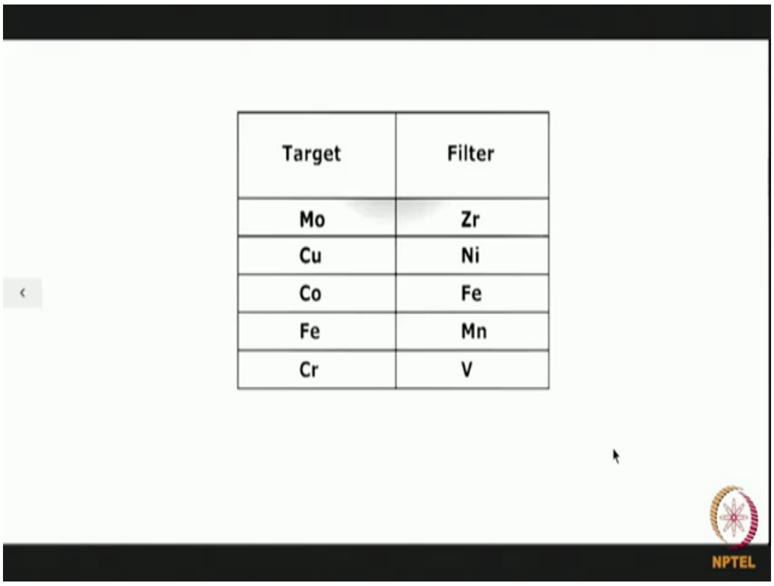

Target	Filter
Mo	Zr
Cu	Ni
Co	Fe
Fe	Mn
Cr	V

So, as you have seen already for copper we can use nickel as a filter material which will filter out the K alpha radiation from all the unwanted radiations. One thing we must remember the filtering action is not perfect, because although K alpha radiation that will come out will be the strongest radiation, there are other radiations also very quick one. So, it is not a perfect filtering then if you have a molybdenum target then use zirconium as a filter material if I have a cobalt target use r n as a filter material. If you have r n as a target use manganese as a filter material, you have chromium as a target you use vanadium as a filtering material.

So in fact, if you look at the atomic numbers of the filter materials and the target materials we will find that the filter material should be such which will have a atomic number one or two different from the target material. For example, for copper it is nickel you know atomic number difference is only one. So, in this way it is possible to figure out when you are using a an X-ray machine with a particular type of target material what should be use which material should be used as a filter material in order to get a more or less monochromatic or single wavelength radiation.