

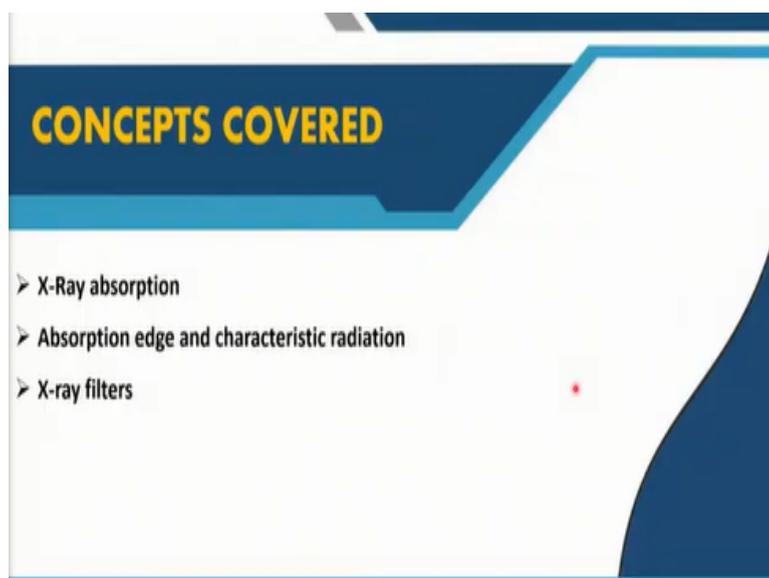
**Techniques of Materials Characterization**  
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**Materials Science Center**  
**Indian Institute of Technology, Kharagpur**

**Lecture - 46**  
**X-ray Absorption and Filters**

Welcome everyone to this NPTEL online certification course on techniques of materials characterization. We have finished 9 modules until up to now and now we are beginning with the tenth module and this one just like the last one this one also will be dedicated to x-ray diffraction. And in the last module we discussed about the history of x-ray, then generation of x-ray by continuous spectrum, characteristic spectrum and all of this.

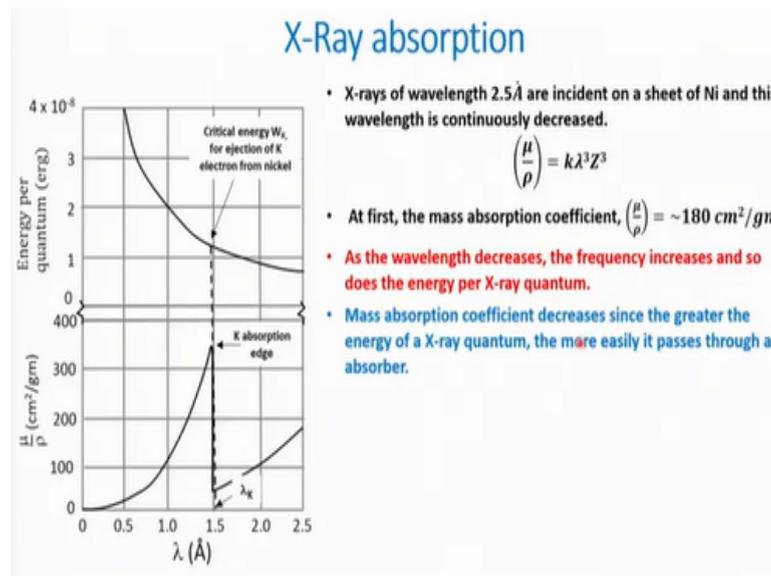
And then we just started discussing about the absorption, x-ray absorption and there we have discussed about mass absorption coefficient, linear absorption coefficient and then also we discussed about the absorption edge how it happens like by scattering by true adsorption and all of this. We discussed about the fluorescent radiation, how fluorescent radiation occurs fluorescent yield and then we discussed about Auger electron generation so on. We will be continuing that discussion about x-ray observe absorption in this lecture as well.

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And we will be looking again x-ray absorption will be discussing about absorption edge and the relationship of absorption edge with characteristic radiation. And if time permits will also be discussing about x-ray filters.

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So, x-ray absorption we have already seen this, how the mass absorption coefficient varies with lambda that is the wavelength of the electrons, wavelength of the x-ray. And what we have seen is that like, this has two branches that mass absorption coefficient variation with lambda. This has two branches one in this side, one in this side and they are separated by sharp discontinuity within a very fixed and very narrow wavelength range where the mass absorption coefficient increases by many fold.

So, if we now consider and this is we told that this is basically for nickel, something like a nickel material. But this is very typical for any other metals and it depends obviously the wavelength depends on the atomic number of the elements but this basic shape and the presence of characteristic, presence of absorption edge. This does not change or this does not depend on the materials the shape.

And the wavelength this may change but the shape does not change for material. All the material most of the metals will have this kind of absorption relationship between mass absorption coefficients with the wavelength. So, the first thing now we can see if we use x-ray of wavelength 2.5 angstrom. So, this is the incident wavelength of the x-ray where we start and initially what we find that this is a nickel. As I said this is a nickel sheet.

So, initially what we find that the x-ray intensity the mass absorption coefficient is continuously decreasing as the wavelength is continuously decrease. Wavelength is decreasing continuously and the mass absorption coefficient is also continuously decreasing and the relationship we already discussed about that  $\mu \text{ by rho} = k \text{ lambda cube } Z \text{ cube}$  where  $k$  is a constant  $\text{lambda}$  is the wavelength and  $Z$  is the atomic number.

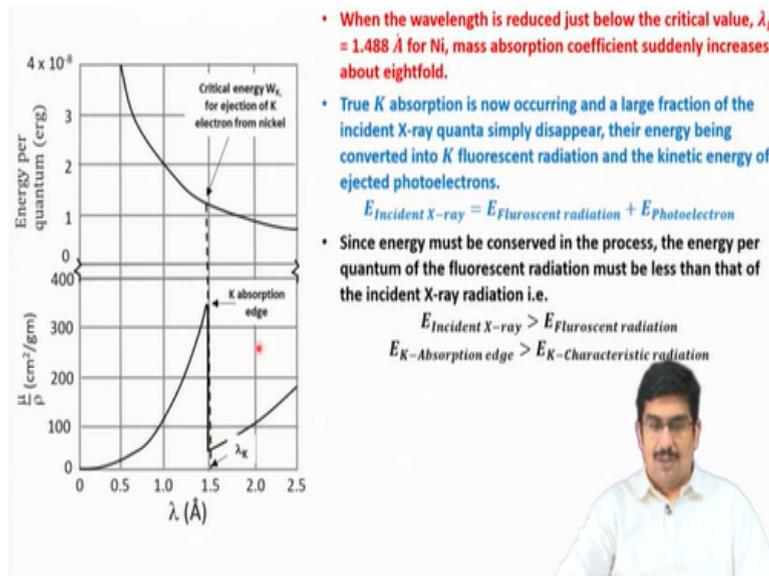
So, at first the mass absorption coefficient here when we begin with around 2.5 angstrom wavelength x-ray source, there the mass absorption coefficient was around 180 centimetre square per gram. So, this is as we discussed that basically this is a linear absorption coefficient and the unit of linear absorption coefficient in centimetre inverse and this is the density. So, the unit of this density is gram per centimetre cube.

And together if we do unit analysis then we will come that dimensional analysis will give us this is to be the kind of unit for absorption coefficient mass absorption coefficient. Now if you decrease the wavelength here. What will happen the energy of the electron will also increase correspondingly? So, it is shown here when we are decreasing this wavelength continuously the energy of the electrons will also goes higher and higher.

Mass absorption coefficient also similarly decreases as per this wavelength decrease as per the increase in the energy because now if the electro or if the x-ray quantum or x-ray photons when they become more energetic, they can easily pass through the absorber the material which is there they can very easily. So, it is like hitting if you have a ball if you have a wall, you are hitting it with some amount some kind of ball.

If the ball has a higher energy, it can just penetrate through it can break the wall and go through on the other side if it does not have that much of energy it will be possibly absorbed within the wall itself so that is that is what is happening. The x-rays when as soon as the wavelength decreases energy of the x-ray increases and those x-ray photons will now be able to pass through the material resulting in a decrease in the mass absorption coefficient.

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Now when the wavelength is reduced below the critical value that means the absorption edge K absorption is and here for nickel this K absorption is  $\lambda_K = 1.488 \text{ \AA}$ . So, as I said this is very narrow the absorption edge is very, very narrow and the wavelength is quite fixed just like the characteristic extra radiation. There also the wavelength is the spread in the wavelength is very, very narrow and it is very well defined for the material.

So, here same thing this is very well defined for any element this does not change if you change the let us say if you change this x-ray the source and then also this remains pretty much basically the same it only depends on the wavelength. The K absorption the mass absorption coefficient; now if you decrease and if you bring the wavelength value close to this K absorption it what you will see is that there is this almost 8 whole jump in the mass absorption coefficient.

And this jump is basically because of the K absorption true K absorption is happening, this is not as we already discussed scattering is another possibility but that is just a possibility for light elements. For heavier element it is mostly the true absorption that happens. So, true K absorption now started happening at this particular  $\lambda_K$  and this transmitted a large fraction of the incident x-ray quanta is taken up or the energy is taken up from the incident extra beam.

And large amount of energy is taken up in this true k absorption process. So, that means the transmitted radiation on the other side that will be having much lower energy or much lower intensity compared to the incident x-ray if the wavelength is false within this K absorption edge. Now this true absorption we know the true absorption process two things happen. Number one a photoelectron is generated.

And second thing and fluorescent radiation is generated. So, the energy of the incident x-ray that is lost here in this K absorption. Near the K absorption edge the incident energy of the incident x-ray which is lost that is we can equate it to the energy of the fluorescent radiation plus the energy kinetic energy of the photoelectron. So, that is how the energy loss happens near this K absorption edge.

From this since this entire energy has to be conserved in the process, now the energy per quantum of the fluorescent radiation that means this fluorescent radiation energy has to be lower than the incident x-ray energy that is lost here because of the K absorption edge. And that is very justified also because it is fluorescent radiation plus the kinetic energy of the electron where this incident energy is going.

This also means that the energy for this K absorption edge if we if we think of that this incident extra energy what the part of the incident x-ray energy what is lost in this K absorption two K absorption process then this K absorption edge the energy required to produce this K absorption edge this will also be greater than the energy required to create a characteristic radiation. Because remember I said the fluorescent radiation is basically nothing.

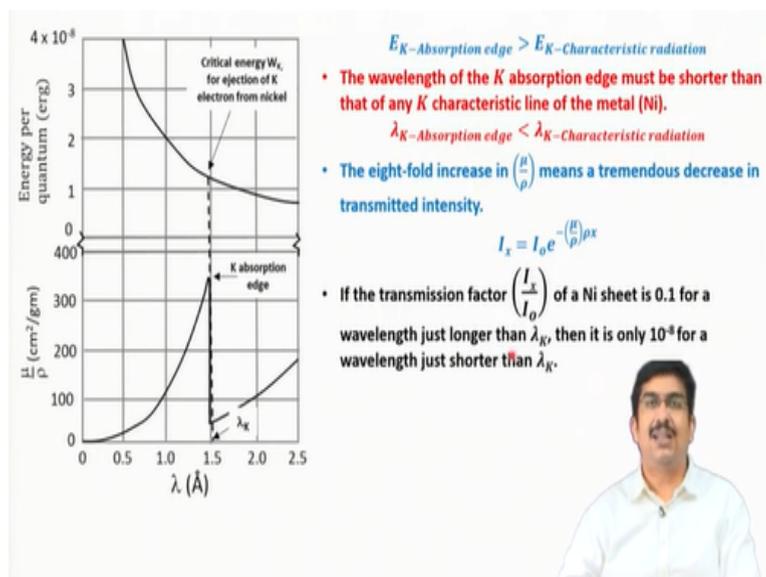
But a characteristic radiation, only difference is fluorescent radiation is caused by an x-ray photon whereas characteristic radiation is caused by bombarding an electron. But the energy between them is basically pretty much the same because they are both generated by k shell vacancy and then another electron jumping from higher energy higher electronic state that is it.

So, the amount of energy between this electronic state decides the energy of this K characteristic radiation or this K fluorescent radiation. So, that is fixed for both of them. So, now if we start from there with that relationship that the incident the energy changes in the K absorption edge is greater than the K characteristic radiation. What we can then confer is that the wavelength of K absorption edge here.

This is the wavelength of K absorption edge this must be shorter than the K characteristic radiation of that particular metal in this case it is nickel. That means the  $\lambda_K$  absorption edge will be lesser than the  $\lambda_K$  characteristic radiation, that means the  $\lambda_K$  characteristic radiation will be somewhere over here just before the K absorption edge because there is this photoelectron.

This part is also involved the photoelectron energy. So, the amount of energy lost in the true absorption or in the absorption process is bigger or is greater than the amount of energy required to produce the K characteristic radiation.

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In the process the absorption edge appears at a shorter wavelength compared to the K characteristic compared to the wavelength, where the K characteristic radiation in or is produced from the same metal. Again, remember the absorption edge is produced by the x-ray signal, whereas characteristic radiation is produced by normally by an electron can be produced by if it is a fluorescent can be produced by x-ray.



So, this is the importance one of the importance for the x-ray absorption edge. Now as we decrease the wavelength below even shorter. So, we started from here, we have seen that when we decrease the wavelength continuously the x-ray continuously the mass absorption coefficient decreases and this decreases purely because x-ray energy is increasing and the x-ray most of the x-ray is just passing through without getting absorbed.

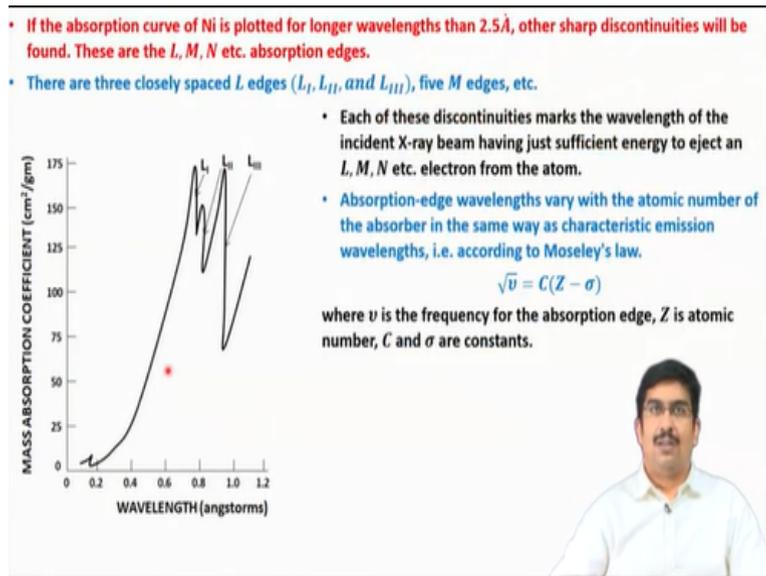
And near to the extra absorption edge when we hit the x absorption a huge increase in the mass absorption coefficient. So, what happens when we decrease the wavelength even further. Now we are the energy is sufficient so, energy reaches the critical excitation critical value and the critical value means the value or the energy of the incident x-ray photon is now enough to produce photoelectron and fluorescent radiation.

So, if we decrease the wavelength even smaller that means if we increase the energy even higher. The process will still continue the production of photoelectrons and production of fluorescent radiation will still go on but the mass absorption coefficient will continue to decrease. And this is because and we can see for the same nickel sheet here that at an wavelength of around one. So, right now here the incident extra quanta is very energetic.

So, the energy of the quanta will be so much that again the same thing will happen it will just pass through the some part of it will definitely cause the true absorption. But most of the x-ray for photon will be so energetic that again the same thing will happen they will just pass through the material without causing any kind of change any kind of true absorption. So, the basically the if you check the mass absorption coefficient of something like one lambda of one angstrom what says something like lambda of two angstrom.

This is pretty much the same the only thing happens between them close to this K absorption edge. And both sides here and here the mass absorption coefficient is decreased because of the increase in energy that is it. Here only the true absorption and scattering all those processes are valid in these two regions it is only decided by the energy of the x-ray. If the energy is too high, they will simply pass through this material without getting absorbed that is it.

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Now what happens if we go in this side? So, we have seen in this side now what happens if we go on this side. If we use an extra signal which is having even higher wavelength then what we can see is that we will be hitting again some other kind of absorption edges. So, this absorption curve of nickel if we plot it for longer wavelengths from compared to 2.5 angstrom.

If we go to higher and higher wavelength then for nickel this is for different material, do not do to continue. So, do not look at the wavelengths here this is for a different material altogether but if we consider only for nickel if we go beyond 2.5 in this direction then what we will be seeing again few other discontinuities. Those are basically L, M, K, N all of this higher order electronic shell or orbitals higher order or primary orbits.

Those absorption because of those electrons. That means in those cases instead of K electron the x-ray photon will have sufficient energy to knock out. And L for example L shell electron or M shell electron and so on and the electronic transition happens between say L between M and L shell N and L shell and so on and so forth. So, we have already discussed this. So, these are also there also it is a true absorption.

But the true absorption process is happening in terms of L shell and higher electronic states not K shell is not involved. So, that is why those processes and we already discussed since the energy of L shell is much lower than the K shell so those processes the energy will be

lower. The energy involved or the energy required for the x-ray photon will also be lower and they will be appearing at a longer wavelength.

So, this absorption for example, here you will be able to see 3 L so there is 3 electrons, 3 orbitals for L shell. And those three corresponding to those three orbitals you will see three different discontinuities or three different absorption edges here. And this absorption edge again it depends on the atomic number we already see the how the atomic number changes or how the characteristic x-ray radiation depends on the atomic number according to Mosley's law exactly the same way.

Because the same process is happening here. The same electronic transition is responsible for characteristic radiation generation and the same electronic transition is responsible for this absorption edge. So, that dependence on the atomic number is also pretty much the same and we can use this Mosley's law for calculating again the lambda k that means the wavelength of absorption edge.

The variation of wavelength of absorption edge with respect to the atomic number, so, heavier the atom so shorter the wavelength for absorption edge. Same thing heavier the lighter the atom and the longer the wavelength for absorption is similar to the characteristic radiation same variation will happen in this case as well.

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### Absorption edge and characteristic radiation

- The measured values of the absorption edges can be used to construct an energy-level diagram for the atom, which in turn can be used in the calculation of characteristic X-ray wavelengths.

$$I_x = I_0 e^{-\left(\frac{\mu}{\rho}\right)\rho x}$$

- The energy of the neutral atom is zero; the energy of an ionized atom (an atom in an excited state) will be some positive quantity, since work must be done to pull an electron away from the positively charged nucleus.
- If a K electron is removed, work equal to  $W_K$  must be done and the atom is said to be in the K state.

Atomic energy levels (schematic). Excitation and emission process indicated by arrows. The insert at top right shows the fine structure of the L state.

So, now the relationship between absorption edge and characteristic radiation, as we said these are pretty much the same process that is happening but of course there are certain distances already we have seen there is a distance difference between the wavelength of the two. The wavelength of absorption edge is shorter than the wavelength of characteristic radiation because of that energetics involved in these two things.

Now the absorption edge is easier to be measured as I already said that in order to measure the absorption edge what we or the wavelength of the absorption edge can be very easily measured. Because what I need to have is an experimental setup where I have an incident x-ray source or incident x-ray with a known wavelength and I have to measure the intensity of that x-ray and on the other side I have to measure the intensity of the transmitted beam.

Then I can put it back here and I can very easily calculate the mass absorption coefficient. And then if I change the wavelength of this incident x-ray, I can repeat this experiment I can measure the intensity of the transmitted beam and I can very well calculate this  $\mu$  by  $\rho$  the mass absorption coefficient. And in the process, I can very easily develop this entire graph the mass absorption coefficient versus the wavelength of the incident x-ray.

This I can very easily get it and from here I can find out that absorption edge very precisely experimentally I can find out the absorption edge. So, point is that calculation of absorption edge or the wavelength of absorption edge is much easier than calculation or finding out the characteristic radiation wavelength of the characteristic radiation. It is experimentally it is much easier to calculate the wavelength responsible for absorption edge.

So, if we can do that if we can measure this absorption edge wavelength of the absorption edge, we can very well then convert it to energy. And we can construct an energy level diagram for the atom, that means we can develop that what is the  $W_K$   $W_L$  and so on from there we can very easily calculate the characteristic x-ray wavelength. Because then we know that if in the process of this electronic transition if we have a characteristic x-ray radiation generation what should be the energy difference.

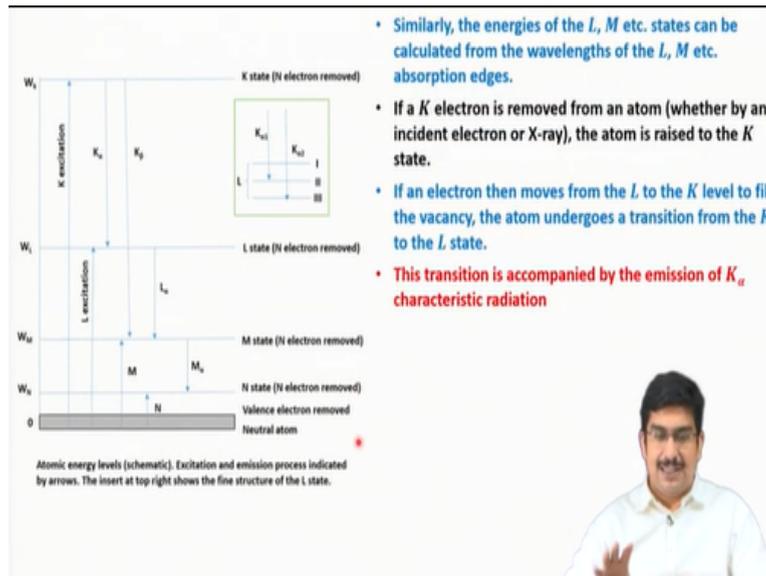
Or what should be the energy change that will involve from there we can measure the wavelength. So, that is what the importance of absorption edge by measuring the absorption edge wavelength we can experimentally which is much easier we can measure the characteristic x-ray radiation theoretically we can calculate that. We can construct this kind of energy level diagrams.

Now in doing this we start with the same thing what we discussed previously when we were discussing about the binding energy. Basically, any atom neutral atom we consider it 0, ground state is 0. And then if an electron is lost from there is the atom goes in an excited state and it will have some positive amount of energy. Because what we consider is some work need to be done to pull this electron away from positively charged nucleus.

So, this goes up to some positively charged state. If we have for example a K electron knocked out then we will have a  $W_K$  amount of energy is there. We think that this much of energy or this much of work done needs to be done in order to knock out a K electron shell. Of course, then we can have a L electron going out then we have  $W_L$  amount of energy required  $W_L$  which are smaller than  $W_K$ .

Because K electrons are much more tightly bonded or the highest amount of binding energy is there for the K electron. So, K electron  $W_K$  state K state is highest. So, there in the K state we have here it should be K electron removed here it should be L electron remove and so on. But this K state is basically where the K electrons are removed. That means  $W_K$  you provide  $W_K$  amount of work or energy in the system in that atom you remove k electron and we call that material now has gone to K energy state.

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Similarly, we can calculate L energy states where it is an L state where  $W_L$  amount of energy is required and you have an L electron removed and so on and so forth. Now if we consider that a K electron is removed from an atom whether by incident electron or by x-ray then the atom raised to the K state. Again, in that process now the atom is gone to an excited state when it tries to come back to the ground state.

Then an electronic transition will happen and the electron let us say moves from L state to K state in the process there is an vacancy created in the L shell. That means the atom we can think of the atom has now undergone from K state to L state. So, understand this so first we started with atom ground state atom we create a K shell vacancy by either incident electron or by x ray whatever it is.

It creates a K shell electron the electron has gone to K state with an amount of energy stored in there if we imagine that it stored there that is  $W_K$ . In order to fill out this vacancy an L shell electron jumps to K shell and in that process the vacancy is now transferred to L shell. That means in that process whatever energy is required to create that L shell vacancy that needs to be there, that that is stored.

So, that amount of energy we can see that this is basically  $W_K - W_L$ . So, that much of energy is stored in the system now and this process if it repeats slowly, slowly, slowly the material should come back to its ground state. So, this when this L shell electron jumps back

to K shell and the material transition material goes from K state to L state this will be accompanied by an emission of a K characteristic radiation.

We have already seen how K alpha 1 generated K beta K alpha 2 all of this. So, that basically this much of energy difference will lead to for example if I have this transition between L and K,

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The slide contains several graphs and text. On the left, there are two spectra: the top one is the 'Figure Spectrum of Ni at 8900 Å line with the x-axis scale' showing intensity vs wavelength, and the bottom one is the 'Figure Spectrum of Cu at 8900 Å line with the x-axis scale' showing intensity vs wavelength. In the center, there are two energy level diagrams. The top one shows energy levels for Ni and Cu, with a vertical line indicating the 'Critical energy  $W_K$  for ejection of K electron from nickel'. The bottom one shows the 'K absorption edge' and 'K<sub>α</sub>' emission line. To the right, there are three bullet points and a formula. At the bottom right, there is a small image of a man in a white shirt.

- Wavelengths of characteristic emission lines can be calculated from the difference in energy between two states.
- Considering  $K_{\alpha}$  characteristic line: The "L level" of an atom is a group of three closely spaced levels ( $L_{II}$ ,  $L_{III}$  and  $L_{IV}$ ), and the emission of the  $K_{\alpha 1}$  line is due to a  $K \rightarrow L_{III}$  transition.
- The frequency  $\nu_{K\alpha 1}$  is given by  

$$h\nu_{K\alpha 1} = W_K - W_{L_{III}}; h\nu_{K\alpha 1} = h\nu_K - W_{L_{III}}$$

$$\frac{1}{\lambda_{K\alpha 1}} = \frac{1}{\lambda_K} - \frac{1}{\lambda_{L_{III}}}$$

where the subscripts  $K$  and  $L_{III}$  refer to absorption edges and the subscript  $K_{\alpha 1}$  to the emission line.

$\frac{1}{\lambda_{K\alpha 1}} < \frac{1}{\lambda_K}$

$\lambda_K$  - Absorption edge <  $\lambda_{K\alpha 1}$  - Characteristic radiation

I will be having a K alpha radiation here characteristic radiation here we have already seen this. So, this is alphabets odd this look little odd here anyway. So, the wavelength of characteristic emission lines can be calculated from the difference in energy between the two state. If we consider that it is between K state and W K and W L, K and L state and we are having L K alpha emission.

So, we just consider that K alpha characteristic line K alpha characteristic radiation is there that means the L level of an atom we have an L shell from an L shell and electron transfers to K state. And this normally K alpha 1 is line is happens between transition between K shell and L 3 shell. So, that that electronic transition basically gives rise to this kind of K alpha 1 radiation.

So, we can write this if the frequency of this k alpha 1 or K alpha 1 radiation which we write it nu k alpha 1. Then the energy of that process in the of that K alpha 1 radiation we can write

it as  $h \nu_{K\alpha 1}$  which is equal to the difference between here. That is this  $K\alpha 1$  energy is basically the difference between  $W_K$  that is the K state energy –  $W_{L3}$  that is the L shell energy and out of the all the L shell it is not all the L shell it is L 3 shell.

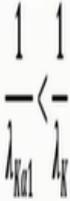
So, this is equated to  $W_K - W_{L3}$  that means here again  $W_K$  what we can write here is  $h \nu_K$ . And  $h$  this new  $K$  is the frequency for K absorption  $h$ . So,  $W_K$  that is the amount of energy required in order to create a K shell electron remember in order to create a K shell electron first you have to knock out a photoelectron and, in the process, you have this radiation this fluorescent radiation generation.

So, that means in the process basically you are creating a K absorption edge that will that energy will be exactly same as the absorption  $h K$  absorption  $h$  energy and correspondingly the same frequency and wavelength and then similar thing for  $W_{L3}$ . So, ultimately what you can write in the terms of wavelength  $1/\lambda_{K\alpha 1} = 1/\lambda_K - 1/\lambda_{L3}$ .

Here  $\lambda_{K\alpha 1}$  is basically the characteristic radiation wavelength of the characteristic radiation whereas  $1/\lambda_K$  this  $\lambda_K$  is the wavelength of the absorption edge. And this  $\lambda_{L3}$  is the absorption edge wavelength of L 3 absorption edge. From here also what we can find out or what we can check is  $1/\lambda_{K\alpha 1}$ . So, if I consider this relationship  $1/\lambda_{K\alpha 1}$  obviously is less than  $1/\lambda_K$ .

So, if I just consider here one by the and from there what I can find out is the same relationship what I previously derived from energetic calculation I have calculated this from energetics of this process.

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- Wavelengths of characteristic emission lines can be calculated from the difference in energy between two states.
- Considering  $K_{\alpha 1}$  characteristic line: The "L level" of an atom is a group of three closely spaced levels ( $L_I$ ,  $L_{II}$  and  $L_{III}$ ), and the emission of the  $K_{\alpha 1}$  line is due to a  $K \rightarrow L_{III}$  transition.
- The frequency  $\nu_{K\alpha 1}$  is given by
 
$$h\nu_{K\alpha 1} = W_K - W_{L_{III}}; h\nu_{K\alpha 1} = h\nu_K - W_{L_{III}};$$

$$\frac{1}{\lambda_{K\alpha 1}} = \frac{1}{\lambda_K} - \frac{1}{\lambda_{L_{III}}}$$
 where the subscripts  $K$  and  $L_{III}$  refer to absorption edges and the subscript  $K_{\alpha 1}$  to the emission line.

$\lambda_{K\alpha 1}$ -Absorption edge <  $\lambda_K$ -Characteristic radiation

$$\frac{1}{\lambda_{K\alpha 1}} < \frac{1}{\lambda_K}$$

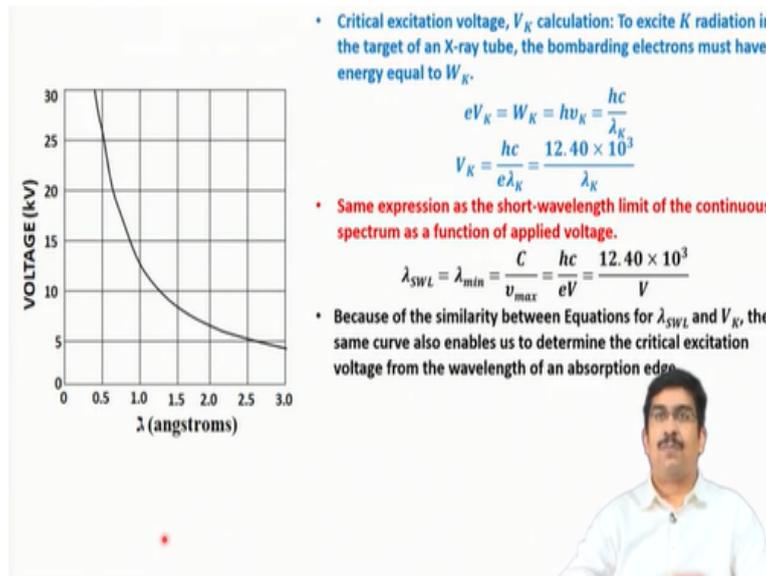
$\lambda_{K\alpha 1}$ -Absorption edge <  $\lambda_K$ -Characteristic radiation



The same thing we can now discover or derive here from this relationship. That is the lambda of K absorption is the wavelength where the absorption edge appears will be at a shorter value or that the shorter wavelength compared to the K characteristic radiation, the wavelength corresponding to K characteristic radiation. So, same thing we can derive again here. Same analogy we can derive.

And from there what we can derive again from this relationship as I already said measurement of this two are pretty easy. So, measuring this absorption is wavelength corresponding to absorption is measurement of that is very easier much easier and same thing we can measure the absorption is for 1 lines and from this value we can calculate the wavelength of this K characteristic radiation very precisely.

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Similar thing we can do to calculate the critical excitation voltage of this characteristic radiation K characteristic radiation and to excite K radiation we know that electrons must have energy equal to  $W_K$ . So, again we go by the same root the energy of the electrons which is given by  $e$  and  $V_K$  where  $V_K$  is the excitation voltage equals  $W_K$  and that  $W_K$  is equals to again  $h\nu_K$  equals  $hc/\lambda_K$ .

All together finally it comes down  $V_K$  the critical excitation voltage for generation of K characteristic radiation. This comes out to be this value  $12.40 \times 10^3$  raised to the power 3 by  $\lambda_K$ . Now again this  $\lambda_K$  is the characteristic or is the wavelength of K absorption edge. So, we can find out not only the wavelength of K characteristic radiation we can also find out the critical excitation voltage for develop for generation of a K characteristic radiation.

So, one thing you must notice that the critical excitation voltage the expression for critical excitation voltage is very similar to that we previously derived for short wavelength limit for a continuous spectrum, short wavelength limit. So, that also has this kind of a shape where  $12.40$  the same terms come here and we have expressed here that short wavelength limit in terms of the voltage.

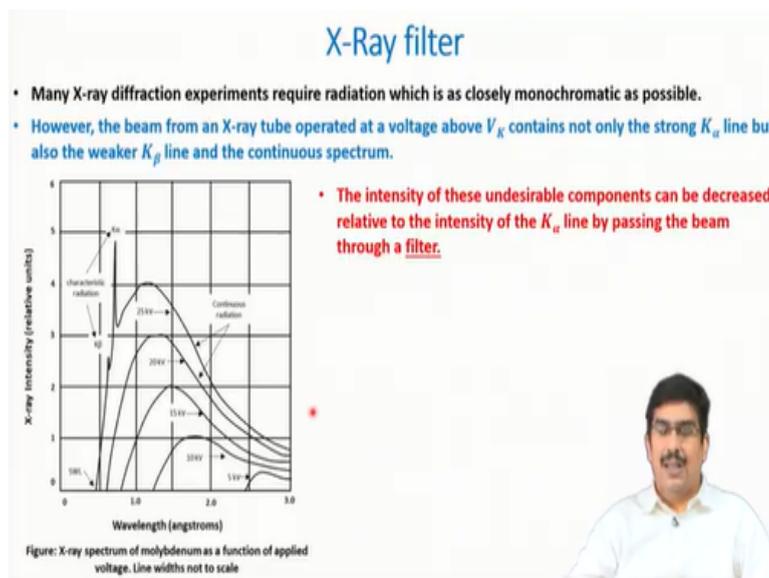
And here we have derived the short wavelength limit or the critical excitation voltage in terms of the absorption, the wavelength of the absorption rate. Basically, all of these

processes is pretty much the same the way electrons are generated the way x-rays are generated the characteristic radiation generated all of them are the way they are absorbed basically all of these are related to electronic transition.

That is why they pretty much look very much the same. And because of the similarity between these two equations for  $\lambda$  SWL and  $V_K$  the same curve that we generate we could generate for one the  $\lambda$  SWL with respect to the voltage applied voltage this from the same curve we can derive the wavelength of the absorption edge and vice versa, if we derive the wavelength of absorption edge from there.

We can derive the critical excitation voltage and from there we can very well derive the  $\lambda$  SWL short critical short wavelength limit.

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So, we will be stopping here and we will continue our discussion about this x-ray filter in the next class. Thank you.