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# Lecture - 45 X-ray Absorption (Continued)

Welcome everyone to this NPTEL online course on techniques of materials characterization. We are still continuing with module 9 and we are discussing now x-ray diffraction. And until up to now we have discussed about the history of x-ray diffraction not only diffraction the history of x-ray then how extra diffraction came in by the Braggs. And then we discussed about x-ray source signal, how the x-ray is generated.

We discussed about continuous spectrum, we discussed about characteristic spectrum. And in the last class we just begin with x-ray absorption and that we will be continuing now we are like in this lecture five.



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And today we are going to cover these few issues x-ray absorption, mass absorption coefficient absorption edge and Auger effect. Auger effect already we have discussed about Auger effect during our lectures on SEM. But again, we will be discussing a little bit about Auger effect in terms of x-ray signals.

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So, this we discussed in the last class x-ray absorption. We said that x-rays encountered any form of matter. Some part of that x-ray will be absorbed by the matter or absorbed by the material and some part goes out. And that is the basis of these radiographs where your flesh is virtually transparent to x-ray signal that means they are not absorbing x-ray. Whereas the bone part which is more dense part they will absorb x-ray most part of x-ray will be absorbed.

And that is why on the back side in the photographic film you will be getting and contrast accordingly. So, wherever the x-ray is fully transmitting not absorbed at all those areas will be appearing in brighter contrast and areas where the x-ray is absorbed. Obviously on the other side the intensity of the x-ray will go down and you will be getting a darker contrast. So, that is the basis of radiography.

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And today we will be discussing from there something else called mass absorption coefficient. And before that we will discuss about linear absorption coefficient. So, this decrease if we now think about any material of finite thickness and this is the x-ray source and this from this side this is the intensity of the x-ray that is hitting this material and on the other side if you measure the xray intensity.

Then what we will be seeing is that the decrease in the intensity of the x-ray beam as it passes through this material this is proportional to the distance it travels. So, this is by simple experiment you can find it out that this is what is happen. So, x-ray the amount of decrease in the intensity of the x-ray between the incident x-ray and the transmitted x-ray, the amount of intensity that is decreased or rather the amount of x-ray intensity that is absorbed by this material.

So, this fractional decrease is basically proportional to the distance or rather to the thickness of this material. So, if I write this down, we will be able to write this kind of a relationship that is minus dI by I. So, dI is basically the decrease in intensity divided by the original intensity this is proportional to the distance that it travels. And the proportionality constant for this relationship mu that is called the linear absorption coefficient.

And this is this linear absorption coefficient as we will be discussing more, this will this depends on the material constant. So, that means this depends on the kind of material, the elements that forms this and the atomic number of those elements and so on. So, basically it depends on what kind of a material it is, the density of the material. So, how dense these material whether this material is only composed of same kind of material or there is another phase is present and so on and so forth.

So, density of material basically how many atoms are there in the path of the x-ray, that is it. And the wavelength of the x-ray, so wavelength of the x-ray means the energy of the x-ray. So, if the energy if it is a very high energy x-ray then obviously that will not be absorbed that much it will be mostly penetrating. So, the energy of the x-ray will also be important. So, these three things will be discussing.

And it will make more sense when we discuss about something called absorption edge and so on. And then we will realize what is the effect of atomic number, what is the effect of density or energy x-ray energy whatever. But to understand this linear absorption coefficient sometimes it is also called linear attenuation coefficient. So, we imagine that there is something like hundred number of x-ray photons which are coming from this side which is an incident x-ray photon.

That is hundred number. And out of that ten number of photons are getting absorbed by this material which is around one centimetre thick and this side we are getting around 90 atoms. So, that means this dI that is I0 - I x basically so this dI of course is 10, I the incident x-ray intensity is 100 here and dx the thickness is 1 centimetre. So, this one finally makes mu that linear absorption coefficient becomes 0.1 per centimetre.

So, that is the unit of mu is basically centimetre inverse. So, this linear absorption coefficient now can be expressed in terms of this inverse distance and it is coming out to be 0.1. If this is the relationship 100 amount of x-ray photons are hitting this material and 10 of them getting resolved, 90 of them getting transmitted. So, the linear absorption coefficient then over a distance of 1 centimetre linear absorption coefficient is 0.1.

So, if we integrate this equation then what we will get is Ix. Of course, Ix is the transmitted intensity in this side equals to I0 that is the initial intensity or incident intensity here x-ray intensity. And Ix = I0 into (e raised to the power - mu x), x is the total distance it travels, mu is the linear absorption coefficient. As we said the linear absorption coefficient of course depends on the density of the material.

So, how dense the material, what is the density? The single phase material multiphase material, what is the density of the material. So, if you introduce the density here in this equation what we see is Ix = I0 into (e raised to the power (mu by rho) into rho x)). So, this is also another constant mu by rho, mu is a constant for any material as we just now discussed and rho is another constant for that particular material in particular condition.

So, this quantity mu by rho is called the mass absorption coefficient. Basically, mass absorption coefficient coming out of the linear absorption coefficient; just we are introducing and normalizing this with respect to the density of material. The linear absorption coefficient normalized with respect to the density of the material that is what is giving the mass absorption coefficient. And this mass absorption coefficient again is a constant for any material.

More importantly it is independent of the physical state of the material whether the material exists liquid solid gas whatever it is independent of that and what we will be discussing it is independent of its state whether it is existing in a composite form mechanical mixing and so on. But if you even if you take this for example let us, say we take nitrogen. We now, we know that nitrogen is basically a gas but if you sufficiently cool it down if you press it.

And sufficiently if you are able to cool it down all the way to - 70 77 k you can make it a liquid. Point is the liquid nitrogen and the gaseous nitrogen both of them will have the same mass absorption coefficient that will not change. Even better; if you take an example of say water. Whether it exists as a water vapour whether it exist as a water as a liquid or as ice in solid the mass absorption coefficient is not going to change. Whatever be the linear absorption coefficient divided by the density of the particular state that will remain constant, that value will be constant. So, that means if the density changes linear absorption coefficient will change accordingly and together it will make this mu by rho constant irrespective of the physical state. We know the density changes when between the water, the water as a liquid and water as a solid ice.

There is a change in density ice is much more lighter than water and that is why it floats over the water so that we all know. So, this density changes accordingly the mass, linear absorption coefficient changes and that makes the mass absorption coefficient constant. So, this is the importance of mass absorption coefficient that is why we are sort of normalizing this on top of the linear absorption coefficient. Linear absorption coefficient changes with the physical state.

But when we normalize with respect to the density what we will see that mass absorption coefficient does not depend on the physical state, that is the point.

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So, now the linear absorption coefficient of course as we understand this is proportional to the density rho. And from there we are getting this relationship and this quantity is of course called the mass absorption coefficient just now we discussed which is independent of its physical state. So, now if we; see this example one more example. We are considering these two material same materials blocks.

And we are seeing that when the 100% out of the incident x-ray 90% is getting transmitted for both of them, 10% is getting absorbed and their thickness or the distance that x-ray beam travels that also is different. But their mass absorption coefficient is different because the density. So, linear absorption coefficient, if I take linear absorption coefficient only depends on the distance it travels and the amount of the absorption. Amount of observe absorption just like what we discussed.

Amount of absorption here is point, 10% the thickness if we take the thickness is one centimetre, linear absorption coefficient is 0.01 centimetre. If we take the thickness of this material slightly longer, linear absorption coefficient will also change accordingly. What will remain constant is basically mass absorption coefficient because the density of the material is changing between these two.

And the density change in density so the density of this block will change accordingly the volume will change and the density will change and we will be getting the same mass absorption coefficient for both of them. So, that is the point or that is the importance of considering mass absorption coefficient instead of linear absorption coefficient.

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Now another important point is mass absorption coefficient of a composite material of a material multiphase material or a composite material containing more than one element. So, wherever whether the substance is a mechanical mixture that means you have two liquids mixing maybe you can the best example you can take a solution where two let us say water and oil solution which is not going to mix or a water and alcohol solution which is a miscible liquid of two miscible liquids forming a solution.

You have a mechanical mixture let us say you have an alloy of any iron based alloy, ferrous alloy or you have a chemical compound. You have taken any of this polymers, you take water for example whatever. And whether that composite or mechanical mixing or mixture or solution or alloy whatever state it exists solid liquid gas whatever state it exists the mass absorption coefficient is the weighted average of mass absorption coefficients of its constituent elements.

So, if you consider for example w 1 and w 2 are the weight fractions of two elements. So, your composite let us say your mixture or your solution what an alcohol solution it is composed of say to for even better if you take something like an alloy of two different elements. So, that two elements let us say you consider a titanium aluminide which is titanium and aluminium. And the weight fraction of these two titanium and aluminium is w 1 and w 2.

The mass absorption coefficient of this two is mu by rho 1 and mu by rho 2. Then the mass absorption coefficient of the entire composite substance entire inter metallics will be just a simple weighted average w 1 into (mu by rho 1) and w 2 into (mu by rho 2) that will give you the mass absorption coefficient of this composite material. So, simply this is how you can derive the mass absorption coefficient of any material just from its constituent element does not matter which state they are, does not matter how they are mixed, does not matter whether they are.

It is like a physical mixture or a chemical mixture nothing. It just depends on the chemical nature of those constituent elements and their weight fraction that is it. So, that means the mass absorption coefficient is a very general concept and very generalized property for any material in terms of x-ray absorption.

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Now let us then see another concept that is called absorption edge. What happens in the x-ray absorption? What is the basis of x-ray absorption? What happens there? What causes absorption? And so on. And how we can use it for working with x-ray or using the x-ray source for characterization? So, the way in which the mass absorption coefficient mu by rho varies with wavelength of x ray.

Remember wavelength and energy of the x-ray is too interchangeably, we will be using these are two interchangeable quantities. So, if something is having a lower x-ray is having a lower wavelength means the energy of the x-ray is correspondingly high. So, if we see that mass absorption variation of mass absorption coefficient with respect to the energy of the x-ray. So, what is we can see? And this is shown for a nickel specimen, nickel absorber.

But it is very typical and this same thing happens for most of the other elements like if they are most of the metal most of the transitional metals. This is the kind of graph you will be seeing for mass absorption coefficient versus the lambda. And this is how again the energy per x-ray quantum versus the lambda this is the relationship. And you can see that when the wavelength is smaller well lower shorter wavelength lower wavelength.

The energy of the x ray beam is correspondingly very, very high. So, in this one the curve shows two distinctly different branches, one is in this side, one is in that side. And this is separated this

side of the curve or this side of the branch is separated from this side of the branch by a very sharp discontinuity means this branch there is a huge jump in the mass absorption coefficient over a very small wavelength range and it increases by many fold.

So, this increase here within a very short wavelength, this increase in the mass absorption coefficient is called the absorption edge. So, this is happening for k absorption edge, K absorption is we will come to know what is K absorption is but this is something happening over a wavelength which is basically belongs to K characteristic radiation or K fluorescent radiation that is why it is called K absorption edge.

But basically, this jump or this sharp discontinuity is called the absorption edge. Now if we consider these two other than this absorption edge if you consider these two branches. Both of these branches the mass absorption coefficient varies with wavelength following this relationship mu by rho = k lambda cube Z cube. So, Z cube is basically the element it also depends on what type of element it is, the mass absorption.

The absolute shape of this one or the extent of variation depends on different material. But basically, the shape of this is pretty much the same. The absorption is the having an absorption edge at what wavelength and all that everything depends on the nature of the material, the atomic number of the material. But this basic shape two branches separated by discontinuity that remains the same for almost all the materials.

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So, if we now see it more one thing, we can quickly realize that the mass absorption coefficient strongly varies with wavelength. And for shorter wavelength if we come to here the shorter wavelength, the mass absorption coefficient is much higher than the longer wavelengths. So, correspondingly if we first thing we understand if we just even do not consider this absorption edge but simply because of that absorption is the presence of absorption edge.

Shorter wavelength mass absorption coefficient of shorter wavelength x-rays are much higher than longer wavelength x-rays. That means x-rays which are much more energetic or high energy x-rays can be absorbed more and less amount will be transmitted or penetrated through anything. So, we can use this information to identify or to differentiate between the short wavelength or soft x-rays versus the hard x-rays as we were discussing in previously.

When we were discussing of x-ray as electromagnetic radiation, we have said that some x-rays some wavelength of x-rays are used for medical purpose and that is called the soft wavelength x-rays. And some of them are used for characterization this x-ray diffraction or XPS or x-ray micro city all of this that is basically the hard x-ray that wavelength of that x-ray is basically the hard wavelength.

The reason for this is softer means the when the wavelength of the x-ray is much smaller then that wavelength that is less absorbing or that is more absorbing compared to the hard x-rays. So,

this is less this shorter wavelength x-rays are having higher energy and they can be their mass absorption coefficient are much higher. So, they can be absorbed more and they can produce this kind of contrast radiographic images.

Whereas the hard x-rays are more or less the wavelength is higher the energy is correspondingly lower and those hard x-rays are basically favourable or they are having less of a absorption which is better for any kind of characterization like x-ray diffraction. You do not want the x-ray signal to be absorbed more by the material itself. It should just do the diffraction; it should not absorb. it should not it should allow the diffraction or scattering rather than absorbing that x-ray.

So, that is possible if you use an hard x-ray where the mass absorption coefficient is pretty much lesser. So, this is the difference between hard x-ray and soft x-ray in terms of the absorption of this x ray signal.

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Now how do this absorption happens? That is the question. So, matter absorbs x-rays by basically two distinct ways, one of them is scattering typical x-ray scattering another one is called true absorption. And these two processes together make or together contribute to the total x-ray absorption. So, between an incident x-ray and the transmitted x-ray whatever the x-ray intensity is lost in the material itself.

That is contributed by both x-ray scattering and something called true absorption. So, scattering we have already discussed in terms of electron scattering there we discussed different processes elastic interaction, inelastic interaction and so on a pretty much the same thing here. You have an incident x-ray electrons and then the x-ray electron either can just get deviated from its original part.

Because of the Columbic interaction it gets deviated or otherwise at special cases it is diffracted as well. So, whatever whether it is a simple scattering or a diffuse scattering that is what it is called diffuse scattering or it is a simple or it is a diffraction or some other kind of inelastic interaction. Whether that part of energy or that part from the incident x-ray that part of energy is lost. So, that is not getting transmitted in this side.

So, we can imagine that this is the incident photon this is called Compton scattering will come to this in the next module. Possibly we will be discussing more about the Compton scattering but basically this is the incident photon and some part of it is just getting lost as a scattered. So, if we collect the transmitted x-ray here definitely this much of x-ray intensity will not be pressed. So, scattering unfortunately it does not contribute much for heavier elements.

It is for a very light element. The scattering is responsible for the absorption or it is having a significant contribution in the total absorption for only for light elements. For heavier elements scattering contributes to very small amount in the total absorption.

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For those kind of material for heavier elements it is mostly something called true absorption. So, what causes the true absorption? True absorption is mostly happening by electronic transitions within the atom. So, this is basically and x-ray this true absorption depends on the x-ray material interaction. So, we have already seen electron material interaction and there we have seen various different processes.

Inelastic interaction and their plasmon scattering; phonons scattering so on and so forth. And one particular process we have seen that is electronic inertial excitation and secondary effects and so on. So, exactly the same thing can also happen when an x-ray photon encounters a material atom. Whatever the electron can do the x-ray also can do because both of them are electromagnetic radiation, there is no difference between at as per their nature.

Of course, electrons are charged particles so there are some other things that happens with electrons but forget about that. But basically, energetically they are both electromagnetic radiation nature wise they are both electromagnetic radiation and they can pretty much do the same thing. So, just like an electron of sufficient energy can knock an K electron out of an atom and that can cause an emission of K characteristic radiation as a secondary effect.

The same thing can be done by an x-ray photon with a particular amount of energy and if it contains certain amount of minimum amount of energy of WK which is basically the binding

energy of the K electron K shell electrons. In this process, basically what happens is that the x-ray photon comes similar to the incident electron. Here it is an incident x-ray that comes that knocks out the K electron from the K shell and creates a K shell vacancy.

And in order to fulfil that then we have an electronic transition from other cell the electrons jumps back and it causes and characteristic radiation. So, two things happens here or two things are generated one an electron which is knocked out that electron is called basically photoelectron and a characteristic K radiation, K characteristic radiation which is called fluorescent radiation. The difference is this K characteristic radiation, fluorescent radiation is caused by an x-ray signal.

And not by an electron signal. So, that is or not by an electron, the source of signal here is the xray not electron that is the difference between a K characteristic radiation and that fluorescent radiation. Now this fluorescent radiation it can go all direction, it can emit in all possible direction. But the wavelength of the K fluorescent radiation is exactly the same as the or wavelength the same means energy also is same.

As the characteristic x-ray K characteristic x-ray radiation which is caused by the electrons in when it encounters any metal target.

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When in the process of generation of characteristic x-ray, the electrons come and hits the metal target exactly the same process. But now we are instead of electrons we are considering the x-ray photons here. So, basically this means an atom emits the same K radiation and it is a x-ray radiation. It is a fluorescent radiation it is called but it is basically an x-ray radiation only. So, this x-ray radiation an atom emits the same K radiation no matter.

How the K shell vacancy was originally created? Whether it is created by the electrons or it is created by an x-ray quantity, it does not matter. All it matters is that this electronic transition should happen because this electronic transition is what is causing. So, this x-ray photon is interacting with the material and causing this photoelectron and K fluorescent radiation. Instead of that if it is an incident electron it will generate an electron.

Knock out an electron and generate a characteristic radiation. But this part is common and the atom does not know whether it is hit by an electron or a x-ray all it knows that this much of electronic transition should happen. And there should be an electron emits and K characteristic emission should happen that is it. And this also this process x-ray absorption phenomena this also we can think it is an x-ray counterpart of photoelectric effect.

That happens in the ultraviolet region where a photoelectron is emitted because of the from the outer shell due to the action of an ultraviolet ray. So, same thing happens here now. Now energy of this incoming x-ray of course just like characteristic radiation there also we have seen that a critical excitation voltage is needed. And unless and until the electrons has a critical or accelerated with through and critical excitation voltage.

That will not be able to produce a characteristic radiation. Same thing happens here that incoming x-ray also must exceed a certain the energy of the incident x-ray photon must have a critical value, must exceed a critical value. There is no acceleration is involved it, just the x-ray photon needs to contain that with needs to hit the atom material atom with that amount of energy incident beam. But the amount of energy the value of that energy remains the same.

So, that is WK if we are considering K characteristic radiation or K fluorescence radiation it is that same WK amount of energy which we can equate it to h mu K. And in the process, we can write hc by lambda K here, lambda K is basically the frequency mu and lambda K the frequency and wavelength of K absorption edge. Instead of calling it K characteristic radiation now we are calling the WK and lambda K, WK remains the same.

WK is the same amount of energy binding energy that you need in order to generate the characteristic irradiation or in order to cause this characteristic or this absorption is to create that absorption. Whatever it is but this lambda K now is the wavelength of K absorption edge.

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One thing we must understand is that instead of fluorescent radiation we can also have an Auger effect. Just the same way we discussed this Auger effect in terms of the electrons electronic transition there also. The same way we can have a Auger effect and we can generate an Auger electron instead of a fluorescent x-ray characteristic fluorescent radiation. Instead of that we can have a Auger electron generated here.

It is a slightly different process altogether because here what we can have is a K shell vacancy created by that incident x-ray photon and then we can have an normal K radiation emission of K characteristic radiation or an Auger electron radiation. In Auger electron radiation what happens

is that the K shell vacancy is filled up from L shell and already I discussed that L shell has various other sub shells or sub orbitals.

So, from any of those orbitals let us say L, two orbital we have this K shell vacancy is filled in from K L to level and then the K radiation that emits basically that K radiation that is also an x-ray radiation it ejects another electrons from L 3 level. So, that electron so instead of K fluorescent radiation coming out of the atom that K fluorescent radiation causes if it has a sufficient energy, it can cause another electron to emit.

In the same process photoelectron, another electron it can knock out and that electron will be known as the Auger electron. So, Auger electrons as that also we already discussed that for lower light elements instead of characteristic emission it is mostly Auger electron emission and for mostly materials above the atomic number is above 31 it is mostly the characteristic radiation which is taking place Auger electron emission is very less.

Whereas less than 31 mostly for very low light element, the characteristic emission is very low and it is mostly the Auger electrons which emits.





And the way we can differentiate between them is called the fluorescence yield. And fluorescence yield also we discussed fluorescence yield depends is basically number of atoms

that emit K radiation versus number of atoms with a K cell vacancy. For a very small light element this is a large this is a very small value, the fluorescent yield is very small value meaning that x-ray emission is very less mostly it is Auger electron emission.

Whereas for heavier elements like copper like Moly this is a very high value fluorescent yield is very high that means mostly the absorption happens by a characteristic K cell K radiation rather than Auger electrons.

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And Auger electrons already we have also discussed this the Auger electrons are very good. Because the energy of the Auger electrons or the wavelength of the Auger electrons is also depends on the electronic transition. So, that generation of Auger electron again is related to electronic transition. So, they can be used for chemical analysis as well. Point is Auger electrons gets very easily absorbed within the material.

So, it is a very much a surface characterization process and very within a depth of around 10 angstrom from which this Auger electron if the electrons are coming from there, they can only escape the specimen surface and then can be detected. So, detection of Auger electrons is also a very big issue altogether Auger electrons is a fantastic way of doing chemical analysis. Only thing the detection and the instrumentation is a problem.

So, we will stop here and we will continue with this absorption edge or x-ray absorption in the next. Bye.