X-Ray Crystallography
Prof. R. K. Ray
MN Dastur School of Materials Science and Engineering
Indian Institute of Engineering Science and Technology, Shibpur
Department of Metallurgical and Materials Engineering
Indian Institute of Technology, Madras

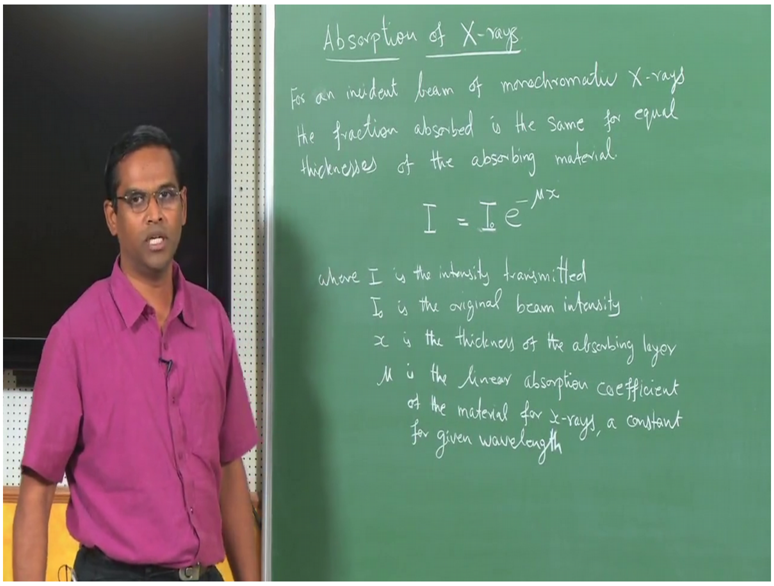
Lecture - 09
Tutorial 03

Hello everyone. Welcome to this tutorial class of X-ray Crystallography course. Today I would like to solve some problems in the chapter of X-ray production. All of you must have seen that Professor Ray, would have clearly demonstrated how the X-rays are being produced, and then the various techniques including the instrumentation, and then filters. So, particularly we will talk about X-ray absorption and then what are the governing equations, and then filtered intensities, and then different target, and filter materials. So, these problems related to this particular chapter and then pertaining to these governing equations.

So, what I will do is, I will just introduce the basic concepts once again in order to have continuity to the problems rather than blindly solve the problems. And then explain the problem content as well as the solution.

So, let me just write down few concepts first and then I will discuss.

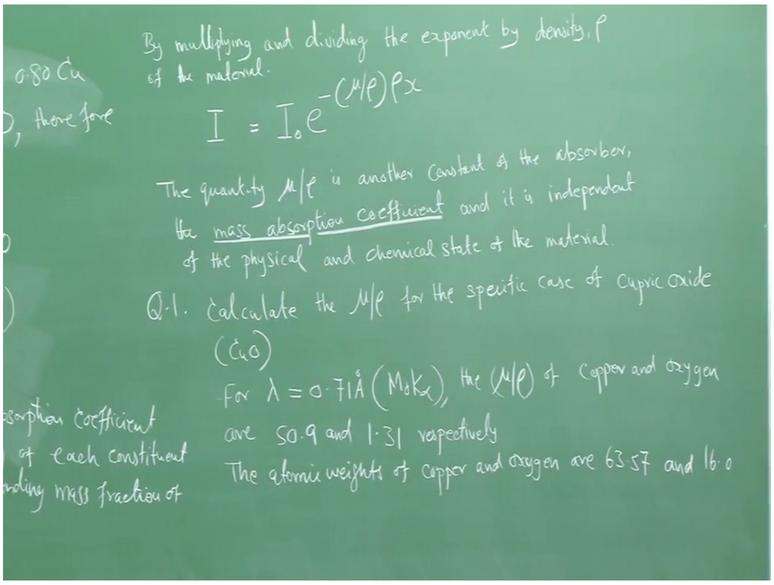
(Refer Slide Time: 01:31)



So, what I have written is for an incident beam of monochromatic X-rays the fraction of absorbed is a same for equal thicknesses of the absorbing material. So, this can be written in the form of equation, which is a well known equation. So, this equation is I is equal to I naught into e to the power minus mu x which you know already. Where; I is the intensity transmitted, I naught is the original beam intensity, x is the thickness of the absorbing layer, and mu is the linear absorption coefficient of the material for X-rays which is a constant for a given wavelength.

But this equation can be put in much more useful form. You can convert this linear absorption coefficient to a mass absorption coefficient, which is much more useful.

(Refer Slide Time: 02:43)



By multiplying and dividing the exponent by density rho this equation can be modified like this: I is equal to I naught into e to the power minus mu by rho which is mass absorption coefficient into rho x. So, this quantity is called Mass Absorption Coefficient which is independent of the physical and chemical state of the material.

Now, we will try to use this equation and try to solve some problems in these chapters. The first one what I will do is try to calculate mass absorption coefficient of some compound, so that you will have some idea how it is done. So, the question here is- calculate the mu by rho for this specific case of cupric oxide. So, what is the way of proceed probably you can just make an observation. So, what is given for this material is. So, these are the given quantities for this problem, where the lambda is about 0.71

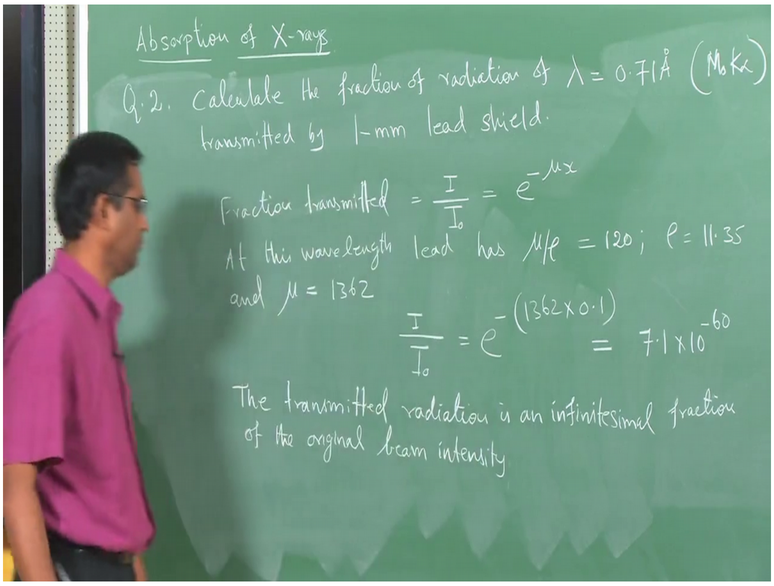
angstrom for the molybdenum. Target and the mass absorption coefficient of copper and oxygen are 50.9 and 1.31 respectively. The atomic weights of copper and oxygens are 63.57 and 16 respectively.

So, for calculating the mu by rho of copper oxide then we have to; for a copper oxide you have to calculate the fraction of each one. So, this is what we have just substituted this for this compound. And then 0.80 of copper and 0.20 of oxygen that is the fraction here. And then for the mu by rho for this you calculate it just sum of the individual mass absorption coefficient multiplied by the weight fraction. So, you just substitute this into this. So, to get the mass absorption coefficient of copper oxide it turned out to be 40.98.

So, that is for any material or any compound or a solid solution or a mixture, the mass of absorption coefficient is equal to the sum of the mass absorption coefficient of each constituent element multiplied by the corresponding mass fraction of the element present. So, this is what illustrated in this step. So, it is simply given idea how to calculate the mass of absorption coefficient for a chemical compound which is having more than one element. Or the same thing is applicable for the solid solutions as well.

We will move onto the next concept

(Refer Slide Time: 06:22)

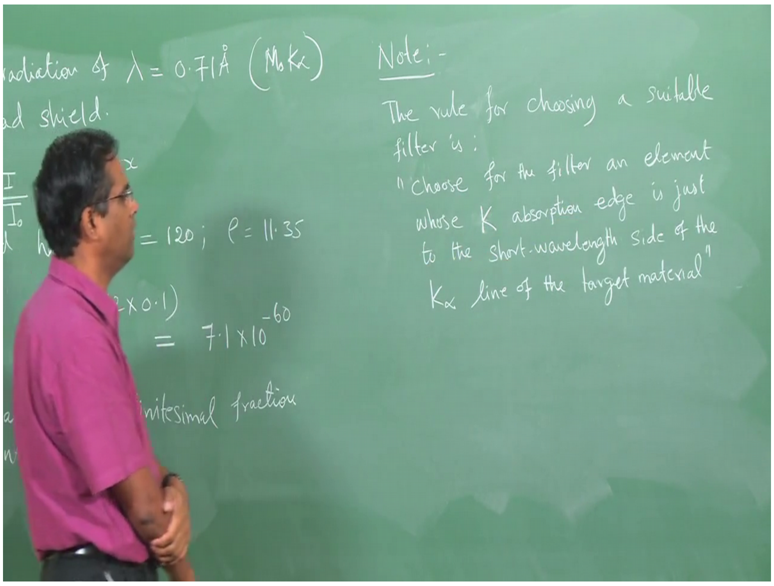


So, you see some of the important application of the governing equations what we have just seen is to find out the: the thickness of the filters that has to be used to obtain a monochromatic X-ray beam, right. So, we will now try to play around with this equation and try to see probably some of the problem, I mean this problem we will try to solve the fraction of radiation coming out of this filter that is a lead filter of 1 mm thickness and then we can go back and then look at other parameters: just playing around these equations.

So, we know the equation can be rewritten to calculate the fraction transmitted I by I naught is equal to e to the power minus mu x. At this wavelength the lead has the mu by rho of 120 where rho for lead is about 11.35 and mu is 1362. So, we will simply substitute this to obtain this value of fraction transmitted. What we have done is- we have just simply substituted this into this, thickness is about 1 mm. So, x in this equation is always given in centimeter. So, you appropriately change that and then you get this value. What you find the number is, it is infinitesimally small compared to the original intensity. So, it is a good filter.

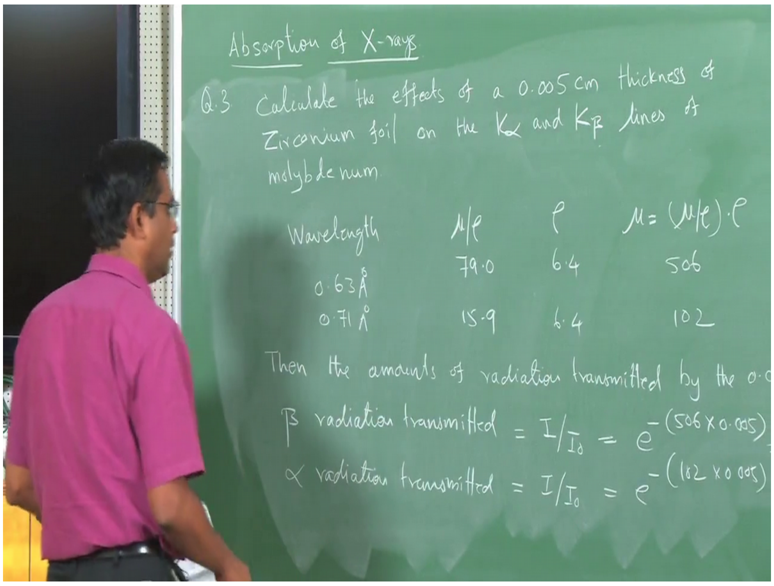
The transmitted radiation is an infinitesimal fraction of the original beam intensity. So, this is the other way of looking at it. And then we learnt just move on to the third problem. So, before even we move to we have note.

(Refer Slide Time: 09:40)



Before we even move into the next problem let us try to get the note. So, the philosophy of choosing the filter: chose for the filter an element whose K absorption edges just to the short wavelength side of the K alpha line of the target material. So, that you will have an effective filtering like you all must have carefully looked at the lecture; it is nicely demonstrated. So, this problem is also we are working around this philosophy only.

(Refer Slide Time: 11:00)

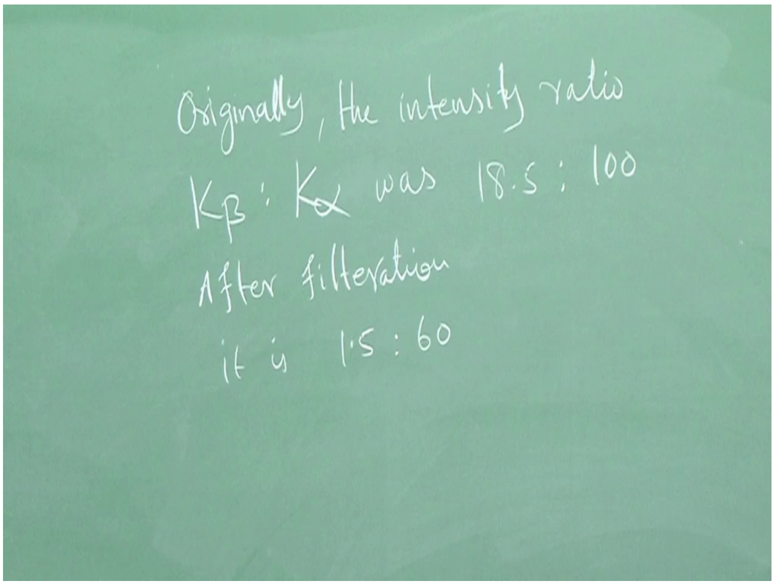


So the question here is: calculate the effects of 0.005 centimeter thickness of zirconium foil on the K alpha and K beta lines of molybdenum. So, basically we are looking at the filtering effect for the given wavelength of zirconium here and the mass absorption coefficient and of course the density data. So, we can calculate the.

So, what we have done here is, we have simply used that the previous equation for calculating the beta radiation transmitted through this formula which is about 0.08, which is nothing but 8 percent. See alpha radiation transmitted according to this calculation it is about 0.6, which is about 60 percent.

So, originally the intensity ratio is pretty high compared to using the zirconium filter probably I will write that t equation here.

(Refer Slide Time: 15:22)

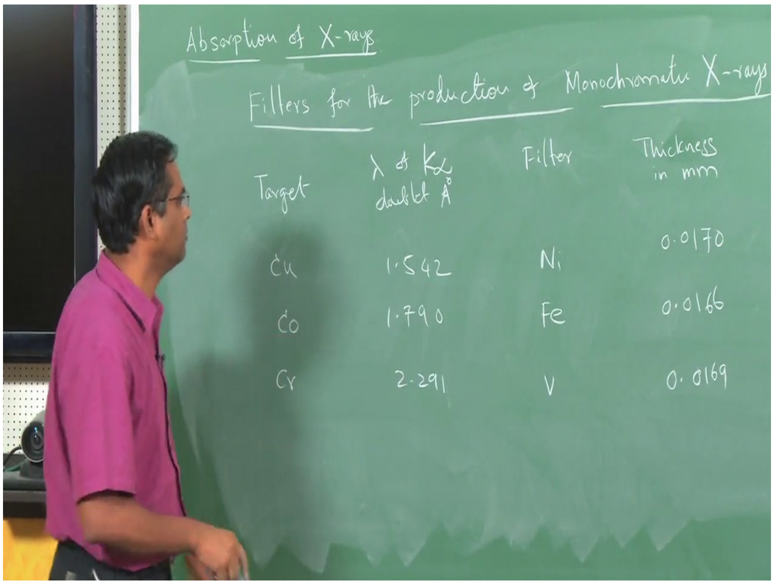


I mean the ratio I will write. So, what is really the intensity ratio of K beta is to K alpha is 18.5 is to 10, after the filtration it is around 1.5 to 60. So, that clearly indicates the effectiveness of this zirconium foil, filter on the molybdenum target.

So, from these three problems at least you have some good idea about how the transmitted radiations are calculated, how the effect of thickness is visualized. And even to start with how the mass absorption coefficients are calculated for a chemical compound.

I will now just list few of the target and filter material based on the philosophy what we have written, which is also you would have seen in the lecture.

(Refer Slide Time: 17:34)



So, what I have just given is a most prominent target material one come across in the X-ray lab. You have the copper target A K alpha doublet wavelength is for a 1.54 angstrom. If we use a nickel filter of a thickness 0.017 mm the filtering K beta filtering will be about 98.4 percent. So, similarly if you use a iron filter for a cobalt target of this wavelength with a 0.016 mm thickness of a filter the effective filtering is about 98.9. And for a chromium target using a vanadium filter of this thickness 0.0169, you have about 99.4 percent of filtering.

So, you see that by choosing an appropriate target for the appropriate thickness the filtering is more effective. Some of these large tables are available in some of the standard handbooks as well as the data books, so can always refer this to select the appropriate filter for making of the obtaining the a monochromatic X-rays for a given target material.

Thank you.