NPTEL
NPTEL ONLINE COURSE

Tutorial – 1
Materials Characterization

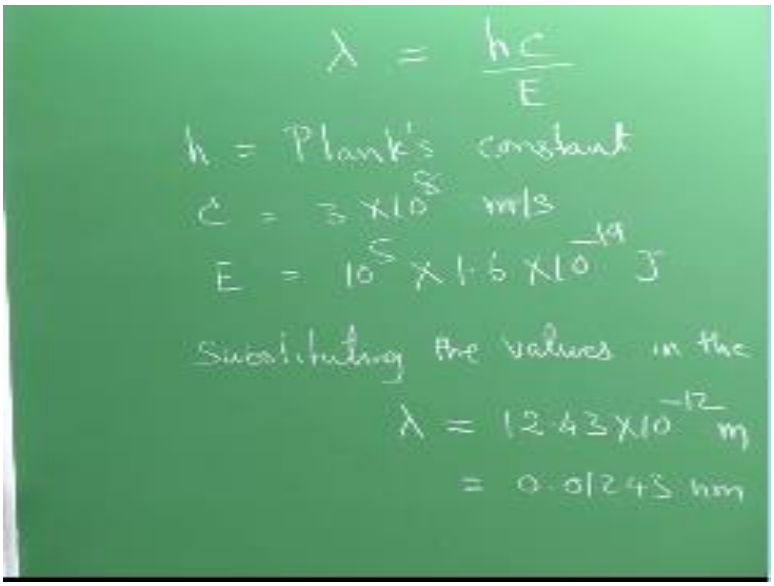
Fundamentals of X – ray diffraction

Dr. S. Sankaran
Associate Professor
Department of Metallurgical and Materials Engineering
IIT Madras
Email: ssankaran@iitm.ac.in

Hello everyone welcome to this online NPTEL course this is part of the x-ray diffraction and transmission electron microscopy course and today we are going to have some tutorials where I would like to give you some numerical examples explaining the concepts which we have covered in the lectures. So I would like to mention that all of you that you have to first clearly understand the concepts what we have discussed in the theory classes and then all this numerical will have direct relation with those lectures.

And if you have any queries you are free to contact us through the discussion forum in the online portal, so I will just start the sum of the numerical problems. So first one is related to the very fundamental nature of electromagnetic radiation.

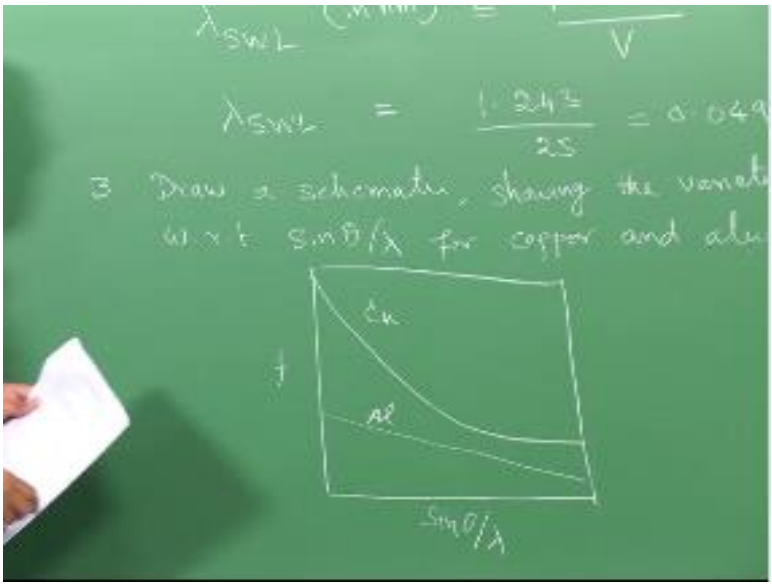
(Refer Slide Time: 01:31)



So the question is calculate the wavelength of an x-ray moving with the speed of light having energy of 10^5 electron volt, so what is the relation what we have learnt in the lectures. So you have this relation λ is equal to HC / E if we can use this relation we will be able to find the answer for this problem where h is Planck's constant see is velocity of light which is 3 $x10^8$ meters per second e is10^5 x 1.6 x 10^{-19} J and if you substitute all these values you get λ 12.4 3 into 10 to the power minus 12 meters or 0. 01243 nanometers.

So it is a simple problem where you would like to see the weather the wavelength is changing with the speed of light which possess this kind of energy.

(Refer Slide Time: 05:18)



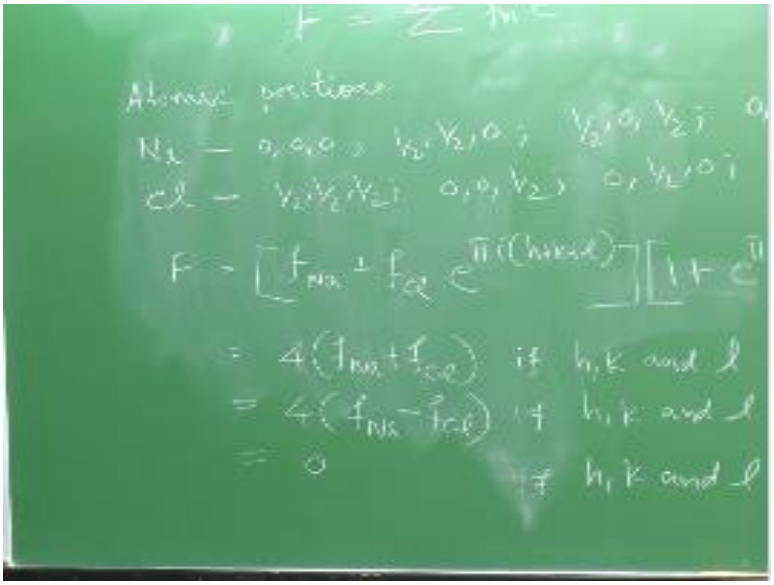
So we will move on to the problem two, so the question is calculate the λ SW gal for the molybdenum when the acceleration potential is 25 kilo volt. So if you recall the beginning of this x-ray lectures some of the first few lectures we talked about this the wave length limit and one can calculate this with this formula you can look at it which is given in nanometers this is in an approximation for 3 x v 1.2 4 3 by v so you have voltage even so it simply substitute this value here.

And then you have lambda s w is equal to 1point 2 4 3 / 25 is equal to 0 point 0for 9 and 0 meter says this is another simple problem where you can find out this wave length limit or for the molybdenum we will slowly move on to the next concept, so the question is draw a schematic showing the variation of atomic scattering factor f with respect to sine θ by λ for a copper and aluminum respectively in the same graph.

So the idea is to illustrate the scattering factor of these two metals and then how they are compared so that is the idea so let us put this is sine theta by λ so the copper atomic scattering factor varies like this with the sine θ whereas your aluminum is varying like this. So this is again just to give you an idea of how these atomic scattering factors are compared between two. So I

hope you will be able to recall the concept of atomic scattering factor and its significance when we when we have discussed in the x-ray class where we talked about the intensity of the x-ray radiation after diffraction we talked about the significance of this and this will be useful in explaining that concept so you can verify the class lectures.

(Refer Slide Time: 12:00)



So now we will move on to other important problem the question is calculate the structure factor f for sodium chloride crystal. So if you recall the lectures on this structure factor so be if you we have first discussed about atomic scattering factor and then how that is influenced by the atom specific atoms in giving the total structure factor of a given crystal system we have solved a few problems in the lectures and if you can recall.

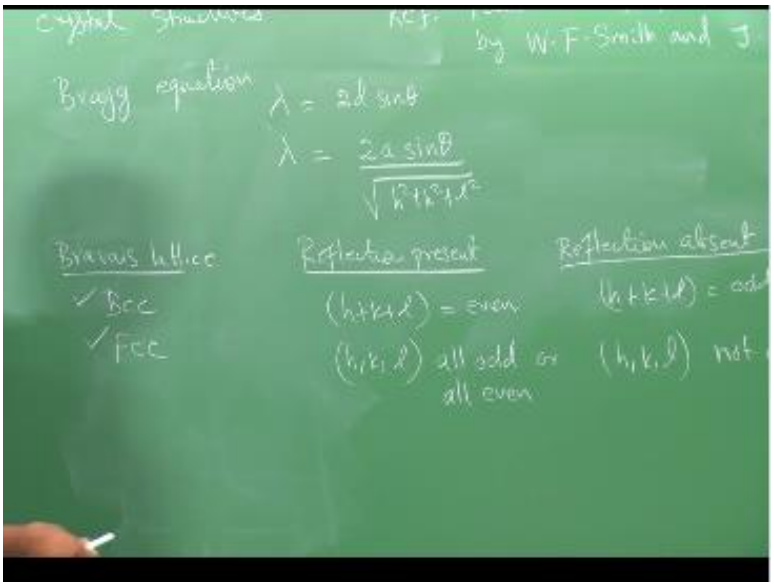
So this if you can try to calculate this in fact this is already solved in the lecture class if I not wrong nevertheless we would like to recall and then try to redo that so the first step is we will write an expression for structure factor f which is summation of all the individual atomic scattering factor of this form, so now we can what is the crystal structure of CL, so if you can write those atomic positions in the unit cells it will be sodium atoms.

So it will be in the cubic lattice and then you can see that sodium atom will be in these positions and similarly we can write chlorine atom positions so they are all exact positions of these two atoms in the cubic lattice and then you just substitute this whole thing in this and then you will get expression like this so since we are talking about individual atomic scattering fact it should be a small F into exponential pi I h + k + L into 1 plush + k +so you will I have not given all the steps but this is a expression you will arrive at if you substitute each one of them and sum it up and take the common factor out you will get the expression like this.

And then we can now write a condition if H K and L all are even then f is equal to four times of n a + f CL and we have another condition if HK and yell all are odd then it is for into F n a minus f CL and we have one more condition f is equal to zero that means the structure factor is zero if HK and L or mixed, so you have three conditions here if hkl all of even then the structure factor is for into fkd a plus f CL if HK and yell are all odd then f is equal to four into find minus f CL your structure factor is zero if H K and L there are mixed indices so.

So like that you can calculate that for other crystal systems and some of them have been shown in the slides during the lecture hours and you can practice it for simple systems we can take simple cubic and body centered cubic face-centered cubic and some other simple compounds like this so you can follow so this is one type. So now we will move on to some of the applications drag law.

(Refer Slide Time: 20:27)

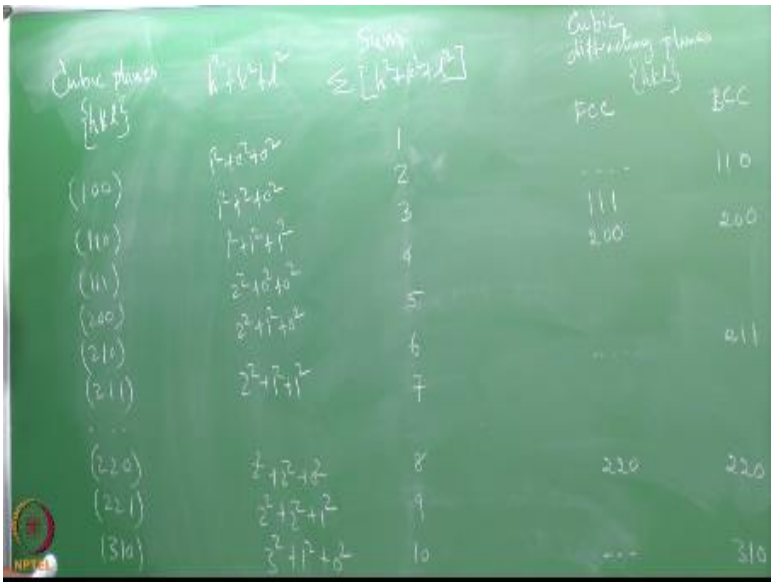


So what we are going to do now look at some of the ideas of interpreting experimental x-ray diffraction data for metals with cubic crystal structures the reference for this exercise is from foundations of material science and engineering by WF Smith and J has hmi, so we look at the some of the parameters or calculation procedures on interpreting this x-ray data so we know then brag equation we will start with the Bragg equation λ is equal to 2 d sine-theta and we can write lambda is to a sine theta divided by square root of H square plus K square plus L square.

So this is you can substitute the expression for D that is a by square root of H square plus K square plus y square and then we can also write some of the basic rules, so these are the rules determining the diffraction planes in the cubic system if it is a VCC Brava is lattice then the reflection will be present when h + k +l is equal to given and the reflection will be absent if h + k + l is equal to art this is for BCC lattice for in the case of FCC Brava is lattice then the reflection is possible where H K and yell are all odd or are all even and the reflection will be absent if hkl not all odd are all even.

So using this rules we can tabulates some of the specific miller indices so that we can interpret them easily I will write few of this values on the board.

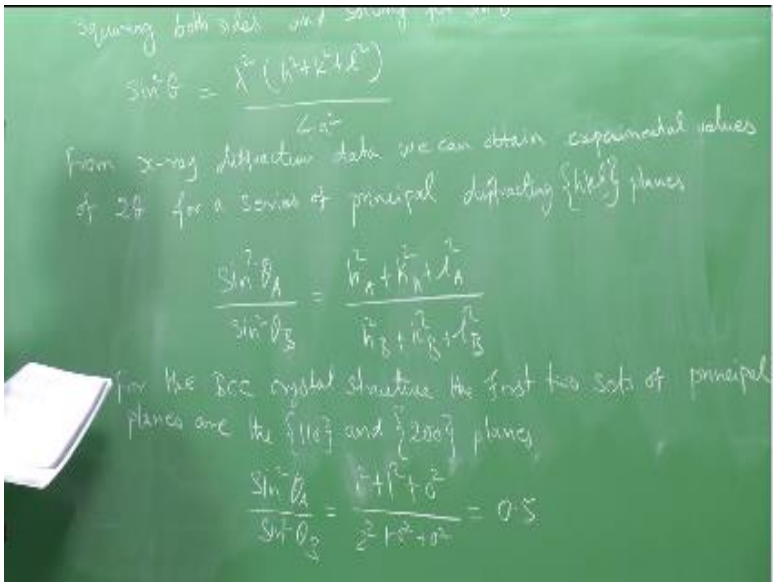
(Refer Slide Time: 26:58)



So what I have done here is putting this all possible hkl values for a simple cubic system that starts from 100 110111 200 210 211 and then you will have a few more possibilities then 220 221 310 and if you can square all of them and then write this summation of the synthesis so you will see that they will all come under the sequence. So now you can see if it is a face that cubic lattice or a BC body centered cubic lattice which are the reflections you will see in an x-ray diffraction according to this selection rule so in the face centered cubic lattice you will see 111 200 220 and so on and BCC you will see 110 200 211 220 and 310 and so on.

So like that if the, if you can keep the stable for a reference it is easy to interpret as a reference so now we will see what are the simple relations.

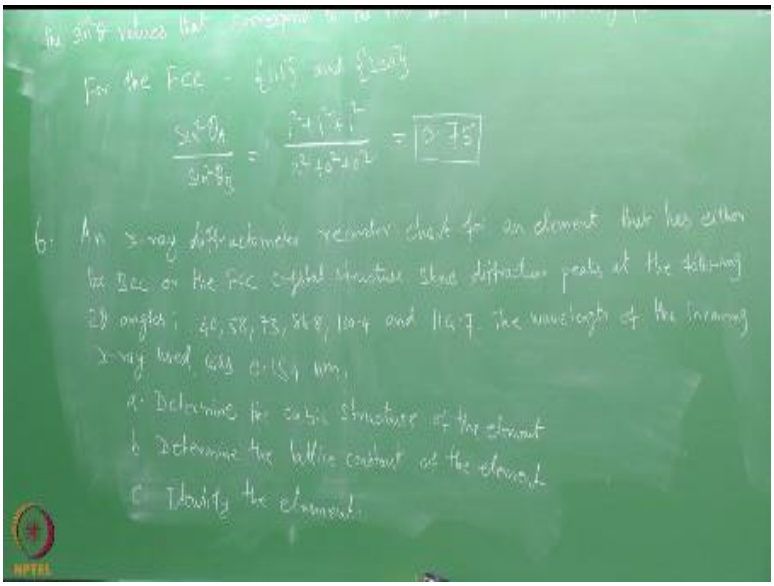
(Refer Slide Time: 32:39)



We can take out from this table so we have written this relation in terms of lattice constant in stuff d spacing. So you see four from the x-ray diffraction data we can obtain experimental values of two θ for a series of principle diffracting hkl planes but the incoming wave length and the lattice constants are constant you can eliminate them and then we can try to get the ratio of two sin θ values.

So suppose if you have the samples which you think that you have both FCC and BCC is there as a mixture to find out the data are interpreting the data coming from such a sample you can we can try to use this kind of relation assuming that one is coming from a one is coming from be so the ratio of this two intensities will be written like this for, so for the BCC crystal structure the first two sets of principle refracting planes are 110 200 so like this from this table. So we can write$1^2+1^2+0^2$ $2^2+0^2+0^2=0.5$.

(Refer Slide Time: 38:42)

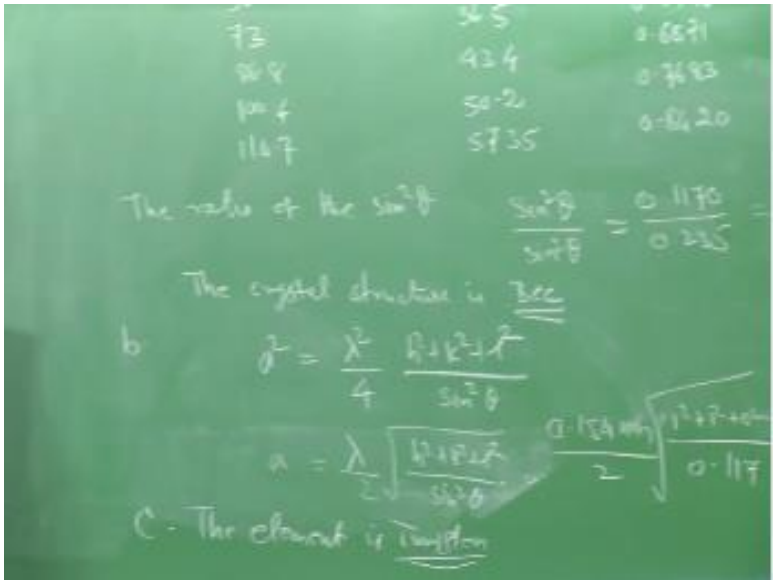


So now we can write from this so from this analysis if the crystal structure of the unknown cubic metal is BCC then the ratio of the sine squared values that correspond to the first two principal diffracting planes will be 0.5, so we can work out the similar for on the FCC the first two principal defecting planes or 111 and 200 then we can write $\sin^2\theta A/\sin^2\theta B$ which is equal to 0.75 so similar to this we can write if the crystal structure of the unknown cubic metal is BCC this is FCC instead of BCC then the ratio of the $\sin^2$ squared values correspond to the first two principal planes will be 0.75 for FCC so based on this all the x-ray diffraction data interpretation we will solve one problem we can take it as problem number 6.

So now let us look at the problem an x-ray diffractometer recorder chart for an element that has either the BCC or the FCC crystal structure shows the diffraction peaks are the following 2θ angles 40, 58, 73, 80 6.8 100.4 and 114.7 the wavelength of the incoming x-ray used was 0.15 for nanometer a determine the cubic structure of the element, b determining the lattice constant of the element, c identify the element.

So since already it is shown as a cubic then we have to find out whether it is BCC our FCC and of course we have to calculate the lattice constant and then we are we also have to identify the element so we will solve this using the known relations whatever we have already discussed.

(Refer Slide Time: 47:46)



So what we have done now is we have the 2θ value given here so now we have tabulated the two θ value and then from that θ value sinθ value and $\sin^2\theta$ value now look at the ratios for the first and second angle so you take first two angles if you take 0.1170/0.23 5 which is 0.498 is approximately equal to 0.5. So since it is 0.5 the crystal structure is so this BCC then we can calculate the lattice constant so we know the relation.

So you can write $a=\lambda/2\sqrt{h^2+K^2+l^2}$ so we can simply substitute this 0.154 for nanometer directed to $\sqrt{1^2+1^2+0^2}/0.117$ so you substitute this into this relation you get about 0.318 nanometers that is a value of a. So since it is lattice constant is 318 and it has got the BCC so from the table we can also find out the element is tungsten, handbook you can find out the element is tungsten that is from this crystal structure as well as the lattice constant value we can find out from the handbook or a reference table.

So what we have seen in this problem if you how to use the sine θ value in determining various parameters corresponding to the given crystal system so the previous relations they were all used here and you can also practice some of these problems where the sin θ values are used to determine the crystal system, so we will stop here we will continue to solve few more problems in the next class, thank you.

IIT Madras Production

Funded by

Department of Higher Education

Ministry of Human Resource Development

Government of India

www.nptel.ac.in