Solid State Chemistry
Prof. Madhav Ranganathan
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture - 45
Review of Week 9, Practice Problems

Now, we will go to the 5th in last lecture of week 9. In this lecture I will do a recap of what we learn this week and then do some practice problems. So, week 9 lecture 5 will be recap of Week 9 and Practice Problems.

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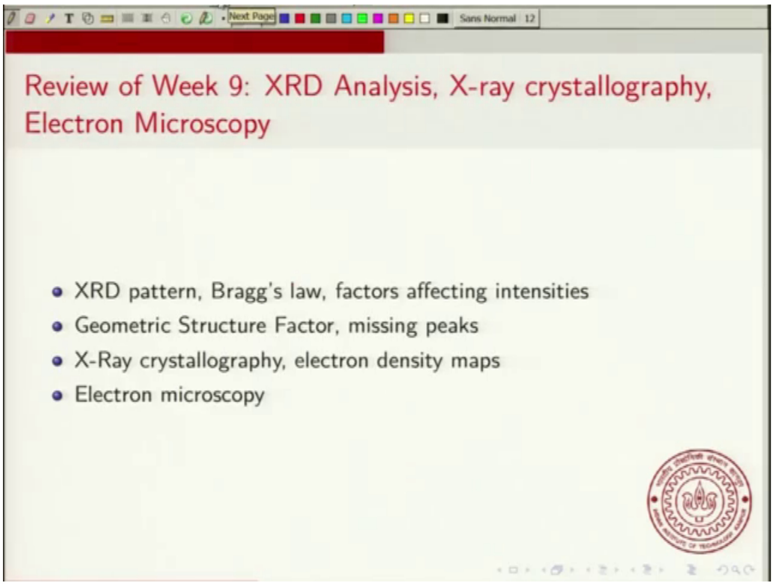

So, let us quickly recap what we learnt. In this week we continued the discussion on X-ray diffraction. In fact, we learnt how to analyse X-ray diffraction patterns and then we learnt we talked briefly about X-ray crystallography and a electron microscopy. So, in more detail we learnt about the X-ray diffraction pattern, we saw how to use Bragg's law and what are the factors affecting the intensities.

Like the temperature factor, the (Refer Time: 00:55) factor, the atomic form factor, the geometric structure factor. And then we saw how to calculate the geometric factor and how the geometric factor can explain missing peaks in X-ray diffraction patterns. Then I talked about X-ray crystallography and electron density maps and finally, we talked briefly about electron microscopy.

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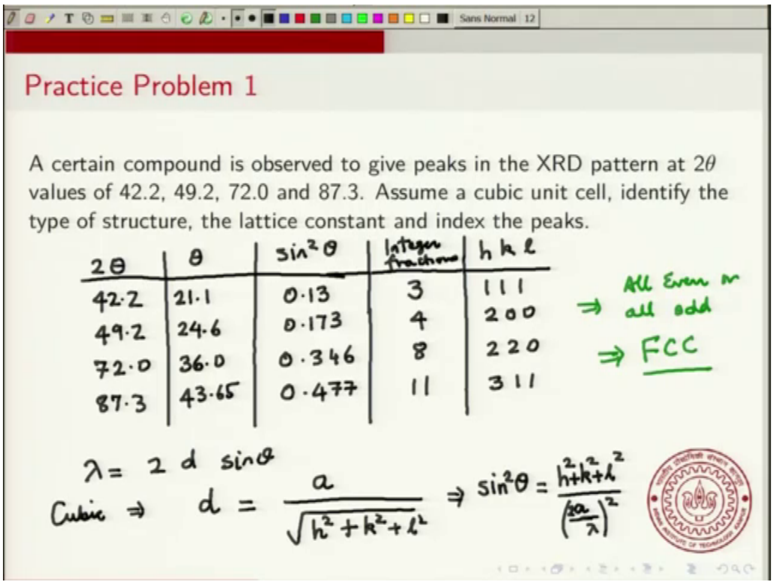

So, now let us do a couple of simple problems that will give you an idea ok. So, the first problem is relates to analysis of XRD patterns. A certain compound is observed to give peaks in the XRD pattern at 2 theta values ok, these are the 2 theta values in degrees. So, you are asked to assume a cubic cell and identify the type of structure, the lattice constant and to index the peaks ok. So, what we have we will make a little table. So, we have 2 theta values we have so, we have 2 theta values of 42.2 49.2 72.0 87.3 ok.

And what we will do is, we will calculate their corresponding theta values that corresponding theta values is just half of this 21.1 24.6 36.0 43.65. Now, what I am going to do is the following remember the Bragg’s law ok. So, the Bragg’s law says that lambda equal to 2 d sin theta and in particular for a cubic crystal; cubic implies d is equal to a divided by square root of h square plus k square plus l square ok.

And so, in other words I can say that so, if I substitute for d and then I multiply out and I can write this in the following way. I can write that sin square theta is equal to h square plus k square plus l square divided by ok, I will just write it as divided by and what I have in here is a by 2 lambda square ok. So, I will just write it this way. So, basically what I want to say is that sin square theta now a is fixed for the lattice, lambda is fixed for the lattice. So, sin square theta is proportional to h square plus k square plus l square ok.

So, what we will do is we will make a table and you will write sin square theta ok, now if I calculate sin square theta. So, for 21.1 degrees if you calculate sin theta and then square it you will get a value of 0.13. For 24.6 if you do the same you will get 0.173, for 36.0 if you do the same you will get 0.346 and for this if you do the same you will get 0.477 ok. So now, at this point you try to identify integer fractions because, what we said is that sin square theta should be proportional to an integer h square plus k square plus l square is an integer.

And so, sin square theta should be proportional to an integer and so, we try to identify integer fractions of each of these ok. Now we notice that you have 0.173 and 0.346. So, clearly this is twice this clearly 0.346 is twice of this ok. Now, but and we see that 0.13 is about three-fourth of this ok. So, if we use 0.042 as a fraction as the divisor then this will be 3 times. So, 0.13 is 3 times 0.042, 0.173 is 4 times 0.042. This is 8 times and this is 11 times ok, so, the integer fractions ok. So, this again we just inspected it and we identified this in integer fractions ok.

And now so, what we identify immediately that h square plus k square plus l square if it is 3 then what; that means, is our h k l has to be 1 1 1; that is a only way h square plus k square plus l square can be 3. Similarly, if it has to be 4 it has to be 2 0 0 2 0 0 or 0 2 0 it or 0 2 0 or 0 0 2, this has to be 2 2 0, this has to be 3 1 1 ok. So, we immediately see that they are either all even or all odd. So, implies it is a face centred cubic structure ok, it is a face centred structure. And since it is cubic so, it is face centred cubic structure ok.

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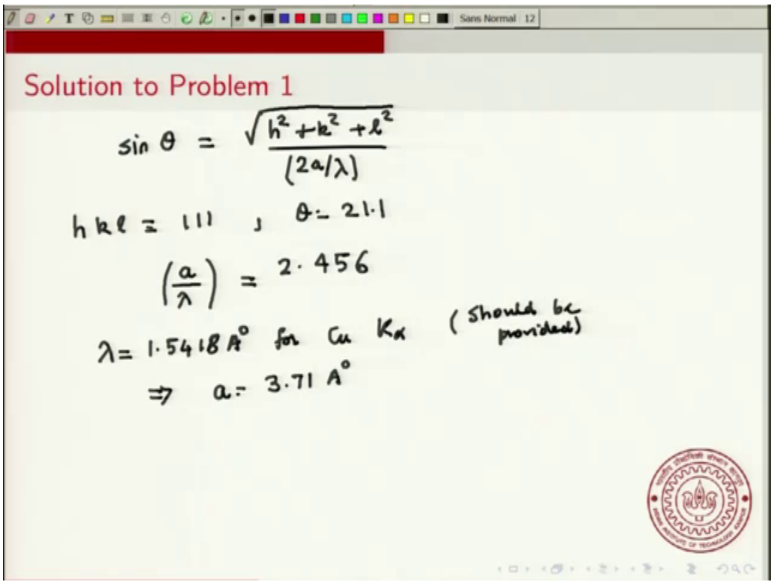

So, just by so, this is how you index a peaks. Now, the remaining part is to calculate the wavelength, no to calculate the lattice parameter. So, again if you use the expression sin square theta is equal to h square plus k square plus l square divided by 2 a by lambda. This should be sorry this should be 2 a by lambda; 2 a by lambda naught a by 2 lambda. Then the what you 2 a by lambda let me write sin theta a square root of h square plus k square plus l square divided by 2 a by lambda ok. And if you work this out you will get; now let us take the case where h k l is 1 1 1 and for that we have theta equal to 21.1 ok.

And if you do this you will get; you will get 2.456 ok, you can where you can verify this. So, basically you will have root 3 and then you will have root 3 divided by 2 and so, that will give you about 2.456 on. And if you substitute the value of lambda for copper K alpha radiation is 1.5418 angstroms for copper K alpha ok. So, that implies and this should be provided should be provided ok. I did not provide this in this problem, but it should have been provided, this implies a is equal to 3.71 angstroms ok. So, we can calculate the lattice parameter in this way ok.

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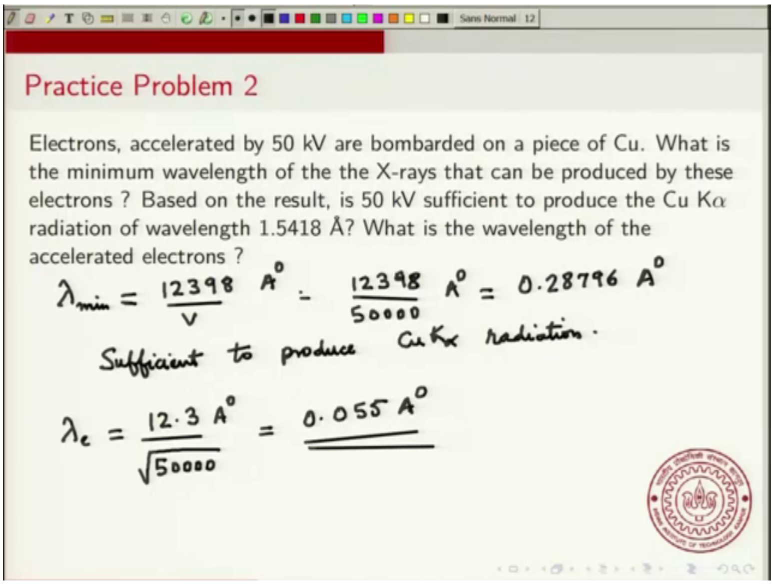

Now, next problem this is a problem which says that electrons are accelerated by 50 kilo volts and these are bombarded on a piece of copper. What is the minimum wavelength of X-rays that can be produced by these electrons? Based on the result is 50 kilo volt sufficient to produce a copper K alpha radiation of wavelength 1.5418. And what is the wavelength of the accelerated electrons? So, we saw when we were discussing X-rays that the minimum wavelength that is produced by X-rays that are produced from accelerating electrons by some voltage is can be written in this way 12398 angstroms divided by v in volts ok.

And so if we substitute 50000 volts so, that gives me 0.28796 angstroms ok. So, clearly the wavelength is much smaller than the copper K alpha radiation. So, this is sufficient so, the wavelength is smaller means the energy is higher than copper K alpha. So, basically this is sufficient to produce Cu K alpha radiation ok. And so, basically 50 kilo volts is sufficient to produce a copper K alpha radiation ok. Since, the minimum wavelength is much smaller than the wavelength of the copper K alpha radiation; remember that smaller wavelength corresponds to higher energy.

So, it has more energy than required for the copper K alpha radiation ok. Now what is the wavelength of the electrons? So, lambda of electrons is equal to 12.3 angstroms divided by square root of v square root of 50000 ok. This works out about 0.055 angstroms and as we said this is much smaller than the wavelength of the X-rays ok. So, with these practice problems I will conclude this lecture and with this I will conclude week 9 of this course. So, in week 8 and week 9 we have learnt; we have learnt a lot about X-ray diffraction. But, we have also learnt about a few other things like reciprocal lattice and some microscopic techniques.

In the next week, I will look at crystal structures of typical materials starting with metals, binary compounds and some interesting oxides ok. So, this will be fairly descriptive ok, but it will be interesting to see what are the various structures that are commonly found.

So, thank you.