Solid State Chemistry
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Lecture – 40
Review of Week 8, Practice Problems

Now, I will go to the 5th and last lecture of week 8 of this course and in this week you have learnt about about Miller indices and about reciprocal lattice, Bragg's law and X-ray diffraction ok. We will continue discussing X-ray diffraction in more detail in the next week ok, but we will review what we learnt this week and then do some practice problems based on the contents of this week in today's lecture. So, week 8 lecture 5 will be, Review of Week 8 and Practice Problem.

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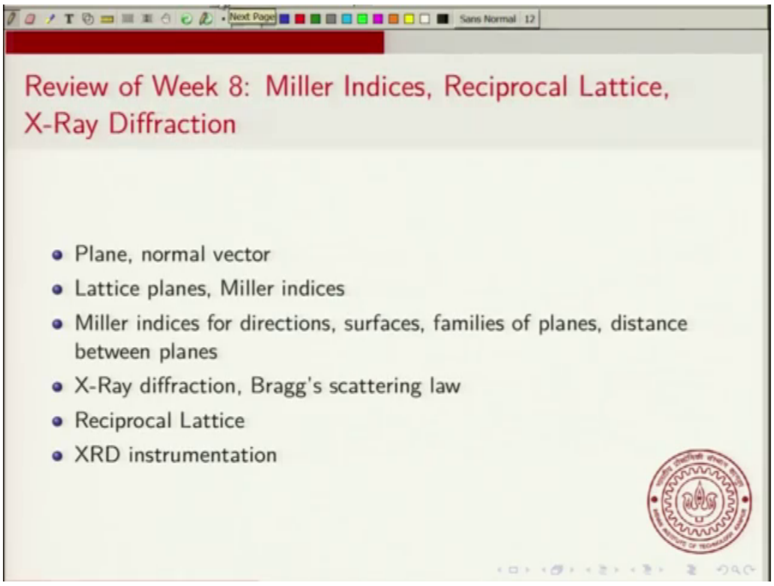

Let us first review what we learnt. So, in this week we learnt Miller indices, reciprocal lattice and X-ray diffraction. So, we learnt how to represent a plane, how to represent a normal vector, we learnt the concept of Lattice planes and Miller indices. Miller indices for directions, surfaces, families of planes, distance between planes and we also showed how to calculate the distance between planes. Then, we learnt about X-ray diffraction, Bragg's scattering law, we learnt about the reciprocal lattice and some details about the instrumentation of the for the X-ray diffractometer ok. So, now let us do a couple of practice problems ok.

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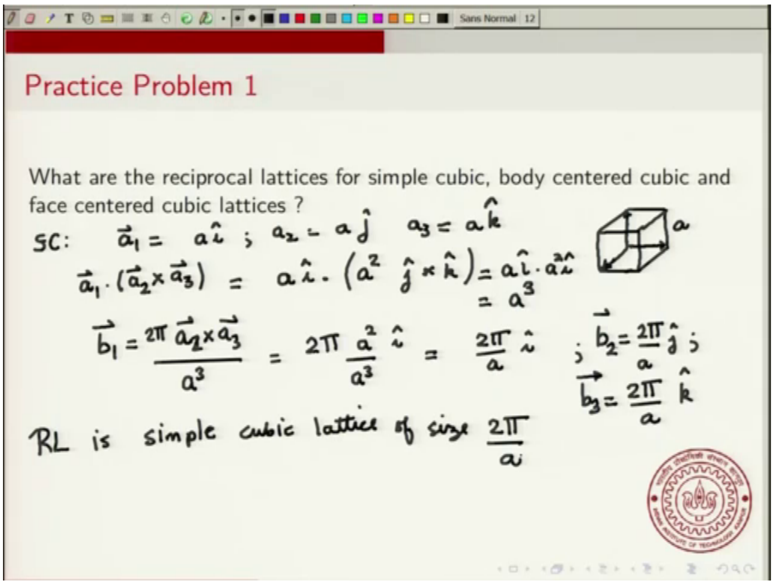

So the first problem ask, what are the reciprocal lattices for simple cubic, body centered cubic and face centered cubic lattices? So, to do this what we need to identify is, so let us first take the simple cubic. So, a 1 is equal to a times i ok. So, if a is the a is the side of the cube, then so clearly you have ok. So, this side is a. So, a 1 is a times i, a 2 equal to a times j, a 3 equal to a times k.

So, what do we get? So, first thing, let us calculate a 1 dot a 2 cross a 3. So, now we can do this quite easily. So, a 1 is just a times i dotted into; now a 2 is a, a times j and a 3 is a times k. So, a 2 cross a 3 can be written as a square multiplied by i cross j. So sorry, not i crossed j it should be j cross k. should be j cross k . Now j cross k is nothing, but i, ok. So, you have so j cross k is i so, this is a i in dotted into a square i. This is equal to a cube, yeah which is the volume of the cell.

So, you can verify that the volume of the cell is given by this. And now so since we know all these cross products, so, a 2 cross a 3 is a 1 ; a 2 cross a 3 is a 1; a 2 cross a 3 is a square i ok. So then, what you can show is that b 1 is equal to 2 pi, 2 pi a 1 cross, no a 2 cross a 3 divided by a cube.

So, this is equal to 2 pi a 2 cross a 3 is a square i by a cube, which is equal to 2 pi by a i; which is what we showed a lot earlier which is what we as should right when we talked about reciprocal lattice. Similarly, you can show that b 2 will be 2 pi by a times j and b 3 equal to 2 pi times k.

Now, so this completes the the reciprocal lattice for the simple cubic and you can see that the only difference between the simple cubic lattice and the reciprocal cubic lattice is that, instead of a that you had in the case of simple cubic lattice you have 2 pi by a ok. So, the reciprocal lattice is a simple cubic lattice of size; cubic lattice of size 2 pi by a ok. So, that is the reciprocal lattice of a simple cubic lattice. So now next let us go to face centered cube ok.

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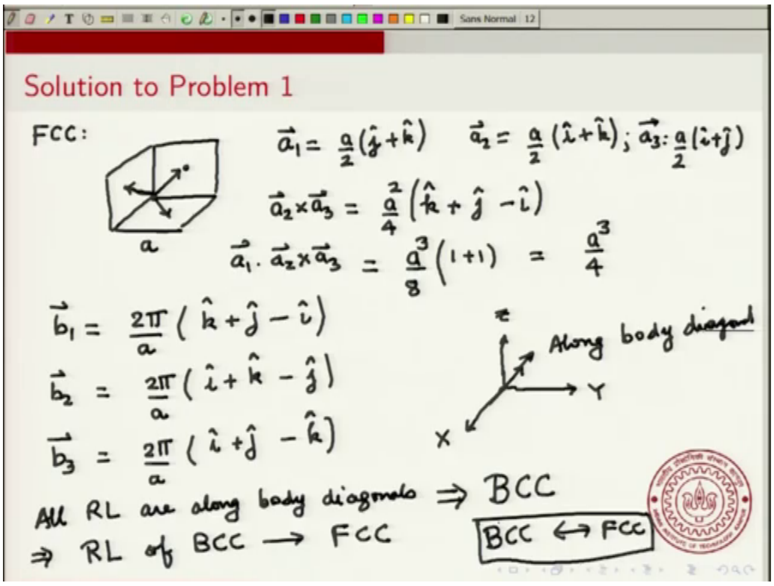

Let us go to FCC. Now in FCC, your primitive translation vectors are the following ok. So, let me draw the FCC cell ok. So, I can take this, this and this as my primitive translation vectors ok. And so, I can take a 1 equal to and if the side is a then a 1 equal to a by 2 times i or I will take it as j plus k; a 2 is equal to a by 2 i plus k and a 3 i plus j. I can take I can take them in any order it does not matter ok.

So, these are my 3 primitive translation vectors. Now you can directly guess what the volume will be ok; the volume of that is formed by these 3 primitive translation vectors, but let us work it out ok. So a 2 cross a 3 is equal to so a by 4, now i cross i is 0; i cross j is k, plus now k cross i is j; k cross j is minus i; k cross j is minus i and now if I take a 1 dot a 2 cross a 3 this will be a by 8 times.

Now, you will have a term j dot j and k dot a. There is no i term so, you will get 1 plus 1 is equal to a by 4 which is what you expect at. You would expect the volume for the volume to be one-forth that of this cube ok. So now, so what do we get? We get b 1 is equal to, now you already have a 2 cross a 3. So, that has a factor of a by 4 and the denominator will also have a by 4. So, we will so it is, it should be a square by 4 a cube by 8. I forgot the a cube by 8 and a cube by 4 ok.

So, b 1 will be equal to 2 pi by a k plus j minus i ok and b 2 by a. And again, you can just do it by permutation. So, you will have for b 2, you will have i plus k minus j and for b 3, i plus j minus k. So you can see by this. So, what do these vectors look like? So what these vectors look like? So, if you take k and let me take this as x, this is y and this is z axis ok. So, k plus j minus i will look like a vector ok.

So that is along the diagonal of the cube ok, but it goes, it basically goes along the diagonal of the cube, from one corner to the opposite corner ok. Similarly, the others so, this is clearly along the body diagonal ok. So similarly, all these will be along body diagonals. So, this basically says that all reciprocal lattice vectors are along body diagonals ok. This implies reciprocal lattices BCC.

So, the reciprocal lattice of FCC is BCC ok, is a BCC lattice and interestingly, this also leads to the result that this implies that reciprocal lattice of BCC should be an FCC. So, by solving the reciprocal lattice of the FCC, we have also solved the reciprocal lattice of BCC because, the reciprocal lattice of a reciprocal lattice is the original lattice ok. So the reciprocal lattice, since reciprocal lattice of BCC is FCC, it follows that the reciprocal lattice is since a reciprocal lattice of FCC is a BCC, it follows that the reciprocal lattice of BCC has to be FCC ok.

So, basically, there is this real lattice reciprocal lattice pair between BCC and FCC. So, FCC forms this real and reciprocal lattice pair ok. So if the real lattice is BCC; if the Bravais lattice is BCC then the reciprocal lattice will be FCC. Similarly, if the Bravais lattice is FCC, the reciprocal lattice will be BCC ok.

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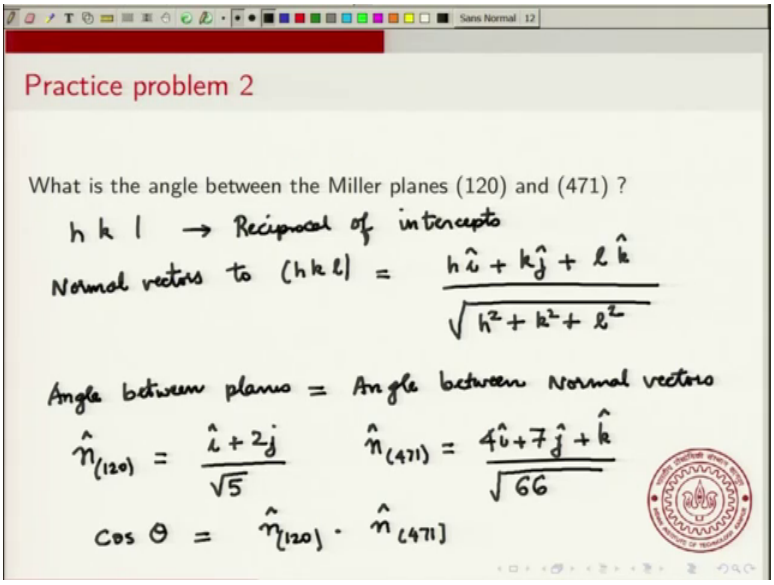

So, next problem is a rather simple problem. What is the angle between the Miller plains 120 and 471? So, we go back to the definition of the Miller indices. So, h k l are their reciprocal of intercepts ok. So, they are proportional to the reciprocal of the intercepts ok. Therefore, the normal vectors to these planes, to h k l is equal to h i plus k j plus l k divided by square root of h square plus k square plus l square that is the unit normal vector to the plane h k l. And the angle between 2 planes is equal to angle between normals.

So, what it immediately follows is that if you want to find the angle between these 2 planes. So, for the normal vector for the 120 plane is equal to i plus 2 j divided by square root of 5. And the normal vector for the 471 Miller planes ok; that is, 4 i plus 7 j plus k divided by 4 square is 16, 7 square is 49 and here in 1 square is 1 so, 50 66 ok.

So, we have these 2 normal vectors. Now we just have to find the angle between these 2 and since these are unit normal vectors, so the angle between them is just the dot product. So, cos of angle between them is equal to n 120 dotted into n 471. So, that is nothing, but the cosine of the angle between them since they are unit normal vectors. So, we can do this easily. So, if you take the dot product you have i into 4 i, and then you have 2 j into 7 j. So, those are the 2 terms that will contribute.

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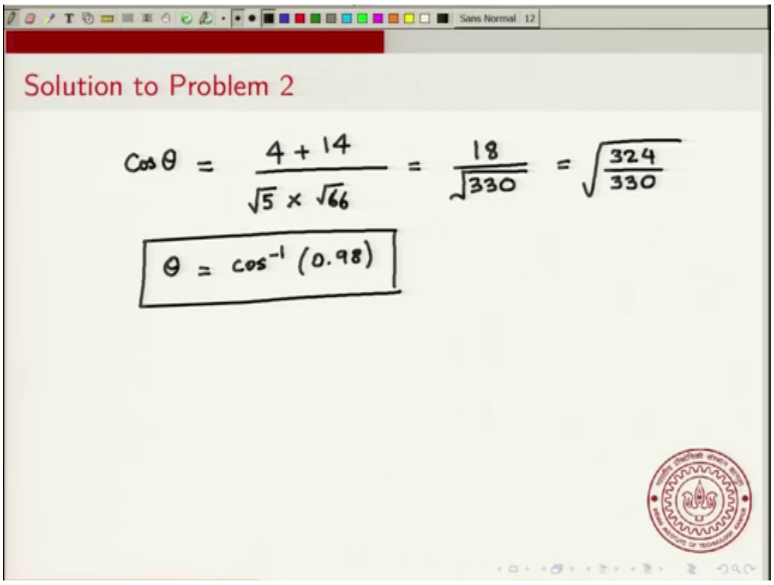

So, cos theta is equal to i into 4 i that is, 4 plus 2 into 7, 14 divided by square root of 5 into square root of 66 that is 1 into 4 4 plus 2 into 7 14. So, that is the dot product and then divided by this square root of 5 into square root of 66 ok. So that is, no sorry 18. Now, 18 square is actually 324 ok so it is actually very close to 1. So, we see that so theta is very small. So, theta equal to cos inverse. This is you know almost about 0.98 ok so, this is the answer. This is the angle between the plane.

So, the angle between the planes this is cos inverse of this will be very close to 0 degrees ok. So, the angle between the planes is extremely close to 0 degrees, ok. So I mean you can find the numerical value of of you can find the exact numerical value, but I will not bother doing that here. But I have illustrated how to calculate the angle between Miller planes. So with this I conclude the 8th week of this course and in the next week we will continue discussing more details about X-ray diffraction ok. And we look at how to actually, how to analyse the X-ray diffraction pattern ok.

Thank you.