Introduction to Reciprocal Space
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Lecture -03
Worked out examples

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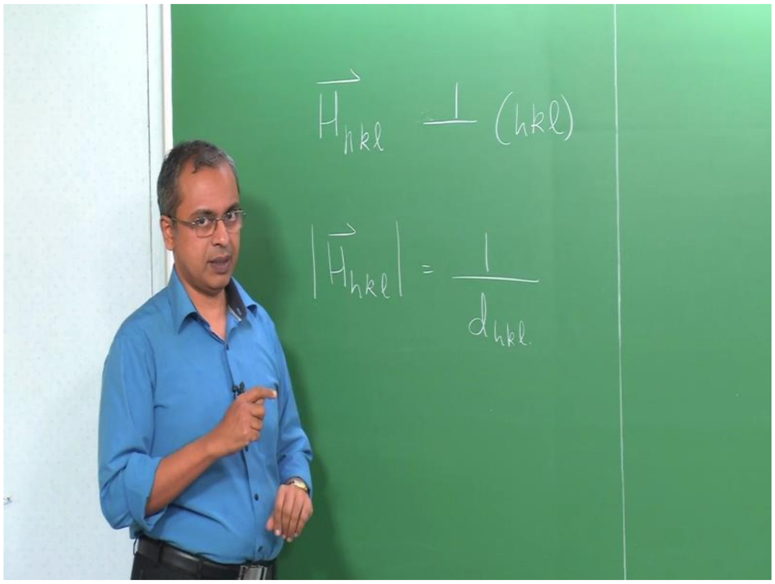

Hello, we have gone over some material on reciprocal lattice. So, in today's class we are just going to look at the three worked examples, about how you would go about drawing a reciprocal lattice based on the few rules that we have understood about the reciprocal lattice okay. So, the two major rules that we put down, are the two rules that I put down here.

We said that the reciprocal lattice vector is designated as Hhkl and that this is perpendicular to the plane hkl. So, in real space you have the plane hkl, the reciprocal lattice vector which is a vector in reciprocal space is perpendicular to the plane in the real space okay. So, this is one rule that we put down for that we derive and we found that you know given our way were defining reciprocal space.

The way we were defining our reciprocal lattice vectors this was one relationship that we arrived at. The other relationship that we arrived at is the modulus of this vector. So, we said the modulus or we found that the modulus of Hhkl = 1 over the spacing of dhkl or 1 divided by the spacing of dhkl right. So, these two rules we arrived at and we just looked at a general triclinic cell.

So, A was not equal to B not equal to C and the angles were all know could have been any angle so there was no great specific specification on the cell, so these rules are general. So, based on this we will do three worked examples. So, the first example we will do is this, we are going to our problem is basically this.

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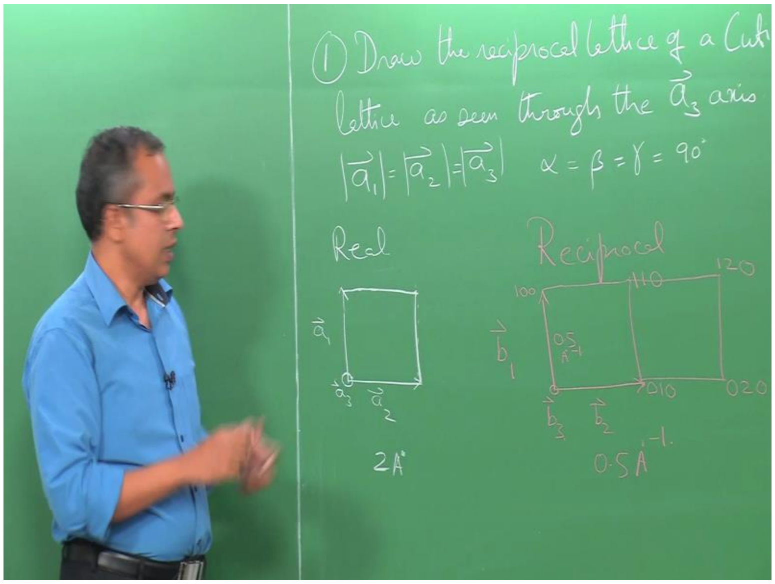

So, we would like to draw the reciprocal lattice of a cubic cell, of a cubic lattice and we will use a two-dimensional representation of it meaning, actually it is three dimensional but we are looking at it from the a3 direction and therefore you only see the a1 and 2, a2 axis so, as seen through the a3 axis. So, this is our problem, so this is the example that we are going to look at, we would like to draw a cubic lattice.

And were going to draw it along the as seen through the a3 direction in other words perpendicular to the a1 and a2 directions and for that we would like to draw the reciprocal lattice. So now as you know for a cubic lattice a1 = a2 = a3 the modulus of these three vectors is the same and alpha equals, so this is the modulus of these three vectors is the same, alpha equals beta equals gamma equals 90 degrees right.

So, this we know about the cubic lattice. So, we will draw the cubic lattice here and we will make some assumptions on the dimensions of a1 and a2 and then on that basis we will come up with the reciprocal lattice. So, let us just draw the cubic lattice as seen, we assume a3 is perpendicular to the plane of the board, so we see a1 and we see a2 okay and a3 is perpendicular to the plane of the board.

So, we simply draw a circle here indicating that a3 is there, but it is perpendicular to the plane of the board right. So now we will complete this lattice, so we just take, so this is how it will be, so it is a cubic lattice and then you can add additional points to fill up the space right. So now we also learnt that through our definition, that you know if you go back to what we define here.

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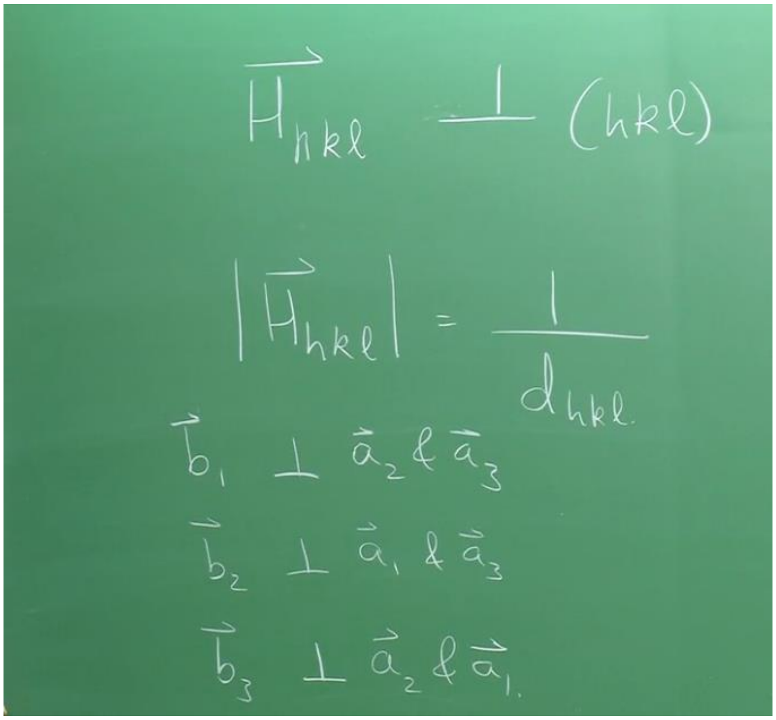

We have Hhkl is perpendicular to 1 by dhkl and Hhkl I am sorry is equal to modulus is 1 by dhkl and the vector itself is perpendicular to Hhkl and therefore we found that, so for example if we have a1, a2 and a3 as the real lattice vectors and b1, b2, b3 as the reciprocal lattice vectors. We had b1 is perpendicular to a1 and I am sorry a2 and a3 and similarly b2 is perpendicular to a1 and a3 and b3 is perpendicular to a2 and a1 right.

So, this is how you would get these things based on these relationships. So that is how we have defined it because it is a2 cross a3 by the volume, a1 cross a3 by volume, a2 cross a1 by volume. So, given that it is naturally perpendicular because of the way we have defined. So now we come back to our worked example.

So, we would now like to draw a lattice which is b1, b2 and b3. So, we see b1 is perpendicular to a3 and a2, so that means it is perpendicular to the a3 axis is here, a2 axis is here. We will assume that these are all about, let us say 2 angstroms which is a very reasonable approximation for many materials. So, we will assume that the dimension a2 is 2 angstroms.

This is 2 angstroms, so on this scale if you look at the idea that the, so first we look at the directions, so and then we look at the magnitude, so our directions are like this, the b1 axis is perpendicular to a3 and a2. So a3 is perpendicular to this plane of the board, a2 is here, so the b1 axis is along this direction, b1 axis is along the a1 direction that we have here.

So, I will just draw the b1 axis here. I will take another colour here to make it clearer for you. So, this is a real space here and this is reciprocal okay. So now along the a1 direction is also b1. So, we are not put a magnitude yet on it, so this is b1, this is the direction of b1 and then b2 will be perpendicular to a1 which is here and to a3 which is in this direction.

So b2 is along that direction which is similar to the direction of a2, so b2 is along this direction okay. So, we got the directions right, based on the idea that it is perpendicular to those planes. The other thing that we know is the value of the reciprocal lattice vector is 1 over the spacing of those corresponding set of planes. So, the spacing between these planes is 2 angstroms right now.

That is the lattice spacing, so that is also the spacing between the set of planes, the spacing between these set of planes. So therefore, the b1 and b2 and b3 are all going to be inverse of 2 angstroms. So that is 0.5 angstrom inverse, so this is 0.5 angstrom inverse and similarly this is 0.5 angstrom inverse okay.

So, if you did that, you can just complete this diagram and so you would get and similarly b3 would be here in the same manner, that will also be 0.5 angstrom inverse. So, they are not drawn actually, they are in different units, so I have not drawn them both to the same scale. But the point is this is 2 angstroms across this is .5 angstrom inverse.

So that is the point and in normal labelling the way we do it is this is simply called 100 without any brackets. This is called 010; this would be 110 and so on. So, you can add actually, you can add the next point also if you wish and this would become this will be 120 and this is 020. So, like this you can add additional points.

And so that is how you would generate the reciprocal lattice of a cubic real lattice, the reciprocal lattice corresponding to cubic real lattice right. So we are now taken a specific case and we have done a worked example, on how you would take a lattice and come up with the reciprocal lattice. We will do a similar example also similarly laid out except that we will relax some conditions here.

So that now this is made it convenient for us because they were all perpendicular to each other. So, we will make it a little bit more difficult for us by relaxing the conditions on the lattice and then see what we get.

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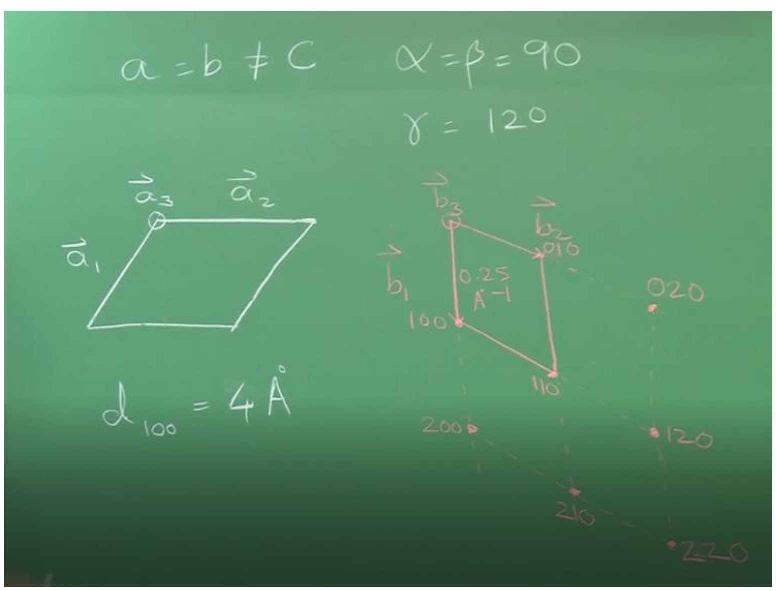

So, we will now look at a hexagonal lattice. So, a hexagonal lattice has the following conditions you have a = b not equal to c and we have alpha equals beta equals 90 and gamma equals 120. So, this is the description we have for hexagonal lattice. So, let us just draw the axis and again we will assume that the c axis is perpendicular to the plane of the board.

Will assume that, so that is the same as a3 axis that we would say a1 this would be a1 this is a2 a3. Will assume a3 is perpendicular to the plane of board and a1 and a2 are along the plane of the board. So, we will simply have this here, I will put something down here, we will say this is 120 degrees right. So, you will have, so that actually yeah, so we will have a1 and then we will come here this is a2 and this would be a3.

So that is how we would do it and incidentally this would then be a right-handed system. So actually, even here we would have to, this is a cubic lattice. So here it did not matter as much but technically this would have to be a right-handed system. So, we should actually have marked this as a1 and this is a2.

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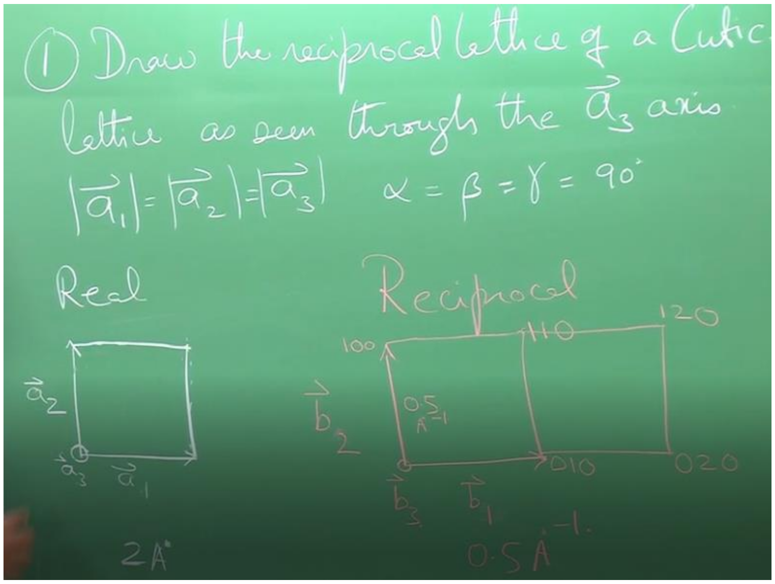

But our basic processes would have been the same. So similarly, this would have become b2 and this would have been b1 to keep it right handed. So just to would keep it right handed that is what it would have been. But basically, it is still all cubic, so it does not really matter here. In any great significance in terms of our result but here also we would look at it the same way a right-handed system.

So, we have a1, a2 and a3 right. So, they are all the same a1 and a2 are the same magnitude, this angle here is 120 degree. So, let us just complete this drawing at this unit cell of the lattice. So, it will be like this, so this is the unit cell we have. Now when you want to draw the reciprocal lattice of this unit cell the same ideas will hold true.

So, we now have the b2 axis as being something that is perpendicular to a3 and a1 okay. So, what is the perpendicular direction here, the perpendicular direction is in this direction right, this direction here is perpendicular to this a3 and a1 is formed this plane a3, a1 plane. This is the direction that is perpendicular to it, so it is in that direction that we will have the b2 axis. So, we just put a dotted line here to just imagine it for ourselves.

And then we just draw that line here, so that is the direction of the b2 axis. The b2 axis which is perpendicular to a3 and it is perpendicular to a1. Similarly, if you look at the b1 axis, the b1 axis is perpendicular to a3 and a2. So, it will actually appear in this direction right. So, parallel to that we will draw a line here that is the b.

So, this is the b3 sorry this is the b1 direction and that is the b2 direction okay. So b2 direction is that side and b1 direction is this side. Now magnitude again we have to see, we will have to make some assumption for inter planar spacing here. So, let us not worry about the lattice dimension directly. We need to worry about the spacing.

Spacing between the planes is the perpendicular distance between these planes and so we just assume that that is say 4 angstroms. We will assume that the planar spacing there is 4 angstroms. So, if you say, if you assume that the spacing here, if you assume that the d for example d100 is equal to the spacing of the 100 planes is equal to, let just say for 4 angstroms okay.

So, then the reciprocal lattice is going to be inverse of this, so that is going to be .25 angstroms, so you will have a reciprocal lattice here where if this is the origin and b3 again would be perpendicular to this. So, this is actually 0.25 angstrom inverse that is the spacing of that vector okay. So, this is b1 and similarly, similar dimension you would have here is b2 would come up to here and then you can complete the lattice.

So, you can just extend this and you can extend this, so this is now the reciprocal lattice of a hexagonal cell and you can extend it. Of course, once you get you know once you get two vectors you have actually you have it is a three-dimensional structure of which we are seeing one planar view we are seeing it face down with this along the b3 direction and that is why you are seeing it like this.

But basically, once you get the three basic vectors which is b1, b2 and b3, you can actually draw the rest of the lattice. So, you can extend here get the next point, you can extend here you can get the next point, so you can see additional points would appear here, this would be a point, this would be a point and you can label them exactly the same way we labelled before.

So, this is b1, so this is 100 and it will just written that way without any brackets this would be 200, this is 010, this is 020, this is 110, this is you go one along this direction, so 120, this is 210 and this is 220 okay. So, this is how you would now get the reciprocal lattice. You are getting the reciprocal lattice of a hexagonal system wherein you have taken one view of it which is convenient for us.

Which is you are looking down the a3 axis and therefore you have gotten this. Similarly, you would have the real lattice spread across space that is how the reciprocal lattice is spread across space. So, you see between this example and the example we did here which is a cubic cell. And there you have done a hexagonal cell.

We see that the two rules that we had, which is that the Hhkl is perpendicular to the plane hkl and these modulus of hkl is one by the, or one over the spacing of dhkl. So, given those two rules the geometry and layout of the lattice we have been able to show here in these two worked examples and in principle you can extend this right.

What we will do is we will do one more worked example, where we will try to complicate it a little bit more further, little further. We basically try to look at a three-dimensional structure and see how best we can manage to draw something. So that at least we understand that it is not an impossible act, you can actually do it and certainly if you have the right kind of software you could probably do it lot easier than what we are doing on the board.

So, what we will do is we take a triclinic cell. We will try to set something up in a three-dimensional sense and then using the two examples that we just did, using what we have learnt from there we will try and solve and see if we can draw the reciprocal lattice corresponding to the triclinic cell.

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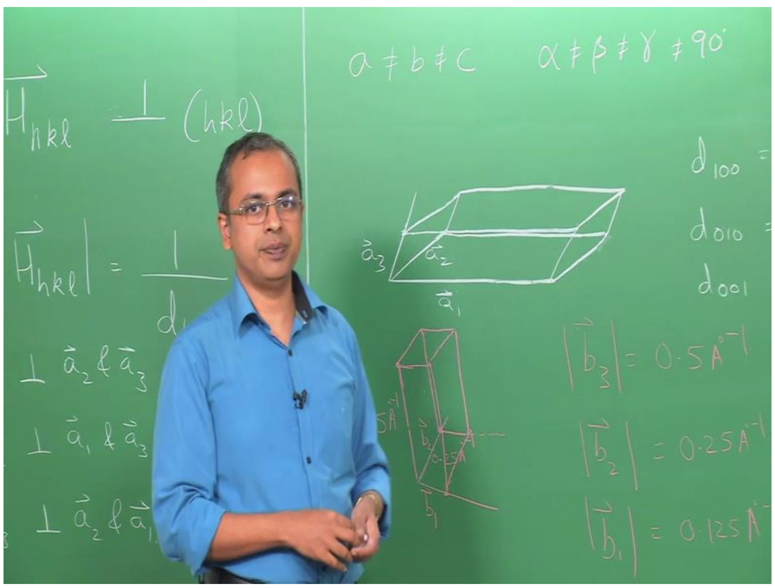

So, to begin with we will draw a triclinic cell. So, a triclinic cell as we already saw in our class has the general restrictions or lack of restrictions, I would say a, is not equal to b is not equal to c and we have alpha is not equal to beta is not equal to gamma is not equal to 90 degrees. So basically, all three axes could be any length the angles could be anything right.

So that is our most general case, so if we are able to draw something for it, presumably we can always work our way back to drawing it for anything that is less you know has less variation in it then this is. So, we just draw something here and work our way through it. So, this is one triclinic cell, so this is a1, this would be a2.

So just to make it easy for ourselves, we will assume that a1 is the longest of them on, a2 is let us say it is half as long as a1 and a3 is half as long as a2. So, we will have a1 a2 so right handed a1 a2 and then a3 is up here okay. So, we will just complete this diagram. So, you will have something like that, So, this is our diagram of a triclinic cell.

Where a1 is not equal to a2 is not equal to a3 and the angles are not all 90 degrees, in fact there they could be anything. It could be basically anything, so we will follow the same logic, we will first figure out the directions then we will try to put in the modulus and so on. We will just make some assumption here, we will simply say that d100, which is along the a, a1 direction. We will simply say that, that is 8 angstroms.

We will say d010 is 4 angstroms and d001 is 2 angstroms, will make some assumption like this and then we will see what best we can do with it. So therefore, if you see here, we need to have the a, as the b3 direction has to be perpendicular to a1 and a2. So, it means it will be straight up, so the b3 will come something like this.

That is the b3 direction, so let us just put on the directions first; b3 is perpendicular to those two b, so the b1 direction will now have to be perpendicular to a3 and a2. So that plane is facing like this, so the perpendicular would come somewhat in that direction, relative to this plane, related to this plane this is how this is the direction in which the perpendicular would come. So, we will just draw the perpendicular like that.

So that is the plane that is perpendicular that is the direction that is perpendicular to this plane. So, we just make it perpendicular and then finally we would need to pick one more plane here, which is the a3 and a1 plane and the perpendicular to that is headed off in that direction, so we will just draw that there.

So, we now have the three directions, which are all perpendicular to those respective planes, so they meet that criteria that Hhkl is perpendicular to the plane hkl, so that criterion we have got.

Now we need to know something about the dimensions. So, we have b3 in this direction and it has to be 1 by, one over the spacing of the 001 planes.

001 planes is 2 angstroms, so 1 over that is .5 angstrom inverse, so just to make it convenient for ourselves, we just make the scale large enough, so that we can draw it conveniently, we just call it say that this is 0.5 angstrom inverse. So, this is b3 up to here okay, then b2 we will see, b2 is actually 1 over the spacing 4 angstroms.

So, it is .25, so that would be half of this and so b2 is now going to be in this direction here. So that is we are going to have .25, so about half this magnitude here, half this magnitude here is what we will put here. So that is b2 okay, so that is .25 angstrom inverse. And finally, we have to have this particular direction; in this direction we have 8 angstroms, so it is going to be .125 angstrom inverse.

Which is half of this and so that is roughly this distance, so about half of that, you just translate it here, so b1 is here right. So, we have b1, so will I just put it down here b3, modulus of b3 is 0.5 angstrom inverse, b2 modulus is 0.25 angstrom inverse and b1 is 0.125 angstrom inverse. So, we got ourselves the three values, we have got the three directions.

So now it is just a matter of completing the lattice. So, we simply have to draw those finish the lattice, so complete the lattice, so it draw the lines that are parallel, so there you go we have the reciprocal lattice. We have reciprocal lattice, so this line goes all the way down here up to here. So that is the reciprocal lattice corresponding to this real lattice.

Which is at a triclinic, very generic triclinic lattice and we have simply used those rules that we have discovered or arrived at through our discussion on the reciprocal lattice. And as you can see one of the things that you immediately notice is that whatever is there in real space is getting inverted into reciprocal space.

So, larger spacing's in real space becomes smaller spacing's in reciprocal space, so you have an inverse relationship and that is why it is called reciprocal space. So, 8 angstroms becomes the lower, the largest axis is there something corresponding to that becomes the smallest dimension here. The smallest dimension here something corresponding to that becomes a largest dimension relatively speaking.

Of course, these are in different units, this is angstrom inverse, this is angstroms, so they are not necessarily you know drawn to the same scale and shown here. But the geometry is what is important; the geometry indicates to you what is going to happen. The units are with respect to that respective to figure. That is how we go about it so right.

So, right with this we will conclude these worked examples, I think these they would give you an idea of how we would go about constructing a reciprocal lattice given some specifications for the real lattice okay. I hope these three worked examples illustrate that to you. Thank you.