Introduction to Reciprocal Space

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Lecture -04
Ewald sphere, Simple Cubic, FCC and BCC in Reciprocal Space

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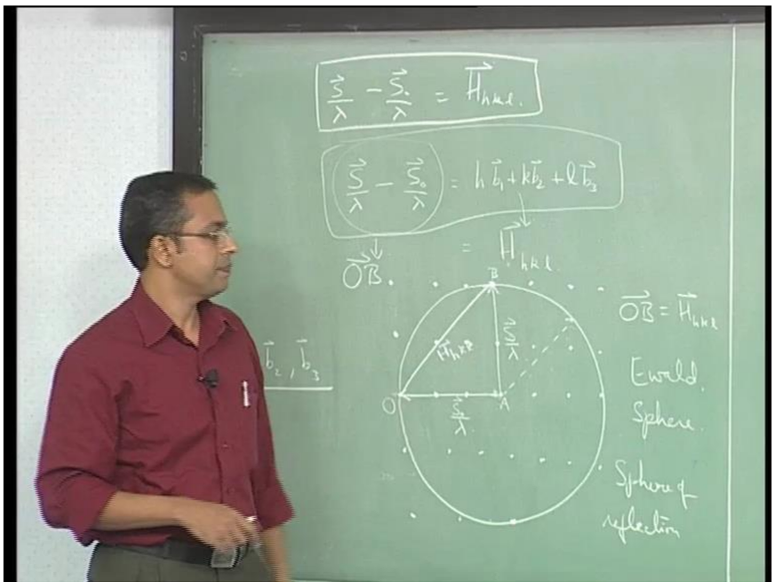

Where we finished off last class is basically we said we looked at the interaction in the reciprocal lattice notation and we specifically found that if you have a unit vector in the incident beam direction given by S naught and 1 by lambda is the magnitude of the wavelength in reciprocal space notation. And S bar, I am sorry S is the unit vector in the diffracted beam direction or in the direction where we are looking to see if there is a diffracted beam.

And again 1 by lambda is the reciprocal of the wavelength and therefore the magnitude of the wave in the reciprocal space notation. Then we find that S, S by lambda -S naught by lambda works out to hb1+kb2+lb3 in the reciprocal space. That is simply based on the notation of reciprocal space. More particularly diffraction occurs when h, k and l are integers and therefore this vector here the difference between these two vectors.

And the resulting vector due to the difference between these two vectors has to be a valid reciprocal lattice vector. In other words, this should be a valid Hhkl okay, so when this happens to be a valid Hhkl, we have diffraction all right. So, this is the condition that we arrived at, at the end of last class and it told us how we would describe diffraction in reciprocal space.

More specifically we will see, let us make a plot of this information and that will further convey to us the important idea that it is conveying to us okay. So, the way that is done is, we take, we draw the reciprocal lattice. So, some point we take as the origin of reciprocal space okay. So, this is arbitrary designated as the origin of reciprocal space.

We take the incident beam vector okay, so that is the incident beam vector and we draw it such that it comes at contacts this reciprocal lattice origin. So, I will call this O and this vector here is this S naught by lambda and we make it contact this origin of the reciprocal lattice space. Now the reciprocal lattice is a series of points right.

So, we will draw those points in just a moment, what we are going to say is, now the we can actually in this diagram what we will simply do is, we will draw a circle with this as the center not the origin. But the end, the starting point of your incident beam as the center. I will just call it A, with A as center, I will draw a circle of radius S naught by lambda all right, so approximately I am drawing it here okay.

So, this is a circle with, S naught by lambda as the radius and A as the origin, as the center of that circle. O is the origin of the reciprocal space. Now supposing I draw a vector like that all right, what is this vector? The magnitude of the vector is the same as the magnitude of this vector right. So, there is no difference in the magnet because it is a radius is a circle of it is the same radius.

So, the magnitude is the same, so the magnitude of this vector is 1 by lambda all right and so if I am and this has a particular direction. So, supposing I want to look for whether or not diffraction is occurring at this direction, in this direction given that the incident beam is in this direction and it is wavelength is lambda.

What I need to do is first I will designate this S by lambda right, simply because first of all this is 1 by lambda that is very clear because it is the same dimension as this vector here and this is the direction in which I wish to see whether or not diffraction is occurring, so I will simply call this the probable diffraction direction S by lambda.

So now if you look at the left-hand side here, we have S by lambda - S naught by lambda that is a vectorial subtraction right. This is S by lambda, this is S naught by lambda, if this is S naught by lambda, if you invert this, if you change, if it go the exact opposite direction that is - S naught by lambda. So, S by lambda - S naught by lambda means this vector simply be inverted this way.

So, you are actually starting from this point going to A, starting from O going to A and then going to be B, let just call this B. So therefore, S by lambda - S naught by lambda which is the left-hand side of this equation is simply this vector which connects the origin O to this point B okay. So, the left-hand side is now this vector OB.

The left-hand side of this equation is this vector OB in this diagram. Everything is consistent with respect to when we have just used a very consistent procedure, we have arrived at this okay. So, S naught by lambda is here S by lambda is there and therefore OB is the left-hand side of this equation.

We are saying that this set of conditions of this incident beam direction, with this wavelength and this diffracted beam direction with the same wavelength. This set of conditions will result in diffraction if the difference S by lambda - S naught by lambda is equal to a valid reciprocal lattice vector. So that difference is now this vector here OB, OB is that vector therefore we are basically saying diffraction occurs when OB equals Hhkl okay.

So, in other words this has to be a Hhkl vector all right, what does that mean? That means there is a valid reciprocal lattice point here, at this point okay. Now I want you to think again for a moment of this particular terminology that I am using a valid reciprocal lattice point and I will use this diagram to illustrate what I mean all right.

There is a difference between simply saying reciprocal space and saying a valid reciprocal lattice point. So, in other words in reciprocal lattice, reciprocal space we have the following unit vectors b1, b2 and b3. These are the valid unit reciprocal lattice vectors, unit vectors in reciprocal space valid unit. So, if I start here, if I go, if this is the origin and if I go, if this let us say this is the positive x direction.

If I go b1, I will get a point here okay, if I travel b1 I get a point here, if I travel again b1 here 2b1 I get a point here, 3b1 I may get a point here, 4b1 I might get a point here, 5b1 and may be this is 6b1 okay. Similarly, if I if we if you say this is the x direction and let us say this is the y direction, so this is x direction this is y direction and z direction is perpendicular to the board okay.

So, if I go b2 in this direction I will get a point here some we do not know what the values of b1 and b2 and b3 are they need not be the same. So, let me just arbitrarily say b2 is little larger, so I will say this is b2 value and this is another b2 value okay. So, something like that and we continue this process okay.

So just for convenience sake, I will just say that okay, for convenience sake we will just say that this coincided with origin. Let us not worry about it, simply because we will get a point there for the purpose of this diagram okay. So, I have actually point made a series of points here they correspond to b1 and b2, b1 along the x direction, b2 along the y direction okay.

So, this is set of points similarly if I know the value of b3, I can continue make the diagram below also below this plane here. So, we can put in a couple of points just for sake of completion, completeness. And it would be very similar the diagrams would be very similar okay. So, like this we would have a set of points let us not worry about it.

About the exact points but it gives us the basic idea because it is just a hand drawn picture okay. So, we have a set of points coming down this way and they are b1 and b2 in the respective direction. If you can, even plot it this way and then you can also plot in the z direction information. If you had a software which would allow you to plot the z direction information you can get it in this direction.

So that is the complete information of this reciprocal lattice that is in fact the reciprocal lattice right. That is a lattice is a set of points right, so these are all points specific points and that is then the reciprocal lattice fine. Any region in between these points is in fact a region in reciprocal space alright but there is no valid reciprocal point in all of those locations fine.

So therefore, there is no reciprocal point here for example, there is no reciprocal point here reciprocal lattice point but it is a region in reciprocal space fine. This is a region in reciprocal space that also has a valid reciprocal lattice point that is the difference. So, wherever you actually end up as a sum of b1 or b2 and b3, b1, b2, b3 some valid, sum of those three integer.

Sum of those three will get you to one of these points. They are valid reciprocal lattice points. Anywhere in the middle it will not be an integer sum of b1, b2 and b3 it will be some fractional sum of b1, b2 b3 that will get you to some in between locations where there is no valid reciprocal lattice point but it is still reciprocal space fine.

So, this circle that we have drawn, is a circle drawn in reciprocal space okay. So, it is in general it is in reciprocal space. At particular locations, it is also touching a valid reciprocal lattice points in this case for example by symmetry somewhere down here there will be a point. If you actually draw it correctly, somewhere down there, there is a point where it will touch the reciprocal lattice point.

So, this circle is independently existing in reciprocal space and at particular locations it happens to touch valid reciprocal lattice points okay. And therefore, those particular locations you will have, you can now define that wave vector S by lambda as, so at that point you not only have the correct magnitude of wavelength which is 1 by lambda.

But you are also having a direction such that this difference between the incident beam vector and the diffracted beam vector is a valid reciprocal lattice vector. Any valid reciprocal lattice point if you connect it to the origin. If you connect the origin to a valid reciprocal lattice point you have a valid reciprocal lattice vector which is designated by Hhkl, it is a valid reciprocal lattice vector.

Anytime the circle also touches that point then it turns out that the difference, that circle is being defined by the difference between these two vectors. So therefore, the circle touching any of these points implies that the difference between these two vectors is now a valid reciprocal lattice vector. And therefore, a circle touching any of these points satisfies this equation, with this being true.

So, it satisfies the equation that S by lambda -S naught by lambda equals Hhkl. This equation is satisfied, I have plotted this in a two-dimensional sense. So, in this two-dimensional figure this equation is satisfied whenever this circle touches any of these points. As you can see clearly there are several points here which are not being touched by the circle.

Therefore, with respect to those points diffraction is not going to occur, that is number one. And number two there is several regions of the circle which are not touching any point okay. So therefore, if you looked at, if you look for diffraction in this direction for example, I will just draw a dotted line here okay.

So, this is an another S by lambda direction. Again the magnitude is still 1 by lambda but it is in a different direction, so a different S okay. So, if you want to call this S1 that is S2, S2 direction. In this direction diffraction will not be visible for us because in this direction there is no, here the circle is not touching a valid reciprocal lattice point.

It is simply touching a region in reciprocal space where there is no valid reciprocal lattice point. Therefore, at this point the difference between these two does not result in a valid reciprocal lattice vector okay. So that is the significance of this equation when it is actually drawn in a reciprocal space notation. Even reciprocal space notation is used and it is actually drawn here this is what you see, this is okay. So, this is what it is.

And the figure I have drawn here is in two dimensions, so in fact when you see here we have a b1, b2 and b3, so actually this information can also be drawn in three dimensions okay. So, when you draw it in three dimensions the, what you see as a circle in two dimensions is actually a sphere in three dimensions.

Because this vector is fixed, OA is fixed, this vector OB can actually go in all directions around it starting from the, with this vector AB with A as center, this B can go in any direction around it. So, what you will see then therefore is a sphere only the length AB is fixed, length AB is 1 by lambda, so that is fixed there is no change in that.

But the direction of AB is free, we can put it in any direction that we wish. In fact, we can put it in all directions. When you put it in all directions or you project it, I mean allow it to go to all directions, all possible directions what you will get is a sphere. You simply have one end fixed and you have a, the other end able to rotate in any possible direction you wish. You will get a sphere.

So, what you see as a circle in two dimensions is a sphere and what I have just shown you a two-dimensional set of points because I only used b1 and b2. So, the reciprocal lattice itself can exist, will exist in three dimensions for a real material. It will exist in three dimensions because you will have b3 also.

So, in the same way you can plot b1, b2, just the way I have plotted b1, b2 you can additionally put b3 points here and below behind the board. So, you will get a three-dimensional set of points corresponding to valid reciprocal lattice points and you will have a three-dimensional sphere. Any place the surface of the sphere touches one of those reciprocal points you have a valid condition for diffraction okay.

This construction is credited to Ewald and is therefore called the Ewald’s sphere. This way of indicating to us when diffraction will occur is credited to Ewald and he is called the Ewald’s Sphere. It is also called a sphere of reflection okay. So, this is a very important construct. It is a construct in reciprocal space.

There is a sphere corresponding to or which carries all the information related to the beam that we are using or the waves that are present that we are considering. And it can and therefore it encapsulate that information and the lattice itself encapsulate the information of the material of the periodicity of the material. So, this is what we have seen okay.

So, we find now we have progressed quite a bit, we understand that the interaction between waves and a periodic lattice can result in diffraction that was something you were already aware of. This is described to us using Bragg notation, that again you are aware of we briefly looked at it in the last class.

It is also something that we can describe in reciprocal lattice notation okay. And independently we have also defined reciprocal lattice and we have, so we understand that, for we define it by saying that for any given lattice, we can define a reciprocal lattice given certain relationships holding too. On the basis of that relationship we can generate the reciprocal lattice.

Now so, we have come this far, what I want to highlight now is that we have in on this diagram I think we have a good feel for the fact that there is a wave arriving in a particular direction which we are simply a designating or denoting by 1 by lambda but the same direction correct direction. And we are looking for the diffracted beam in some direction.

Which we are designating by S and 1 by lambda is the magnitude. So that part I think we have a good feel for. What I would like to improve our feel for is the reciprocal lattice itself okay. So, in the next few minutes through the rest of this class we will look at the reciprocal lattice and understand certain aspects of it.

So that we have a better feel for this whole picture because intuitively we have a better feel for real space. To have a feel for reciprocal space is not that intuitive for us so that is what we will look at okay.

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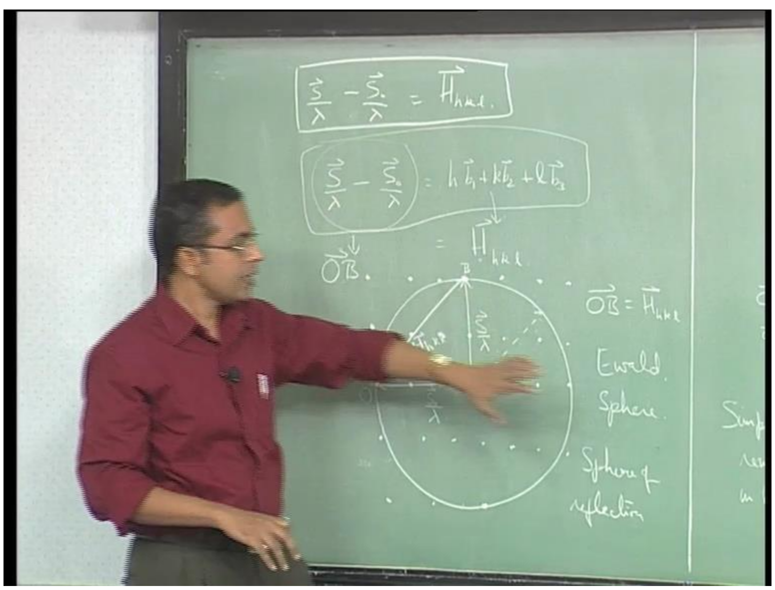

Now the point, so far, we have simply said a1, a2 and a3 are real lattice vectors which then give us a reciprocal lattice, set of reciprocal lattice vectors which are b1, b2 and b3. Based on the relationship that b1 is a2 cross a3 divided by the volume which is simply a1 dot a2 cross a3 okay, volume of when you have three vectors and if you want to calculate the volume of that region described by the three vectors.

This is the formula for it, a1 dot it is a triple product a1 dot a2 cross a3, so you will get the volume. So, this is all we have done, we have we just stated it like this and on that basis, we created the reciprocal lattice, we kept that as a independent entity and then we have looked at diffraction.

So, these are all to some degree these are all independent pieces of information possibly for another class we will still continue to look at independent pieces of information with or at least information where the links between them seem a little loose at this moment. But it will all tie in together in a class or so. So therefore, you have to be a little patient and proceed on that basis.

Now what I want to draw your attention to is that right now it is simply a1, a2, a3 b1, b2, b3 okay. So, it seems like something that is detached from our standard discussion. In real materials what do we have? We have crystal structures, we have you know we can say it is simple cubic, we can say it is face centered cubic; we can say it is body centered cubic and so on.

So, when you take a real sample we want all the discussion we are doing we are trying to do so that we can carry out, so that we can understand something about a real material okay. Real material and what its properties are why its properties or whatever it they are and how can we understand that these are the reasons why the property is what it is.

So, we have a real material, a real material may have one of these I mean it may have several structures we just illustratively we look at say simple cubic, face centered cubic and body centered cubic. So that is what is being described by a1, a2 and a3. When you say something is simple cubic correspondingly there will be an a1, a2, a3.

If you say it is FCC or face centered cubic it will have an a1, a2, a3 and BCC will similarly have a corresponding a1, a2, a3. When you take that real material and you want to consider you know what is happening with respect to diffraction in it, how is that real material interacting with some radiation. What is the result of that interaction and so on.

We have just seen that we can plot all this information in reciprocal space and then we get the sphere and with respect to that we can say a lot of things. Therefore, we have to do two things first is that the material itself okay, we have to depict this material in reciprocal space. That is the first thing we have to do.

And that is simple that simply means that for the a1, a2 and a3 that we have here, we have to get b1, b2 and b3. Once we get b1, b2, b3 the way I just currently, in our previous plot here where we looked at here, we looked at plotting b1, b2, b3 we can do that. We can plot b1, b2, b3 and of course once you know the wavelength of the radiation and which direction the radiation is coming in we can incorporate that information in here.

And we have all the information we want fine, so we have to get here. So therefore, we need to have a better understanding or better feel for how a1, a2, a3 relate to b1, b2, b3. The equation is given here that is fine, the equation is definitely given here and in fact this is the equation we will use. But we will look at these three specific cases of simple cubic, face centered cubic and body centered cubic.

And see what does this equation do I mean is that something that we can physically understand about what this equation has done with respect to these three structures and what is the result of it. In other words, given those three structures, if you get b1, b2, b3, what will we really have? So, let us start with simple cubic. So, a good way of describing it is a1 is simply ax okay.

So, we will say ax, a in the x direction, x cap, a2 is ay cap and a3 is az cap. Where, these are unit vectors in those directions x y and z okay. Now we would like to get b1, b2 and b3, so we have taken a simple cubic lattice, so the magnitude of the vectors a1, a2 and a3 are the same a, a and a that is why it is simple cubic okay, it is cube it is a cube so also sides are a.

So, in all three directions we have the same magnitude a, only the direction differs it is in x direction, y direction or z direction that is all we have fine. So, given this lattice what is the reciprocal lattice that we will get? So, first thing we will need to do is we need to calculate this bottom part which is the volume of this reciprocal lattice.

So, we will we will do that we need a1 dot a2 cross a3, what is a2 cross a3, a2 I mean we will the magnitude simply is a square right, a square a2 cross a3 a square, it is y cross z, y cross z is x, xyz if you have three coordinate system y cross z is x. So therefore, this is simply a1 is still the same ax cap dot a2 cross a3, we will pull out the two a's, so we get a square and y cross z is x. So, this is simply a cube.

Which of course, we know for a simple cube if you have a side a, the volume is a cube, so that is what it is. Except that we find that when you use the vectorial notation, we are able to, we are getting an answer that is consistent with what we already know a cube we have. So now we need to simply calculate b1, b2 and b3, b1 will put it here, b1 is a2 cross a3.

Which we already just calculated as a squared x divided by this volume a1 dot a2 cross a3 which is a cube okay. So, therefore b1 equals 1 by ax, x cap okay. So, in other words b1 the reciprocal lattice vector has the dimension of 1 by a, and the direction is still x. And then similarly b2, so b1 equals 1 by a into x cap, b2 if you did the same analysis you will have a3 cross a1, a3 cross a1 is z cross x.

Which is y, so it will become y cap 1 by a, and b3 will become z cap 1 by a. So, what do we have here, we have the directions are still x, y and z. The unit vector are still in the x, y and z directions, magnitudes have become 1 by a, 1 by a, 1 by a all right. So, if you take a simple cube, a simple cube of side a, its representation in reciprocal space will continue to be a simple cube.

Because the dimensions the magnitudes are the same right it is 1 by a, 1 by a, 1 by a, the magnitude is still the same. So, we have three mutually perpendicular directions x, y and z, three mutually perpendicular directions along which we are travelling the same distance 1 by a, 1 by a 1 by a. So, we are, we continue to have a cube.

So, a simple cube in real space remains a simple cube in reciprocal space. It is only that the dimension of the cube has changed. Where the dimension of the cube was, it was a cube of side a, it is now a cube of side 1 by a. So therefore, if you were to plot, if you have a real material, a real material which has a simple cubic structure okay.

A simple cubic structure will then consist of points which are cubically arrayed. So, you will have an origin, an atom at a, another atom at a there, another atom at there and that is the way you will build the simple cubic structure. This same material, if you want to understand what is happening with respect to, how it is interacting with waves, especially electromagnetic waves.

We will have to first represent this in reciprocal space. Its representation in reciprocal space will continue to be a simple cube, except that the dimensions will now be 1 by a. So, you will now make 1 by a, 1 by a, and 1 by a, in three directions and you will build the lattice. Now that is a reciprocal lattice of the original material you were discussing, you are trying, you are interested in okay.

So, whatever is the original material you are now created its reciprocal lattice. It is now a simple cube of side 1 by a. So that is what, that will form the set of points here and whatever way we are talking off that will that will independently from the sphere. So, this sphere is independently form based on the radiation you have chosen.

The set of points that are there which are reciprocal lattice points are based on the material you have chosen which happen to be simple cubic. Therefore, the reciprocal lattice also happen to be simple cubic and then you see the interaction based on this relationship you know when diffraction occur or when it will not occur okay. So, this is with respect to simple cube. We will also look at face centered cubic and body centered cubic.

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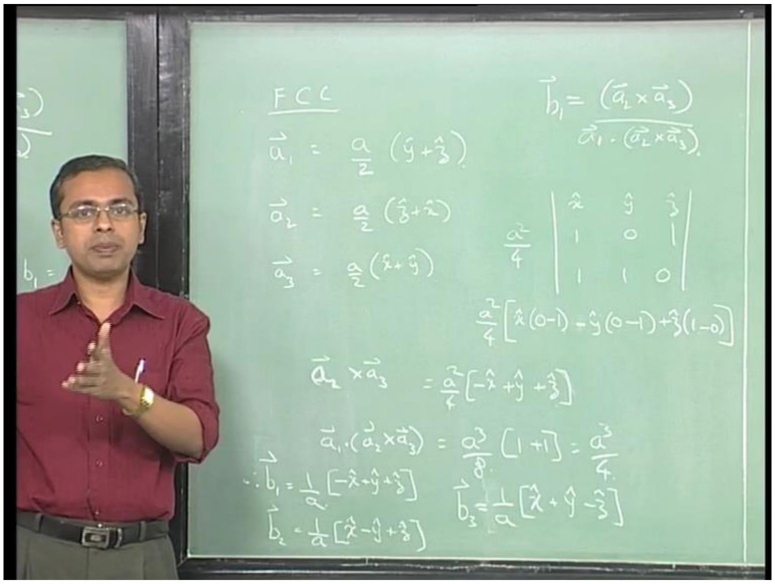

So, we will start with face centered cubic. Here by convention a1 is designated as a by 2 y+z then a2 a by 2 z +x and a3 a by 2 x+y. Initially, immediately may be these do not, these vectors do not immediately convey to you the sense of a face centered cubic structure that you are more familiar with. But actually, if you take a moment you realize that in fact it is.

What we have plotted is these are vectors which connect the origin of the face centered cubic structure to the three phase centers, those that is what these vectors are this vector goes to a phase center that is halfway between, if you travel half the distance along y axis and half the distance along the x axis, half a unit vector along y axis and half a unit vector along x axis.

Then you find that you have reached a face centered location. So, on the origin connecting it to the three phase centers, so that is what we have three phase centers, that then forms the unit cell that we are interested in. And on that basis, you can build the rest of it okay. So therefore, this is fine, this is the, these are the unit vectors that we would select in real space corresponding to a face centered cubic structure.

Given this, what is the reciprocal lattice we will get, b1, b2, b3 okay. I will, we will do the calculation of b1, b2, b3 and then we will see what it comes to. So again, we want the a1 dot a2 cross a3 that is the volume that we want similar. So b1 is still the same thing a2 cross a3 by a1 dot a2 cross a3 okay.

So, what do we have here we will just look at this a2 cross a3. So a2 cross a3, this is what we have to do, so of course these two will get multiplied, so we would have a square by 4. And then we have to write this down here, so we will do that we will write x cap, y cap, z cap, z+x would mean, we will write it as 101 and then x + y we will write as 110.

So, we can evaluate this, this is a square by 4 times x cap into 0 -1 all right, +y cap into I am sorry -y cap this is just a standard expansion of what we have here -y cap 0 – 1,0 - 1 + z cap into 1-0 okay. So, this is simply a square by 4 into -x cap + y cap + z cap, this is simply the cross product a2 cross a3 okay.

Now we will do a dot product with, so this we already have the numerator, so we already got the numerator. The denominator is simply this a2, same a2 cross a3 dot a1, so the denominator is going to be dot product of this and a1 here. So a1 dot a2 cross a3, so this is what we have here is simply a2 cross a3 okay. So that is what we already have a1 dot a2 cross a3 is this dot product.

So, this is, this will become a cube by eight right and then we have y +z okay. So, y +z, so it is basically 011 and we have -111, so y times y will become 1 and z times z will become 1 and the dot product, so therefore this is a cube by 4, so this a cube by 4 is the volume that we have for this unit cell and this is the unit vector I mean this is the vector a2 cross a3.

So, if you divide a2 cross a3 by this volume here you are simply dividing this entire term here by a cube by 4. So therefore, b1will be actually 1 by a because that if you divide by a cube by 4, the four and four will get cancelled, you will have a square by a cube which is one by a times -x cap + y cap + z cap, so this is b1 okay.

Similarly, if you do the calculation, by symmetry you will find that you know b1 gets you a -x+y+z, b2 will get you a -y +x+z and b3 will get you -z +x +y okay. So, for example we just write it here, b2 will simply be the same 1 by a +x - y +z and b3 will be +x +y -z okay. So, we have, we once again find that the dimension is 1 by a, so that part is still the same.

So, we have in that sense, we understand that you know in terms of magnitude, we have gone from a scale of length to 1 by length. So that is consistent with our feel for what reciprocal space is. So, 1 by a, we have one and these are the unit at the vector directions -x +y +z, x -y +z and x +y –z. In fact, if you actually plot this up, if you make a plot of this.

You will find that it is the same as a body centered cube where in these are vectors going from the origin to the three body centers okay, to three neighbouring body centers, is what, is where it is headed. So that is how we are getting the three body centers and then you can build your structure around it.

So, in other words I mean right now we have to just take my word for it, but if you just plot it, you will find it, if it is x+y, you are going along x direction + y direction, so you are getting to a point –z. So, you are going down, so you are getting to one body center in that location. If you went only x+ y, you would get to the face center right x + y and with some constant.

So, in fact a by 2 x+y, would get us to the face center which is what this is, a by 2 x+y, gets us to the face center, a by 2 z+x gets us to the next face center, a by 2 y+z gets us to third face center. So, these are face centers right, so along the x direction you can go the full a, instead you are going only half the a.

And another y direction also you can go the full a, you are going only half the a, so in between this x half a and the other y half a, you can come to the face center. So that is why these are face center locations. This x, - x + y +z would simply mean you are coming halfway and then you are going down also one more and that therefore you are reaching a body center.

So, these three therefore represent body centers. Although the scaling factor is different but you have now gone to the reciprocal space so it is 1 by a, at the moment. So, we have to just let us not worry about the scaling factor, but the general layout of those three points is as though you are reaching out to three body centers okay.

So, what we find is, if you take a face center cubic structure in real space, in other words you take a material okay, so you take silver, you take copper or whatever some face centered cubic material and then you see you represent this materials crystal lattice in reciprocal space you will actually be representing it in the form of a body center okay.

So that is something you would understand a simple cubic structure represented in real space being represented in reciprocal space continues to remain a simple cubic structure. Whereas a face centered cubic structure, when you try and represent it in reciprocal space, it is being represented as a body centered cubic lattice okay. So, this is an important thing we have to note. The last thing we will do is for the BCC structure itself.

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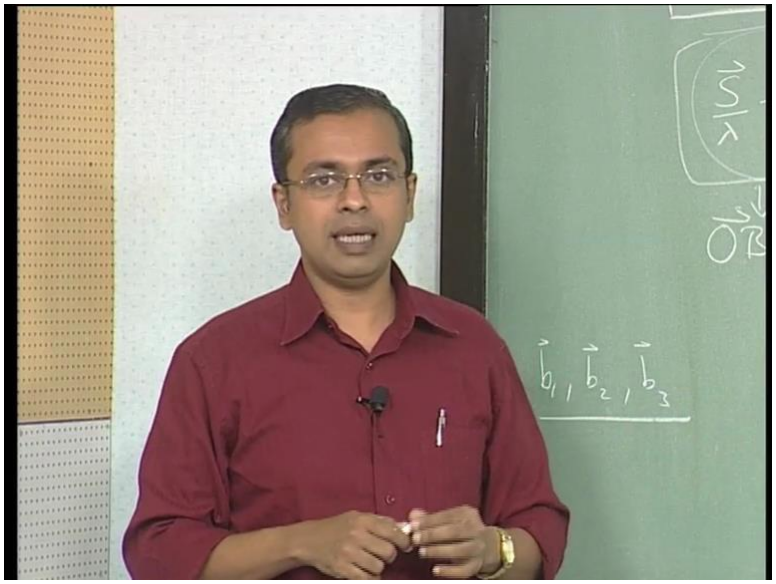

So, we are starting with a BCC structure okay, here we started with an FCC structure and we have arrived at a BCC structure, so this our result here is BCC okay. It is in reciprocal space that is why we have 1 by a, so that I just mentioned it let us not worry about 1 by a. In BCC in fact we would have a1 is a by 2 -x +y +z, a2 is a by 2 x-y+z and a3 is a by 2 x+y+z, I am sorry –z.

As I mentioned you know this is very clearly going from the origin to the three-body centered, the body centers. This is a by 2 which gives you the dimension that you are not travelling half the distance of that valid reciprocal lattice length, I mean, I am sorry valid lattice length, I am sorry so this is a lattice length or lattice vector a is a and so you are travelling a by 2, a by 2 and then you are travelling halfway between.

So, you are travelling in the y and z directions to half that length and then down the x direction half the length that will get you to a body centered location. Similarly, this will get you to a body centered location; this will get you to a body centered location. So, these are three vectors that are go from the origin to the three body centers fine. So therefore, this is body centered cubic structure this is representation of body centered cubic structure.

Directly you can see that this looks very similar to where we finished off here. Exactly the same vectors you see here, only difference is the scaling factor. So, the scaling factor we need not worry about, but it is a geometry that we are interested in here. The geometry that was face centered cubic as we started out with when we converted that to a reciprocal lattice notation it became a body centered cubic.

Please keep in mind as I mentioned right at the beginning this is only for our convenience okay. In the sense, this is just a notation we use to serve some purpose. The material is still face centered cubic nothing has happened to the material. It is not that the material suddenly became body centered cubic, material still remains face centered cubic.

When we want to understand how it is interacting with a radiation we would and we want to use the reciprocal lattice notation to see how it is interacting with radiation, we see what does the structure, how is the structure represented in reciprocal space? It is simply a representation of the face centered cubic structure in reciprocal space that is all.

The material still remains FCC that is the thing you have to remember. We will do the same thing now for BCC, we will do a2 cross a3, so we have to do b1 is a2 cross a3 by a1 dot a2 cross a3, what is a2 cross a3, we have to take a cross product of these two that is again a2, a by 2, a by 2 will become a square by 4.

And we can write x cap, y cap, z cap and this is +1-1+1 and this is +1+1-1, 11-1 we expand this what do we get, we get a square by 4 x cap this will become +1-1 -y cap -1 -1 + z cap 1 + 1, so this is therefore a2 cross a3 equals a squared by 4 this becomes 0, so this term goes away, this becomes -2 times -1 becomes + 2 2y +2z.

So, it is basically a square by 2 into y +z that is the cross product a2 cross a3 and the denominator is a1 dot a2 cross a3 okay. So that is simply the dot product of this a1, a1 that we have here and this a 2 cross a3 that we have already seen here. Dot product there is an x component here; there is no x component there.

So that goes away, so this irrelevant to us, there is a y component and a z component, y component and a z component. So, y dot y will be 1, +1, z dot z will be +1, so we simply you get +2 and a by 2 into a square by 2 will become a cube by 3. I am a cube by 4, so this is a cube by 4 times +1 +1 is two, so this is a cube by 2.

So therefore, the denominator in this b1 is a cube by 2, the numerator is a square by 2 times y+z. Therefore, b1 is, if you divide this by a cube by 2, you are simply going to get 1 by a, y+z. By symmetry you see 1 you want to see y and z, so if you see 2 you only see z and x, you will if you take 3 you will only get x +y that is by symmetry if you actually did it you will get it.

Because they are symmetric there is nothing, there is no preference to any one of these axis. Whatever result you see everything will symmetrically change for the other two. You can do the calculation, you can simply carry out for b2 and b3 just the way we have described the way we have, except correspondingly these vectors will change.

We select b2, this would be a3 cross a1 this denominator will remain the same, denominator will still come to the same thing. It does not really matter which way you do it, you always get a cube by 2 right. So, the denominator is not going to change in any significant manner is going to remain the same. In fact, it is not going to change going to remain the same. Only the numerator will change.

For b2, you have to look at a3 cross a1 and for b3 your to look at a1 cross a2. So, if you do this you will get the answers. You will find b2 is 1 by a, x + z and b3 is 1 by a x + y, this is what you will get, if you look at what we have got here, if you compare with something that we started out just a few minutes ago.

We will have the FCC structure we defined as this a by 2 y+z, a by 2 z+x, a by 2 x+y. These three directions, the magnitude is something else, let us not worry about the magnitude. Look at the three directions that we have here. We have the same dimension in three directions and those three directions are listed here, if you go to our result just now, we have the same directions here y +z, x+z, x+y.

Those directions are the same and it is one magnitude regardless of what the magnitude is. In this case the magnitude is 1 by a, the same magnitude in those same three direction, so this is a representation of BCC, I am sorry this is a representation of FCC okay. So, what have we reached, what have we done here today.

We have really looked at a few things; first of all, we understand that we can represent diffraction as a process. Diffraction is simply the interaction of waves with electromagnetic waves with a periodic crystal structure. So that is a concept right, we can represent it in real space and write an equation which tells us under what conditions diffraction is occurring. That is Bragg's law.

You can represent the same information in reciprocal space and see you under what conditions diffraction is occurring that is the Ewald's sphere construction. So, either way it is the same information, it is the same material, it is just being represented either in real space or in reciprocal space. That is a piece of information we understand.

Now we also want to understand that if you are given a real material and it has a certain crystal structure, what will, how will you represent that crystal structure in reciprocal space so that you can now see the diffraction process in reciprocal space. We find from that the discussion that we have had that if our original material happens to be a simple cubic material structure happens to be simple cubic.

Then its reciprocal lattice the b1, b2 and b3 that we calculate, the layout of those reciprocal lattice vectors is simple cubic in geometry. It is the same magnitude in x direction, +y direction, +z direction. So, it is one single magnitude that happens to be in the x direction, y direction or z direction, in three mutually perpendicular directions.

So therefore, the layout of this information of a simple cubic material in reciprocal space continues to be simple cubic, only the magnitude has changed because we are now gone to reciprocal space. If we start with the face centered cubic material and we take the three characteristic vectors that represent face centered cubic material.

And we run through the calculations corresponding to reciprocal space. We find that the reciprocal lattice that is generated that corresponds to a real material having an FCC structure happens to have the vectors which are similar to the vectors of a body centered cubic structure. So therefore, if you have a sample that is face centered cubic, you will have to plot the points in reciprocal space.

The manner you would do for a body centered cubic material okay. It is, we are only talking of geometry. Geometry in real space is face centered cubic, this same material when represented in reciprocal space will have to have a geometry that that is similar to that of a body centered cubic material okay.

So, the layout of the points when you make these points in this figure here when you lay out those points of the body of the face-centered cubic, real material has face centered cubic when you plot this reciprocal lattice points here b1, b2 and b3 when you plot them those b1, b2, b3 will have a layout which will look very similar to body centered cubic, will be identical to a body centered cubic layout okay.

So that is the thing, third thing we did we did the other structure which is body centered cubic here. We took the characteristic vectors that represent body centered cubic atoms. We looked what would happen if we just went through the standard, we are enforcing the rules of reciprocal space, reciprocal lattice, we said that b1, b2, b3 have this relationship to a1, a2 anda3.

If we enforce those relationships we find that the vectors that result, are these vectors which have a layout that is identical to face centered cubic. So, if you have a real material which is body centered cubic okay, so you have a real material that is a body centered cubic and you want to represent it in reciprocal space, so that you can see its interaction with waves.

Then its representation in reciprocal space will have some dimension 1 by a, and the layout of those vectors will be identical to face centered cubic material okay. So that is what it is. So, to finish this class I want to just highlight a few points that I made throughout this class. The first is that the reciprocal lattice notation which is represented in the form of this Ewald sphere.

Tells us how the matter is really interacting with the radiation and therefore or waves in this case. And tells us when diffraction will occur and when diffraction will not occur. It gives us a nice elegant geometrical look at how when and when diffraction will occur when it will not occur okay.

So that is one information and we have also seen in this class that when you do this transformation from real space to reciprocal space some structure that has a certain geometrical layout in real space may have a different geometrical layout in reciprocal space. In the case of simple cubic it happens to have the same layout.

In the case of FCC and BCC it has a different layout in reciprocal space. The information is still the original materials information it is only the representation in reciprocal space that has a certain type, certain layout. And by, it so happens by chance that when you take face centered cubic material its representation in reciprocal space happens to be that of a body centered cube.

And if you take a body centered cubic material its representation in reciprocal space happens to be a face centered cubic. So, these are all independent pieces of information that we will keep in mind okay. Later on, we will see that, so when we go from real space to reciprocal space we understand that structures can change.

So, it is not something that we should feel afraid of or confused about, we also understand how we can figure out what has happened to the structure. Those are the calculations we have done and we also understand that having come to reciprocal space we have the understanding of how to figure out, what is happening with respect to interaction of waves with that structure okay. So, these are all independent pieces of information.

Finally, we when we go back to, when you go to our next classes, next few classes when we look at electron waves and how they interact with matter. It is all these concepts that will be pulled together okay. And that stage again as and when necessary I will highlight those salient points which will help us relate to this material.

I will only finish off by one, with one other comment which is basically that in this last couple of classes and maybe the next class or too we are talking of some independent pieces of information and then looking at them in great detail. So please feel free to review this information when you come to one of the later classes when we pull this information together.

So that you can understand, in case you are having some difficulty following at that stage in terms of how they are coming together come back and check one of these classes, see what this information is as an independent entity. You will be able to relate it to our discussion data much better okay. So, with this we will halt for today. Thank you