Electronics.

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Lecture No. # 29

Reciprocal Space 3

Ewald sphere, Simple Cubic, FCC and BCC in Reciprocal Space

Hello, And welcome to the twenty ninth class in our course the physics of materials. In the last class we looked at the diffraction process as it occurs in real space and the kind of description, you would use for that and as it would occur in reciprocal space and the kind of description we would use for that. As I mentioned on the whole there is a material and there is an interaction of that material or the atoms in that material with the incoming electromagnetic radiation or with electromagnetic radiation in general. So, that interaction is whatever it is. So, the description that we used whether it is real space or reciprocal space, you simply something that is for our convenience we are creating these spaces and examining the interaction within the frame work of that space.

And the reason we do that is a for certain types of analysis, one description of the interaction works out more convenient than the other. So, that simply what it is. So, there is no greater purpose to the analysis in that sense. So, but at the same time we have to understand these approaches because in the subsequent classes. We will use the those approaches to further analyze the impact of the interaction of electromagnetic radiation or of waves electron waves with the periodic structure of the material. And that interaction we will look at in the reciprocal lattice notation, because that gives us some insides which are very useful to us. So, it is in that context that we looked at interaction, now where we finished off last class? Is a basically we said we looked at the interaction in the reciprocal lattice notation and we specifically found that if we have.

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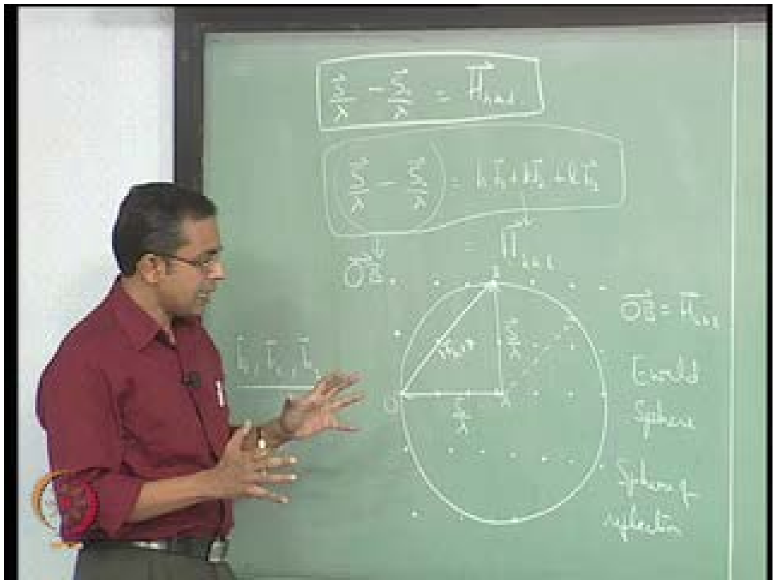

If you have a unit factor in the incident beam direction given by S naught, and 1 by lambda is the magnitude of the wave length in the reciprocal space notation. And S bar I am S is the unit vector in the diffracted beam direction or in the direction where we are looking to see if there is a diffracted beam. And again 1 by lambda is the reciprocal of the wave length. And therefore, the magnitude of the wave in the reciprocal space notation, then we find that S by lambda minus S naught by lambda works out to h b 1 plus k b 2 plus l b 3 in the reciprocal space that is base simply based on the notation of reciprocal space more particularly a 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 as to be a valid reciprocal lattice vector in other words this should be a valid h h k l.

So, when this happens to be a valid h h k l we have diffraction already. So, this is the condition that we arrived at the end of last class and he told us, how we would describe a fraction in reciprocal space? More specifically we will see let us make plot of this information and that will further convey to us the important idea that is convey into us. 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. So, this is the arbitrary designated or origin of reciprocal space we take the incident beam vector so that is the incident beam vector and we draw it such that it comes at contact 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 reciprocal lattice is a series of points.

So, we will draw those points in a just movement what we are going to say is? Now the we can actually in this diagram what we will simply do is we draw circle with this as the center not the origin, but the end the starting point of the our incident beam as a center I will just call it a with a as the center I will draw a circle of In radius S naught by lambda alright. So, approximately I am drawing it here. So, this is the 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, alright what is this vector? The magnitude of the vector is the same as the magnitude of this vector. So, there is no difference in the magnitude, because it is a radius is a circle of as same radius. So, the magnitude is same. So, the magnitude of this vector is 1 by lambda alright, and so if I am and this as the particular direction. So, supposing I want to look for a whether or not diffraction is occurring at this direction in this direction given that the incident beam is in this direction and its wave length is lambda.

What I need to do is? First I will designate this as S by lambda. 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 wished to see whether or naught diffraction is occurring. So, I will simply call this the probably diffraction direction S by lambda. So, now if you look at left hand side here we have S by lambda minus 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 minus S naught by lambda. So, S by lambda minus S naught by lambda means this vector would simply be inverted in this way.

So, you are actually starting from this point going to a starting from O going to a and then going to b let us say call this b. So, therefore S by lambda minus 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. So, the left hand side is now this vector O B, the left hand side of this equation is this vector O B in this diagram. Everything is consistence with respect to when we have just used a very consistent procedure we arrived at this ok. So, S naught by lambda is here S by lambda is there and therefore, O B is the left hand side of this equation we are saying that this set of conditions of this incident beam direction with this wave length and this diffracted beam direction with the same wave length. This set of conditions will result in diffraction if the difference S by lambda minus S naught by lambda is equal to a valid vectorial reciprocal lattice vector.

So, that difference is now this vector here O B, O B is that vector. Therefore, we are basically saying diffraction occurs when O B equals H h k l. So, in other words this as to be H h k l vector alright what does mean; that means, there is a valid reciprocal lattice point here at this point. Now I want you to think again for a moment this specific particular terminology that I am using a valid reciprocal lattice point and I will use this diagram to illustrate what I mean. 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 b 1 b 2 and b 3. These are the valid unit reciprocal lattice vector units vector 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 say this is the positive x direction if I go b 1. I will get a point here, if travel b 1 I will get a point here, if I travel again b 1 here 2 b 1 I get a point here 3 b 1 I may get a point here, 4 b 1 I may get a point here, 5 b 1 and may be this is 6 b 1. Similarly, if I if we say this is the x direction and let say this is the y direction. So, this is x direction. So, this is y direction and z direction is perpendicular to the board. So, if I go b 2 in this direction I will get a point here some we do not know what the values of b 1 and b 2 and b 3 are they need not be the same.

So, let us be just orbital say b 2 as little larger. So, I will say this is b 2 values, and this is another b 2 value. So, something like that and we continue this process. So, just for convenience sake I will just say that for convenience sake, we will say just that this coincided with the origin. Let us not worry about it simply because we will get a point there for the purpose of this diagram. So, I have actually point made a series of points here they correspond to b 1 and b 2, b 1 among the x direction b 2 along the y direction. So, this is at a point similarly if I know the value of b 3 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 completeness and it would be very similar, the diagrams would be very similar. So, like this we would have 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. So, we have set of points coming down let say and they are b 1 and b 2 in the respective direction, if you can even plotted this way, and then you can also plot in the z direction information. If you had a softer which would allow you to plot this z direction information you can get it in this direction.

So, that is the complete information of this reciprocal lattice that is. In fact, reciprocal lattice that is lattice is set of points. So, these are all points specific points and that is then the reciprocal lattice fine. Any region in between this points. In fact, a region in reciprocal space alright, but there is no valid reciprocal point in those entire 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 as a valid reciprocal lattice point that is the difference. So, wherever you actually end up as a some of b 1 or b 2 and b 3 b 1 b 2 b 3 some valid some of those 3 integer some of those 3 will get you to 1 of these points. They are valid reciprocal lattice points.

Anywhere in the middle it will not be an integers some of b 1 b 2 and b 3, it will be some fractional some of b 1 b 2 b 3 that will get you to some in between locations where there is no valid reciprocal lattice point. But it is reciprocal space fine. So, this circle that we have drawn is a circle drawn in a reciprocal space. So, it is in general it is an reciprocal space at particular locations it is also touching valid reciprocal lattice point. In this case for example, by symmetry somewhere down here there will be a point if you actually draw it correctly somewhere down there is a point where it will touch the reciprocal lattice point. So, this circle is a independently exiting in reciprocal space and at particular locations it happens to touch valid reciprocal lattice points. And therefore, those particular locations you will have you can now define that wave vector S by lambda.

So, at that point you not only have the correct magnitude of wave length which is 1 by lambda, but you are also having a directions, 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 connected to the origin, if you connect the origin to a valid reciprocal lattice point you have valid reciprocal lattice vector which is designated by H h k l. It is a valid reciprocal lattice vector, any time this circle also touches that point then it turns out that the difference the 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 too. So, it satisfies are the equation that S by lambda minus S naught by lambda equals H h k l. 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 see clearly there are several points here which are not being touch 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. So, therefore if you looked at if you look for diffraction in this direction for example, I will just draw dotted line here.

So, this is another S by lambda direction, again the magnitude is still 1 by lambda, but is a different direction different S. So, if you want call this S 1 that is S 2, S 2 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. So, that is the significant of this equation when it is actually drawn in a reciprocal space notation where even reciprocal space notation is used and it is actually dawn here this is what you see this is.

So, this is what it is? The figure I have drawn here it is in 2 dimensions. So, In fact, when you see here we have a b 1 b 2 and b 3. So, actually this information can also be drawn in three dimensions. So, when you draw it in three dimensions the what you see what you see as a circle in two dimensions is actually as three are in dimensions, because this vector is fixed O A is fixed this vector O B can actually go in all directions around it, starting from with this vector A B with A as a center this B can go in any direction around it. So, what you will see then therefore is a sphere only the length A B is fixed length A B is 1 by lambda. So, that is fixed there is no change in that, but the direction of A B is free we can put it in any direction that we wish.

In fact, we can put in all direction when you put it in all direction or you projected in a normally it go to all direction all possible directions what you will get as sphere. You simply have one and end is fixed and you have the other end able to rotate in any possible direction, you do you get a sphere. So, what you see as a circle in two dimensions is actually as sphere and what I have I will just shown you two dimensional set of points, because I only used b 1 b 2. So, the reciprocal lattice itself can exist will exist in three dimensions for a real material it will exist in 3 dimensions. Because you will have b 3 also. So, in same way you can plot b 1 b 2 that is the way I plot b 1 b 2 you can additional put b 3 points here and below beyond the both. So, you will get a 3 dimensional set of points corresponding to valid reciprocal lattice points and you will have 3 dimensional sphere.

Any place the surface of the sphere touches 1 of those reciprocal points you have a valid condition for diffraction. This construction is credited to Ewald and therefore, call the Ewald sphere, this way of indicating process when diffraction will occur is credited to Ewald and he is called a d p Ewald sphere it is also called sphere of reflection. So, this is the very important construct it is a construct in reciprocal space, there is a sphere corresponding to all 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, in encapsulate that information and the lattice itself encapsulate the information of the material of the periodicity of the material. So, this is what we can see. So, we find now we have progress quite a bit we understand that the interaction between weaves and periodic lattice can result in the diffraction that was something.

You already aware of this is describe was using brag notation that again you are aware of we briefly looked at in the last class it is also something that we can describe in reciprocal lattice notation. And independently we have also define reciprocal lattice and we understand that for we defined it by saying for any given lattice we can define a reciprocal lattice given certain relationships holding to. On the basis of that relationship we can generate the reciprocal lattice now. So, we come this part what I want highlight now is that we have 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 have simply a designating or denoting by 1 by lambda, but the same direction correct direction.

And we are looking for the defecated beam in some direction which we are designated by S and 1 by lambda is the magnitude. So, that part in think we have good feel for, what I would like to improve our feel for is the a reciprocal lattice itself. So, in the next few minutes through the rest for this class we will look at the reciprocal lattice and understands 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 now the point.

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So, for we have simple said a 1 a 2 and a 3 are real lattice vectors which then give us a reciprocal lattice set of reciprocal lattice vectors which are b 1 b 2 and b 3 based on the relationship that b 1 is a 2 cross a 3 divided by the volume which is simply a 1 dot a 2 cross a 3 volume of we have three vectors. And if you want to calculate the volume of that region describe by the three vectors, this is the formula for it a 1 dot it is a triple product a 1 dot a 2 cross a 3. So, you will get the whole. So, this is all we have done we just stated it like this among that basis we created the reciprocal lattice we kept that as an independent entity and then we have looked at diffractions. So, these are all to some degree these are independent pieces of information possible for another class we still continue to look at independent pieces of information with or at least information where the links between them see a little loss at this movement. But it will all tie into together in class also. So, therefore, we have to be a little patient and proceed on that basis now I want to draw your attention to is that right now it is simply a 1 a 2 a 3 b 1 b 2 b 3.

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 simply cubic, we can say it as face center cubic, you can say its a body center cubic and so on. So, when you take a real sample we want all the discussion we are doing we trying do so that we can carry out. So, that we can understand something about real material, real material, and what its properties are? Why its properties are? Whatever they are? And how can we understand that these are the reasons? Why the property is what it is so? We have real material real material may have one of these I mean it may have several structures we guess illustratively we look at say simple cubic face center cubic and body center cubic. So, that is what is being describe by a 1 a 2 and a 3 when you say something is simple cubic correspondingly there will be a 1 a 2 a 3 if you say it as FCC or face center cubic it will have an a 1 a 2 a 3 and BCC will similar have a corresponding a 1 equate. When you take that real material and you want to consider you know what is happening with respect to diffraction entity.

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 these information in reciprocal space and then we get this sphere and with respect to that we can say lot of things. Therefore, we added two things first is that the material itself we have to debt this material in reciprocal space, that is the first thing we have do. And that is that simply means that for the a 1 a 2 and a 3 that we have here we have to get b 1 b 2 and b 3, once we get b 1 b 2 b 3 the way I just currently in our precious plot here. Where we looked at here we looked at plotting b 1 b 2 b 3. We can do that we can plot b 1 b 2 b 3 and of course, once you know the wave length 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 get here. So, therefore, we need to have better understanding or better feel for how a 1 a 2 a 3 relate to b 1 b 2 b 3 the equation is given here, that is fine the equation is definitely given here and. In fact, this is the equation we were used, but we will look at these three specific cases of simple cubic, face center cubic and body center cubic. And see what does this equation do is that something that we can physically understand about what this equation as done with respect to these three structures.

And what is result of it? In other words even those three structures if we get b 1 b 2 b 3, what will be really happen? So, let us start with simple cubic. So, a good way of describing it is a 1 a simple a x. So, we say a in the x direction x cap a 2 is a y cap and a 3 is a z cap where these are unit vectors in those directions x y and z. Now we will like to get b 1 b 2 and b 3. So, we have taken a simple cubic lattice. So, the magnitude of the vectors a 1 a 2 and a 3 are the same a, a and a, that S why it is a simple cubic. So, it is a cube it is a cube. So, all sides are a. So, in all three directions. We have the same magnitude a only the direction differs it is a 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 do that we need a 1 dot a 2 cross a 3, what is a 2 cross a 3 a 2 I mean will the magnitude simple a square right a square a 2 cross a 3 a square it is y cross z, y cross z is x , y z if you have three coordinate system y cross z x.

So, therefore this is simply a 1 is still the same, a x cap dot a 2 cross a 3 will pull out that 2 a. 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 we have a side a volume is a cube. So, that is what it is expect that we find that the when use the vectorial notation we are able we are getting the answer that is consistent with what we have already known a cube we have. So, now, we need we need to simply calculate b 1 b 2 and b 3, b 1 we put it here b 1 is a 2 cross a 3. Which we already just calculated as a square x divided by this one volume a 1 dot a 2 cross a 3 which is a cube. So, therefore p 1 equals 1 by a x cap. So, in other words b 1 the reciprocal lattice vector as the dimension of 1 by a, and direction is still x. And then similarly b 2 so b 1 equals 1 by a into a x cap b 2 if we did the same analysis you will have a 3 cross a 1 a 3 cross a 1 is a z cross x which is y. So, it will become y cap 1 by a and b 3 will become z cap 1 by a.

So, what do we have here? We have the directions are still x y z and unit vectors are still in the x y and z directions, magnitudes are become 1 by a 1 by a 1 by a. So, if we take a simple cube, a simple cube of side a its representation and 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, 3 mutually perpendicular directions along which we are traveling the same distance 1 by a 1 by a 1 by a. So, we are we continue to have cube. So, a simple cube in real space remains a simple cube in reciprocal space.

Its only that the dimension of the cube as changed where the dimension of the cube was it was cube of side a, it is a now a cube of side 1 by a. So, therefore if you evaluate to plot if you have a real material, a real material which has which has a simple cubic structure a simple cubic structure will then consist of points which are cubically arrived. So, you will have an origin an atom at a, another atom at a there, another atom at a there, and that is the way you will build the simple cubic structure. This same material if you would not understand what is happening with respect to how it is interacting with waves a specially electromagnetic waves. We will have to first represent this in reciprocal space, its representation in reciprocal space will continue to be a simple cube expect that the dimensions will now by 1 by a. So, you will now make 1 by a and 1 by a in 3 directions and you will build the lattice. Now that is a reciprocal lattice of the original material we were discussing you are try you are interested.

So, whatever is the original material you now created its reciprocal lattice it is now simple cube of side 1 by a. So, that is what that will form the set of points here, and whatever wave you are talking of that will that will independently form the sphere. So, the sphere is independently formed 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 happened to be central cubic and then you see the interaction a based on this relationship you know when diffraction occur or when it will not occur. So, this is with respect to simple cube we will now also look at a face center cubic and body center cubic.

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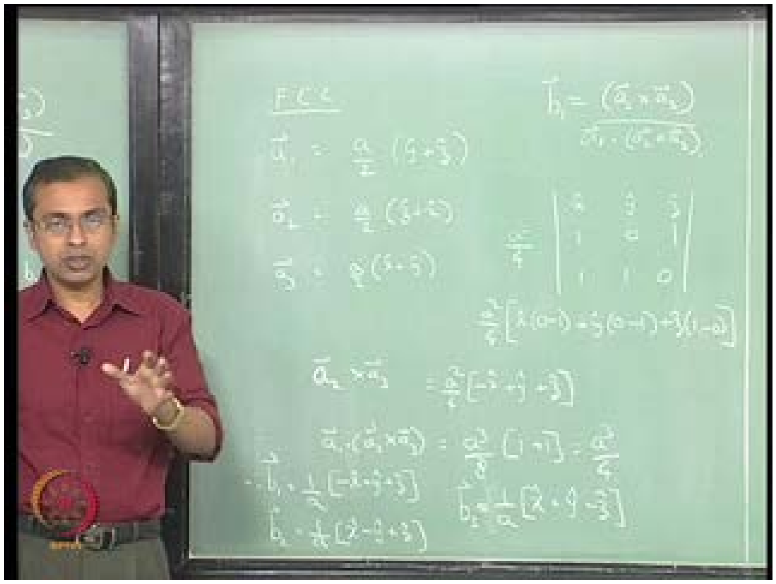

So, we will start with face center cubic, here by convention a 1 is a designated as a by 2 y plus z a 2 a by 2 z plus x and a 3 a by 2 x plus y, initially immediately may be this do not this vectors do not immediately convey to you the sense of a face centered cubic structure. That you are more familiar with, but actually if you take a moment we 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 face centers. Those that is what this vectors are, these vector goes to a face center that is half way between a if you travel half the distance along the 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 face centers.

So, that is what we have three face centers that then forms the unit cell that we are interested and on that basis you can build the rest of it. So, therefore this is fine this is the these are the unit vector that is we would selected in real space corresponding to a face centered cubic structure. Given this what is the reciprocal lattice? We will get b 1 b 2 b 3 I will we will do the calculation of b 1 b 2 b 3 and then we will see what it comes to. So, again we want the a 1 dot a tow cross a 3 that is volume that we want similar. So, b 1 is still the same thing a 2 cross a 3 by a 1 dot a 2 cross a 3. So, what do we have here? We will just look at this a 2 cross a three so a 2 cross a 3 this is what we have do.

So, of course, these three will get multiplied. So, we will have a square by four and then we have write this down here. So, we will do that, we will write x cap y cap z cap z plus x we will write it as 1 0 1 and then x plus y we will write as 1 1 0. So, we can evaluate this is a square by four times x cap into 0 minus 1 plus y cap into minus y cap, this just a standard expansion of what we have here minus y cap zero minus 1 zero minus 1 plus z cap into 1 minus 0. So, this is simple a square by 4 into minus x cap plus y cap or z cap this is a simple the cross product a 2 cross a 3. Now we will do a dot product with so this we will already have the numerator actually. So, we already got the numerator the denominator is simple this a say a 2 cross a 3 dot a 1.

So, the denominator is a going to be dot product of this and a 1 here. So, a 1 dot a 2 crosses a 3. So, this is what we have here a simple a 2 cross a 3. So, that is what we already have a 1 dot a 2 cross a 3 is this dot product. So, this is this will become a cube by 8 right, and then we have y plus z so y plus z. So, is specifically 0 1 1 and we have minus 1 1 1. 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 a 2 cross a 3. So, if you divided it a 2 cross a 3 by this volume here we simple dividing this entire term here by a cube by 4. So, therefore, b 1 will be actually 1 by a because that if you divided by a cube by 4, the 4 and 4 will get canceled.

You will have a square by a cube which is 1 by a times minus x cap plus y cap plus z cap. So, this is b 1. Similarly, if you if you do the calculation by symmetry you will find that you know b 1 gets you a minus x plus y plus z b 2 will get you minus y plus x plus z and b 3 will get you minus z plus x plus y. So, for example, we just write it here b 2 will simple be the same 1 by a plus x minus y plus z and b 3 will be plus x plus y minus z. So, we have we once again find that the dimension is 1 by a. So, that parts 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 2 1 by length.

So, that that is a consistent with our feel for what reciprocal spaces. So, 1 by a we have gone and these are the unit the vector directions minus x plus y plus z, x minus y plus z and x plus y minus z. In fact, if you actually plot this up if you make a plot of this you will find that is this the same as a centered cube where in these are vectors going from the origin to the three body centers. So, 2 3 neighboring body centers what is where it is haven. So, that is how we are getting three body centers and then you can build your structure around it. So, in other words I mean now you have just take my word for it if you just plotted you will find it its x plus y your going along x direction plus y direction.

So, you are getting a point minus z. So, you are going down. So, you are getting to 1 body center in that location, if you went only x plus y you would get to the face center x plus y and with some constants so. In fact, a by 2 x plus y would get face center which is what this is a by 2 x plus y gets us to the face center at by 2 z plus x gets us to the next face center A by 2 y plus 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 half the a and another y direction also you can go the full as you are going only half a. So, in between this x half a and the other y half as you come to the face center.

So, that is why these are face centers locations this x minus x plus y plus z would simple mean you coming half way and then you're going down also one more and then therefore, you are reaching a body center. So, these therefore, a represent the body centers although this scaling factor is different, but you do not gone to the reciprocal space. So, it is 1 by a at the movement. So, we will have to just let us not worry about this scaling factor, but the general layout of those three points is as though you are reaching out to three body centers. So, what we find is if we take face centered cubic structure in real space in other words. You take a material. So, you take silver you take copper 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 body center.

So, that is something you have to understand a simple cubic structure represented in a in real space being represented in reciprocal space continuous to remain a simple cubic structure whereas, a face centered cubic structure when you tried an presented in reciprocal space it is being presented as a body centered cubic lattice. So, this is an important thing we are not the last we will do is for the BCC structure it is a.

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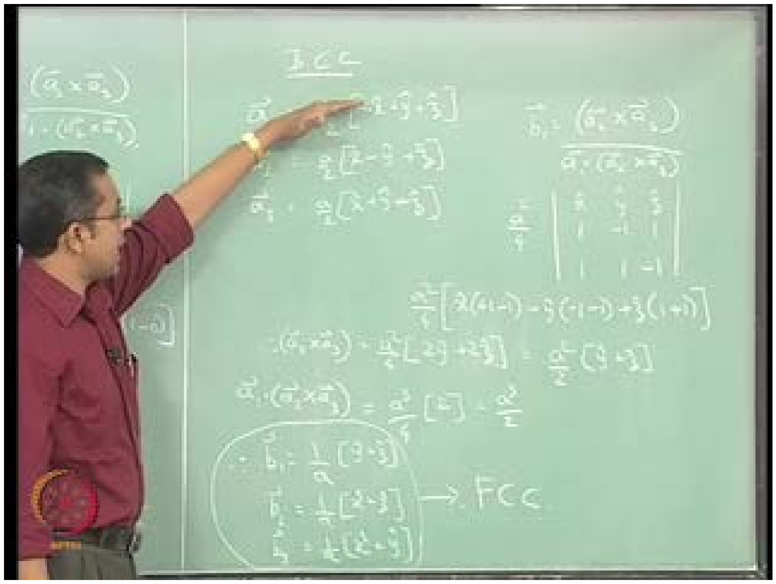

So, we are starting with a BCC structure here, we started with an FCC structure and we have arrived at a BCC structure. So, this our result here is BCC, it is in reciprocal space that is why we have 1 by a. So, that I just mentioned it lets not worry about 1 by a in BCC. In fact, we would have a 1 is a by 2 minus x plus y plus z a 2 is a by 2 x minus y plus z and a 3 is a by 2 x plus y plus z minus z as I mentioned you know this is very clearly going from the origin to three body centered the body centers this is a by two which gives you the dimension. That you would not be traveling half the distance of the recite valid reciprocal lattice length. I mean valid lattice length. So, the lattice length lattice vector a is a and. So, you're traveling a by 2 a by 2 and then you're traveling half way between. So, you're traveling in the y and z directions to half that length and then down the x direction half the length that will get to a body centered location.

Similarly, this will get to a body centered location this get you to a body centered location. So, these are 3 vectors that are go from the origin to the 3 body centers fine. So, therefore, this is body centered cubic structure this is representation of body centered cubic center. Directly you can see that this looks very similar to where we finish of here exactly the same vectors you see here only difference is the scaling the 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 center cubic where we started out with when we converted that to a reciprocal lattice notation, it become a body centered cubic. Please keep in mind as I mentioned right at the beginning this is only for our convince, in the sense this is just a notation we used to serve some purpose the material still face centered cubic nothing as a happened to the material.

It is not with the material suddenly become body centered cubic materials still remain face centered cubic, when we would not understand how it interacting with radiation. We would and we want use the reciprocal lattice notation to see how it is interacting with radiation we see that does the structure. How is this structure represented in reciprocal space? It is simple a representation of the face centered cubic structure in reciprocal space that is all the material still remain FCC that is the thing you have to remember. We will do this same thing now for BCC we will do a 2 cross a 3. So, we have do b 1 is a 2 cross a 3 a 1 dot a 2 cross a 3 What is a 2 cross a 3? We have to take cross a these 2 that is again a 2 by 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 plus 1 minus 1 plus 1, And this is plus 1 plus 1 minus 1 one 1 minus 1. We expand this what do we get? We get a square by 4 x cap this will become plus 1 minus 1 minus y cap minus 1 minus 1 plus z cap 1 plus 1.

So, this is therefore a 2 cross a 3 equals a square by 4, this becomes 0. So, this term goes away this becomes minus 2 times minus 1 becomes plus 2 two y plus 2 z. So, it basically a square by 2 into y x z that is the cross product a 2 cross a 3, and the denominator is a 1 dot a 2 cross a 3. So, that simple the dot product of this a 1, a 1 that we have here and this 2 cross a 3 that we have already seen here dot product there is an x component here there is no x component there. So, therefore, that goes away. So, this irrelevant to us there is y component and z component y component and z component. So, y dot y will be 1 plus 1 z dot z will be plus one. So, simple will get plus 2 and a by 2 into a square by 2 will a cube by 3 I mean a cube by 4. So, this is a cube by four times plus 1 plus 1 is 2 so this is a cube by 2. So, therefore the denominator in this b 1 is a cube by 2 the numerator is a square by 2 times y plus z. Therefore, b 1 is if you divided if you divided this by a cube by 2 you are simple going to get 1 by a 5 plus z by symmetry you see you see 1 you only see y and z. So, if you see two.

You will only see z and x you will if you take 3 you will only get x plus y that is by symmetry if you actually did it you will get it, because there symmetry there Is nothing there is no preference to anyone of this axis whatever result you see a everything symmetrical change for the other two. You can do the calculation you can simple carry out for b 2 and b 3 just the way we have describe the way we have expect correspondingly this vectors will change. We select b 2 this will be a 3 cross a 1 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 will always get a cube by 2. So, the denominator is not going change in any significant manner it is going to be remain the same. In fact, this not going to change. Its not going to remain the same only nominator will change for b 2 you have to look at a 3 cross a 1 and for b 3 you have look at a 1 cross a 2.

So, if you do this you will get answers you will find b 2 is 1 by a x plus z and b 3 is a 1 by a x plus 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 few minutes ago we will have the FCC structure we defined as this a by 2 y plus z a by 2 z plus x a by 2 x plus y. These 3 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 a result just now we have the same directions we here y plus z x plus z x plus y, those directions are the same and its one magnitude, regardless of what the magnitude is? .In this case the magnitude is one by a the same magnitude in the same three directions.

So, this is a representation of BCC, this is representation of FCC. So, what are reach what have we done here? Today we really looked at few things first of all we have we understand that we can represent diffraction as a process diffraction is the simple the interaction of waves with electromagnetic waves with periodic crystal structure. So, that is the concept right we can represent it in really space and write an equation which tells us under, what conditions diffraction is occurring that is brags law you can represent the same information in reciprocal space and see under what condition diffraction is occurring that is the Ewald sphere construction. So, either way it is the same information it is a same material it S just being represented either in real space or in reciprocal space that is the piece of information we understand.

Now we also want to understand that if you are given a real material, and it as a certain crystal structure, what will our how you will represent that crystal structure in reciprocal space? So, that you can now see the diffraction process in reciprocal space, we find from 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 b 1 b 2 and b 3 that we calculate the layout of those reciprocal lattice vectors is still simple cubic in geometry. It is the same magnitude in a x direction plus y direction plus z direction. So, it is one single magnitude that happens to be in the x direction y direction was z direction in three mutually perpendicular directions. So, therefore, the layout of this information of a simple cubic material in reciprocal space continuous be center cubic only the magnitude as changed because we 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 real material having an FCC structure happens to have the vectors which are similar to the vectors of the body centered cubic structure. So, therefore if you have 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 its we are only talking about geometry in real space is face centered cubic.

This same material when represented in reciprocal space we will have to have geometry, that is similar to that of a body centered cubic material. So, the layout of the points when you makes these points in this figure here, in this figure here when layout those points of that body of the face centered cubic real material. Real material as face centered cubic when you plot this reciprocal lattice points here b 1 b 2 and b 3 when you plot them those b 1 b 2 b 3 will have layout which will look very similar to body centered cubic we will be identical to body centered cubic layout. 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 will look what would happen if we just went through the standard we are we are enforcing the rules of reciprocal space reciprocal lattice, we said that b 1 b 2 b 3 have this relationship to a 1 a 2 and a 3.

If we enforce those relationships we find that the vectors that result are these vectors which have layout that is identical to face centered cubic. So, if you have real material which is body centered cubic. So, you have real material to the body centered cubic and you want representative reciprocal space. So, that you can see its interaction with waves then its representation in a reciprocal space we will have some dimension 1 by a and the layout of those vectors we will be identical to face centered cubic material. So, that is what it is? So, to finish this class I want 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 interacting with the radiation.

And therefore, or our waves in this case and tells us when diffraction will when diffraction will not occur, it gives in a nice elegant geometrical look at how and when and when diffraction will occur when it will not occur. So, that is one information. And we also see we have also seen in this class that when you do this transformation from real space to reciprocal space, some structure that as 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.

In case of FCC BCC it as a different layout in reciprocal space the information is still the original materials information, its only the representation reciprocal space that as a certain style 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 body centered cube, and if you take body centered cubic material its representation in reciprocal space happens to be face centered cubic. So, these are independent pieces of information that we will keep it in mind. Later on we will see that so when we go from real space to reciprocal space we understand the structure 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 as happen to the structure we are that those are the calculations that we have done. And we also understand that having reciprocal space we have the understanding of how to understand figure out, what is happening with respect to interaction of a waves with that structure. So, these are all independent pieces of information finally.

We when we go back to when you go to next classes I mean next few classes, when we look at electron waves and how they interact with matter. It is all these concepts that we pull together and at that stage again as an when necessary I will highlight those silent points which will helps relate this material. I will only finish off by with one another comment it is basically that in these last couple of classes and may be next or two 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 that stage, in terms of how they are coming together come back and check one of these classes see what this information is as a independent entity you will able to rewrite to our discussion later much better. So, with this we will allot for today. Thank You.