Solid State Physics

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Lecture - 28
Reciprocal Lattice (Contd.)

So, we are discussing about the application of reciprocal lattice. Today, we will see the Bragg law in reciprocal lattice or basically in different form in reciprocal lattice.

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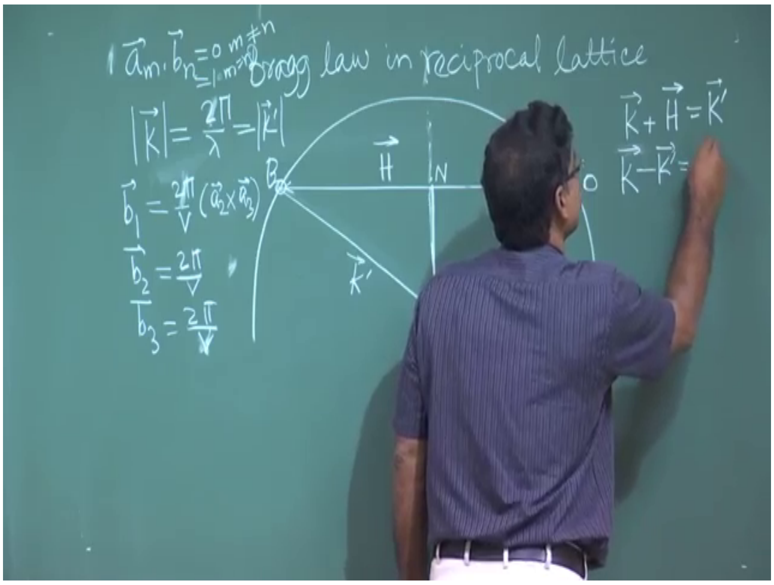

Reciprocal lattice, we have discussed the Ewald construction. What was that? See if you take a vector along the direction of the incident x-ray; say this is the incident x-ray, so from any point, if you take the magnitude 1 by lambda in such way that it ends at the 1 reciprocal lattice point.

So, this length is basically 1 by lambda, then if you construct a sphere with this radius, then that sphere will intersect the reciprocal lattice points. If you draw a sphere with this say, this way if you draw a sphere, and then it say intersect some reciprocal points at different places. So, if you add 1 of them with this origin, this value we will take origin of the reciprocal lattice, because this is a lattice point; if you take origin of the reciprocal lattice point this one, if you add, connect from this origin to the lattice point which on this sphere or here on 2 dimension circle.

If you add them, connect them, then this will be the perpendicular bisector of crystal plane and this will be the direction of the diffracted ray or reflected ray. So, that is the Ewald construction. If we follow this Ewald construction, this is the direction of incident x-ray and we have chosen this length 1 by lambda, now this will be the perpendicular bisector of a crystal plane, direct crystal plane, real crystal plane. I think it is, I have to draw slightly this, so this 2 angle should be same. This, it will be bisector of a crystal plane, so, crystal plane will be; so, let us take this is point A, this is B, this N.

So, here already we have discussed about this Ewald construction; to show the Bragg law in reciprocal lattice, I need this figure again. This is, we are telling, say K vector this is K dash vector and this is another vector say O B. So, from Vectorian rule, we can write that K plus O B; now, O B is we can say this is the vector, reciprocal vector H, because that is the definition of reciprocal vector. So, it is the basically bisector, normal bisector of the crystal plane and here it is same. This will be O B, is basically we can write H. So, this is H vector. So, this plus this will be this. That will be equal to K dash that we can write from this Ewald construction.

So, here K we have taken 1 by lambda, now I have to tell you one additional information that in definition of reciprocal lattice axis b 1, b 2, b 3; what was the definition? So, 1 by V then a 2 cross a 3 etcetera and another relation we used that was, a m dot b n equal to 0, when m is not equal to n and this was 1, when m equal to n.

So, here 1 we have written, but one can write 2 pi also generally crystallographer they use just 1, but in solid state physics we use 2 pi instead of 1. But, everything is valid whether you take 1 or 2 pi; but 2 pi physics wise I one should take 2 pi, because, here this K equal to 1 by lambda, but it will be momentum vector, if I write here instead of 1 or wave vector, then wave vector is 2 pi by lambda. So, then this K we can treat as a wave vector, momentum vector, reciprocal vector. That is why, it is a, if you use 2 pi, then this K will be it is a wave vector and in general this wave vector this in physics we use 2 pi by lambda. So, here we use 2 pi; when you used 2 pi here, this definition just you have to include 2 pi so, here other whatever.

So, generally also people use 2 pi whenever necessary otherwise just 1 by lambda or in this case one can proceed, but wherever necessary to include 2 pi, one can include 2 pi. So, this K is basically wave vector and it is defined by this. Here, instead of 1 pi, one can consider 2 pi. We can take 1 pi 1 by lambda, but in sometimes when you are writing equation etcetera there you can just 2 pi, that way also we can deal.

So, this equation is basically for reciprocal lattice, here K equal to 2 pi by lambda and it has direction. If I write magnitude wise, this is the 2 pi by lambda and magnitude of K dash also same, 2 pi by lambda, but direction are different. So, they are different in direction having same magnitude.

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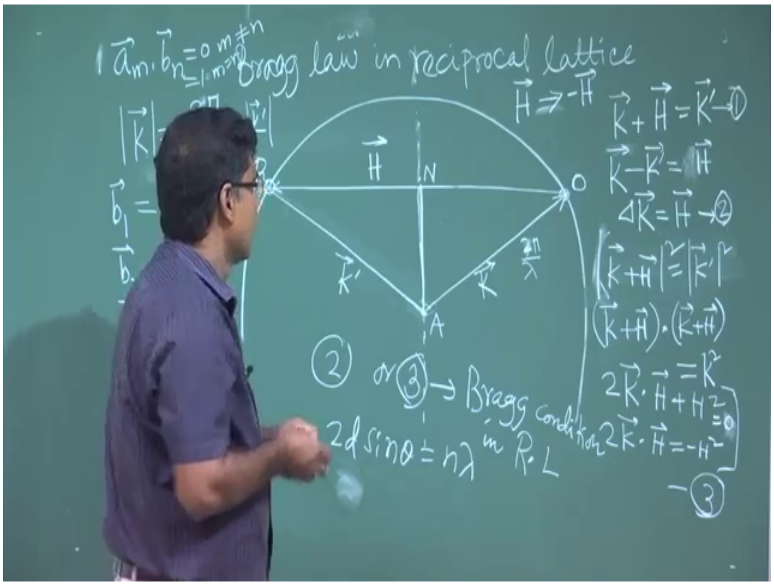

So, here I can write K minus K dash equal to minus H. Now, whenever in this direction say H is here, there must be another lattice point on the other direction. So, whenever plus H this direction is there, other direction exist. Its equivalent; minus H and plus H with direction, that is one can write. Basically, whenever your H is there, there must be existence of minus H. So, that is why do not need to use this negative sign. So, this one can write delta K del K equal to H, so this is a equation 1 or this same thing is coming in other form, say equation 2. Also, if I just in other form also we can write K minus K dash equal to right. These basically if you take dot product of this 2, we will get square of magnitude. So, this you can write I think I will take this one, from here I can get this and another form from here another we can get another form. Basically I can write K plus H magnitude square equal to K dash magnitude square.

So, this is nothing but, we can take dot product. If you take dot product, we will get, let me write, that will be equal to H K dash square; K dash square is nothing, but magnitude

K square, so I can write this K square. From here dot product we will get K square plus 2 K dot H or a is dot k this both are same and H square; K square K square will go. So, what will get, 2 K dot H plus, H square equal to 0. So, we can write either this or you can just keep the other one this other direction side this can be minus H square.

So, this is another form. This if it is 2, then I can say this is the form basically 3. This is the, this is called the Bragg law in this reciprocal lattice. Already from this configuration I have showed that we can get the Bragg law. So, from here to Bragg law in direct lattice that I have shown you.

So, this configuration Ewald, that we have tested the Ewald construction and now we are using this construction we got this condition in vector form. This form is basically is still Bragg law in reciprocal lattice. So, either form 2 or 3, it is a Bragg condition in reciprocal lattice or Bragg law in reciprocal lattice. I am writing R L, reciprocal lattice.

So, one can use 2 d sin theta equal to n lambda, also that is for direct lattice. Also reciprocal lattice, one can use either 2 or 3, this condition for diffraction. This is nothing, but, the condition for diffraction. We have given this Bragg diffraction, Bragg law that is condition for diffraction, constructive diffraction; this also condition for constructive diffraction, because this is the direction in which direction x-ray will be reflected and gives a, what I should tell this the Bragg intensity or Bragg peak or interference maxima or diffraction maxima.

So, this form is very useful for different calculation. We will see this, some calculation where this will be; this form will be very useful. So, let us see this other parameter which we can calculate and they are very useful for not only determination of crystal structure, but also to learn about the different physical properties of solids.

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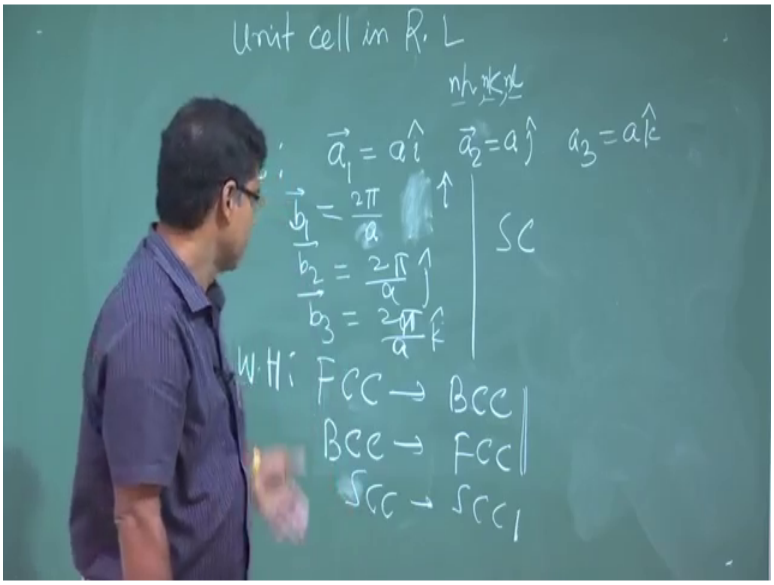

So, let us see that reciprocal lattice and unit cell in reciprocal lattice. So, reciprocal lattice R L. So, just we are deriving the similar things for reciprocal lattice whatever exist in direct lattice, crystal lattice, real lattice, everything similar things can be defined for reciprocal lattice. In direct lattice, reciprocal lattice, they are in different space that we will understand after some more discussion. Here, in direct lattice they are basically one can use coordinate; we use coordinate x, y, z coordinate. The space whatever we define the space or point in a space using coordinate x, y, z.

So, in reciprocal lattice also we look at the point, reciprocal lattice point and that reciprocal lattice point, how we have identify or we locate, that already we have discussed that; that is h, k, l. So, h, k, l parameter I have written, but it is better in reciprocal lattice this coordinate it is better to write n, because this h, k, l this nothing, but Miller indices and as you know that in Miller indices we have removed the common factor. But, in reciprocal lattice common factor has importance, because in reciprocal lattice that distance is just inverse or reciprocal. So, whatever the in half distance in direct lattice, here it will be double just because of the inverse of the distance or reciprocal of the distance.

So, that is why, we write here this include the common factor, one can include the common factor n. So, that n basically in case of 2 d sin theta equal to lambda, n was the diffraction order. Here also, it is significant is similar. It is similar fact, that in reciprocal lattice we are getting additional points, that additional point it is now if they are coming from same planes, but giving additional points. So, whatever the order in direct lattice and here it is giving points, reciprocal lattice point; additional this is reciprocal lattice point for same sets of planes; parallel planes. So, we will get many. If it is just one point, n equal to 1, this n equal to 2, it will be this point, n equal to 3 it will be this point. So, on a line whatever the many points we are getting they are from each parallel planes.

In direct lattice, we have represented with h, k, l; which represent as I told, that a set of parallel planes having same spacing and here this is h, k, l point, this is 2 h k l; 2 h 2 k 2 l, 3 h k l. So, this equivalent it is also equivalent to diffraction order. Why I mentioned that one, because we will see if I get information about this point or if I consider only this point not others, then I will not miss anything because whatever I will get from first order Bragg peak, same thing I will get from the second order, third order. So, I can use one that will give me all information, I do not need basically higher order; but it appears it is there.

So, unit cell, that you know this, same to same. Let us consider simple cubic. In direct lattice, we can represent this on for in case of simple cubic, a 1 equal to basically a i. So, i, j, k if I take along the a axis a 1, a 2, a 3, its magnitude a i then a 2 will be a j and a 3 will be a k.

Now, in reciprocal lattice what will be the unit cell? So, I can use this b 1, I have to find out basically b 1, b 2, b 3. You can know this takes, so here I have to take 2 pi; 2 pi by volume and a 2 cross a 3 means a square j cross k, j cross k means direction will be i and volume will be a cube. So, basically 2 pi by a i, similarly b 2 will be 2 pi by a j, b 3 will be 2 pi by a k. So, here I am getting b 1, b 2, b 3 just along the a 1 direction, a 2 direction, a 3 direction, having the same magnitude as here.

So, for simple cubic in direct lattice it is when it is simple cubic in reciprocal lattice also it is simple cubic. So, in reciprocal lattice we are getting simple cubic. So, because why I started from direct lattice and going to the reciprocal lattice, because they are connected it is not arbitrary. Because they are connected to this direction that b 1, b 2, b 3 we have defined in terms of a 1, a 2, a 3, so, this is simple cubic.

And these are homework, your homework, just check it. In direct lattice FCC show that, so that BCC in reciprocal lattice and BCC in direct lattice it is FCC in and simple cubic I showed here. So, this I showed and these you can just take as a homework and do it.

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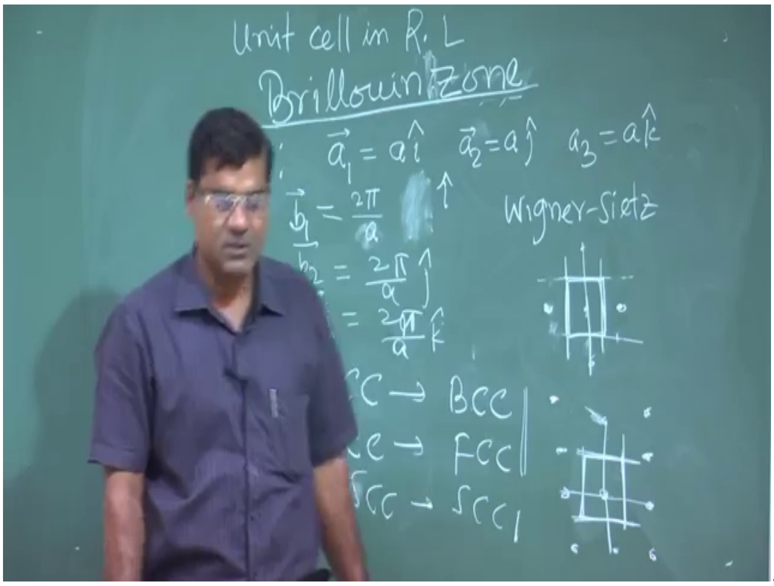

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So, unit cell as I mention that Seitz with the Seitz cell is a primitive cell Wigner-Seitz is primitive cell for any lattice one can find the Wigner cell. How it was found? That nearest neighbour lattice point, just take normal bisect sorry one has to take half if it is lattice point take, this is the lattice point.

So, this is the Wigner-Seitz cell, that way primitive cell one can find out in direct lattice. Similarly one can find out the unit cell in reciprocal lattice and that is similar way one can find out. In reciprocal lattice, lattice points are there; in reciprocal lattice take bisectors, normal bisector. So, in this case, normal bisector; in this case normal bisector. So, these will be the similar to this Wigner-Seitz cell, but it is called Brillouin zone. Brillouin zone is basically equivalent to the Wigner-Seitz cell in direct lattice. So, similar unit cell in reciprocal lattice it is called Brillouin zone; unit cell equivalent to Wigner-Seitz cell that is called Brillouin zone reciprocal lattice. So, in next class I will discuss about more. So, I will stop here.

Thank you.