Introduction to Solid State Physics
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Lecture - 38
Reciprocal lattice vectors and Laue's condition for diffraction of waves by a crystal
Part-I

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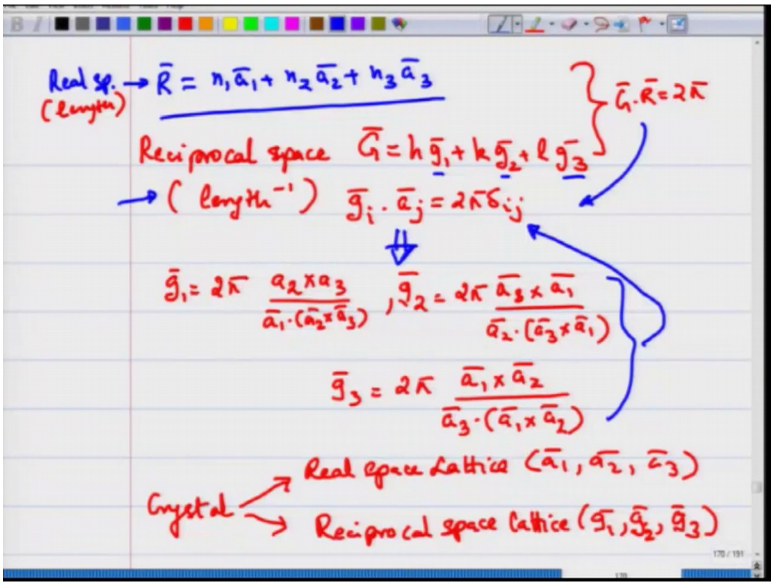

So, in the last lecture, we introduced the concept of a reciprocal lattice, where if you have a crystal, then from that crystal you can generate a Bravais lattice using your real space translation vector R, which is written as linear combinations of a 1, a 2, and a 3. This is your real space translation vector.

So, from your crystal, you can generate your Bravais lattice in real space. You can also generate for the same crystal another set of points which is in another space not in real space, but in another space which is called as a reciprocal space where distances are measured in inverse of length. So, it is another space which is called as a reciprocal space, and in that space you can generate a set of points which correspond to the same crystal, but you are drawing it in another space which is called as a reciprocal space using these fundamental vectors g 1, g 2 and g 3 in the reciprocal space. And you can generate a set of points corresponding to the crystal using linear combinations of g 1 g 2, g 3 where these are integers h k and l.

And g 1, g 2, g 3 are the fundamental translation vectors in the reciprocal space. And the two translation vectors are related by G dot R bar is equal to 2 pi; one is in the real space, one is in the reciprocal space. And from here, you can also link your fundamental translation vectors in the two spaces g i dot a j is equal to 2 pie delta i j. And this gave us a way to calculate g 1, g 2, g 3. And therefore, help us to draw the equivalent reciprocal lattice, where g 1 g 2 g 3 are related to a 1 a 2 a 3 by these forms which satisfy all of these forms satisfy this expression. And so each crystal has a real space lattice in real space a 1, a 2, a 3 you can also construct s reciprocal space lattice.

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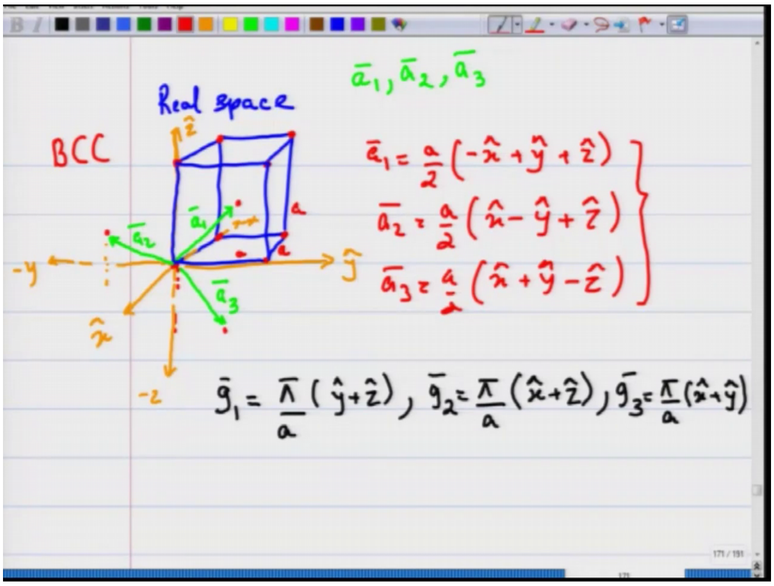

So, let us try and do one example where I can take first a body centred in real space. Let us take a body centred cubic lattice. So, in real space, if you have a body centred cubic lattice, you have points which are at the edges of a cube, but there is one point which is sitting in the centre of this lattice ok. And let us define my coordinate axis. So, my coordinate axis, this is my let us take this as my z-axis; this as my x-axis; and this as my y axis.

And you would recall that in some of my earlier lectures, I have already drawn the fundamental one way to choose the fundamental translational vectors in real space a 1, a 2, a 3 for the body centred lattice as these points. One is of course, this; this is your origin. The second point is a body centred point which is sitting for a lattice which is in the x z plane I mean the face of the square or the cube is on the x z plane, and the body centred point is sitting along this axis. So, this is a point which is sitting in the x minus y direction and plus z direction.

And the third point is sitting, so you have a point which is going this way. And there is another point which is sitting here. So, this is in the minus z direction, this is in the minus the z direction, minus y direction, of course this is your minus x direction. One point here, one point in the minus y plus x and plus z direction, this point is in the minus z plus x plus y direction. So, this is your third vector a 3; a 1, a 2, a 3 these are actually a primitive vectors for your body centred cubic lattice.

And you can write these vectors a 1, a 2, a 3 as a 1 as if the cube has sides of length a, then a 1 is a by 2, this point is minus x cap plus y cap plus z cap, because this point is along the minus x cap direction plus y plus z; a 2 is equivalently plus x cap minus y cap plus z cap direction; a 3 is a by 2 x cap plus y cap minus z cap direction a 3.

So, these are your fundamental translation vectors for a body centred cubic lattice. So, using a 1 a 2 and a 3 we can write down r vectors in reciprocal space the fundamental vectors in reciprocal space g 1 which is pi by a y cap plus z cap; g 2 which is pie by a x cap plus z cap; and g 3 which is pie by a x cap plus y cap. And now we can actually sketch what is this type of a lattice that you can generate with g 1, g 2 and g 3. So, this was your body centred lattice we had a BCC lattice in real space. And from the BCC lattice we are now generating another lattice corresponding to the BCC lattice in reciprocal space. What is that lattice, let us find out.

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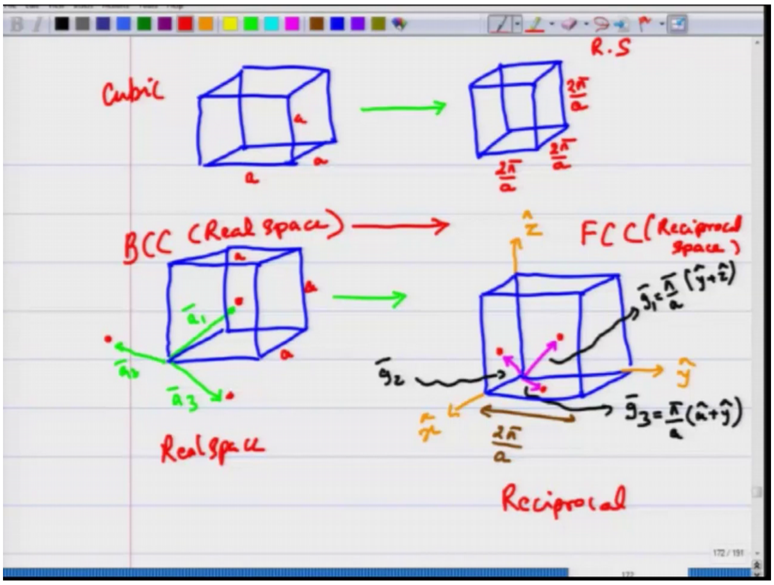

So, if you have a cubic lattice with lattice spacing a or lattice constants a, we know that it transforms in reciprocal space two these with lattice spacing 2 pi by a. Now, this is your BCC lattice which we had drawn earlier in real space. This is in real space;. And this is reciprocal space. These are lattice constant a. So, this cube will go into a first this cubic structure will actually going to a cubic structure with size 2 pi by a. These were your BCC points which defined your primitive lattice vectors a 1, a 2, a 3. And from there, we got g 1, g 2, g 3 which are half of 2 pi by a y cap cross z cap. So, this gives a point in the y z plane.

This gives a point which is half way on the x-axis, half way on the y-axis; and this give a point on this face; this gives a point on the face. So, what do you have here you have a face centred cubic structure. So, the BCC lattice in real space goes over into an FCC lattice in reciprocal space. So, corresponding to a crystal which can have a BCC lattice in real space you can also construct geometrically construct the reciprocal lattice corresponding to that lattice and that turns out to be for a BCC structure, it is FCC. And similarly you can find out for others lattices also. So, with this concept of reciprocal lattice, let us see where is it useful.

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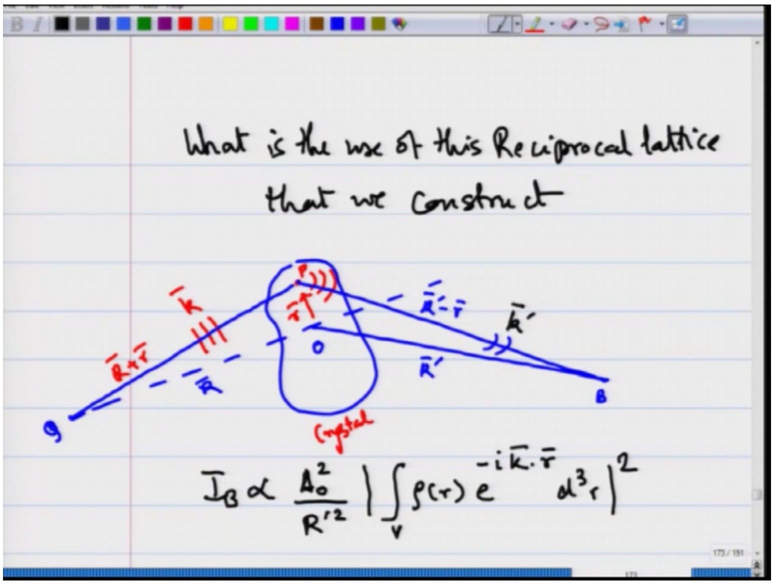

So, let us look at what is the use of this reciprocal lattice that we construct. And here let us recall our discussions of X-ray diffraction, where we had considered the following. You have a source Q which is very far away, and you have a crystal. And we looked at the plane waves which were reaching this crystal with a wave vector k, which were reaching this point p on the crystal. This is of course R plus r, where this is the position of the point in the crystal.

So, this is our crystal. And then the X-ray from here starts diffracting. So, each point out here becomes the secondary source; and it starts deflecting light from this point. So, you start getting secondary wave spherical wave fronts. And as a result you get a diffracted beam or a scattered beam. At another point B, R prime, and this is where you are measuring the scattered beam and this is of course, R prime minus r, and you are getting the wave fronts reaching point B.

And we had found that if I write the intensity at point B using the electric field that are heating point P and then diffracting out and integrating over the entire crystal, then it was proportional to the square of the initial amplitude of the way which is coming divided by inverse square of the distance of B from the crystal, the intensity dies down as square of the distance from the crystal you naturally expected. And there was an another term which was a Fourier transform of the density of points in the crystal that was rho of r e raise to minus i k dot r d cube r the whole square.

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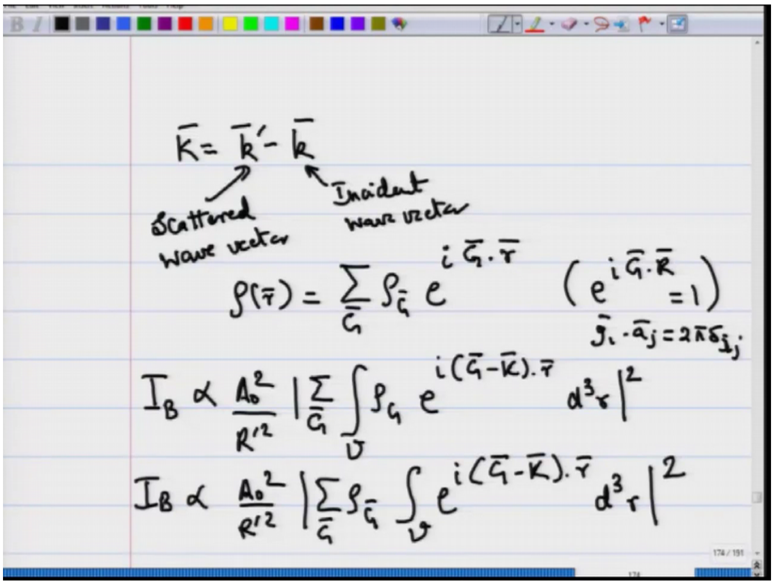

Where this scattering vector K was equal to k prime minus k, where k prime is the wave vector of the scattered wave. So, this is the wave vector of the scattered waves and your scattering vector is written as k prime minus k. This is your incident wave vector; and this is my scattered wave vector.

Now, let us look at this intensity. And you know that rho of r, you can now Fourier expand in your reciprocal space and so you can do and expansion of this density in also reciprocal space rho of G because of periodicity of the lattice and translational invariance. We saw that rho of r can be expanded in the reciprocal space, and you can write it as e raise to i G bar dot r bar, where e raise to i G bar dot capital R becomes equal to 1. So, translational invariance allows you to write this in terms of this, and your reciprocal lattice vector satisfy this condition.

So, this we can put it back in the intensity. And you can get your intensity at point B, the scattered intensity at point B is A naught square by R prime the whole square, summation over the reciprocal lattice vector, integral over the volume of the crystal rho G e raise to i G minus K dot r bar d cube r the whole square. Or I B is proportional to A naught square by R prime the whole square summation over all the reciprocal lattice vectors in a reciprocal lattice rho of G integral over the volume of the crystal e raise to i G minus K dot r bar d cube r.

So, now we have introduced our reciprocal lattice vector. For a given lattice, we construct the reciprocal lattice and that is associated with reciprocal lattice vectors. And now in our scattered intensity, this reciprocal lattice is appearing explicitly.

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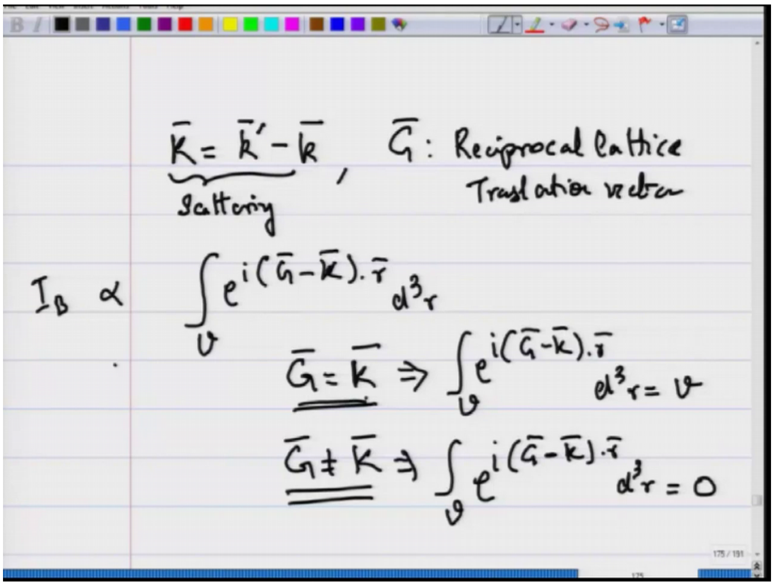

How does it help, if I write down my scattering vector. This is my scattering vector K, and G is my reciprocal lattice translation vector. And my scattered intensity depends on this integral the value of this integral e raise to i G minus K dot r bar d cube r, we have seen that my scattered intensity at point B is dependent on this value. If you look at this integral for G equal to K, mainly for reciprocal lattice translation vectors which are equal to the scattering vector G equal to K the above integral e raise to i G minus K dot r bar d cube becomes equal to v, because this will become equal to 1 if you integrate over the volume of the crystal this will be related to the volume.

And for G not equal to K, this integral v is e raise to i G minus K dot r bar d cube r. Now, these factors are just sines and cosines. And if you integrated over this entire large volume of the crystal, this will average out to 0, because these are just sines and cosines which are spread over a distance r with these wave vectors. So, if you integrated over a reasonably large crystal this integral will be equal to 0 if G is not equal to K and it will be equal to 1 or it will be this integral will equal to the volume of the crystal if it is equal to K.

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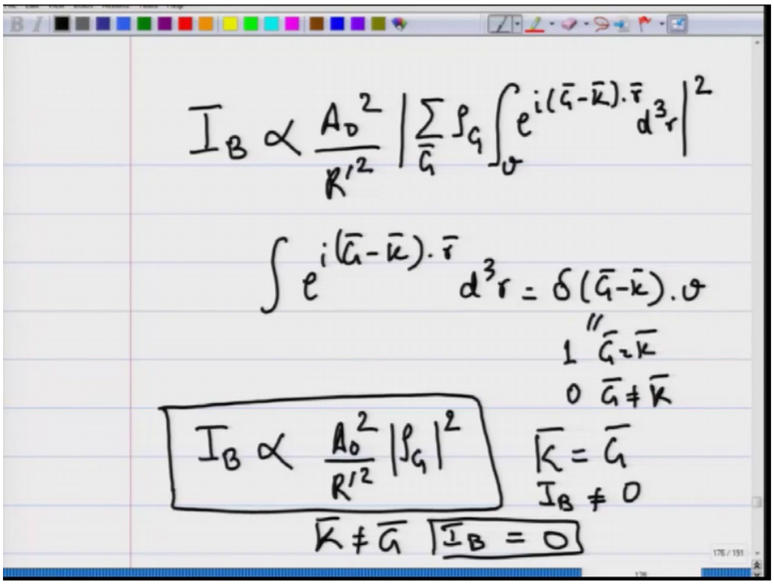

So, this scattered intensity which is written as A naught square by R prime square summation over all lattice vectors rho g integral of e raise to i G minus K dot r bar d cube bar the whole square over the volume.

This integral e raise to i G minus K dot r bar d cube r can be written as delta of G minus K into the volume, where this is equal to 1 if G is equal to K or K is equal to G, and is equal to 0 for K not equal to K. This is equal to 1 if K is equal to G, it is not equal to and is equal to 0 for K not equal to G so your intensity at point B becomes proportional to A naught square by r prime square rho g square.

So, my intensity at a given point in the lattice becomes maximum if my scattered wave vector becomes equal to G, then I get a finite intensity I B is not equal to 0. If K is not equal to G, if my scattering vector K is not equal to G, my I B becomes equal to 0. I get no scattered intensity.

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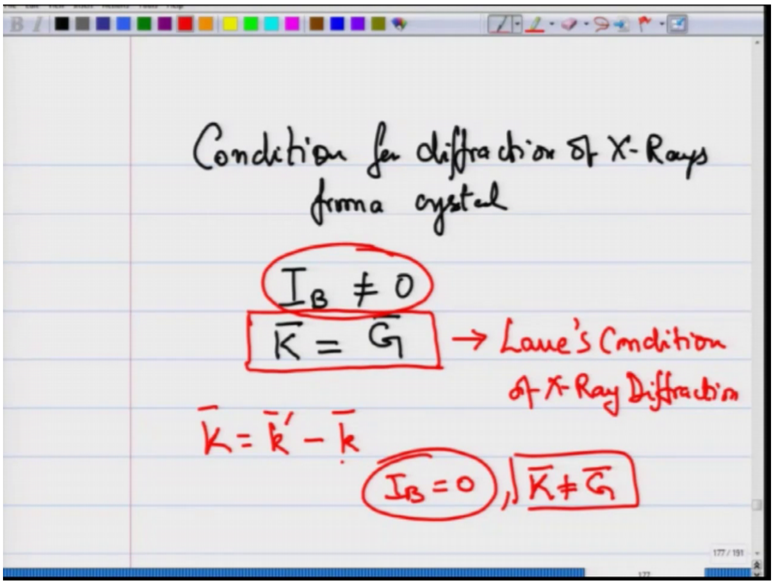

And this is the condition for diffraction. The condition for diffraction of X-rays from a crystal namely under what conditions I b the intensity at any scattered point is not equal to 0, the intensity at a scattered point or any other point the scattered intensity at any point is not equal to 0 if my scattering wave vector is equal to my reciprocal lattice vector.

And this condition of the diffraction is called as the Laue's condition of X-ray diffraction this scattering vector is the difference between the scattered wave vector minus the incident wave vector. If the scattering vector is equal to the reciprocal lattice vector only then my scattered intensity is not equal to 0, namely I will get a finite bright point at that location. And intensity at that point will be equal to 0 if the scattered vector is not equal to this namely I will get low intensity or the average intensity at a point B will turn out to be 0, if the scattering vector is not equal to your reciprocal lattice vector. And we will see the interpretation of this in the next lecture.