Introduction to Solid State Physics
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Lecture - 39
Reciprocal lattice vectors and Laue's condition for diffraction of waves by a crystal
Part-II

In the last lecture, we looked at the Reciprocal lattice vector and how we can apply it. And one of the places where it gets applied is when you are looking at the diffraction or scattering of waves electromagnetic waves specifically x-rays from crystals.

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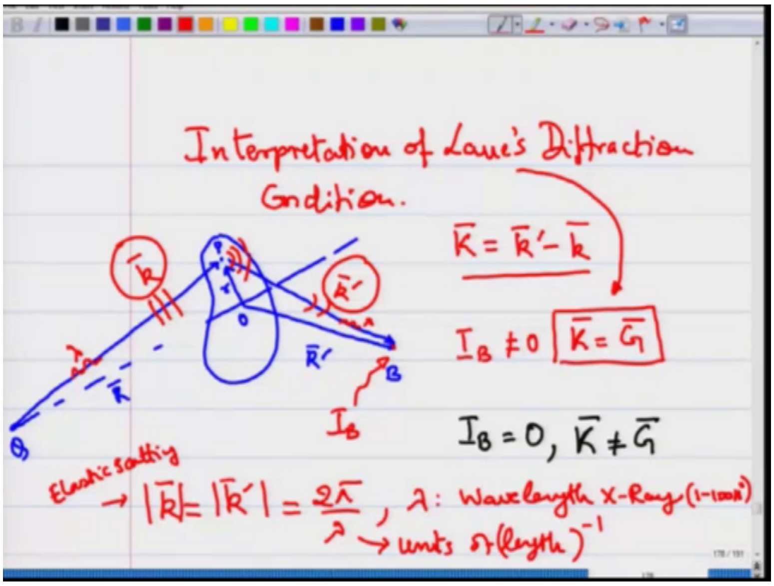

And there we saw that if you are looking at an incident wave with a wave vector k and it gets scattered with a wave vector k prime. Then the intensity at the detector point that intensity will be nonzero or will be maximum if the scattering vector k is equal to the reciprocal lattice vector. And this is your Laue's diffraction condition that: to get a maxima at the point B of your the detection point B your scattering vector which is the difference between the scattered wave vector and the incident wave vector.

If that scattered vector is equal to your reciprocal lattice vector you will get a maxima at point B. And there will be no maxima or 0 at point B, if this condition is not satisfied. So, this is the Laue's condition and we will see how to physically interpreted.

Now before we go into a physical interpretation let us recall that d is wave vectors; the incident wave vector k and the scattered wave vector k are given by 2 pi by lambda. The magnitude of these scattered wave vectors; incident wave vector and the scattered wave vector they magnitude is 2 pi by lambda because its elastic scattering, we have just looking at elastic scattering.

The wave length of the wave which is coming is lambda and the wave length of the scattered wave is also lambda. That is not changing there is no change in the energy of the beam which goes in and comes out which gets scatted out, only the directions are changing.

So, because its elastic scattering the incoming and outgoing wave vector magnitudes are 2 pi by lambda, where lambda is the wave length of the x-rays. Typically it is you know it has to be of the order of automatic spacing's. So, they will go from 1 to 100 youngstorms. That is the typical wavelength of the x-rays that you use.

And what you can see is that the units of wave vector are in units of length inverse. So, if you have to take a space where you can plot this wave vectors, the space where you can plotted is your reciprocal space because in reciprocal space you actually sketch things in units of length inverse. And you know for every crystal you can draw its reciprocal lattice in the reciprocal space. So, in the reciprocal space not only can you draw the reciprocal lattice, but you can also draw the incoming and outgoing wave vectors. And that is what is the Ewald's sphere?

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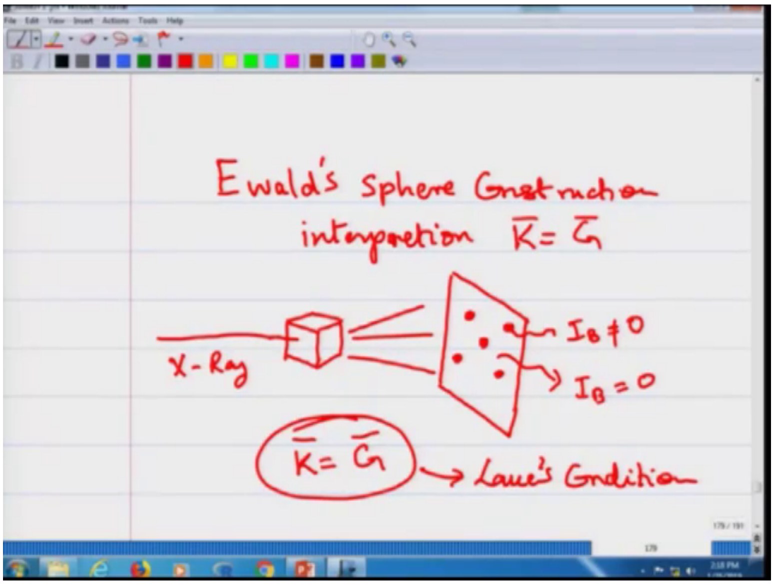

That was the Ewald's sphere construction; Ewald's sphere construction which gave the interpretation to the Laue's condition K is equal to G. So, for that I would like to show you the following slide.

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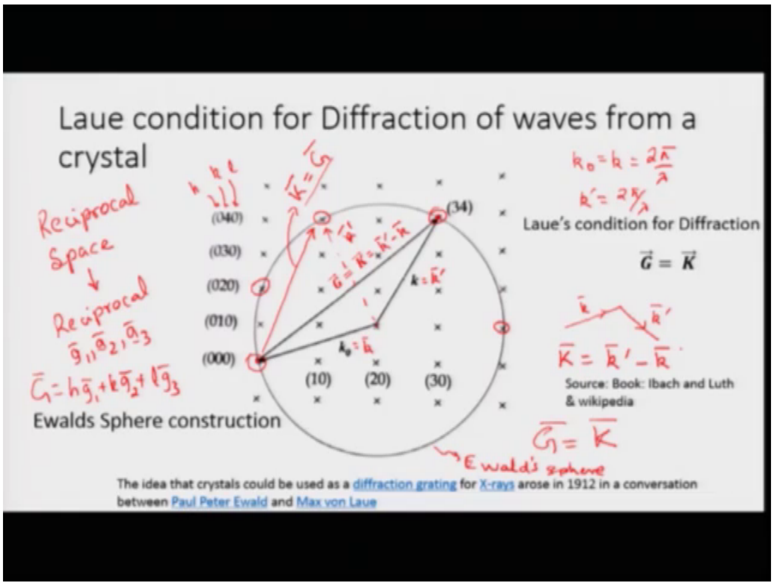

That this is in your reciprocal space, now we go to our reciprocal space. And in our reciprocal space for a given crystal you can make your reciprocal lattice using g 1, g 2, g 3. Combinations of g 1, g 2, g 3 you can generate your reciprocal lattice points. So, for example, in this 2-d space you have your reciprocal lattice points which are shown here.

And these are just the indexes h, k and l for each of the points. So, if you recall the reciprocal lattice vector can be written as h times g 1 plus k times g 2 plus l times g 3. So, these indexes h, k and l are the reciprocal lattice points.

Now, in this reciprocal space which is in length inverse, I can draw my incident wave vector. The incident wave vector has a magnitude; the incident wave vector k naught which in my terminology is k is 2 pi by lambda. So, this incident wave vector you can draw it in the reciprocal space as a vector which is shown here. You can choose any point as the centre, you can choose any point in this reciprocal lattice as the centre and from that point you can generate or you can draw a vector whose length is the incident wave vector 2 pi by lambda. And it has some direction you can draw it in any direction.

And you can also draw the scattered wave vector k with respect to the incident wave vector you have a scattered wave vector. So, you know that it comes in one direction and then it gets scattered out. So, once you know your incident direction you know you are scattered direction also. But the magnitude of the scattered vector is nothing else, but 2 pi by also lambda. But you know its direction, so you can draw this other scattered vector.

So, this is your incident wave vector, this is your scattered wave vector, this is your scattering vector K which is the difference between k prime minus k. This is equal to k in my terminology, and this is equal to k prime in my terminology. So, this vector which I have drawn here is vectorially the difference between k prime minus k. The difference between the scattered wave vector and the incident wave vector.

And this vector you can see is joining two points on the reciprocal lattice. This point and this point it belongs to the reciprocal lattice. So, the condition that this vector k, the scattered vector which is k prime minus k is equal to g means that this vector should fit between two points in your reciprocal lattice. If this scattered wave vector connects two points on the reciprocal lattice, then you will get finite intensity of scattered wave from these point in the reciprocal lattice.

And these are not two unique points, because what you can do is that keeping this point as a centre and this has the radius you can draw a circle. And for any points of the reciprocal lattice which are sitting on this circle you can show that they will satisfy the Laue's condition: G is equal to K. For any points, like these points which are sitting on your circle which is called the Ewald's sphere; this sphere is called the Ewald's sphere. For any point which is sitting on this your k minus k prime will be connected.

So, if I draw a k prime out here for a scattered wave k prime in this direction, this is your scattering vector k and that you can see is connecting two points in the reciprocal lattice. So, even this will give rise to a finite intensity at your point of observation. So, these are the different points which was start generating a diffraction pattern. So, when you come in with an incident beam of light you will get a collection of spots bright spots in your screen and that corresponds to these points on the reciprocal lattice which are satisfying this condition and this is your Laue condition.

So, if you recall that we had seen if you have an incoming beam of X-rays which is falling on a crystal, then this beam scatters. And if you look at the distribution of points on a screen you will see a bright spot, and you will see a set of bright spots. These are the points where the intensity is not equal to 0, this is the scattered intensity is not equal to 0, and in between the scattered intensity is equal to 0. So, only at these points, which are these bright spots the scattered intensity is not equal to 0. And it is at these points where the scattered wave becomes equal to the reciprocal lattice points.

So, these are your reciprocal lattice points from where which are satisfying this condition, which we have seen is coming when you look at the Ewald's sphere. So, which points are going to give you finite intensity or diffracted beams are going to be governed by the points in the reciprocal space which are sitting on the Ewald's sphere. And this is your interpretation of your Laue's condition.

So, actually you start mapping your reciprocal lattice space, with X-ray diffraction what you are actually doing is that you are actually mapping the points in your reciprocal lattice.

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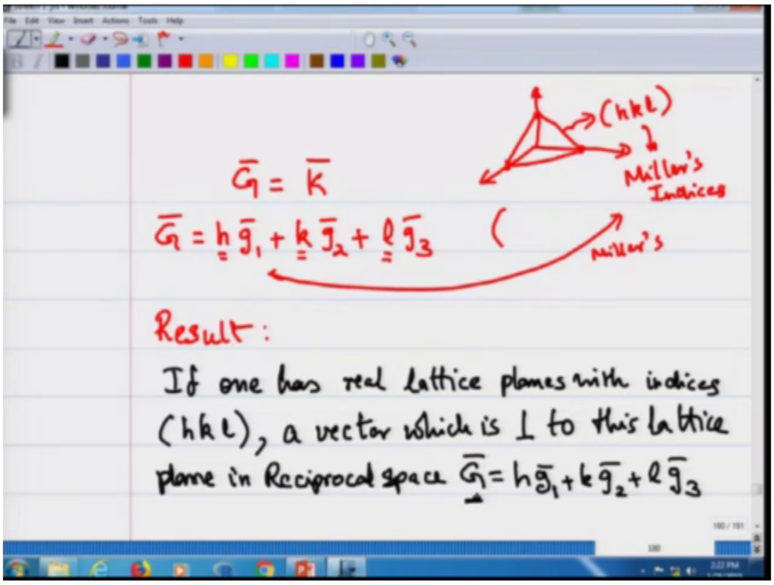

Now, let us look at the condition. The Laue's condition G is equal to K a little bit more closely. Without getting into the derivations I would like to state a result for you. So, you know that you have a reciprocal lattice which can be constructed with this h g 1 plus k g 2 plus l g 3. Now, you might be wondering why I am giving these indexes h, k and l.

Because if you look at my lectures on crystals you recall that lattice planes; atomic lattice planes in the real space if I had a real space and if I was looking at atomic lattice planes or lattice planes in the real space. Then these lattice planes in real space were indexed by something called as millers indices, which were given this combination of indices h, k and l ok; combination of integers which are h, k and l.

So, a real plane of lattice points and parallel set of lattice planes have an index which is given by h, k and l. My reciprocal lattice is also generated with g 1, g 2, g 3 and you have these indexes which are written as h, k and l. Is there any connection between these indices and millers indices? Do you have any connection between the points in the reciprocal lattice space and the miller indices which are there in the real space.

So, here is a result which I will state without giving a proof and the result is as follows. The result says that if one has real lattice planes with indices h, k and l. If one has real lattice planes with indices h, k and l, a vector which is perpendicular to this lattice plane in reciprocal space is G; which is given by the same indices a g 1 plus k g 2 plus l g 3. Alternatively stated, that in reciprocal space if you have this vector G which is written as h times g 1 plus k times g 2 plus l times g 3, then h, k and l are the millers indices of real lattice planes which are perpendicular to this vector G.

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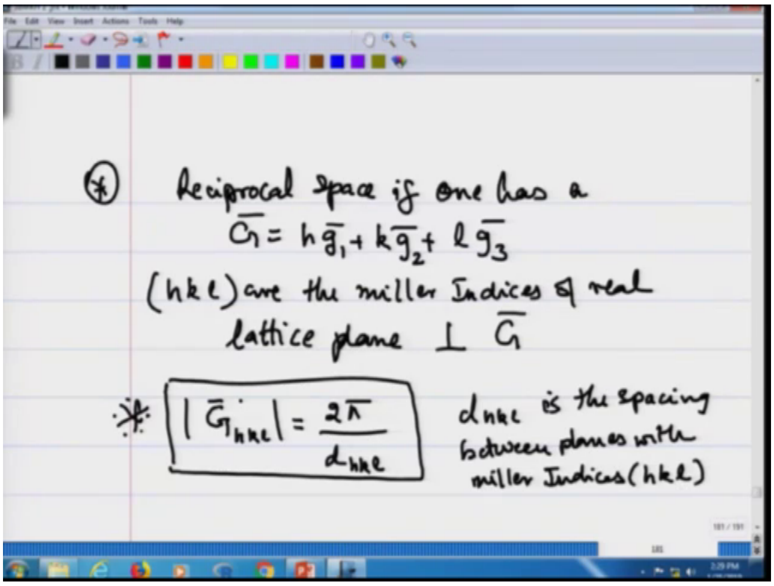

So, in reciprocal space if one has a vector G which is given by h g 1 plus k g 2 plus l g 3; where h, k and l are integers. Then these h, k and l are the miller's indices of real lattice planes which are perpendicular to this vector G in the reciprocal space. And this gives you a way to connect the real space and your reciprocal space. And for that let me again show you a slide which makes this slightly clear.

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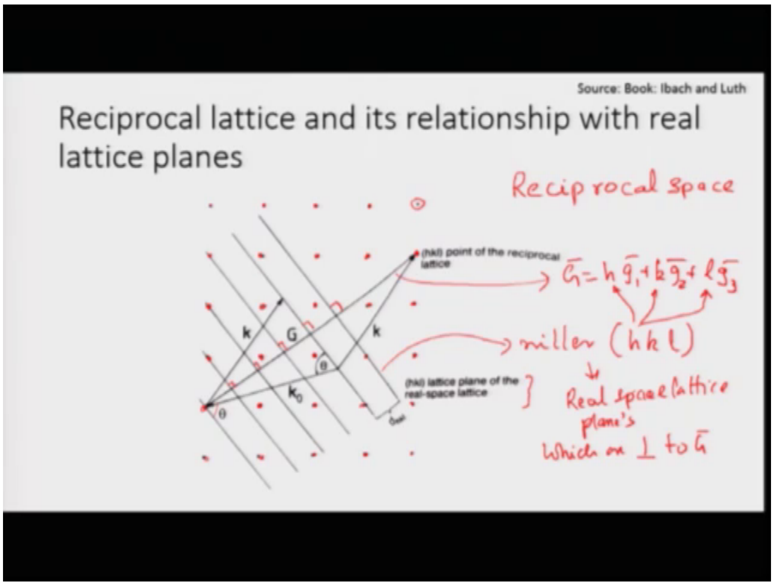

Is that this is my points in my reciprocal space. So, these are my points in the reciprocal space. So, this is all in the reciprocal space, this vector G which is connecting one point in the reciprocal space with another point in the reciprocal space. This vector G is written in some combination of h time's g 1 plus k time's g 2 plus l time's g 3. So, here you have your points in the reciprocal space which are generated by combinations of this g 1, g 2 and g 3.

Now, if we consider this vector which is given as some particular combination of h, k and l, this vector is some particular combination of h, k and l then the lattice planes which are these black lines which are drawn these are atomic real space lattice points. These are the real space lattice planes which have miller's indices h, k and l corresponding to this. These are miller's indices of real space lattice planes which are perpendicular to G. If you can see that all these lattice planes are perpendicular to this vector G.

So, given a vector G you can construct lattice planes which are perpendicular to the G. And from this vector G, the indices of these vectors or the components of these vectors h, k and l will form the miller's indices for these lattice planes which are perpendicular to G. So, this is an important result which shows the relationship between points in the reciprocal space and vectors in the reciprocal space with real lattice planes.

And another result which is related to this is that you can show that the magnitude of G which is characterized by some of these indices is 2 pi divided by the perpendicular distance between the lattice planes which are characterized by h, k and l. So, if I go back to the slide once again this is your reciprocal lattice vector which is characterized by components h, k and l, and these give the lattice planes whose miller's indices are also h, k and l. Now these lattice planes, all these parallel lattice planes which are perpendicular to g have the same miller's indices. The spacing between these lattice planes is d, h, k and l. This is the atomic lattice planes, this is in real space.

These lattice planes, all of these lattice planes have the same miller's indices and the spacing between them is d, h, k and l. So, from this result one knows that the relationship between this lattice vector which has components h, k and l in the reciprocal space is related to planes with millers indices h, k and l which are perpendicular to G, having a planner spacing d h k l is the spacing between planes with millers indices h, k and l. This is an extremely important result

However, this can be proved, but I am not going to get into the proof. These are the two very important results that one should understand. That one is the relationship between this vector G in the reciprocal space which has components h, k and l. And these components h, k and l correspond to the miller's indices of lattice planes which are perpendicular to G. And the magnitude of this g is 2 pi divided by the spacing between the planes which have millers indices h, k and l.

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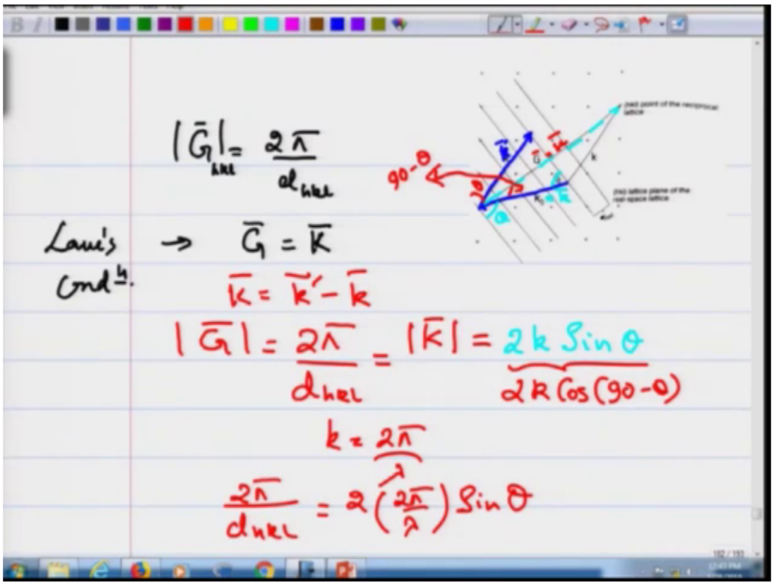

Now, with this result in mind now recall that your Laue's condition for Bragg diffraction or for diffraction of x-rays; the Laue's condition for diffraction of x-rays is G is equal to K. And here in this diagram G is equal to K; where k is the scattered wave vector minus the incident wave vector.

Now, the condition that we had got that your reciprocal lattice vector G is going to be perpendicular to a set of real planes which are space by d, that condition is G is equal to 2 pi by d h k l. Where, d is the spacing between the planes and this is equal to the magnitude of the scattering wave vector K. And this magnitude K in this diagram you can see that in the reciprocal space my incoming scattering wave vector is this, which is making an angle theta with this lattice plane and it is getting scattered with this wave vector small k which is written as k prime. And k minus k prime is your vector, capital K the scattering vector which should be equal to the reciprocal lattice vector for a diffraction and this is the angle theta.

So, now this vector K which is your scattering vector which is k naught minus k prime or incoming vector k minus k prime; this is also equal to what I am writing it as k out here small k. This capital K which is the scattering vector can be written as 2 times k. The magnitude of this is nothing else, but 2 times k times sin theta, because this angle theta that you draw here because the lines are parallel, this is also equal to this angle theta. And therefore, this is 90 minus theta; this angle which I have drawn here is 90 minus theta.

So, this total distance will be twice; this will be essentially twice of k cos of 90 minus theta because that will be equal to this. And that is nothing else but this. And you know k is 2 pi by lambda. And this gives me my relation, so 2 pi by d h k l will be 2 into 2 pi by lambda sin of theta. Where, theta is the angle of the incident wave vector with the lattice plane and it is also the angle with the scattered wave vector; k prime makes with the lattice plane or the reflected wave vector k prime.

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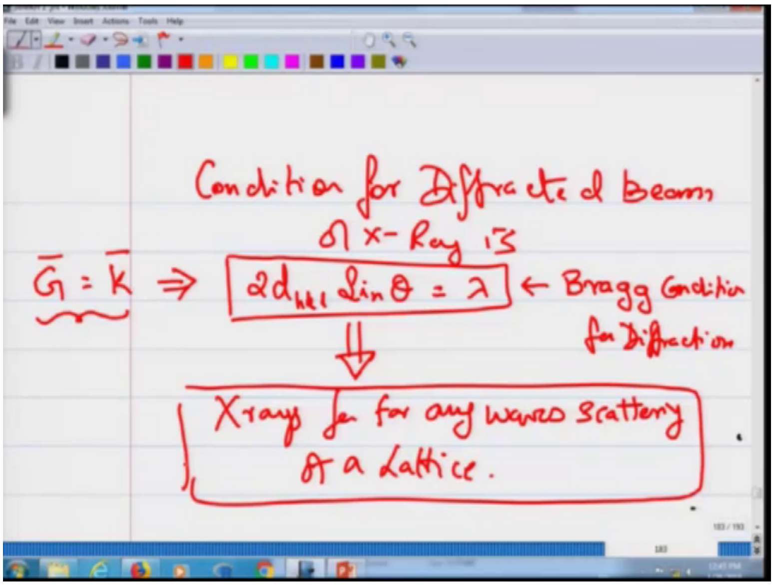

So, you can show therefore, that the condition for diffracted beams of X-ray is that: 2 d h k l sin theta is equal to lambda.

So, the Laue's condition G is equal to k can be rewritten as this; where d is the spacing between the real atomic lattice planes. So, a condition in the reciprocal lattice can be rewritten as the condition in the real space. Where, d is the spacing between the real lattice planes which are perpendicular to g, sin theta is the angle between the incident wave vector with the lattice plane, and lambda is the wavelength of the X-rays. And this also known as the Bragg's condition for diffraction. And this condition is not only true for X-rays, but for any waves scattering of a lattice. We have done it for X-rays, but this is true for any waves which are scattering of a lattice.