Introduction to Solid State Physics
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Lecture - 40
Reciprocal lattice vectors, Laue's condition, and Bragg's law for diffraction of waves by a crystal

So, in our last lecture we had seen the concept of a reciprocal lattice, and you can define points in the reciprocal space which is the Fourier transform of the real lattice.

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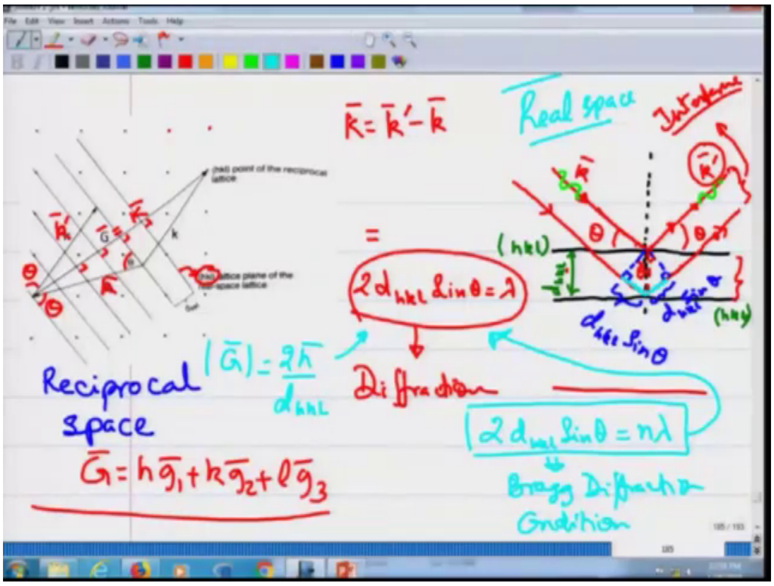

And we are identified your reciprocal lattice vectors G, with which you can draw these points. So, for every real lattice you can also make a geometrical construction of a reciprocal lattice. And the entire scattering process can be described in the reciprocal lattice. For example, the incoming x-rays is represented with a vector whose length is your incoming wave vector k and whose direction is the direction of the incoming wave vector. And it gets scattered out with a wave vector k prime whose magnitude is the same as k direction is different. So, in the reciprocal space you can draw this other vector which is representing your k prime vector.

And in the reciprocal space we came across the result that the real lattice planes which are shown here as solid lines are cutting your reciprocal lattice vector perpendicular to it.

So, your perpendicular reciprocal lattice vector G, this vector is perpendicular to reciprocal lattice planes with millers indices h, k and l.

So, if you have real lattice planes with millers indices h, k and l, the reciprocal lattice vector G which is given by G is equal to h g 1 plus k g 2 plus l g 3 is going to be a vector perpendicular to these lattice planes. If theta is the angle between the incoming wave vector and the lattice plane then we showed that the Laue's condition gives us the condition for diffraction of the scattered beam. The 2 d sin theta is equal to n lambda where d hkl is the distance between the parallel set of planes which are characterized by a millers indices h, k and l.

So, the Laue's condition gave us this condition for diffraction. And this condition also came to be known as the Bragg's law for diffraction of waves. So whereas, all of this was done in the reciprocal space you can also look at this phenomena in real space. And in real space what you have is these two planes which are have millers indices h, k and l; have a spacing of d hkl. The incoming wave has got a wave vector k and the outgoing reflected wave has a wave vector k prime. Theta is the angle between the incoming wave vector and the lattice plane, and the reflected wave also has the same angle.

Now, you have another wave which is parallel and strikes the parallel layer below it, which is at a distance of d hkl from the upper layer, and so it gets also reflected. And then these two waves will undergo interference. And whether you will observe a maxima or a minima the diffracted beam, whether it will be a maxima or a minima will depend on the path difference between these two beams.

And what is the path difference? This if d hkl is the distance which is also equal to this distance between the planes, then you can show that the path difference between these two beams will be twice of this distance. This is the extra distance which the beam is traveling. With respect to the upper beam, this beam which is striking the lower plane is traveling this extra distance. And this extra distance you can show is d hkl sin theta. So, the extra distance travelled is 2 d hkl sin theta, and the condition for constructive interference is n lambda.

So, 2 d sin theta is equal to n lambda, this will give you your Bragg Diffraction Condition which is also what we have obtained from our Laue's diffraction. From the reciprocals lattice consideration when we wrote that the magnitude of the vector G should be equal to 2 pi by d hkl. Then this gave us also, this condition which is nothing else for the Bragg diffraction condition which we have seen in the real space.

So, the two are exactly equivalent and identical. And this for n is equal to 1 n is some integer; n is equal to 1 it gives the first order maxima, the first maxima in your diffracted beam. So, you see the importance of the reciprocal lattice and how to describe diffraction of waves in this reciprocal lattice. Whatever I tell you for x-rays holds true for any waves, whether they are coming from outside or are waves which are generated inside the solid itself. And these type of waves you will study further. For example, one set of waves is called as a phonon which is related to vibration of atoms inside the lattice. Another type of waves which is not coming from anywhere outside, but it is there inside the material are electron waves; which are related to propagation of electrons through the material and these are like plane waves.

So, how do they scatter of the atomic lattice or the lattice which is present inside the crystal; that is also described by similar set of features, And similar set of laws which govern the diffraction of those waves also. aAnd in relation to this scattering of waves the final an important aspect which I will introduce now is something called as the Brillouin.

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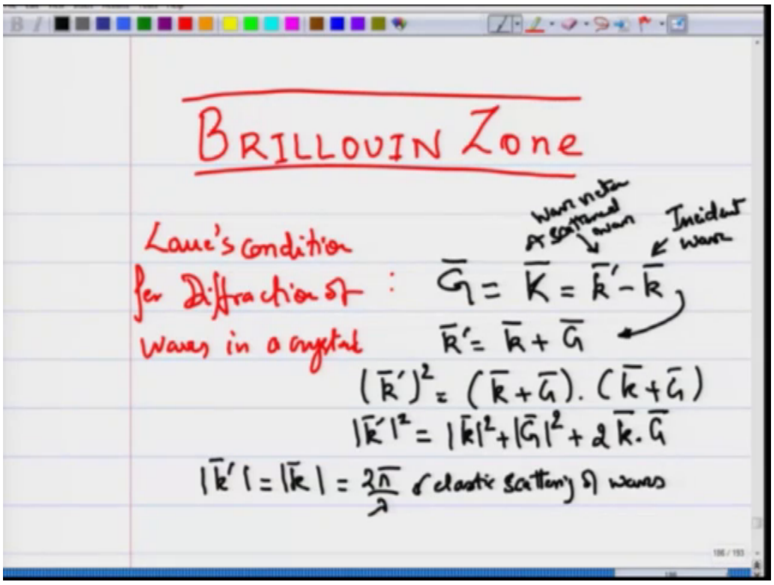

The concept of a Brillouin Zone. So, what is the Brillouin zone? Before we take a look at what is the Brillouin zone let us go back again to our Laue's condition for diffraction.

The Laue's condition for diffraction of waves in a crystal; and what is that condition? The condition states that the reciprocal lattice vector has to be equal to the scattered vector K scattering vector K which is equal to k prime minus k; k is the wave vector of the scattered wave vector of scattered wave and this is the wave vector of the incident wave.

And so, I can rewrite this expression as k prime is equal to k plus g. And if I take the square of this; so from here I can write this. And if I take the magnitude of both sides then I will get k prime square is equal to k plus G dot k plus G. And you will get k prime the whole square is equal to whole square plus. But the magnitude of k prime is equal to the magnitude of k which is equal to 2 pi by lambda, because we are looking at elastic scattering of waves.

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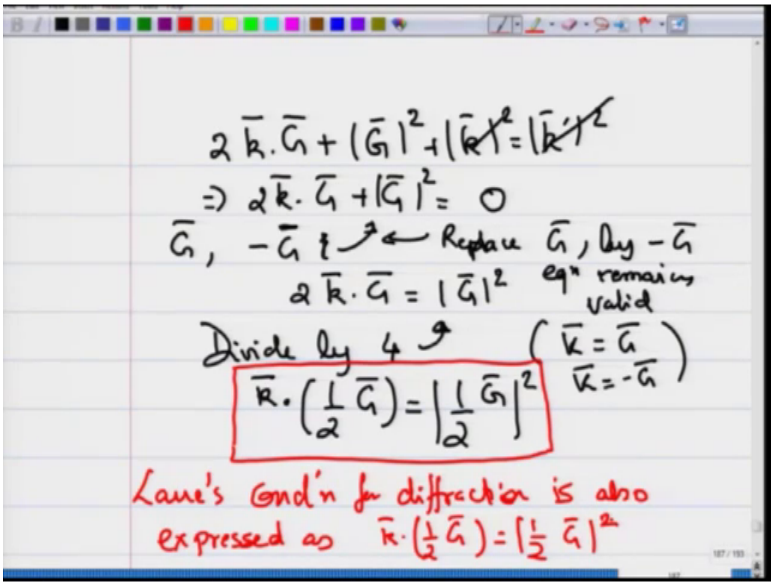

And therefore, you will get 2 of k dot g plus k square is equal to k prime square; these two will cancel which will give me 2 k dot G plus whole square is equal to 0. Now whatever this expression, whatever is satisfied by G is also equivalently satisfied by minus G.

So, in a reciprocal lattice whatever is satisfied by the wave vector G is also satisfied by negative of that wave vector. So, if you substitute that here you can write this as 2 of k dot G. So, you replace G by G prime, you replace G by minus of G the equation remains unchanged equation remains valid basically because the Laue's condition is valid whether k is equal to G or k is equal to minus of G in both conditions is valid. So, this a trick becomes convenient to write this as once you replace minus G out, you will get a minus sin and therefore it becomes possible.

Now, divide it by 4 this equation and you will get the condition that k dot half of G is equal to half of G the whole square. So, the Laue's condition for diffraction; the Laue's condition for diffraction is also expressed as k dot half of G is equal to half of G whole square.

So, let us look at the physical interpretation of this equation.

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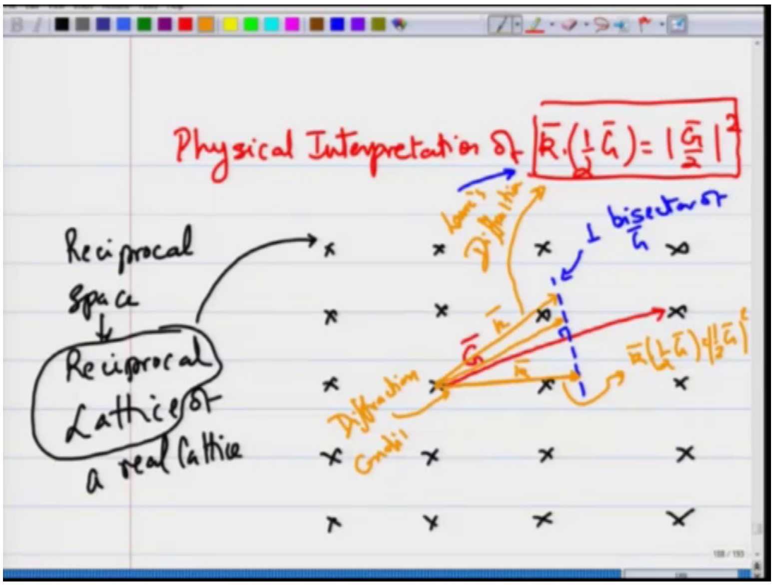

So, what is the physical interpretation of k dot half of G is equal to G by 2 the whole square or half of G the whole square? The Laue's condition, what is the expression what is the physical interpretation of this Laue's condition.

So, let us go to the reciprocal space and look at the reciprocal lattice of a real lattice. So, given a real lattice corresponding to some crystal you have a real lattice and you can also make its reciprocal lattice. So, let us look at the reciprocal lattice of a crystal.

so let us For example, into dimensions I am just making a simple reciprocal lattice as an example. So, these are all reciprocal lattice points. And now in this space from any point I can draw a reciprocal lattice vector G. So, two points in my reciprocal lattice are connected by the reciprocal lattice vector G, then this condition that k dot half of G corresponds to all the wave vectors which fall. So, I can draw the perpendicular bisector of this reciprocal lattice vector. So, this is my perpendicular bisector of G.

The Laue's condition which is given here suggests that for any vector k; starting from this point any vector k of a wave which terminates on the perpendicular lattice vector, this wave is going to get scattered following the Laue's condition or this wave we will undergo a diffraction.

So, all the wave vectors which terminate on this line which is the perpendicular vector of G, all these wave vectors will satisfy the diffraction condition. Namely, this is just one wave vector, but I can have multiples of wave vectors; I can have another wave vector like this ok. All these wave vectors which are terminating on this perpendicular bisector we will satisfy, all these k's we will satisfy this condition namely they will give rise to diffraction Laue's diffraction. So, they will all give rise to Laue's diffraction. All of these wave vectors which are satisfying we will satisfy the equation k dot half of G is equal to half of G the whole square.

You can show that all these vectors which are terminating on all this wave vectors which are falling on this perpendicular bisector of g satisfy the Laue's diffraction conditions. So, these waves which are going to get reflected from here we will undergo a diffraction as they get reflected from this plane.

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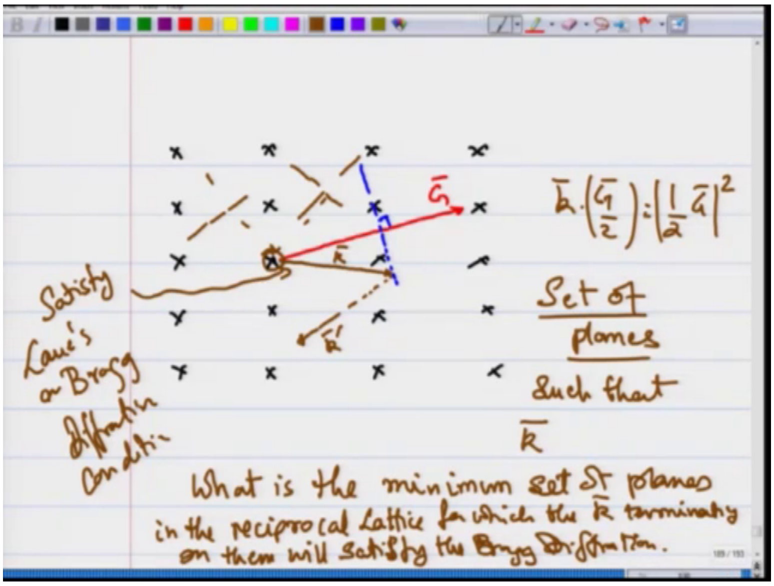

So, the idea is that if you have these lattice planes in the reciprocal lattice, if you have these points in the reciprocal lattice. Then, if this is your reciprocal lattice and you draw the perpendicular bisector of the reciprocal lattice which divides it into two equal parts and is a perpendicular to this reciprocal lattice vector, then all the waves which are falling on this line which is the perpendicular bisector of G; all the waves with a wave vector k which terminate on this line satisfy the. All these wave satisfy the Laue's or equivalently the Bragg's diffraction condition. And they will get scattered of with k prime.

So, all of this k's we will satisfy this equation. And what is the minimum set of planes? So, in this direction I can draw this, and similarly I can get multiple set of planes which I can draw and different directions in this reciprocal lattice. I can take different directions and I can draw reciprocal lattice vectors from each of from this point, I can draw different reciprocal lattice vectors in different directions. So, I can draw in this direction, I can draw, and I can draw perpendicular bisectors, and I will get a set of planes. I will get a set of planes such that wave vectors which terminate on these set of planes which I will be drawing if they terminate on these set of planes then they will satisfy the Bragg diffraction condition, So, what is the minimum set of planes set of planes in the reciprocal lattice for which the k's terminating on them we will satisfy the Bragg's diffraction. And that is given by a construction which you are already familiar with.

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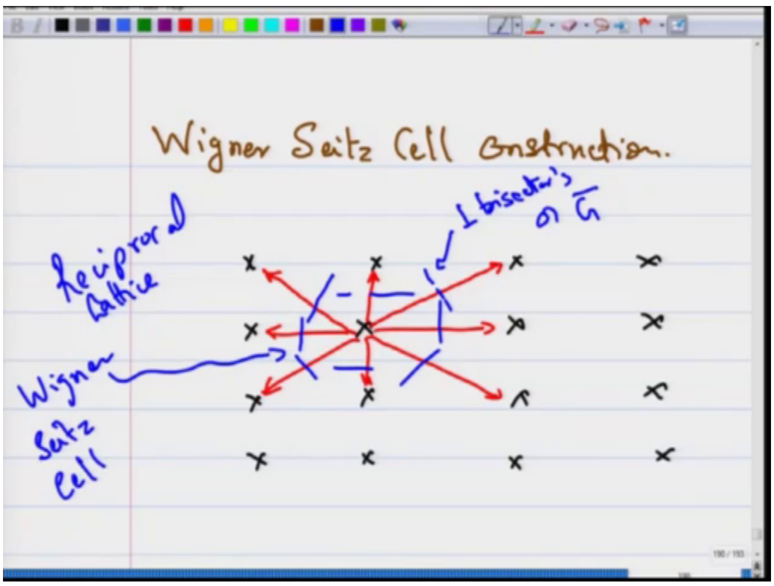

And that is the Wigner Seitz Cell Construction. Whereas, I had shown you in the earlier when we were discussing crystals the Wigner Seitz cell for a real lattice, now we will construct the Wigner Seitz cell for a reciprocal lattice.

And again the construction is exactly identical. What you do is: if you have reciprocal lattice, then from any point you join to nearest points and then you make the perpendicular bisectors. If you recall: this was a Wigner Seitz cell construction you make a perpendicular bisector, and you will describe your Wigner Seitz cell. But now, this we do in the reciprocal lattice. And these are the perpendicular bisectors of the vectors that I am drawing.

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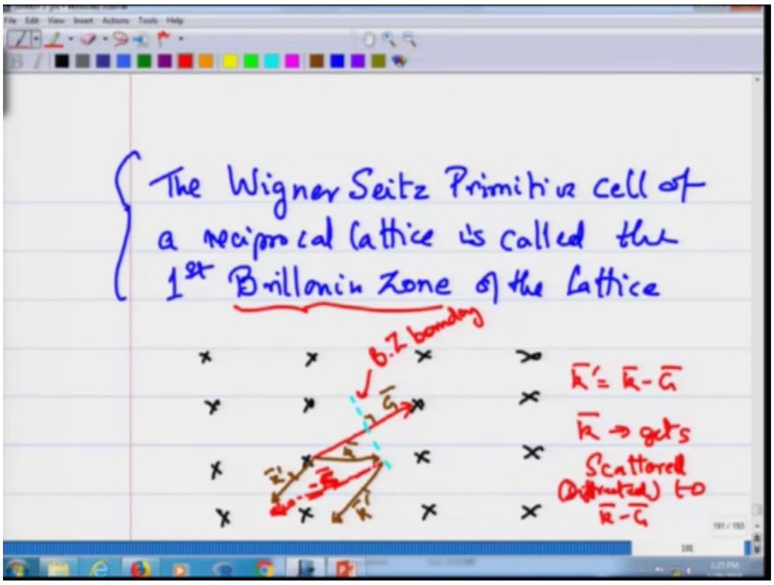

And this zone that we define or this surface that we define: the Wigner Seitz primitive cell of a reciprocal lattice is called the 1st Brillouin Zone of the Lattice. The Wigner Seitz primitive cell of a reciprocal lattice is the 1st Brillouin Zone of the Lattice.

So, let us look at an example.

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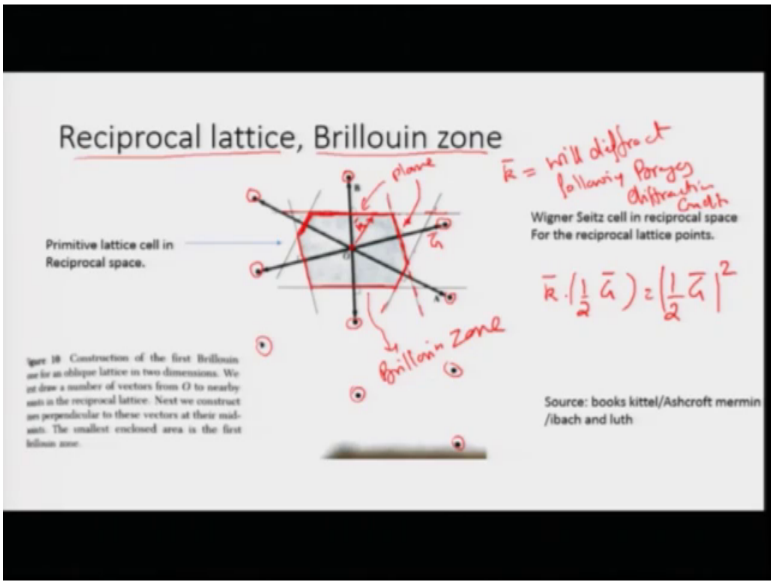

So, here in the reciprocal lattice, we will look at the 1st Brillouin zone. So, this is the reciprocal lattice of an oblique lattice ok. These are the reciprocal lattice points of an oblique lattice. These are nothing else, but the reciprocal lattice points. Each point I am connecting it with the nearest neighbor point by drawing this vectors, and then I am drawing the perpendicular I am drawing my perpendicular bisectors. These are all my perpendicular bisectors,

And if I draw my perpendicular bisectors then I define set of planes. If you can see I have defined a set of planes which are all part of perpendicular bisectors of the reciprocal lattice vectors. And these set of planes which I have defined. As I said for any vector wave vector k which is terminating on this plane or on this plane these wave vectors will diffract following Bragg diffraction conditions.

So, this is the minimum set of planes which you can define through the Wigner Seitz cell construction, which will define your 1st Brillouin zone. For waves with a wave vector k which are impinging and reflecting of these set of planes they will undergo Bragg scattering or they will undergo diffraction.

And those waves we will certainly satisfy k dot half of G is equal to this Bragg diffraction condition or the Laue's diffraction condition. These waves will satisfy this diffraction condition. And this is called as the Brillouin Zone; the 1st Brillouin Zone of your Crystal or of your Lattice. And waves which diffract of the 1st Brillouin zone undergo Bragg diffraction.

So, this is an important step to define

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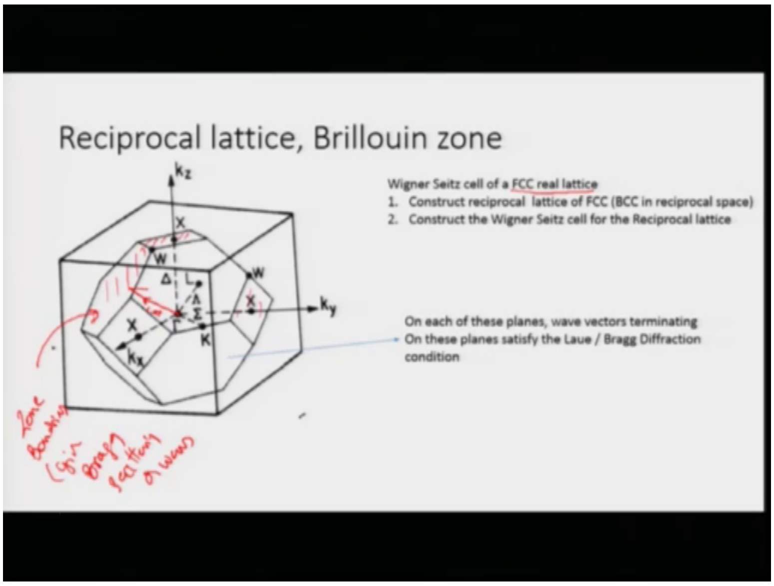

Now this is a more complicated Brillouin zone; the 1st Brillouin zone for an FCC lattice. So, if you take an FCC real lattice you can actually construct the reciprocal lattice of the FCC which is the BCC lattice. And then once you construct the BCC lattice this is your body centered point and then you can construct the Wigner Seitz cell, from each of the body centered point you can connect the. And these are the planes these are the planes which are perpendicular to the nearest neighbour reciprocal lattice vectors. And then you can get this surface which is the Wigner Seitz cell in the reciprocal lattice ok.

And for waves which are getting diffracted from these planes. So, wave which is getting diffracted from this plane, these waves will undergo Bragg scattering. So, waves which are undergoing a diffraction from these planes which are which is the zone boundaries this planes are also called as zone boundaries; they will undergo they give rise to Bragg scattering of waves. And different directions in this reciprocal lattice are given in terms of this tau x sigma delta directions to define different directions in the Brillouin zone; the by convention you take certain directions tau is taken as the zone centre. And then you have a sigma direction, you have a lambda, you have a delta, you have a x point and so on. All these are the by convention, these are certain directions which are define for the Brillouin zone.

So, before I end I would just like to tell you that if you have a reciprocal lattice vector; if you have these reciprocal lattice points and this is my reciprocal lattice vector, this is the perpendicular bisector of the reciprocal lattice vector. Then a wave k which is diffracted from this the wave falls on this on this plane which is the perpendicular bisector; the wave falls on this plane in blue which is the perpendicular bisector of G ok. This wave will undergo a Bragg scattering ok.

And so, this wave will obey; the scattered wave will obey your Laue condition k prime will be a Laue condition. So, I can read draw it as: this is in the minus G direction, this is your minus G, and this is my k, this is my k prime, this is my minus G direction. And then this part of the diagram I can rewrite it has so a wave which is scattered took k prime k prime is equal to k minus G. So, k gets scattered to scattered or diffracted to k minus G from the Brillouin zone boundary. So, far waves which are scattering from the Brillouin zone boundary they will get scattered to k minus G. This is the minus G direction, and this is the Brillouin zone.

So, this is to not only for diffraction of x-rays, this will also be true as I said; all this rules are going to be true for not only electromagnetic waves which are coming from outside or waves which are coming from outside like we are sending and x-rays, these are also true for waves which are present inside the solid. For example, phonons which are generated because of vibration of atoms inside the solid or they are also related to they also satisfied by electron waves which are scattered from within the crystal. These electron waves correspond to propagating waves of electrons inside the metal itself, they also satisfy these conditions. And therefore, Brillouin zone is a very important concept which will govern the scattering of these waves inside the crystal.