Solid State Physics

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Lecture - 29
Reciprocal Lattice (Contd.)

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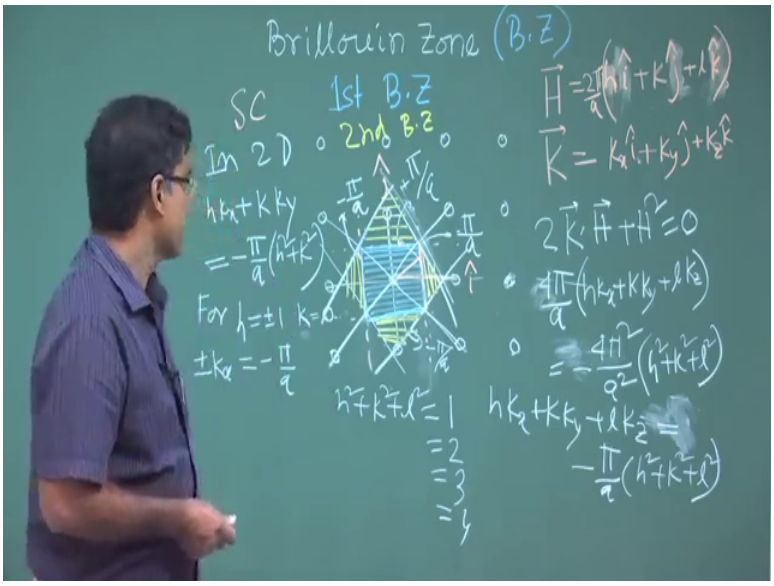

So, I will discuss about Brillouin zone, in reciprocal lattices which is equivalent to Wigner Seitz cell Wigner cell in direct lattice. So, as I mentioned in last class that, that this total lattice point reciprocal lattice point.

So, this is the reciprocal lattice point; and this how to construct Brillouin zone as I mentioned this equivalent to Wigner Seitz cell. So, you just take one point and then one has to take bisect, normal bisect of the nearest point equidistant point of course, ok.

So, here, these are nearest point and if I take normal bisector of these lines connected lines. So, this is found right now these you can use. So, this is the area, this is the area in 2 dimension of course, if it is in 3 dimension you have to you have to follow accordingly. So, this is basically is Brillouin zone, this is Brillouin zone and this called first Brillouin zone; it is called first Brillouin zone first.

If I write B, Z Brillouin zone just abbreviation. So, I can tell this is first Brillouin zone. So, what it is just look at it? If you look at it; so these each edge what it is, this one is the basically if I take this is a origin in one point in reciprocal lattice.

So, if I connect with any other lattice points. So, this is basically reciprocal vector this is basically reciprocal vector H right. Now this edge is nothing but the bisectors of this one reciprocal lattice vector reciprocal lattice vector reciprocal vector right or other way I can say from here you can see that this edge is non perpendicular bisector of edge

So, this edge is perpendicular bisector of edge reciprocal lattice what is that? In all construction we have seen that it is nothing but then this is nothing but the crystal plane right in direct lattice or lattice plane crystal plane in direct lattice. So, this boundary of this zone, this each one are basically it is crystal plane right.

Which crystal plane? The inside x-ray reflected from that crystal plane and generated the points reciprocal points right because reciprocal point is connected with the x-ray, x-ray wavelength direction right. So, these planes are the crystal planes, here line in 2 dimension 3 dimensional if things, ok

So, this we can represent with this H what we have taken H equal to hb 1 plus kb 2 plus l b 3 right. So, as I told that this is the crystal plane and from this crystal plane x-ray are reflected or diffracted right. So, any incident x-ray is falling on this boundary any x-ray is falling on this boundary that will be reflected right that will be reflected and this incident x-ray or reflected x-ray that is basically represent with the k vector right k vector.

So, k vector now if I give the direction this is say i direction this is j direction and this other one is k direction or b 1, b 2, b 3 right. So, now, let us take this simple example again this simple cubic simple cubic right, if it is simple cubic lattice as you know for simple cubic both are in reciprocal lattice and direct lattice both are same right it will be simple cube.

So, these are simple cubic lattice reciprocal lattice and b 1, b 2, b 3 if a direction is I j k. So, this I can write that is b 1 the direction I can write by i and magnitude was 2 pi by a right. So, b I can write 2 pi by a. So, 2 pi h by a right and again here basically 1 instead of h 1 should right n h, as I told this in reciprocal lattice that is in have significant.

So, one can write nh. So, for the time being you just write h whenever necessary we will put n and. So, I can. So, this all are magnitude 2 pi a just here it is j and here it is k direction. So, there are many k in miller indices k web vector k right and image vector also you have taken k. So, do not be confused.

And now this momentum vector right incident x-ray it has its the defecting its deflecting plane right it is a deflecting plane. So, whenever its index will fall on this it will be reflected right. So, it is it has K vector. So, it will have 3 components if I write kx ky kz. So, this k vector I can write Kxi plus Kyj plus Kz k right, ok.

So, it is in reciprocal lattice it is in reciprocal lattice right and here this reflection these are reflecting planes incident x-ray getting defection deflected right and now we have this reciprocal vector. So, so in the reciprocal what is the Bragg condition?

So, you want to see the diffraction right. So, what is the Bragg condition; 2 K dot H plus H square equal to 0 that is the Bragg condition in the reciprocal lattice right. So, I can use this 1 K dot H, K dot H will give you K dot H will. So, 2 K dot H. So, 2 pi by a. So, I can write 4 pi by a right.

So, I can write hkx plus kky plus l kz right just if I take dot product I will get it plus H square. So, if you take the other side minus H square. So, let me take other side minus H square. So, minus H square H square means H dot H I have to take dot product. So, H square dot product if you taken the 4 pi square by H square I have to take minus sign right equal to h square plus k square plus l square, right.

So, this condition has to satisfy for getting reflection right. So, from here, from here we can write 4 pi here this 4 pi square by a square. So, I can write h kx plus kky plus lkz equal to pi by a; so minus pi by a.

So, let me write here, because space is not there. So, minus pi by a h square plus k square plus l square right. So, this is for 3 dimension. Just here we have line of in second 2 dimension. So, just let me that I take the things in 2 dimension the same way. So, I can write basically just if we do not take l and Kz. So, it will be 2 dimension. So, basically 2 dimension in 2 dimension we can just to compare it.

So, what I am getting? I am getting h kx plus kky equal to minus pi by a, h square plus k square for 2 dimension. So, here for all possible value of hkl or in this case hk, we will get different value of kx ky means a k ok.

So, we are getting different k means we are getting different reflected rays right k represent the reflected rays here from these Bragg plane. For different h scale means for all possible h scale means for all possible planes crystal planes, we will get different k value means different deflected rays right. So, so let us take h scale value.

Generally here the that is a importance lowest h scale, h square, k square l square that value H square plus k square plus l square value if you see it become 1 2 3 4 5 6 7 8 etcetera. So, 1 may be missing somewhere this one has to see, but is this way. So, its smallest value is 1 right that is for 0 0 1 or 1 0 0 etcetera etcetera right

Second value is 2 it is for 1 1 0 or 0 1 0 sorry 1 0 1 or 0 1 1. So, for this plane it is a so; that means, in this 2 case this is 1 right. So, that is for 0 0 1, 0 0 1 plane. So, H value is 1.

So, what we can take for h equal to plus minus 1, k equal to 0 right what we will get kx here to satisfy this condition this is one means it has to pi by minus pi by a. So, here this is one means k x for this we will get kx H is plus minus 1 we will get plus minus kx equal to this is 0 equal to minus pi by a and this is for all value of ky because this is k 0. So, it can take any value.

So, in 3 dimension one you can see if h is plus minus 1 and other is 0. So, it will be plus minus kx for all other value of ky and kz. So, in this case it is kx equal to minus pi by a or plus pi by a right it is representing basically you see in what is this distance? In simple cubic what is this 2 pi by a right in reciprocal lattice this is simple kv this 2 pi by a and this is intersecting right perpendicular bisector, ok.

So, this magnitude is pi by a right kx, kx value along with this distance it will be pi by a other direction minus pi by a this one, this one will be minus pi by a right similarly if you consider this k equal to plus minus 1, but h equal to 0 and l equal to 0 for 3 dimensional case ok.

So, it will represent this 2, it will also be this same value minus this say plus pi by a and this is minus pi by a for. So, in 3 dimension these will be plane right h for 1 0 0 plane, it has 6 you will get 6 combination 6 planes you will get you know these these and other is these and other side. So, it will it will form a cube of 6 faces right and these the this will be the first Brillouin zone if this square or this cube in 3 dimension.

So, and important is that here from Bragg condition in reciprocal lattice we are able to show that these are reflecting plane crystal reflecting plane from where this x-ray reflected and I do not show it is a unit cell right it is a unit cell first Brillouin zone right and if I consider the first Brillouin zone, I can get all information I do not need a to consider a other points because this second (Refer Time: 22:26) mentioned here earlier these on this line whatever other point we are getting this point is nothing but the second order diffraction point right then third order forth order other side also similar way as I told this whatever information I will get from first order.

So, this point is nothing but whatever this points for a particular crystal plane. So, this in reciprocal lattice whatever the points we are getting that is coming second order is nothing but it is coming from the it has contribution from second plane, third plane fourth plane, fifth plane etcetera right which we told incase of direct lattice this. This from all these planes whatever this will get one peak that is called first order we will get second peak that is called second order, ok

So, these are information are coming from all sets of plane they are equivalent plane equidistant plane number of lattice points in that planar planar density of number of points are same for all planes. So, that is why this whenever to calculate some properties like electronic property when electrical property when you study you will see that we are considering the only this first Brillouin zone, we are not considering the other Brillouin zone.

So, all information we will get from the first Brillouin zone what is second Brillouin zone. So, second layer is neighbour of this. So, these the second nearest neighbour take bisector sorry take bisector second nearest neighbour take bisector. So, here you are getting you see. So, this is the zone, ok.

Now, this additional zones this. So, whatever yellow colour I have used. So, this additional zones first zone it is there already. Now, this total it is including first zone. So, if you leave this first zone these additional zones yellow colour whatever we are showing that is the second Brillouin zone that is called second Brillouin zone. So, this is the concept of Brillouin zone which coming from this following the Bragg condition in reciprocal lattice ok.

So, one can calculate this whatever I have calculated for simple cubic, one can calculate for BCC FCC. So, that is take as homework if you do not calculate there is no problem because one suggest if you get just definition of Brillouin zone and these simple way to tell you that is may be good enough for you.

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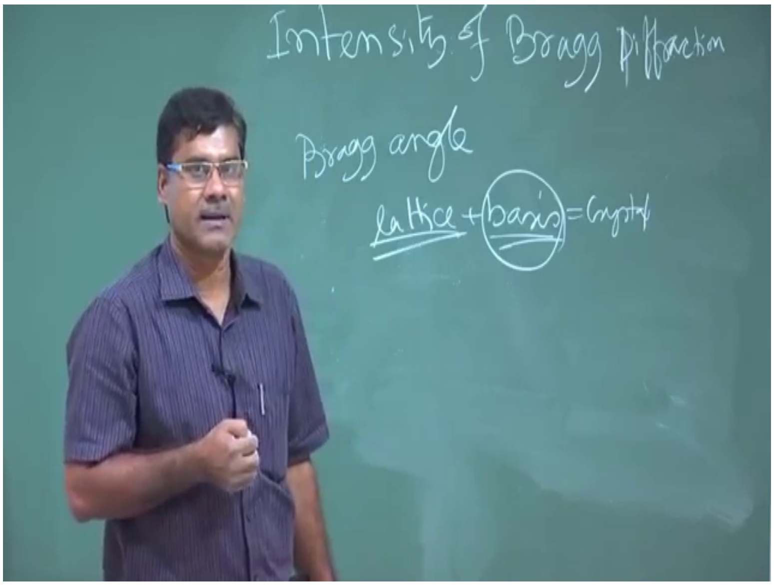

So, let me tell some other shortly I will tell, just I want to tell you about the intensity of Bragg peak and what is its significance; intensity of Bragg peak or Bragg diffraction.

So,. So, far we discussed and used only the about the Bragg angle and I have showed you how to get the lattice structure Bravais lattice for a crystal from this Bagg angle right.

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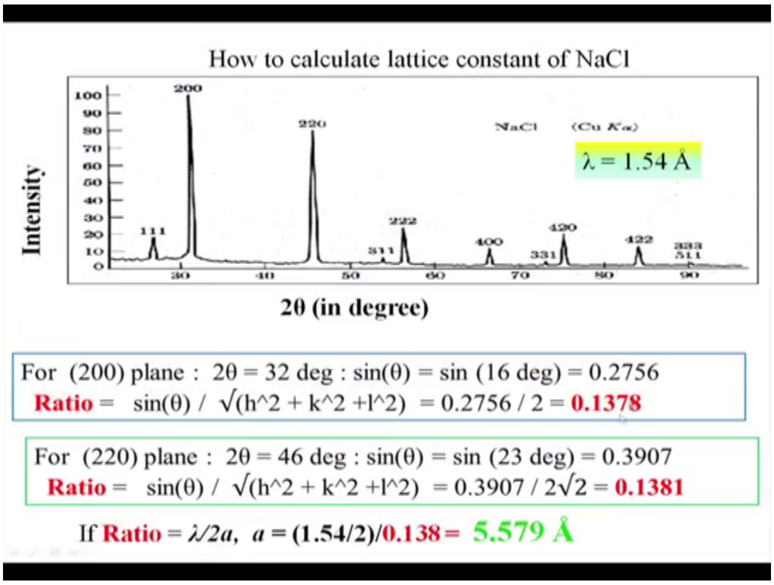

So, here if I show you that already you have seen that that is the x-ray diffraction from sodium chloride crystal and here you are seeing many peaks this 1 1 1 peak, this 2 0 0, this is 2 2 0 right. So, many peaks you are seen.

Now, question is why these different peaks are intensity are different what is the reason, because it is diffracting from different plane crystal planes and different crystal planes having the different number of lattice point right. So, planar densities of lattice point are different for different plane.

So, now with each lattice point basis are connected basis are included there. So, lattice plus basis lattice plus basis that is the crystal. So, from Bragg angle what we are getting information about the lattice, we are not getting information about the basis right. So, in a crystal structure in a unit cell, that is defined by lattice Bravais lattice.

Now in these, lattice basis are distributed in case of sodium chloride. So, sodium chloride are distributed in these lattice in a particular following a particular pattern right. So, same FCC structure, they say sodium chloride FCC structure. So, this other materials having the same structure right, but their basis are different.

So, because of the type of basis and distribution of basis this intensity of the Bragg peak varies. See in case of sodium chloride here basically mainly basis are same, but their distribution the intensity variation of intensity in different Bragg peak, it is because of the position because of the position or distribution of this basis in this lattice.

So, position of the basis 2 important factor, if you take FCC it is FCC structure, but it is of other material say probably iron, iron may be. If the iron is or copper is having the bcc structure say as for example, I am not sure, but other material have this FCC structure. So, for that material you will not get the same Bragg angle it you will get different because the lattice constant will be different that is fine.

So, you will get intensity variation different than this sodium chloride, 2 reason 1 is basis are different. So, that is why you will get and distribution of the basis it will be in more or less similar pattern right.

So, in case of sodium chloride you are getting the intensity variation because of the distribution of the basis same basis in this particular lattice Bravais lattice and intensity variation you will get for different materials having the same Bravais lattice. So, that is because of the different type of basis.

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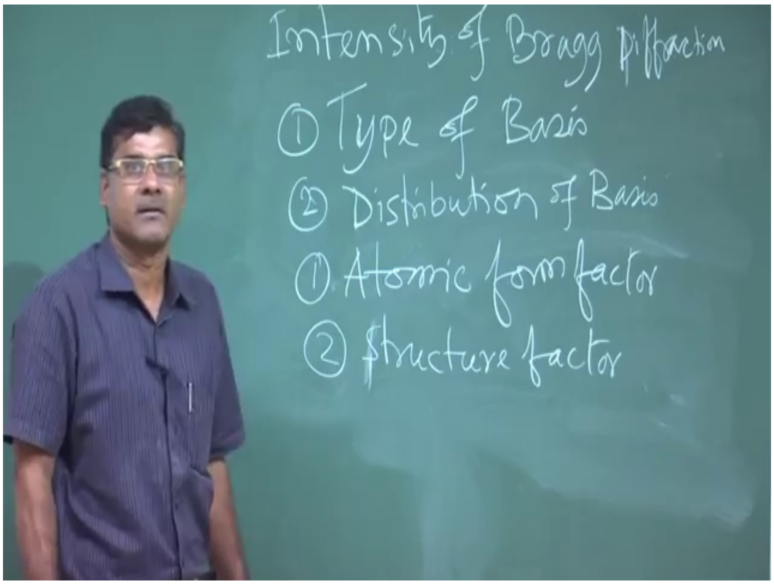

So, intensity depends on the type of basis; type of basis one is type of basis and another is distribution of basis. So, these both are very important and analyzing the intensity actually one can find out the type of basis and distribution of basis; that I will not discuss in details, ok.

So, just I mention the fact. So, from Bragg angle we can find out the Bravais lattice, but from intensity Bragg intensity we can find out the type of basis and distribution of basis. So, the just why it depend on that, just because of this 2 factor you know one is called atomic factor atomic form factor and another is structure factor.

So, this atomic form factor, actually what happens that x-ray scattered. So, when x-ray is falling on crystal x-ray actually scatter from electron. X-ray scatter from electron this is gas scattering center.

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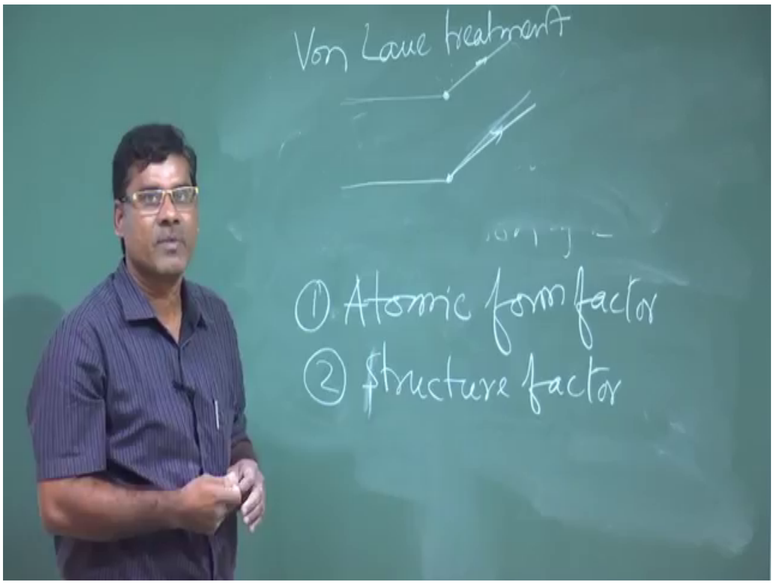

So, when x-ray is falling on it. So, electron its oscillate with same frequency same wavelength frequency and it radiates since it is charge it radiates this radiation or if it is x-ray it radiates x-ray with the same wavelength same frequency in all directions.

So, if you consider another electron. So, it will do same thing in all direction. Now you are getting basically diffraction is taking at a particular direction whether you all get the diffraction maximum or not. So, take at a particular direction a set of parallel reflected x-ray and just calculate the path difference and show that if this condition is full filled then you will get.

So, this is the formula I have not discussed this Von Laue treatment, I have not discussed this one, but this is the concept general way Von Laue find out the condition for diffraction. So, I think I will discuss in next class. So, let me stop here.

Thank you very much.