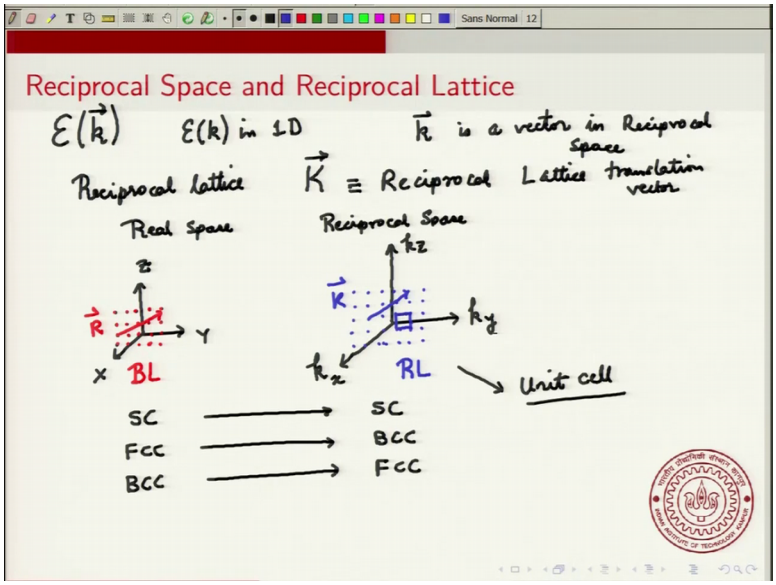
**Solid State Chemistry**
**Prof. Madhav Ranganathan**
**Department of Chemistry**
**Indian Institute of Technology, Kanpur**

**Lecture - 54**
**Bands in Higher Dimensions**

In this lecture, I will briefly describe a Bands in Higher Dimensions. We will not be able to do too much quantitatively here ok. So, I will just show it very schematically ok. So, week 11, lecture 4 will be bands in higher dimensions.

(Refer Slide Time: 00:35)




So, to understand bands in higher dimensions recall that the band structure. Band structure is basically given by energy as a function of k ok; energy as a function of k ok. In 1 D, this k vector was just k in 1 D ok. Now, in 2 D and 3 D, k will be a vector ok. So, now, what can you say about this vector ok? So, k is a vector in the space of all wave vectors. So, the space of all vectors is called reciprocal space ok. So, reciprocal space is like the space of all possible k vectors ok, just as the real space is a space of all possible r vectors ok. Now, the reciprocal lattice is a lattice in reciprocal space, just as a Bravais lattice is a lattice in real space.

So, reciprocal lattice is a lattice in reciprocal space and it is characterized by lattice translation vector K; K is a reciprocal lattice translation vector and we know that reciprocal lattice is also a Bravais lattice. So, what does that mean? That means that if

you are looking in this reciprocal in the space of all wave vectors so, instead of having so in real space so, this is real space ok.

You have your coordinates X Y Z rather I will put this as X Y Z and you have this lattice in real space, Bravais lattice in real space. Some lattice I am just showing a few points, just to indicate that there is a Bravais lattice in let me show it in a different color, it will be better. This is your Bravais lattice, in real some Bravais lattice in real space ok.

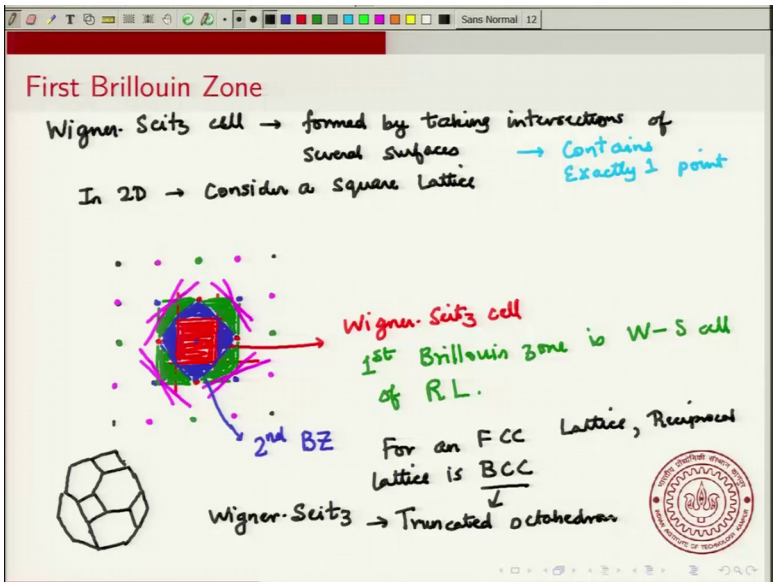
So, this is the lattice, which is the ordered arrangement of points in real space. So, this is called the Bravais lattice. Now, in reciprocal space it is actually, exactly the same thing; exactly the same thing. I mean, when I say exactly the same thing, I actually mean, it is almost it is pretty much identical. In the in reciprocal space, you have kx, ky and kz instead of having x, y, z, you have kx, ky and kz and again you have some lattice.

We just call the reciprocal lattice ok, this is supposed to be a lattice and it is just like a Bravais lattice. It is an array ordered arrangement of points and each point is identical to the other ok. So, this is our reciprocal lattice and essentially just as the Bravais lattice is characterized by a lattice translation vector R ok, this is that this is characterized by a lattice translation vector K ok. So, K so, essentially the reciprocal lattice and the Bravais lattice are the same thing, only thing this is in reciprocal space ok. Now, where things get interesting is that, corresponding to a Bravais lattice ok, there is a reciprocal lattice.

So, corresponding to a given Bravais lattice, there is a reciprocal lattice ok. Now, if your Bravais lattice is simple cubic, then the reciprocal lattice is also simple cubic, if your Bravais lattice is FCC, then the reciprocal lattice is BCC, if the Bravais lattice is BCC, then the reciprocal lattice is FCC ok, but whatever it is some lattice reciprocal lattice is some lattice and if it is a lattice, then it has a lattice translation vectors ok, but there is also a unit cell and you can choose unit cell of your choice.

So, there will always be a unit cell for this reciprocal lattice. So, I can just show some unit cell ok, that might be the unit cell and depending on what the reciprocal lattice is you can choose the; you can choose different unit cells ok.

(Refer Slide Time: 06:11)




Now, one particular unit cell ok, which is of interest to us is called the Wigner Scitz cell and so, this Wigner Scitz cell is a unit cell that is formed by taking intersections of several surfaces and just to show you in 2 dimensions ok. So, let us show in 2 dimensions ok. So, the way you form the Wigner Scitz cell is ok, let us consider a square lattice.

If you have a square lattice, let me show one more set of points ok, let me show this set of points. Now, let us take the point, how do you construct the Wigner Scitz cell. So, we take any one point ok. Let us say this point ok, Wigner Scitz cell by the way it contains only one point contains exactly one point and it has all the symmetries of the lattice.

So, it contains exactly one point and it has all the symmetries of the lattice. So, how do you construct it? So, suppose you take this point at the center ok, then you see that its closest neighbours or this atom. So, now, if you take; if you take this segment joining the atom, draw joining the center atom to its nearest neighbour and you bisect it ok, you bisect it with a line in the in 2 D.

It is just a line ok, you will get something like this ok. Now, you do this again, in this you do this for the next neighbour, you will get another line like this, you do it for the third neighbour you will get a line like this, you do it for a fourth neighbour you will get a line like this ok. Now, you do the same for the next nearest neighbour.

So, here let me emphasize that we bisected each of these four nearest neighbours ok. So, we bisected the segment, joining these nearest neighbours and we got a grid like this. Now, if you take the next two nearest neighbours that is these, these 4 atoms are the next two nearest neighbours and now you bisect this segment ok, then you will get something like this; you will get something like this ok.

Then you go to the next to next nearest neighbours and that is these are the next to next nearest neighbours ok. Now, if you bisect the segment joining the central atom to these, you will get something like this ok. And now, I will just I mean, I do not, I will just show one more that is quite illustrative ok. Let me take the next to next nearest neighbour. So, I will take this one.

So, after this the now, there are there are not only 4, but there are 8 next to next to next nearest neighbours ok. Now, you consider this segment, joining this to the central atom and you bisect it and what you will get is something that looks like ok. So, I just by, I just bisected the segment joining this atom to this atom and I will get this purple line, I do the same for these two atoms and now, I will get another purple line that looks like and you can do the same you will get; you will get a purple line that looks similarly, you will get 2 purple lines and you will get on this side also ok.

Now, you ask what is the intersection of all these? And the answer you will get is this. This is the intersection of all these and this intersection is the is called the Wigner Scitz cell and this is also called the first Brillouin zone. So, Wigner Scitz cell and the first Brillouin zone is the Wigner Scitz cell, is Wigner Scitz cell of reciprocal lattice. So, it is a Wigner Scitz cell of the reciprocal lattice is called the first Brillouin zone ok. So, what you imagine is that this is in k space.

So, you have k x k y and we are looking in at this reciprocal lattice ok. Now, the second Brillouin zone is the set of points that are next to nearest from the first. So, all the points in this red region are closest to the center point than any other points. So, they are nearer to the center point than any other point ok.

So, if you take all the points in the red region all the points any point inside this red region will be closest to the through to the central atom. Any point in the blue region will have one atom that it is closest to and the second closest atom will be the center atom ok.

So, this is called the 2nd Brillouin zone and you can similarly, you can go and identify the 3rd Brillouin zone.

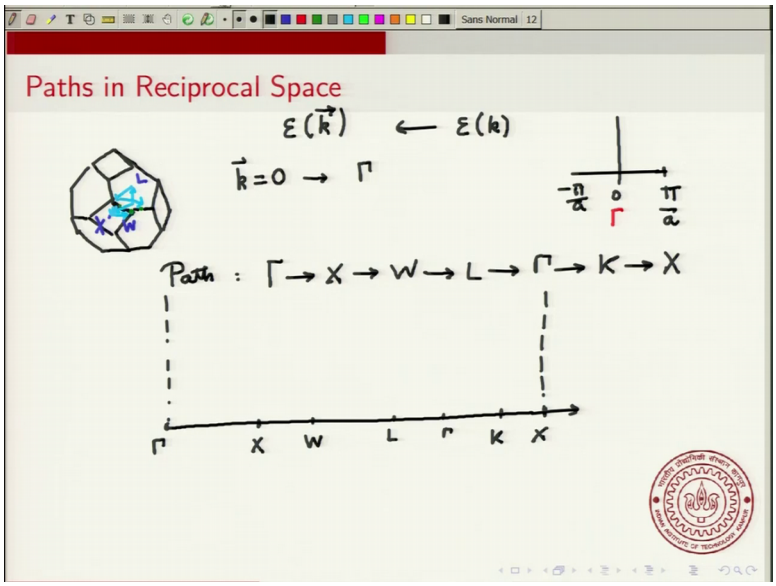
Now, the 3rd Brillouin zone becomes a little more tricky in this case actually the 3rd Brillouin zone is just this region. So, all the points that are two other points that are closer to it than the central point. So, everything is with respect to the central atom and you can define the 1st 2nd 3rd and you can go on, you can define the 4th Brillouin zone, the 5th Brillouin zone and so on ok.

I am just showing the construction, you should actually try this yourself and identify each of the Brillouin zones. So, the first Brillouin zone in a 1 D lattice, the first Brillouin zone was just a region from minus pi by a to plus pi by a, but in 2 D if you can see it is a for a square lattice, it is a square region ok. Now, the Wigner Scitz cell of a. So, for an FCC lattice; for an FCC lattice the reciprocal lattice is BCC ok. So, the reciprocal lattice of FCC is BCC and for a BCC the Wigner Scitz cell actually becomes quite complicated.

So, the Wigner Scitz cell for BCC is not a simple cube, it is in fact, a truncated octahedron ok. So, I will just tell what it looks like. So, you have this kind of so, I mean we have these hexagons and these diamonds forming a truncated octahedron.

So, I am just showing it approximately, but it looks like this object ok, which is a three dimension like a ball ok. It is like an octahedron, but you chop off the sides using this kind of piece and you get a truncated octahedron, which is the Wigner Scitz cell of a BCC. So, if you take a cell of this shape and just take it around any atom in a BCC ok, if you keep repeating that you will fill up the space ok. So, the unit cell for this BCC is actually quite complicated ok.

(Refer Slide Time: 17:54)




So, now, what do we have, if earlier if we wanted to show bands ok, we just showed energy as a function of k ok, but now, you have energy as a function of k vector ok. Now, in this case you could just plot from minus pi by a to pi by a ok, passing through 0 and that was the first Brillouin zone ok. Now, in this case, in higher dimensions, you have this truncated octahedron ok. Let us say for an FCC lattice ok, you have a BCC reciprocal lattice, whose unit cell is a truncated octahedron. So, it is truncated octahedron, I am just showing approximately the shape. Now, the center of this truncated octahedron ok.

So, the center of this truncated octahedron is called so this point where k equal to 0, 0 k vector is 0 is called the gamma point gamma ok. So, gamma is one point that is there right at the center of this unit cell. So, it is there deep inside ok, do you have this gamma point ok. So, gamma is right in the center I am not showing that point. Now, in the case of 1 dimension so gamma is like the 0 in 1 D ok.

So, the equivalent point is a 0 in 1 D and now in 1 D you just needed to go from 0 to pi by a ok. In this case, things are more complicated, because you could go from the center of the Brillouin zone to the edge of the Brillouin zone that is to the surface of this Wigner Scitz cell, but there are different points you can go, you could go to a point that is at the center of the hexagon, you could go to a point that is at the center of this rhombus, but you could go to a point that is located somewhere on the at the intersection of these

points, you could go somewhere here and in each case your band structure will look different ok.

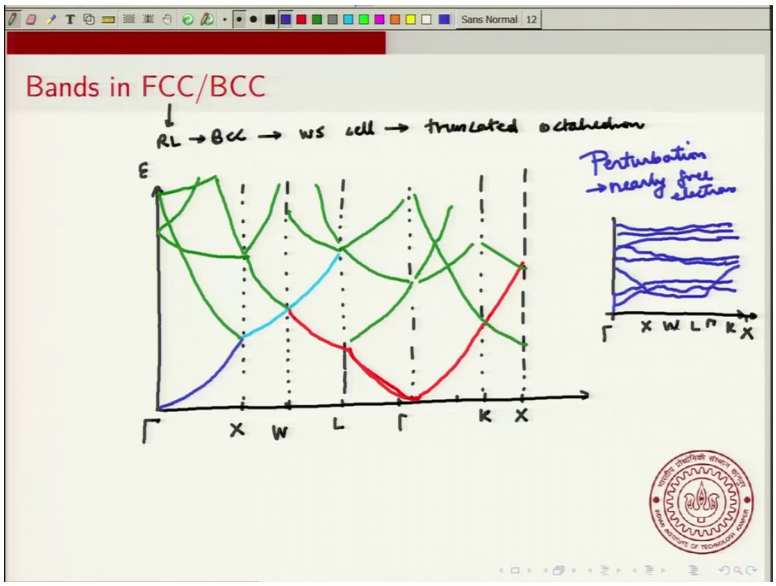
So, what is done traditionally is each of these points are given a name. So, this point is called X or chi point, this is called the L, this is W and this is K ok. These are capital Greek letters and so when you show the band structure, what is done is you typically show from the gamma point ok. You construct a path in reciprocal space ok.

So, the path in reciprocal space will tell you, in which way you will show the bands. So, here, in the 1 D case you just went from minus pi by a to plus pi by a. So, here in 2 D you will go from the gamma. So, one example of a path is gamma to X to W to L to gamma to K to X; that means, what you do is in your axis in your X axis ok, you start at gamma this is your K axis. So, you start at the gamma point then you go along; that means, you go from the center you come out to the point X. So, you come out to the point X on along the straight line then from X, you go to the point W again along a straight line. So, let me show this path.

So, you have the gamma point you come to X, then you come to W, then you go then the path actually goes to L ok, then it goes back to the gamma point which is deep inside and then it comes to K and then it comes to X. Let me show an alternate K point that is write here oh sorry. Now, this is a K point, so, W to L to X and then to K and then back to X ok; so, W to L to gamma and then to K and finally to X.

So, this is the path on which you are going to show the band structure and the band structure will be shown in this path ok. So, if you look at a typical band structure of let us say an FCC ok.

(Refer Slide Time: 24:00)




So, let us take an FCC. So, the reciprocal lattice is BCC and Wigner Scitz cell is a truncated octahedron and again so the band structure so, the important thing is that you have energy axis and this axis you have K and the variation of K, you start at the gamma point that is at K equal to 0 and then you go to the X point.

And let me put a dashed line here, then from X you go to W and then to L, you just go along straight line paths ok. What is that? From gamma to W is not a straight line path and only gamma to X is a straight line path, X to W is a straight line path W to L L to gamma back to gamma to K and K to X and I am just showing these lines for reference ok. Now, let us show the case of the free electrons ok, if it is nearly free electrons, there will be some perturbation.

So, you will have some band that looks like this ok, from gamma to X just like your free electron band ok. Now, this is going to intersect some other band and basically, because these are not straight lines ok. So, the band might be in a different direction.

So, for example, it might intersect a band, that makes it go like this ok. Now, there could be another band ok, that goes from X to W and that might go say this way ok. Now, there would be another bands, let us imagine that there is a band that goes like this. This is again the gamma point and now, you will have at this gamma point, you will have this parabolic behaviour and then from gamma to X you will have some other ok.

And what I am trying to show is that you have a fairly call, you have a fairly complicated band structure ok and I again this is just schematic ok, I am just showing schematically what the typical band structure look like and what is amazing is that all this is got just from the free electron model ok. So, this whole band structure that I am depicting here is all based on the free electron model ok. In the sense I did not take any interactions, I do not have any band gap and you have several lines here ok.

So, you have all these this kind of complicated structure and you will find this in, if you read any journal you know or any if you look at any book in solid state physics, you will find such things. And in fact what would happen due to the non free nature of the bands due to the non free nature of the electrons, because the electrons are not truly free electrons ok.

What you will get is this band structure, will look slightly more complicated gamma X W L gamma K X ok. What will happen is that each of these bands will actually, because of the repulsion, they will go to something like this. So, you will have a band structure that looks something like this and it is actually in analysing this band structure. So, this is if there is perturbation, nearly free electrons ok and in general the band structure will look something like this ok.

So, the whole point of this whole exercise is to show, how you can get bands both in 1 D and in higher dimensions and again I have just shown this schematically, but you can actually plot the free electron levels for this BCC and you can actually show what the bands look like. So, with this I will conclude this 4rth lecture of week 11. In the next lecture, we will do some practice questions ok. I will keep it short lecture, where we will basically, just revise what we did and do a couple of practice questions.

Thank you.