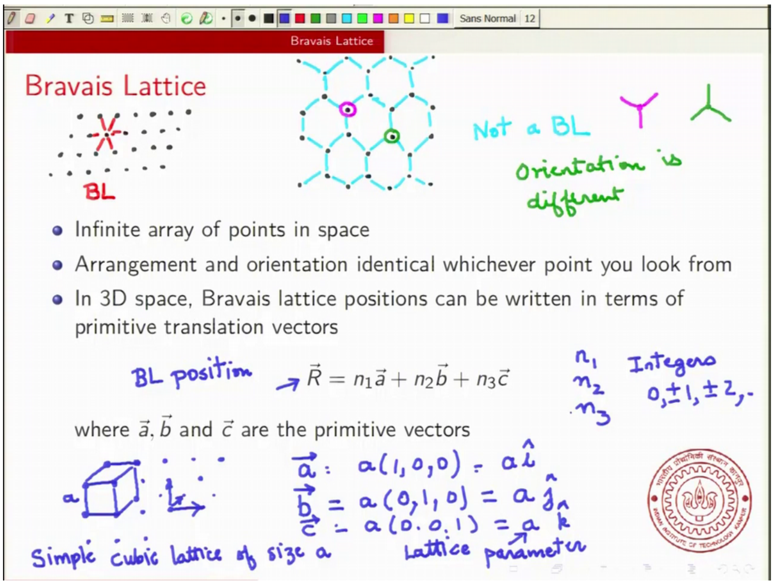
Solid State Chemistry
Prof. Madhav Ranganathan
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture – 08
Bravais Lattices

In the last two lectures, we learnt about the concept of a unit cell and what a primitive and a conventional unit cell is and, during this lectures, we kept referring to points in space we said that on each you we talked about points and which can be atoms or molecules.

Now, in today's lecture I am going to formalize this discussion of points and in formal language this is referred to as a Bravais Lattice. So, today's lecture and the next lecture we will also be focused on Bravais lattice. So, let us go to a Bravais lattice.

(Refer Slide Time: 01:10)



What is a Bravais lattice? So, a lattice and a lattice is an infinite array of points in space. So, any arrangement of points in space, any ordered arrangement of points in space is referred to as a lattice, ok. Now, for a Bravais lattice the arrangement and orientation should be identical for each point. So, whichever point you sit and you look from you should see the same arrangement and orientation, ok.

So, let us look at some examples, ok. So, and an again I will be using 2-dimensional space to show an example, but you can do the same in 3-dimensions. So, let us construct an array of points. So, let us take one set of points. So, it has to be an ordered arrangement of points. So, this is an arrangement of points in.

So, you arrange all these points on a line then let us say you arrange some points here ok. This is an ordered arrangement of points and notice that each point is completely identical; that means, if you sit on any point you see exactly the same thing. So, if you sit on this point you will see it has neighbours in these directions, neighbours in these direction and some additional neighbours in this direction, and you see the orientation is also identical, ok.

So, this is an arrangements of points, so, this is a Bravais lattice. This is a Bravais lattice I will use BL for short Bravais lattice. Now, let us take another arrangement of points, another ordered arrangements where the orientation is not identical and an example of this is the hexagonal lattice in 2 in 2-dimensions. If you take hexagonal lattice ok, you take one hexagon, you take another hexagon, you translate, you take another hexagon you keep you keep doing it in all directions, ok. This is and on this side you have this hexagons. So, it looks like this.

This is referred to as a honeycomb lattice in 2-dimensions and you have seen this structure in the in the honeycombs of bees, ok. Let me I will just for reference I will draw some lines connecting these points, so that you can see how what the hexagonal honeycomb lattice is. So, this honeycomb lattice in 2-dimension, it is an ordered arrangement of points and you can see that the points are it is an infinite arrangement you can extend these to infinite infinity and you get this arrangement of points.

Now, now this is not a Bravais lattice. This is not a Bravais lattice and the reason it is not a Bravais lattice is the following if you sit on this point, and you look at the arrangement of points surrounded and I will show it over here. So, if you this point you will see that there is one point directly below it. So, that is shown here. There is one point that is in this direction and there is another point in this direction. So, this is the arrangement like a Y.

Now, if you do the same thing at let us say you do at this point, ok, what you notice is that you have this point now; you have a point above it and two points. So, it is like an inverted Y, ok. So, the arrangement of points the orientation around these two points is different, and therefore, this is not a Bravais lattice, ok. So, the orientation is different, ok. So, a honeycomb lattice in 2-dimensions is not a Bravais lattice.

Now, in 3D space you can write a Bravais lattice positions in terms of primitive translation vectors, ok. So, the Bravais lattice positions are expressible. So, if R refers to a to a Bravais lattice position; that means, it is one of the points on the Bravais lattice. It is a coordinate of one of the points on the Bravais lattice, ok. So, it is the 3-dimensional coordinate of one of the points on the Bravais lattice and n 1, n 2, n 3 are integers, are integers. So, that means, they are the so; that means, they can be 0 plus or minus 1 plus or minus 2 and so on. So, they can be any positive or negative number, or they can be 0, ok.

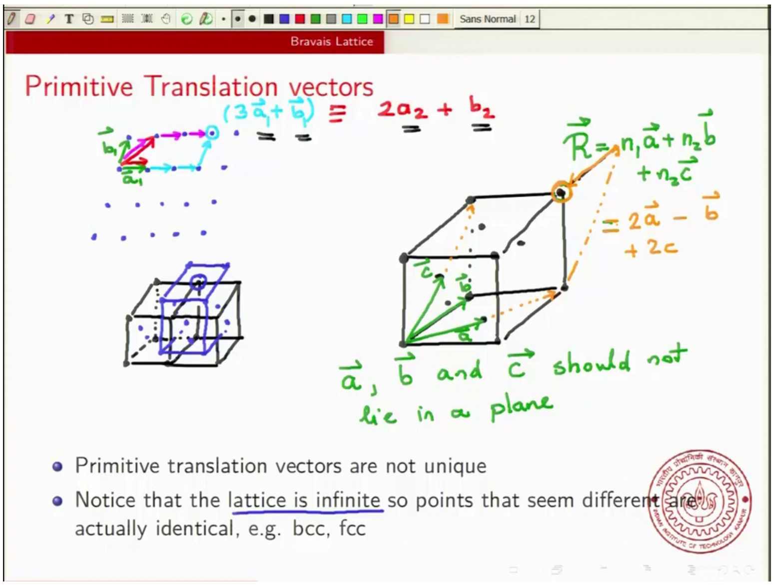
Now, so, you can write any lattice position in terms of these primitive translation vectors and you can easily see is suppose you have a simple cubic lattice suppose you have a simple cubic lattice in 3-dimensions, then you can you can choose. So, if you have a simple cubic lattice of size a and let us say the length of this lattice is a then this complete the cube and imagine that you have a lattice. So, this is really extending to extending in all directions. So, it is extending in the in the three co-ordinate directions, so, it is along x and so and so on, ok. I will not bother drawing the whole thing.

But, you can easily see that if I take lattice translation vectors like this, like this and like this, so, along the coordinate directions. So, my lattice translation vectors a will be equal to a into 1, 0, 0 that is along the x-axis. So, in other words I can write this as ai plus bj plus ck where i, j, k are unit ai plus ai, I can just write it as a i there is no j and k. So, i is a unit vector along the x-direction.

Similarly, the lattice translation vector b looks like a 0, 1, 0. This is for a simple cubic lattice only for a simple cubic lattice and I can write this as a times j. So, keep in mind we are considering simple cubic lattice of size a; that means, the dimension of the size the lattice parameter is a, and c looks like a times 0, 0, 1 or I can write it simply as a times k hat where k is a unit vector along the z-direction.

So, now this quantity a is referred to as the lattice parameter and we can see that in a cubic lattice there is only one parameter. So, the simple cubic lattice has only one lattice parameter ok. Now, what is important is that you can write any point as a linear combination of these vectors and that is very easy to see in the simple cubic lattice. So, if you have any point it will be either some linear combination of these where some integral linear combination of these, and we will look at this more closely.

(Refer Slide Time: 10:21)



So, so, let us look at the primitive translation vectors. So, let us take an example and I will take I will take 2D as an example because you can see that 3D is not very easy to draw. So, so let us take a lattice that looks and I will take a lattice I would not take a I would not take a square lattice I will take a slightly I will take an oblique lattice. So, these are the points on the oblique lattice and that should be sufficient, ok.

Now, I can take one choice of primitive lattice translation vectors is this. I take this as a now I have only two primitive translation vectors in some looking at a 2D lattice and let us say I take a and b as my lattice translation vectors and let me call it a 1 and b 1 just for convenience, ok. Now, you can see that any point. So, if I take let us say I take this point, ok. I can write it as 1 2 3 times a plus b. So, this is this I can write it as 3 times a plus b, ok. So, it is written exactly as an integer linear combination of these primitive translation vectors, ok.

Now, I said that this combination is not unique, so, what is meant by that? Ok. So, let me take exactly the same thing ok, but I will choose two different I will take a different choice for the translation vectors, ok. So, let me take a let us be a little extreme let us take this and let me take let me take this, ok. So, so in this case a remains the same. So, or or I should I should use a 1 and b 1 in the first case I had a 1 and b 1, ok

Now, I have a 2 is same as a 1, but b 2 is not the same as b 1, and in this case I can write the same point as 2a 2 plus b 2, and you can see this let me use a different colour. So, let me use the violet colour. So, you can see that if I do this plus this plus this. So, you can clearly see that a 2, a 2, a 2 plus a 2 plus b 2 gives you this lattice point, and I should I should mention that this is the origin. So, the origin is same as 0 a 1 plus 0 b 1 or 0 a 2 plus 0 b 2, ok.

So, you can see that the primitive lattice translations are not unique,. So, you can express them and you can write as you can you can choose I can choose either a 1 a 2 as the primitive translation vectors or I can choose a 2 b 2 as the primitive translation vectors, and what is important is that the set I mean the lattice is actually infinite, ok. So, that is so, lattice is infinite. So, the points extend everywhere in space, ok. The other thing to keep in mind is that since the lattice is infinite points that might look different are actually the identical.

So, let us take a very typical example. You take an fcc lattice. So, fcc is actually a lattice and if you take this fcc lattice now, you might say you might be tempted to say I will let me draw the fcc lattice. So, I have a cube you have a cube and you have all its face centered points. So, and you have you have all the face centers. So, let me let me write draw the face centers in a different colour. So, these are the six face centers. So, imagine you have a lattice you have a set of infinite points where infinite cubes and their centers, ok. This is the back face ok.

So, if you have a now you might think that, this corner point the corner of a cube. So, you have the corner of the cube the point and black and in the face centre which is shown in blue and you might naively think that these two points are actually different, ok; one is a corner, one is a face center. However, if you keep in mind, that the lattice is infinitely extended in all directions, ok. We will just extend and I will show this by extending the blue points which are the face centers.

So, if you take this blue if you if you take this blue point and you have a blue point on the neighbouring unit cell ok, it will appear here this point. If you take a blue point on the neighbour of this blue point, so, it will appear somewhere here this blue point on this neighbouring cell. Let me draw the let me draw the cube, ok. So, this blue point will be at the center of this face ok.

Now, you have a blue point that is in the center of this face and in the center of this front face and that I will show it here and you have a blue point that is centre of the rare face and that I will show it here, ok. Now, you can see this that if I take these blue points. If I take this blue point connected to a blue point in the neighbouring neighbouring face neighbouring cell and make this connection, and now you also keep in mind that there will be there will be point there will be a cell behind this directly behind it, and you can see what I am trying to say that if you take all these points, there will be another cell behind this and cell behind this you will take all these blue points from the from the cells and you will and it will appear that there are the corners, and now the black points are actually they appear to be at the face centers.

So, the black points which are originally the corners, so that is most easily seen here. So, you can see that this point ok, is now appears like a face center point, ok. So, the point is just by shift shifting the cube a little point that was at the corner of the cube now becomes a face center, ok. What we are trying to say is that whichever point you sit on you will see the same orientation, and you can convince yourself. So, you look around this point you will see you will see four neighbours along these directions. So, you look around this point you see four neighbours four in plane neighbours.

So, essentially all the lattice points are identical ok, even though they appear to be different and in fact, in fact this is the definition of the Bravais lattice, ok. You can you can also verify this for the for the bcc case for the bcc lattice also you can verify that that all the points are identical. So, so there is no difference between the corner point and the body centered point. And, as I said you can use many different primitive lattice translation vectors to describe to describe the points. So, let me just show you the primitive translation vectors for an fcc lattice.

So, if you have an fcc lattice and I will draw it again and I will draw it slightly bigger here just illustrate the point. So, one choice I can take is the following I can take point I can take this choice I will show it in green. So, one would be this and so, I can take two others let me take. This and let me take a third one along this, and you can show that any point can be written as a linear combination of these points. Any lattice points can be written as a linear combination of these points, ok. This is one choice you could take other choices also, ok.

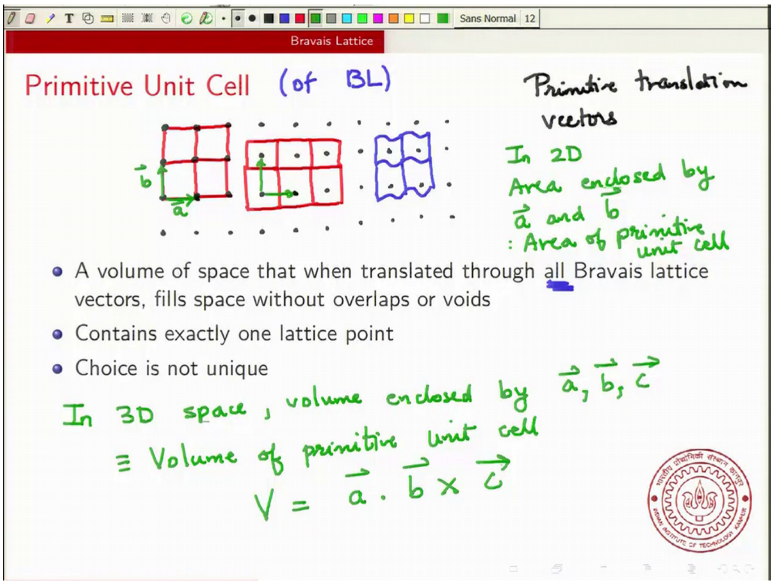
So, what is you could take many other choices what is important is that a, b and c should not lie in a plane, and you can convince yourself that if you take if you make sure that this so, to construct your primitive translation vectors you can just take translation vectors ok, if when I say translation vector I mean they go from one lattice point to another lattice point, ok. So, you can take translation vectors and you take any three translation vectors that do not lie in a plane and they can be lattice translation vectors and what they mean what you mean is that you can write any lattice point any Bravais lattice point which is denoted by R as n 1 a plus n 2 b plus n 2 c, ok.

So, for example, if using these lattice translation vectors if you want to express this point this point on the other corner ok, then you can you can see that that you can translate it you can see that let me let me give names to this. So, let me call this a, b and c ok; then, yes so, you can see that this can be written as. So, I will show it I will show it in a slightly different colour. So, I can write this as 2a, ok. So, if I take 2a then I will get somewhere here, and if I take 2c ok, 2c gives me this, and if I add these two you can see that you will end up in corner that is one you will end up in the corner of the neighbouring cell.

So, if I take 2a I will end up here. Now, if I take 2c from here so, c takes along this side face so, now, this will be of the neighbouring cell, so, it will leave you it will take you to this to this point 2c ok. So, this 2a plus 2c it will take me to the point on this neighbouring cell on the on the still that is directly behind and then I bring it back here. So, that is minus b, ok. So, 2a minus b plus 2c will correspond to this point.

So, this point and I let me show it in orange ok, is 2a minus b plus 2c and you write any lattice point in a combination of these of these primitive translation vectors , ok.

(Refer Slide Time: 23:37)



Now, what is the primitive unit cell? A primitive unit cell and let me emphasize that here we are referring to the primitive unit cell of the Bravais lattice, ok. So, of the Bravais lattice. So, we are referring to the primitive unit cell of the Bravais lattice. This is the volume of space that when translated through all the Bravais lattice vectors, it fills the space without overlaps or voids, ok. It should fill the space without overlap or voids, and what; that means, is that it should contain exactly one point.

Because, if you take all if you if you make all translations then you should get all the Bravais lattice points, and so, the number of translations that you have ok, it should be it should be as many as the number of lattice points, ok. And, so, the number of primitive cells that you should have should be there the number of Bravais lattice points. So, therefore, each primitive cell should contain exactly one lattice point and again the choice is not unique. Let us look at an example just to be just to get things clear and let us let me take the example of a square lattice.

So, in 2D again I am working in 2D just because it is easier to represent on the screen. So, if you take a square lattice in 2D, and you imagine that imagine that I have a have a primitive cell I will show I will show at least three different ones. So, so this can be a primitive cell, ok. This contains exactly one point, ok. You can see that each of these lattice points contributes one fourth to this cell because they are part four of these cells and you can see that if you translated. So, if I take the cell and translated by a multiple of the primitive translation vectors then I will fill up the entire space, and I fill it up without any without any voids or any vacancies or any overlaps.

So, it fills up the space without voids or overlaps and you can see this quite easily. So, this is one choice, ok. Now, let me show you another choice and I will just extend the lattice here just to illustrate the choice. Now, let me take a cell that looks like this and you can see that if you extend it you again fill up space without any voids or overlaps, and you can again see that you fill up the space without any voids or overlaps, ok. You can make things more I mean these as it looks you do not have your cell does not have to be square, you can take different shapes of cells.

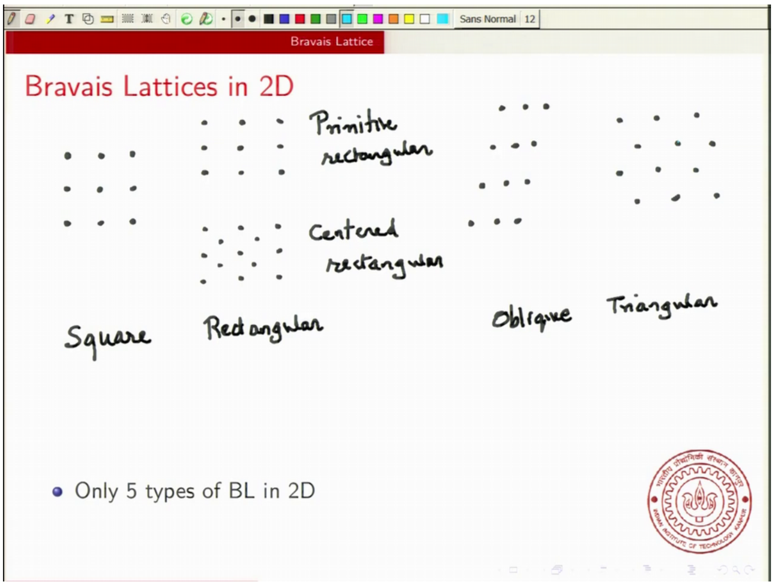
For example, let me take a shape let me take something like this, and again again you can see that if I take the same cell same cell shape and I translated here ok, then I translated downwards, and so on, and I can again fill up space without any voids or overlaps. So, it can translated either to the side or vertically, ok. So, the choice is not unique, ok. Now, there is a nice relation between the primitive between the lattice translation vectors and this primitive unit cell, ok.

Now, it turns out that since the primitive cell contains exactly one point ok, you can define this primitive translation vectors. So, you can define primitive translation vectors some, so these are special primitive translation and I will just illustrate this here, ok. So, these are let us say here this is a example, you can you can you can do use the same month for this also, and the idea is that is that if you have this if you have this primitive translation vectors, then you can get the size of the primitive cell by looking at the at the space enclosed by these, ok.

So, in 2D ok, you can you need the area enclosed by a and b, ok. So, that will give you the area of the unit cell area of primitive cell primitive unit cell, ok. So, the area of the primitive unit cell will be given by the area enclosed by these special translation vectors. So, so, now, these are not arbitrary lattice translation vectors, these are some specific translation vectors which help you define the area of the primitive unit cell.

In 3D; so, so I will write it right here. So, in 3-dimensions you need the volume enclosed by now you have three vectors a, b, c, and this volume is the volume of the is equal to volume of primitive cell primitive unit cell and what is important is that this is a volume that contains exactly one point, ok. This is a volume that contains exactly one point. So, if you take the volume of the primitive cell I can write it as a dot b cross c. This is the volume of the primitive unit cell and this is the volume that contains exactly one point.

(Refer Slide Time: 31:03)

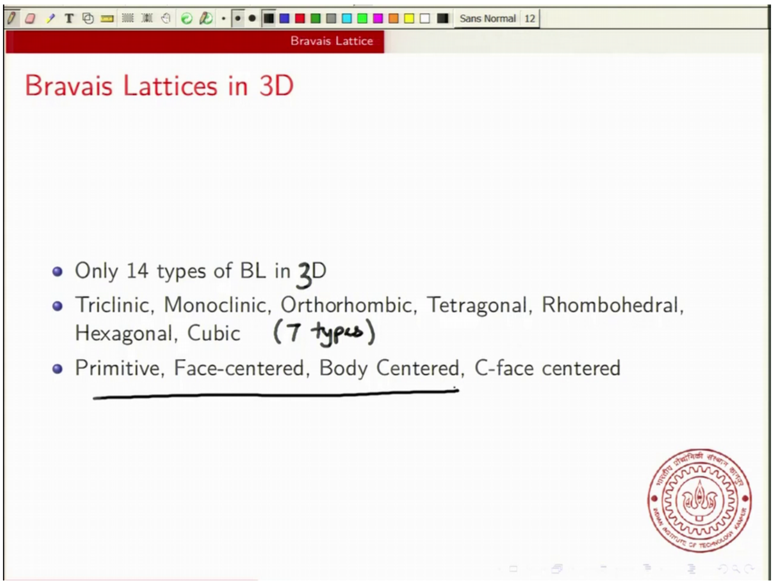


Now, what are the Bravais lattices in 2D? In 2D there are exactly five types of Bravais lattices; and I will just illustrate them, ok. So, they are the square. So, the square lattice is where the points exactly form a square ok, then there is the rectangular lattice and in this rectangular you can have two types of rectangular lattices, you can have what is called this is referred to as a primitive rectangular, but you could also have you could also have something called as centered rectangular this is a centered rectangular and I do not have to tell you I mean the shape of rectangles and so on, ok. But, you can see again that each lattice point is identical ok.

There are two others, ok. So, you have these three there are two others, one is one is called an oblique lattice and we already saw some of these. So, so here you have you can you set of points and they are at some angle. So, it is an oblique rectangular lattice, and here you can only have primitive, ok. Then the last one is a triangular lattice where you essentially take equilateral triangles, and you make a lattice with these equilateral triangles.

So, these are the only five types of lattices. Now, now you might say that oh this seems very restrictive, but remember the oblique lattice can take all kinds of angles. Similarly you can have rectangles of all kinds of aspect all different aspect ratio. The other point note is that is that we said that we said that you know we said that the honeycomb lattice is not a Bravais lattice. This is a triangular lattice which looks like a hexagon with a center. So, it is like a centered hexagon, that is a in fact Bravais lattice and you can easily see that each point is identical, ok.

(Refer Slide Time: 34:32)



Now, in 3D it turns out that there are only 14 different types of Bravais lattices should be in 3D in 3D, now these 14 different types of lattices are the triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral, hexagonal and cubic and within each of them there are different kinds there are primitive face centered, body centered or C -face centered, ok.

Now, now we will we will discuss each of these in detail in the next class, but you already notice that there are seven types triclinic, monoclinic, orthorhombic, tetragonal, rhombohedral, hexagonal, cubic. So, this gives you seven types and this you recall the seven shapes of unit cells that we learnt, and this is again related to that ok, but each of them some of them like you can have a primitive cube, you can have a face centered cube, you can have a body centered cube, ok. So, not all of them can have a all these all these different types, but many of them can have these multiple types, ok.

So, we will start looking at Bravais lattices in 3D in more detail in the next class, ok. So, in this class I have introduce the concept of a Bravais lattice and at this point the Bravais lattice is just a mathematical construct. So, it just a construction of various points in space and the only condition is that these points have to be arranged and their and their arrangement around each point and the orientation around each point is identical. So, in other words you cannot distinguish one point from another ok. So, in the next class we will look at Bravais lattices in 3D in more detail.

Thank you.