Solid State Chemistry
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Lecture – 09
Bravais Lattice, Basis and Crystal

Now, let us go to the 4th lecture of this second week. And in this lecture, I will talk little bit more about Bravais lattices, and I will introduce the concept of a lattice translation vector, and then we will define the crystal in terms of lattices with a basis. So, we will go to this 4th lecture and after this lecture the 5th lecture of the week will be a review of the week and practice problems. So, let us go to the lecture.

So, I am going to be talking about Bravais lattices, basis and crystals. And just we already saw what Bravais lattice is in the previous lecture.

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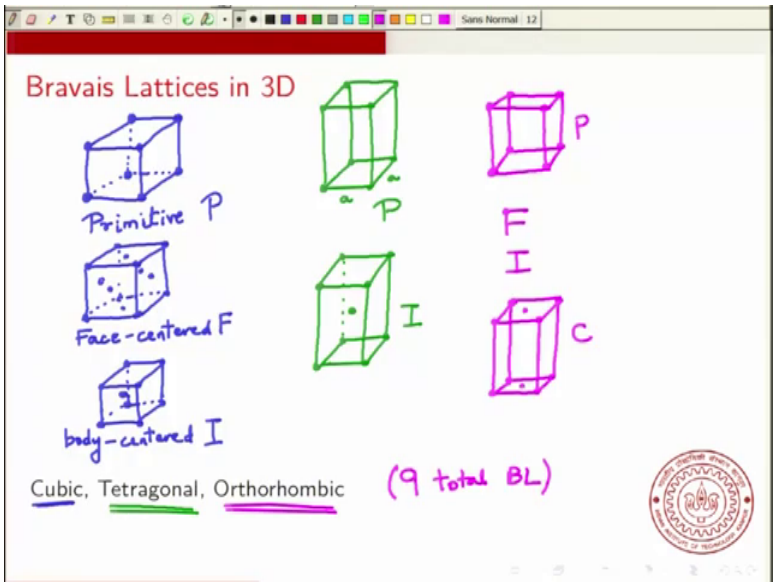

Now, let us look at the Bravais lattices that we see in three-dimensions and I will just quickly go through them, you can find these in any standard book, ok. So, I will not spend too much time on them. But I will just I will just order them in a particular way. So, there are 14 Bravais lattices in 3D, ok. Now, if you classify based on the crystal system you have cubic tetragonal orthorhombic and corresponding to these there are Bravais lattices which are, there is a set of cubic Bravais lattices, ok. So, let me show a typical cubic cell.

So, I am just showing the unit cell for these cubic lattices and I want; so, these are the. So, this is called primitive unit cell or we simply use the symbol P, ok. Then you can have face center, units a face centered cubic unit cell where you have all the atoms which are there in the primitive and in addition you have atoms at the face centers. So, at each of the face centers there is, I should emphasize points not atoms. So, at this point at here there they refer to points. So, you have points at the corners of the cube and at the face centers of the cube and this corresponds to a face centered or we use the symbol F, ok.

You could also have a body centered cubic lattice, ok. So, you have a cube and you have points at the corners of the cube and you have a point at the body center and this is denoted by the symbol I, you use I for body centered because there is a inversion center in the crystal, ok. So, these are in the cubic you can have these types. So, in the cubic we saw that we can have these kinds of lattices.

Now, what about the case of tetragonal? So, in the case of tetragonal, the difference between a cube and a tetragonal cell is that in the tetragonal one of the dimensions, so one of this a, b, c is different. So, if you look at a unit cell for a tetragonal lattice you will have two of the dimensions be the same. So, these two are a and a third dimension is slightly greater.

So, in this case you have a cuboid, but what we see is that 2 of the faces are squares and 4 of the faces are rectangles. In a tetragonal if you have a tetragonal cell you can have a primitive and you can have a body centered you can have a body centered. So, body centered tetragonal lattice.

And these are the only two lattices; only two Bravais lattices, that are possible for a tetragonal for a hetragonal system. So, there are only two tetragonal Bravais lattices a primitive and a body centered. Now, you can ask why is there no face centered in this case, and you can easily see that one of the criteria is that each lattice point should be identical to every other lattice point. So, all the lattice points should be identical.

Now, if I put a face centered then you can clearly see that an atom on this face will have these 4 atom, these 4 points that are closest to each other whereas, a point on this face will have these points and they are not they are much further apart. So, it sees a different environment. So, in the case of tetragonal lattice you can have primitive or body centered, you cannot have face centered.

What about the case of an orthorhombic? So, now, in the case of orthorhombic you have all the three a, b, c are all distinct ok, and in if each of these are distinct, ok. Then you can have, in this case you can have the primitive as usual, you can have in this case you can have a face center, ok. So, the face centered orthorhombic cell is also Bravais lattice and this and have a face centered, you can also have a body center, ok. And in addition, in the case of the orthorhombic lattice, you have a 4th type of lattice which is referred to as a C center or a C face center. So, in this case only one of the face is contingent contains an extra point, only one or rather two of the faces, ok. So, these two phases this is called a C centered orthorhombic, ok.

Now, this is there only in the case of the orthorhombic cell and the reason it is there only in the case of the orthorhombic cell is that or if you can ask a question the other way why is it not there in the case of a cubic, cubic cell why do not you have a C centered cube. It turns out that you can have a C centered cube, but it will be identical to one of these other choices, ok. It will be identical to a primitive tetragonal cell. So, it turns out to be identical to a primitive tetragonal cell, ok. So, that is the reason you do not have a C centered in the case of a cube, but you can have it in the case of this orthorhombic cells.

So, what we notice right here is that in the cubic or tetragonal and orthorhombic you have a total of 7 or you have a total of 4 plus 2 plus 3 that is 9, 9 Bravais lattices. So, 9 out of 14 lattices are already represented in this, ok. So, there are only total of 14 Bravais lattices in 3D, and 9 of them can be brought by just stretching a cube. So, you take a cube and you stretch it in one direction you get a tetragonal cell, you stretch it in two directions you get an orthorhombic cell, ok. What about the remaining 5? So, what do the remaining 5 look like.

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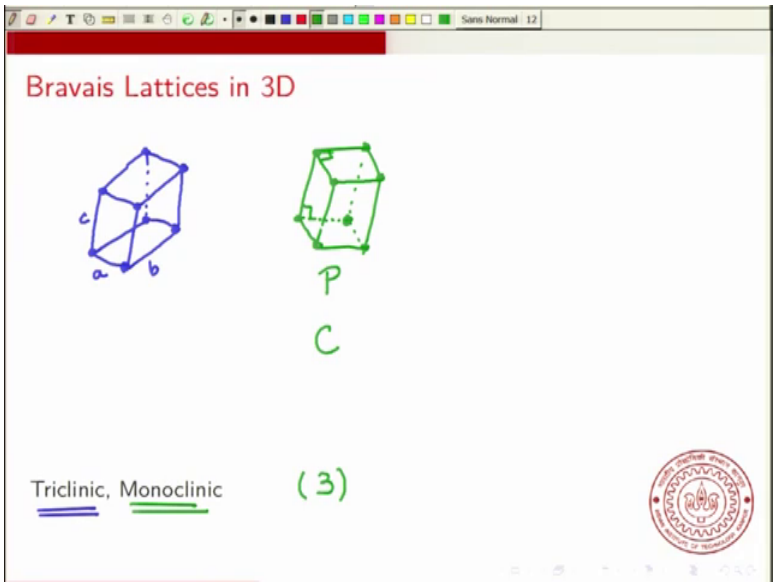

We can we can see this, so there are two that are referred to as triclinic and monoclinic, ok. So, in this case the triclinic case you can, in this case all the sides and all the angles are distinct. So, you have, I should show it a little elongated and just to show that the angles. So, in the case of triclinic you can only have a primitive triclinic. So, you can only have a primitive triclinic, ok. So, this is triclinic where you have a, b and c and all the angles none of the angles are 90 degrees.

In the case of the monoclinic, monoclinic cell, now the unit cell for monoclinic has the characteristic that two of the angles are 90 degrees, and one of the angles is not 90 degrees. So, in this case you can show it in this manner. So, essentially, I am choosing this angle as 90 degrees, I am choosing this angle as 90 degrees and additionally I am choosing one of these angles as 90 degrees. So, for example, I could take this angle as 90 degrees, ok.

And in this case, you can have either a primitive monoclinic or you can also have a C centered monoclinic, you can also have a C centered monoclinic or C centered. You cannot have a face centered or a body centered, that would not be a Bravais lattice, but you can have a C centered monoclinic Bravais lattice, ok.

So, there are 3 more that are done here, ok. So, we had 9 which were based on stretching of a cube and then there are 3 more which are due to triclinic and monoclinic. In monoclinic you have the primitive and the C centered, ok.

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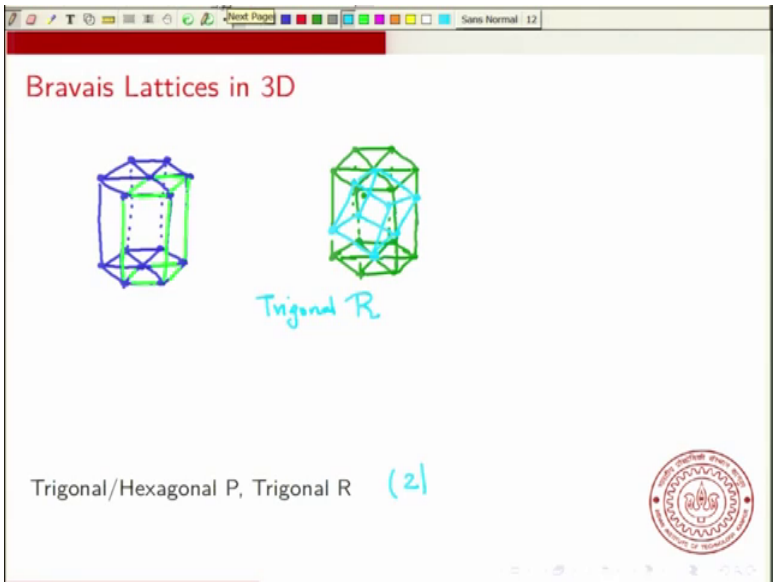

Finally, you have two more, which one of them is called trigonal hexagonal P and a trigonal R, ok. And these you can get them from a hexagonal cell, ok. So, these are both related to the hexagonal cell. So, the hexagonal cell looks like this. So, you have a regular hexagon, and you have another regular hexagon here and there, ok. So, this is the hexagonal; and here, here this is referred to as a trigonal hexagonal or hexagonal P, and you can understand it by looking at this as a unit cell.

So, we choose this as the unit cell, even though its it does not seem to the cell itself does not have the 6 fold symmetry that is there in a hexagon, and you know in a hexagonal cell, but this is a cell that is used, and here you can see that that the angle between these two is exactly 60 degrees, ok. So, this angle is exactly 60 degrees, ok.

So, this is the trigonal hexagonal P, it is primitive in this sense. The other interesting Bravais lattice and this is the last Bravais lattice, that we have is what is called the trigonal R or its also; again you can get this from the hexagon, from the hexagonal cell. So, we have exactly the same as the primitive hexagonal cell, but you have some additional points, ok. So, what are these? What are those additional points in addition to these, ok? You have some additional points and where are the additional points, ok. So, these are what are called the R centers, and again I will not discuss this in too much detail here, but basically you can show that they should be, they will be they are located somewhere around here. There is a point, ok.

There are very very specific points and then there are two points that are located here, and there is another point and there is a 4th point that is located along this line. So, the way this turns out to be a Bravais lattice is if you look at the point in the following sense, ok. So, you look at this, this, maybe we should use a different color. Let me just draw it again and let me show it somewhere around here.

So, now the R hexagon, the R hexagonal cell and R hexagonal lattice can be obtained from the hexagonal lattice, through the following many points. So, you consider, I will just mark these in light blue you consider this point you consider the point located here, there is a third point located in the front edge, ok. So, this is the edge on the front face, and there is a 4th point, this is also located on the front face right here, and. So, you form the cell in this manner and then you need 4 more points and those points are located here, here, and you have two more points, one is located on this face and that is it and you have one more that will be located right along this face. So, that will be located right here.

So, this, it is a hexagonal cell with these 4 additional points, and these 4 effectively each of them. So, it actually has 6 additional points, ok, but each of them contribute only one-sixth. So, each of them contribute one-third. So, this is called an R centered hexagonal or it is called a trigonal R. So, this can be obtained from the hexagonal cell, and this is the 14th Bravais lattice, ok. So, there are there are total of 14 Bravais lattices in 3D and let us just refresh.

So, 9 of them you can get from taking a cube and stretching it by keeping the angles at 90 degrees the 5 of them you can get from this monoclinic cell, and from this triclinic and in terms of triclinic and monoclinic, and the last two we explained in terms of the hexagonal cell, ok. Now, you have a maximum of 14 possible Bravais lattices in 3D, and it is you can take any lattice, any regular arrangement of points where each point looks identical will fall into one of these 14 lattices. And remember the criterion is that every point should have the same environment same arrangement and orientation around it, ok.

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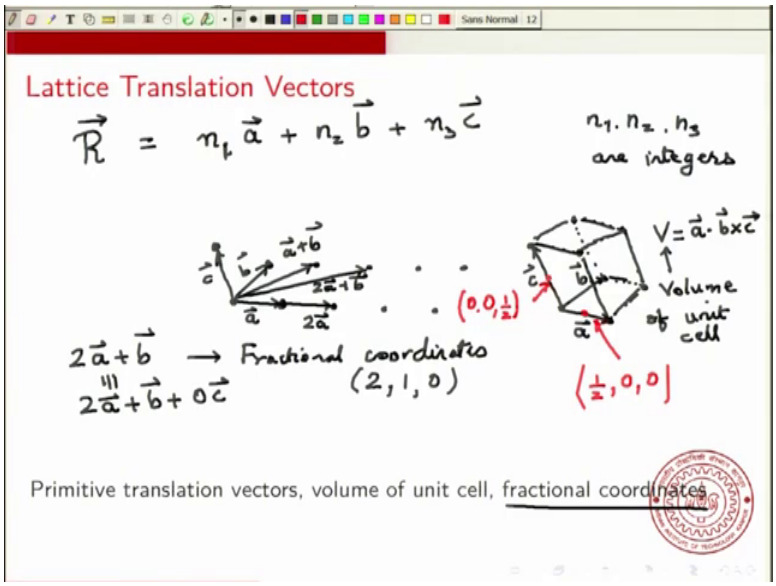

Now, let us talk a little bit about lattice translation vectors, and so, these are the; these refer to these refer to the translation vectors of the unit cell. So, for example, what we have been talking about a, b, c, ok. So, these are the translation vectors of this lattice, ok. And by combinations of these translation vectors we can generate all the points, ok. So, again just to emphasize, so we had a Bravais lattice point written as n 1 a, n 1 a plus n 2 b plus n 3 c, ok. So, what is R? R is a vector from one lattice point. So, we said n 1, n 2, n 3 are integers; that means, they can be 0, plus minus 1, plus minus 2 etcetera.

Now, you can have, what we said is that the set of all n 1, n 2 n 3 will generate the entire lattice. So, if we have let us say n 1 equal to n 2 equal to n 3 equal to 0, you will get let us say the origin of that, ok. And let us mark out our translation vectors, so if you have a b b and let us say c, then if you take n 1 equal to 1 n 2 and n 3 are 0 then you will get this point. If you take n 2 equal to 1 n 1 and n 3 are 0 you will get this point, if you take n 3 equal to 1 n 2 and n 1 are 0 you will get this point, ok. And, now if I take n 1 equal to 2 then I will get the next point n 1 equal to 2 n 2 and n 3 are 0 I will get a whole set of points. So, if I keep n 2 and n 3 equal to 0 I will get a whole set of points, ok. And notice that this vector this R is a vector that that goes from this origin which is also a Bravais lattice point to some other point, ok.

Now, suppose I take n 1 equal to 1, n 2 equal to 1, n 3 equal to 0, then you can see that I will get a plus b which will give me this point, ok. So, this point, the translation vector is

a plus b. What about this? This one the translation vector is 2 a, this is 3 a and so on. What about this point? This point is 2 a plus b, ok. So, this translation vector is 2 a plus b. And you can see you can you can put the c dimension also I am not showing this, but essentially what you can show is that with these translation vectors they are essentially lines that join one point on the Bravais lattice to other points, ok.

And now, let us look at the primitive translation vectors this a, b and c, ok. So, this a, b and c are the primitive translation vectors. Now, if you just take a, b and c, a and I had b and if I take c, ok. Now, if I imagine that I construct a volume using a, b and c using these 3 vectors I construct some sort of volume. So, this is the general parallelepiped that we have been using so far to represent unit cells, ok. So, this unit cell that we have this parallelepiped, ok.

Now, if you are asked what is the volume of this parallelepiped; what is the volume of this parallelepiped, that corresponds to this unit cell. So, the volume can be expressed in terms of a, b and c as a dot b cross c or it is the scalar triple product, ok. This is called the scalar triple product. And basically, if you have 3 translation vectors a, b and c then the volume of this unit cell can be expressed in terms of a scalar triple product of a, b and c, ok.

Now, the next concept that will be using very very frequently is that of fractional coordinates, ok. So, what a fractional coordinates? So, now, suppose I ask you the coordinate of this point, ok. So, this point is 2 a is the x coordinate or rather if I ask if I ask the coordinates of any point, ok. Now, then what you have to do is to you have to convert this vector into Cartesian coordinates you have to convert the vector 2 a plus b into Cartesian coordinates, and you will get the coordinates of that point. But it turns out that it is much more convenient to use fractional coordinates that are defined as follows.

So, suppose you have a point 2 a plus b, ok. So, this in fractional coordinates it becomes 2, 1 and 0, ok. So, the 0 is the c coordinate. So, I could have written this as 2 a plus b plus 0 c. So, this is equivalent to equivalent to 2 a plus b plus 0 c, ok. So, this is represented by 2 1 0 in coordinate in this fractional coordinate system. And actually, their fractions if I want to write the coordinate of any point inside this unit cell within the unit cell, ok.

So, suppose I want to take a point that is let us say here this is let me show it in red. So, this point in red will have fractional coordinates half 0, 0. So, it is along the a a vector, and it is half of the entire distance. So, this will have coordinates half, 0, 0, ok. Similarly, a point that is let us say it is located here will have fractional coordinates 0 0 half. So, it is located along the c direction. So, the a component is 0, ok, but c component is half a and b components are 0. So, this fractional coordinates are actually fairly useful, ok. And in the case of they are most useful for cubic cells cubic or cubic tetragonal or orthorhombic cell when each of these vectors are mutually perpendicular, but they can also be used for other cells, ok.

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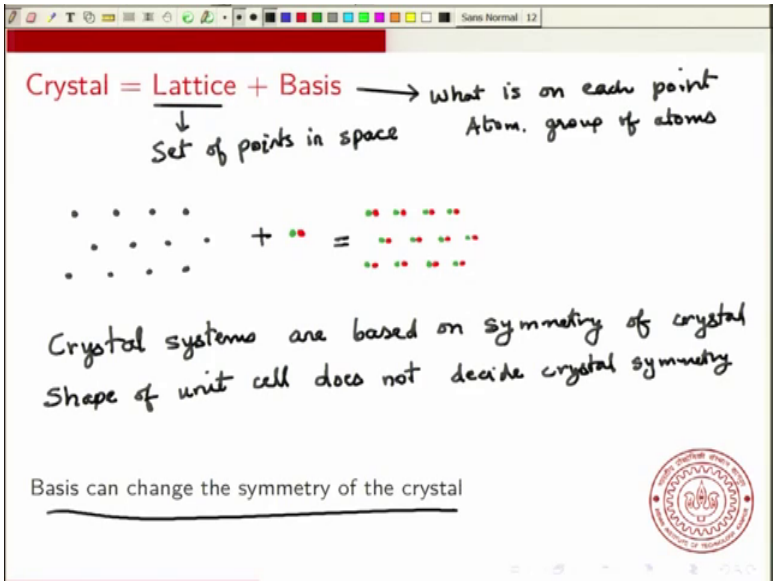

So, we have been talking about lattices, ok, now crystal formally consists of both a lattice and a basis. So, a crystal is a combination of a lattice and a basis, ok. Now, we want to emphasize here is that your lattice is just a set of points, arrangement of points; in space and the basis is the what is at each point. So, for example, let me illustrate this in 2D, ok. So, suppose you have a lattice that looks let us consider the triangular lattice in 2D.

So, if I have a lattice and now let me put a basis, so on each of these I can put some object, and some object, let me put just to show something extreme I will put one green dot and a red dot. So, I will put both these on each side, ok. So, then my crystal looks like this. So, I have on each of these sides I have a red and a blue dot, and I can extend

this, so I can extend this every all over and I will get my crystal. So, I will first do for the red dots and then I will do for the green dots, ok.

So, this becomes my crystal, ok. So, the crystal consists of some basis and some lattice, ok. And, now this basis can be either an atom. So, basis can be an atom or a group of atoms, ok. So, you might put one atom or you might put a whole set of atoms, you might put a pair of atoms and so on. And what is to be noted is that the basis actually changes the symmetry of the crystal, ok. So, now see if you see the triangular lattice that has a I mean it has a six fold axis, ok. So, if you rotate it by 60 degrees you get the same thing. But if you take this and rotate it by 60 degrees, the crystal you will not get the same thing because the basis is actually forcing it is giving it a direction. So, the basis actually changes the symmetry of the crystal, ok.

And what is important is that crystal systems are based on symmetry of crystal, ok. So, the crystal systems are based on the symmetry of the crystal of the overall crystal symmetry and this depends on both the lattice and the basis, it depends on both the lattice and the basis. And sometimes we choose, so the shape of unit cell might have different symmetry or actually I should say the shape of unit cell that itself does not decide crystal symmetry, ok. So, if you had a crystal like this, this crystal, its symmetry is not is not that of a triangular lattice, it is very different, it has a very different symmetry than a triangular lattice, that is one important key thing to keep in mind. So, the symmetry of the lattice and the crystal might be entirely different, ok.

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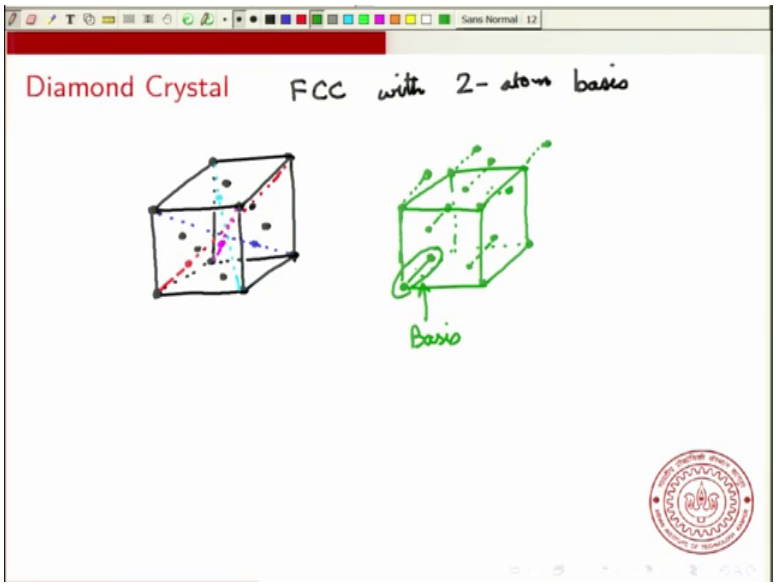

Now, let us take one example of a diamond crystal, and this will just illustrate my point about lattice and a basis. So, a diamond crystal, can be thought of as FCC with 2-atom basis, ok. So, I will just show it quickly. So, you have a diamond. So, you take an FCC, ok. So, this is your FCC crystal, but you put a 2-atom basis, so you put one out here at let us start with one of the corners. So, you put one at a corner and the next one you put along the body diagonal at one-fourth, one-fourth, one-fourth. So, if I take, so I put quarter of the way along the body diagonal. So, it will be located somewhere here, this will be inside the cell, one-fourth along the body diagonal, but let me slightly, ok.

Then what I am going to do is to take this body diagram and put one-fourth along the way, and there is a prescription that, ok. So, what I want to say let me show this in a different color. So, if you put one along one-fourth along this body diagonal then you have to put along one-fourth of the next body diagonal, ok. So, now, a let me take another body diagonal that is this and here I will put one-fourth along this side, ok. And then and then you will take a third body diagonal that is let us say this way and you put one-fourth along this side and you take a 4th body diagonal that is this and you will put one-fourth along this, ok.

Now, I specifically chose these 4 and you can actually generate the same thing, ok. So, it is one-fourth along the body diagonal. So, 4 of these what are known as tetrahedral voids, ok. So, but you can also think of it as you take this FCC and at each point you put

2-atoms. So, I will just I will just illustrate this and then, so at each point you put these two atoms, then you have meet my FCC, ok. So, what I am thinking of it is as an FCC with a 2-atom basis. So, instead of putting one point at the corner I put one at the corner and one at you know one-fourth, one-fourth, one-fourth along this direction.

So, now at this point if I put one-fourth, one-fourth, one-fourth it will go outside the cell, so we do not I mean it will be in the neighboring cell, ok. Now, if I take this point then the one-fourth, one-fourth, one-fourth will correspond to this and that is exactly the point that we showed here in this blue color, ok. And you can again show that all the points on the top face, they will go the second point will be on the neighboring cell, ok. So, in this case will be here, ok. So, all these will be outside the cell.

Similarly, for all these points they will go outside to the neighboring cell, but if you take this point this face center, the second point will be along this body diagonal, so it will be somewhere here, ok. And in this way, you can show that if you take each FCC point and you put this 2-atom basis you will generate the diamond crystal. So, this is an example of a, so if you take this as the basis and you put this unit on each of the points of the FCC lattice you will get a diamond crystal, ok.

So, I will conclude this lecture here, and in the next class I will talk about, we will summarize what we did in this week and then we will do a few practice questions.

Thank you.