Introduction to Materials Science and Engineering
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Lecture – 28
Structure of Diamond

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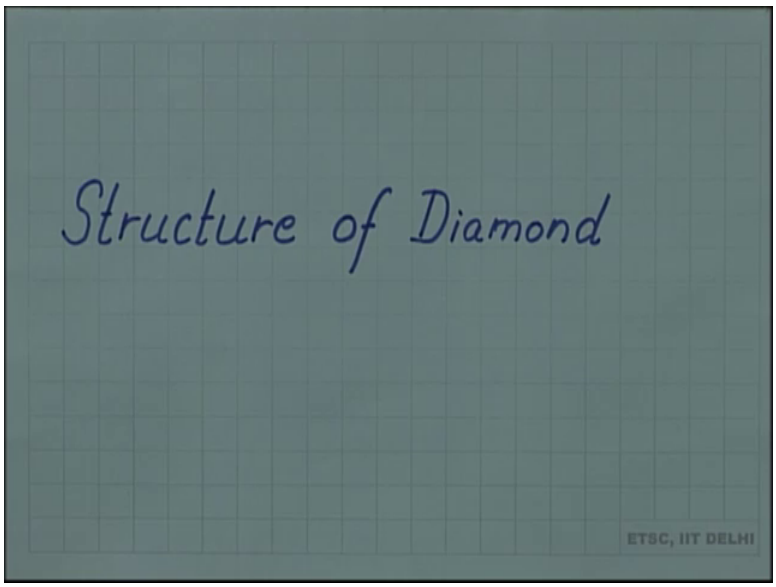

Hello and welcome. So, today we will discuss the structure of diamond, we have discussed various forms of carbon like graphite we or I have already discussed. So, today let us look at what is the structure of diamond which is also a form of carbon. So, diamond basically has the diamond cubic crystal structure.

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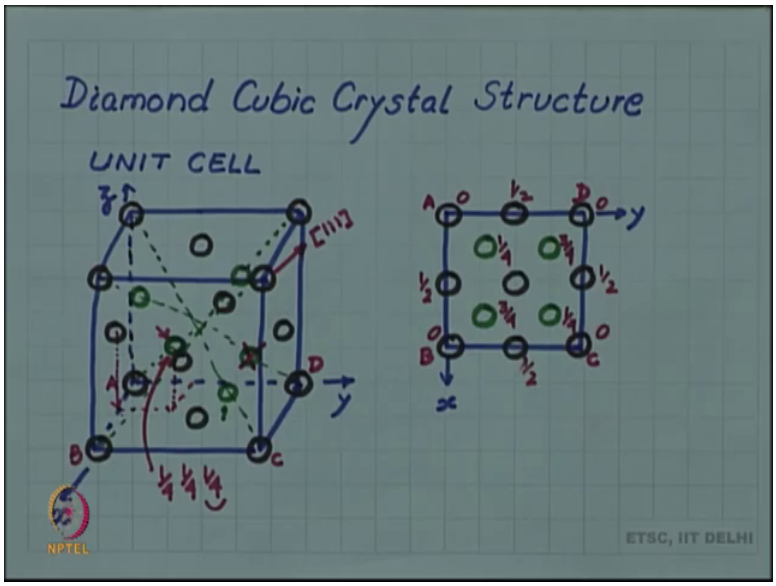

So, this diamond cubic structure let me try to draw the unit cell of the diamond cubic structure for you.

So, let us begin with the cube it is a cubic crystal. So, has a cubic unit cell. So, I'm beginning with the cube this is a skeleton cube and will become diamond cubic, when we populate it with I mean properly located atomics. So, let us place the carbon atoms now we place the carbon atoms at all the corners of the unit cell. So, that is the 8 atoms at the corners, it is a face centered cubic unit cell.

So, we place atoms at face centers also top and bottom face center and left and right face center we need to place the front and back also, front face center and the back-face center. So, we have got for 6 more atoms so, 8 at the corner 6 at the face centers and at the moment it will be a face centered cubic crystal, but diamond cubic crystal is not a face centered cubic crystal it has additional atoms and we place those additional atoms, at the body diagonals those additional atoms are located at the body diagonals. So, let us identify the body diagonals.

So, one body diagonally is emerging from here and on each of the body diagonal the atom is either at 1 4th or 3 4th location. So, starting with this let with this corner I have drawn a body diagonal and I have located an atom at 1 4th of the total length of the body diagonal, then I go from this a at this corner from this corner another body diagonal emerges, on that body diagonal I place an atom which is 3 4th from the bottom. So, it is

now 1 4th from the top. So, it comes somewhere there, then cyclically I go to the third body diagonal here. So, I started with this body diagonal placed 1 4th then this next body diagonal I placed 3 4th, the third body diagonal I again place 1 4th atom, and the final 4th and the last body diagonals on this body diagonal I'm sorry my diagonal this time has become a little more curved anyway. So, I place another 1 4th one there.

So, the whole thing also has 4 additional atoms. So, diamond cubic crystal structure has all the atoms for a face centered cubic crystal, plus 4 additional atoms one sitting on each of the 4 body diagonals, and the way it sits I have already shown you that on one body diagonal it is at 1-4th, then on an adjoining body diagonal starting from an adjoining atom at the base adjoining corner of the square base square base. So, there it is at 3 4th, then again 1 4th, and then again 3-4th. So, alternately it goes 1 4th and 3 4th location, I'm sorry I have made a mistake here. So, let me cross this out. So, 1 4th on the first diagonal 3 4th on the second diagonal, then 1 4th on the 3rd diagonal and again this one I have placed 1 4 this should have been on with 3 4th location. So, that comes there.

Now, it is. So, the whole appearance looks little complicated. So, sometimes little bit a better clarity comes, if we draw it in the projection. So, let us try to draw the unit cell in the projections. So, we will project the unit cells on the x y plane, on the base plane. So, let us try to draw that the base plane of course, is a square. So, I draw a square this is my x axis, this is my y axis, this is a 2-dimensional projection so, z axis is not shown, z axis is perpendicular to my projection plane.

So, this is the square if we label it let us say let me try to label this as a b c d. So, the base of the unit cell a b c d is what you are seeing here as this is square. Now you can see that this square itself is populated with atoms. So, all those atoms be placed. So, atoms are at the corners, and atom is at the face center. So, these atoms are as they are in the original unit cell, other atoms are not on the base plane they are above the base plane and we will project them onto this base plane.

So, for example, let us look at this face center this one here. So, if I project it vertically downward it will come exactly on the middle of the a b edge. So, on the middle of the a b edge, I have another atom projected, which is representing the atom which in the original unit cell was a center of the left face. So, the left face center got projected here, similarly the front face center will get projected in the middle of this edge, the right face

center will get projected there and the back-face center will get projected there. So, we have projected all the vertical face center and we already have the atoms on the base plane, the top now only atoms left are those which are on the body diagonals and on the top face, the top face atoms when you will project will coincide exactly with the corners and the face center of the bottom face. So, no new locations are generated by that. So, we leave that out.

Now, let us look at the body diagonal one. So, this particular atom this particular body diagonal one, which is located at 1 4th of this body diagonal. Body diagonal is starting from a so, what is it is coordinates. So, since it is 1 4th of the body diagonal, and a body diagonal direction if you find the miller indices is a 1 1 1 direction. So, it is equally inclined to all the 3 axis. So, along this all the 3 coordinates are equal, and since it is 1 4th of the entire body diagonal, the coordinate of this particular atoms coordinate of this particular atom is 1 4th along x, 1 4th along y, and 1 4th along z. So, when I will project this it will show 1 4th along x, and 1 4 along y and z component of course, will not be seen in the projection. So, if I now project this particular green atom on the body diagonal, I will get at 1 4th 1 4th and here.

Similarly, if I project this one this particular one will come here, the third one will go there and 4th one will go there. So, this completes the projection, but the standard crystallographic projection, the convention is to show the z fractional coordinate, the z fractional z component because x y component can easily be re-read. So, I know for this atom because it is 1 4th of this side and 1 4th of this side it is x and y coordinate is 1 4th 1 4th, but since it is projected I do not know the z coordinate. So, the z coordinate can be explicitly written on the projection itself.

So, let us do that you let us write the z coordinate of all the atoms. So, these a b c d of course, were on the plane itself. So, their z component worth 0, I write 0 for them, the one on the vertical face center, this one was to one to a half of the total height of the unit cells. So, I write one 2 to indicate that that it is at half height half the height of the unit cells. So, these 4 atoms the front face center the right face center and the back-face center all these are at half height.

And then the 4 on the body diagonal you saw that this one was 1 4th 1 4th 1 4th. So, it is z component was 1 4th so, I write 1 4th to indicate that the height above the projection

plane is 1 4th similarly this one which is this here is 1 4th, and the other 2 on this diagonal since you have an atom at 3 4th distance it is height from the basal plane also is 3 4th alright 3 4th. So, this completes the projection.

And so, sometimes you can see this also gives you the 3-dimensional view, this gives the 2-dimensional projection, but sometimes it is clearer to see things in the projection, and sometimes it is better to use this isometric view. So, you can use whatever way you like both are giving you exactly the same information that the diamond cubic unit cell even itself is a cubic unit cell, with atoms at the corners and the atoms at the face centers and for atoms located appropriately one each on the 4 body diagonals.

So, that completes the description of the unit cell; however, we have described all crystal structures we have seen this and this been has been our theme we have done this for graphite also that all crystal structure should be described as a combination of lattice and motif. So, we have drawn the unit cell, but what is it is lattice? And what is it is motif?

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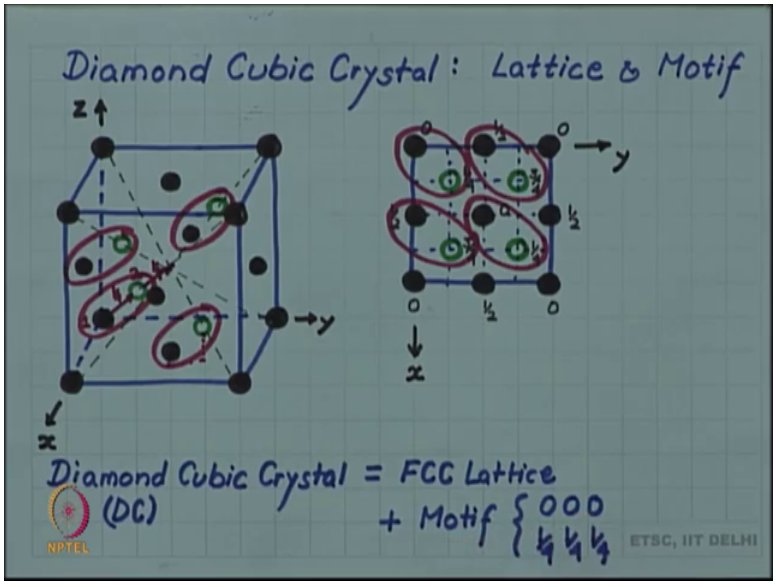

So, let us try to look at that we already know that face centered cubic is a lattice. So, which means that the face centered cubic unit cell all the black atoms which are located at the face centered cubic, all are equivalent in the lattice sense. So, they are forming a lattice there is no problem; however, the additional 4 atoms whether they are at lattice points or not is what we have to check. So, let us look at let us look at let us go in this direction let us start with this as my lattice point one lattice point.

So, one and from this I go along the body diagonal, and I find this green atom and I travel a distance 1 4th along the body diagonal. So, one has a neighbor and let me locate in a call this atom 2. So, one has a neighbor 2, in this body diagonal direction at this distance if I travel the same distance from 2 that is if I travel another 1 4th distance along the body diagonal, then I would have traveled half the distance of body diagonal half the length of body diagonals, and I will end up in the center of the cube, but please note that we have not placed any atom at the center of the cube.

So, which means the green atom does not have a neighbor in the same direction at the same location as the black atom, which clearly shows that the green if 1 is the lattice point 1 is considered as a lattice point 2 cannot be considered as a lattice point. So, what we have to do is to associate 2 to the lattice point. So, our motif should at least be 2 atoms, 2 has to be associated to the lattice point at one.

So, let us propose or consider this as our possible motif. Now if since each lattice points are equivalent each motif also has to be equivalent and if we have given a motive atom to this lattice point, similar motive atom should be there for all the lattice points. So, let us consider this face center one. So, from here we went 1 4th along x 1 4th along y and 1 4th along z to find the motif atom, this from here if we start we are already at the face center. So, we will go 1 4th along this, 1 4th along y and then 1 4th z. So, exactly we will come to the location of this atom at the other body diagonal.

So, we can see that the motive is actually repeated at this atom at the face center also, similarly if you look at this vertical face center from here if you go 1 4th along x, 1 4th along y, and 1 4th along z, you will come to this atom which is sitting at 3 4th recall that this center atom is already at half height. So, if you go further half 1 4th height up, you will come to 3 4th and this atom was the 3 4th atom.

So, this is also associated with this and this one is associated with the back-face center. So, easier to see probably in the projection that this 1 4th atom is associated with that lattice point, this 1 4th 3 4th atom is associated with this face center at the back, this 3 4th is associated with the face center at the left, and this 1 4th is associated with the face center at the bottom. So, every now we are finding that we have accounted for all the extra 4 atoms, all of them are associated with their corresponding lattice point. So, we do not need any more.

So, the motif is 2 atom motif. So, we can write the diamond cubic structure that the conclusion of this analysis is that diamond cubic, briefly we can write d c diamond cubic crystal. So, recall that lattice is only the green atoms are not contributing to the lattice. So, lattice is only defined by the black atoms. So, the lattices face centered cubic, it is FCC lattice plus of course, it has to have motif, and we have seen that motif has 2 atoms, one black and one green now how do I give the coordinates of the motif atom. So, remember the coordinates of the motif atom is given as displacement coordinates with respect to the lattice point.

So, the black atom is sitting at the lattice point. So, it is not displaced. So, it is coordinate is o o o, the green atom is displaced with respect to the lattice point as you have already seen now by translations 1 4th along x 1 4th along y and 1 4th along z. So, the second atom in the motif is given coordinate 1 4th 1 4th 1 4th. So, we have successfully analyzed the diamond cubic crystal as a lattice plus motif, the crystal structure is diamond cubic lattice is FCC.

FCC lattice, but unlike we saw FCC crystal also cubic close packed crystal contrast this with cubic close packed structure CCP which we have already seen, which also had FCC lattice, but it had only one atom motif, only one atoms were sitting only at the lattice point, in diamond cubic since additional atoms are sitting beyond lattice points we get a motif of 2 atoms, one at the lattice point and one displaced by this vector 1 4th, 1 4th, 1 4th with respect to the lattice point.

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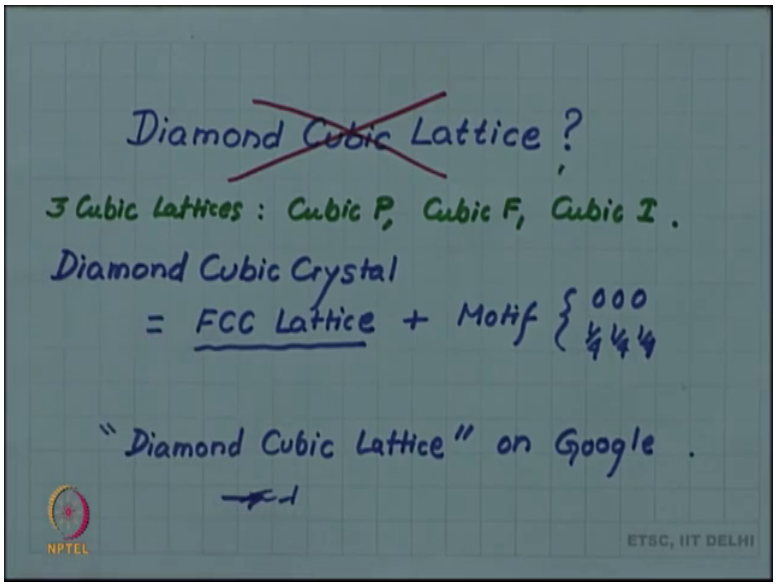

So, an interesting question comes and it is a widespread confusion in literature as well as on the web is there anything called diamond cubic lattice. So, we have already seen the crystal of diamond is a diamond cubic crystal. So, it is not diamond cubic lattice, but diamond cubic crystal, and when we analyzed it we found that the lattice was FCC, FCC lattice. So, there is no lattice called diamond cubic lattice, but diamond cubic is a crystal having FCC lattice with a motif of 2 atom at o o and quarter, quarter, quarter. So, diamond cubic lattice is a wrong phrase and should not be used, I trust that after this video you will not be using this incorrect phrase diamond cubic lattice which is quite common on the internet.

I think if you search if you do an exact phrase search, please do this exercise do an exact phrase search time and cubic lattice on Google, and it will happily throw you thousands of website which will which will be using phrase diamond cubic lattice which is incorrect. So, do this on the Google, you can also see why this is incorrect we have already met 14 bravais lattices.

So, out of those 14 bravais lattices there are only 3 cubic lattices, and they are simple cubic you may recall, that the 3 cubic lattices, or cubic p simple cubic, cubic f, face centered cubic, and cubic I, the body centered cubic. So, there is no such diamond in cubic lattice if you introduce a phrase like diamond cubic lattice; that means, you are talking of 15th bravais lattice which is an incorrect terminology. So, never use diamond

cubic lattice if you are use diamond cubic adjective should be used only for crystal and not for the lattice diamond cubic crystal having an FCC lattice.

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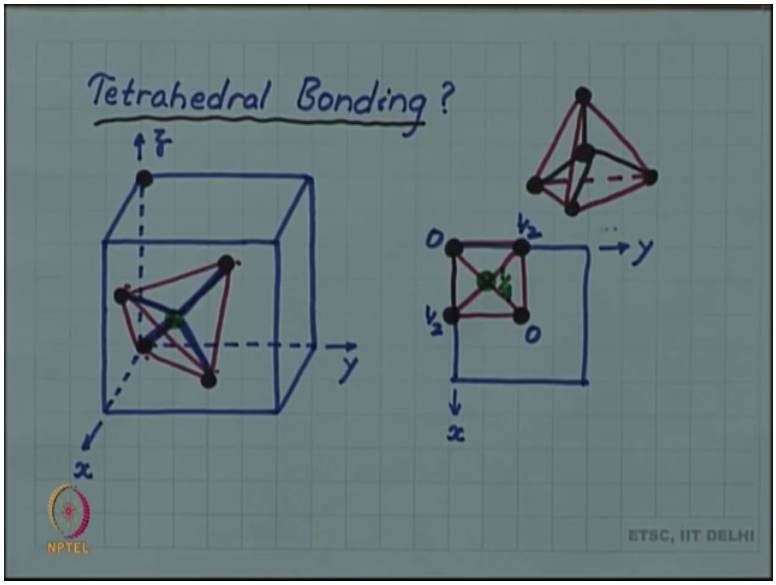

We also know we have ah from our previous studies that there is a tetrahedral bonding of carbon, each carbon atom is bonded to 4 other carbon atoms located on the corners of a tetrahedron in diamond. So, if I take a carbon atom in diamond, it is supposed to be bonded to 4 other carbon atoms, and these 4 carbon atoms if I join they are on the vertices of a tetrahedron, they are forming a tetrahedron. So, where is this tetrahedron in our unit cell so, this was something which was not obvious. So, I want in this slide I want to show you where is this tetrahedron in the diamond cubic structure, diamond cubic crystal structure.

So, let us look at this 3-dimensional picture of the unit cell first, and we see that every corner in a in an FCC send a structure we have already seen in the cubic close packed case that you have tetrahedral and octahedral void. So, a tetrahedron is formed by any corner atom if you look at this corner atom let us say, this one and at that at each corner 3 faces meet and if you look at so, at this corner left face back face and the bottom face is meeting, consider the center face centers of all these 3 phases which are meeting. So now, you have 4 atoms the corner one and the 3-face center, you can show you have shown already in when we were studying the cubic close packed structure that these 4

atoms form a tetrahedron they form a nice tetrahedron. And then this 1 4th 1 4th 1 4th atoms on the body diagonal you can show is exactly the centroid of this tetrahedron.

So, this is where this green atom the one sitting on the body diagonals then forms, a tetrahedral bonding with all the 4-neighboring carbon atom. So, the red lines which I have drawn are not carbon bonds, they are the reference lines to show the tetrahedron, and the blue lines here are the actual carbon bonds.

So, I have done this for this 1 4th atom in this unit cell, if you do this for other atoms you will find that each atom is at the center of a tetrahedron.

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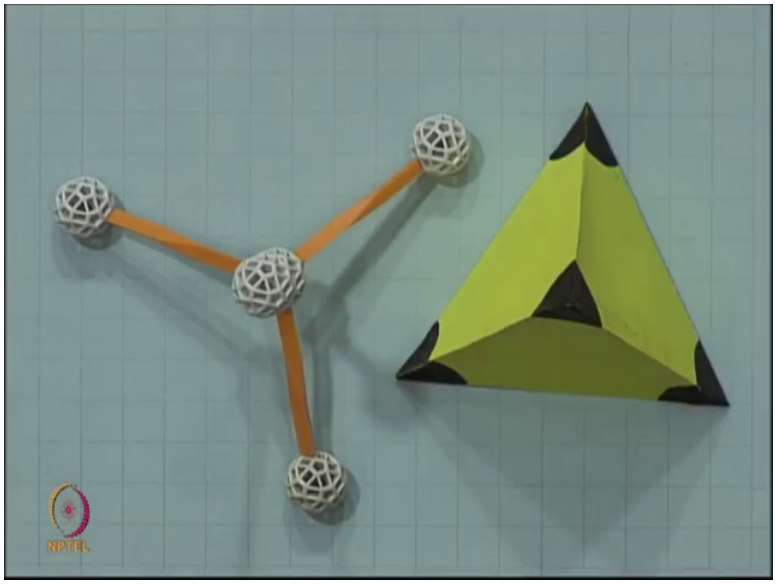

So, this is what makes the 3-dimensional diamond structure and I have a model here to show you. So, this this carbon atom is at the center, of 4 atoms it is bonded to 4 atoms you can see one atom there, one atom here, one down there and another down there of course, it is not easy I can see it is not easy to see on a video like this you have to have a model to play with, but then such a structure will continue and if I just separate my model to show you, this just one tetrahedral unit I am trying to separate now from my 3 dimensional structure. So, that looks like this.

So, this is probably easier to see you can see the 4 atoms on the center one connected with 4. So, and so, you can model it with the tetrahedron here is the tetrahedron solid. So, if I place it then like this. So, you can see that there is a base of 3. So, and the and

these lines these lines are the edges of the tetrahedron these lines are here like this and they are not the or like this. So, this edge this bottom edge is actually not a bond, but that is the edge of the tetrahedron. So, if I place it like this. So, that is the edge of the tetrahedron.

So, tetrahedron can be seen you can see the tetrahedron can be seen in 2 ways one is this a standard way in which case the there is a base of 3 atoms, and one atom is sitting on the top of that base. So, the vertical axis in this case is a 3 fold axis if I look at this axis that is the 3 fold axis whereas, the other way of looking at the tetrahedron is to stand it on edge.

If you stand it on edge then you see you have to bottom atoms, which I am now holding by my hand and there are 2 atoms on the top and the orientation of the line of these atom the bottom is oriented one way, and this is oriented orthogonal to the bottom atoms. So, the 2 lines are at 90 degrees to each other. So, this is another way of looking at it tetrahedron in this case the vertical axis is a 2fold axis, you can orient the tetrahedron either as with 3-fold vertical or you can orient the tetrahedron with the 2fold vertical in this way.

So, in the in the projection if you try to find the tetrahedron. So, you can see this was the 1 4th atom and there are 4 atoms here. So, this one was let me write the coordinates half this one was 0, 0 and this particular one was the 1 4th. So, you can see that the 2 atoms below 0 0, then 2 atoms above half, in my this tetrahedron orientation 2 atoms below, and 2 atoms above and they are at 90 degree and they are at 90 degrees.

So, that is what is forming a tetrahedron. So, these 4 atoms the black atoms are forming the tetrahedron, and this 1 4th atom is at the centroid of the tetrahedron, in this case if I outline in red the tetrahedron is shown here, the projected tetrahedron will look like a square like this with the green atom in the center. So, we have seen how the tetrahedral bonding of diamond fits in in the unit cell and we have also seen how the diamond structure the diamond cubic crystal structure can be analyzed or discussed in terms of lattice and motif, and we have emphasized that there is nothing like diamond cubic lattice there is only diamond cubic crystal which has an FCC lattice and there are 2 atom motif. So, with this we end the video.