# X-Ray Crystallography
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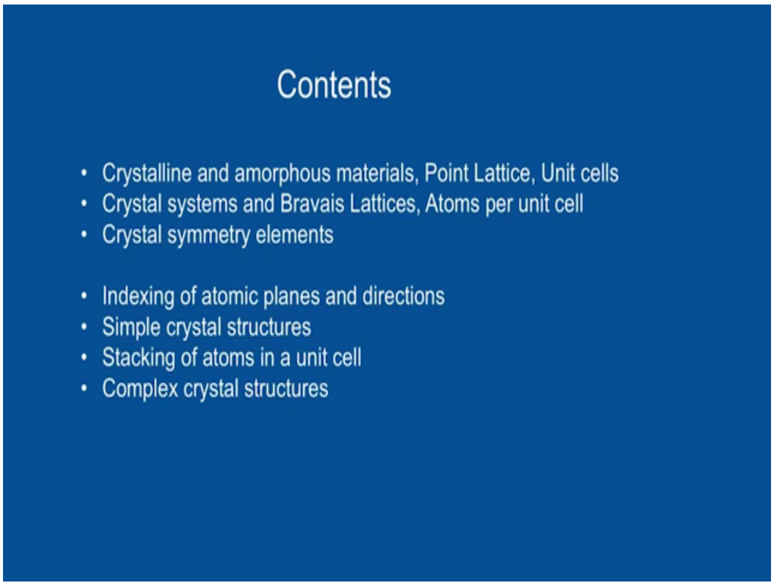
## Lecture - 2
## Geometry of Crystals (Continued)

(Refer Slide Time: 00:16)



Contents

- Crystalline and amorphous materials, Point Lattice, Unit cells
- Crystal systems and Bravais Lattices, Atoms per unit cell
- Crystal symmetry elements

- Indexing of atomic planes and directions
- Simple crystal structures
- Stacking of atoms in a unit cell
- Complex crystal structures

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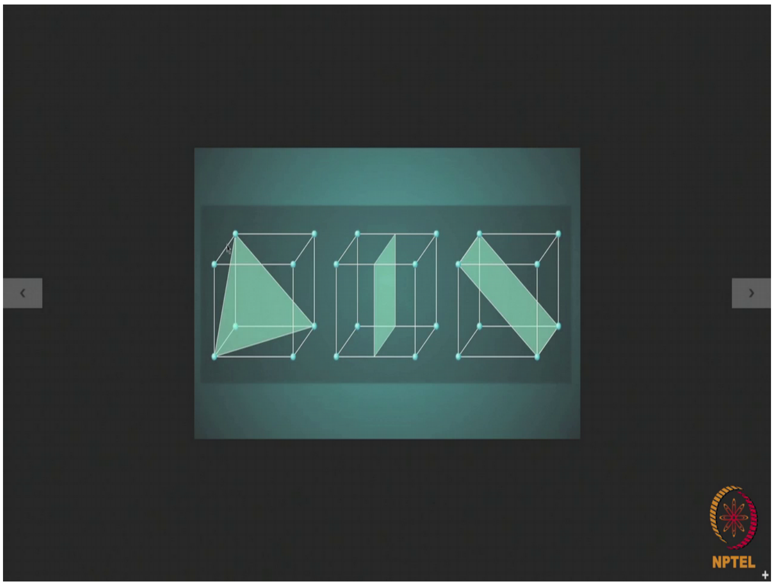

In this diagram three unit cells of the primitive cubic material are shown. For example, this is an atomic plane as you can see passing through the atoms here, here and here, this is also an atomic plane passing through the atoms here, here, here and here and this plane is not an atomic plane, but it lies midway between the two atomic planes given by this as well as this. Now the question comes how can we name an atomic plane or a plane in the unit cell so that you can identify easily. The method that we follow in naming a plane was given by Miller and that is the reason why the nomenclature goes by the name Miller Indices.

Now, let us see how they hold this tongue. So, the first step in the naming of a plane is to find out the actual intercepts which the plane makes on the X Y and Z axis.

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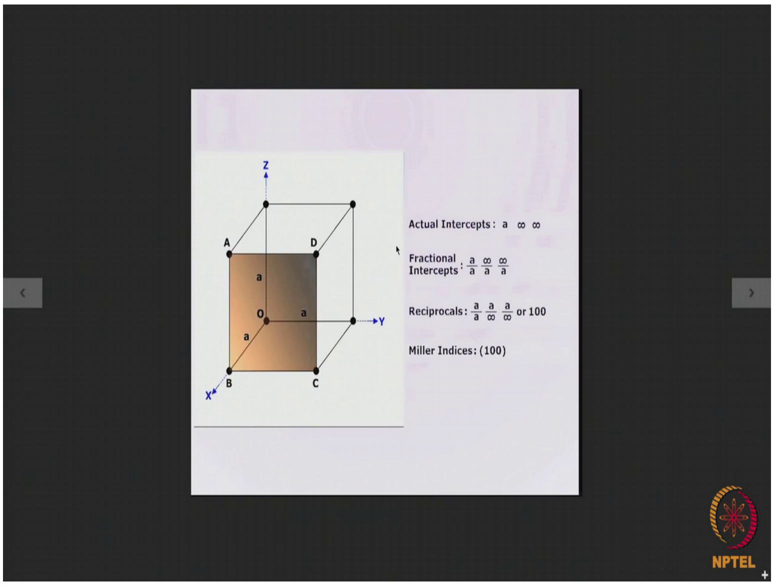

Actual Intercepts : a ∞ ∞

Fractional Intercepts : $\frac{a}{a}$ $\frac{\infty}{a}$ $\frac{\infty}{a}$

Reciprocals : $\frac{a}{a}$ $\frac{a}{\infty}$ $\frac{a}{\infty}$ or 100

Miller Indices: (100)

Now, if we want to name this front plane here A B C D what are the intercepts this plane makes on the X Y and Z axis as you can see the intercept is a on the X axis; however, the plane does not intersect the Y axis at all neither does it intersect the Z axis. Now if it does not inspect the Y or the Z axis we can say that the intercepts made on the Y and Z access are infinity; that means, the plane A B C D is such that it has an intercept of a on the X axis, infinity on the Y axis and infinity on the Z axis.

Now the second step is to find out the fractional intercepts this is done by dividing the actual intercepts by the relevant that is parameter. So, the fractional intercepts in this particular case will be a by a, infinity by a, infinity by a. The third step is to take the reciprocal of these values. So, the reciprocals will be from here to the a by a, from here it will be a by infinity, from here it will be a by infinity or it will be 100.

Now, the next step is to put this number in a first bracket 100 within the first bracket. So, that indicates that this is displaying A B C D. So, the A B C D plane is written as the 100 within first bracket and this is how the Miller Indices are found out for this particular plane.

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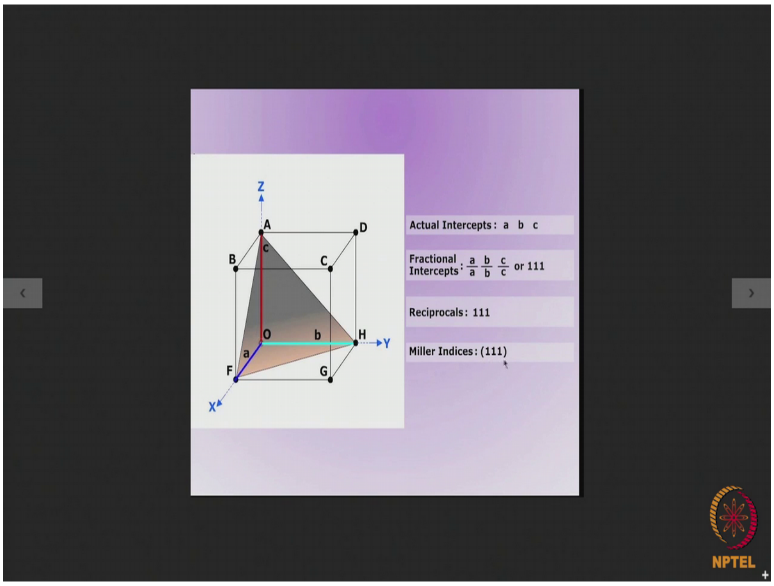

Actual Intercepts: a b c

Fractional Intercepts: $\frac{a}{a}\ \frac{b}{b}\ \frac{c}{c}$ or 111

Reciprocals: 111

Miller Indices: (111)

Say for example, we want to find out about this particular plane in the simple cubic unit cell. So, this is a plane which makes the actual intercepts on X at a distance a and makes an intercept of b on the Y axis and an intercept of c on the Z axis. So, the actual intercepts are a b and c on the X Y and Z axis respectively. So, what are the intercepts? Fractional intercepts rather we will divide the actual intercepts by the relevant lattice parameters the relevant lattice parameters say over here are A B and C. So, what we do? We divide the actual intercepts by a by a, b by b, c by c or it becomes 111.

Now, we take the reciprocal it remains the same as 111, put a first, put these numbers within the first bracket. So, these become the Miller Indices for the plane A F and H.

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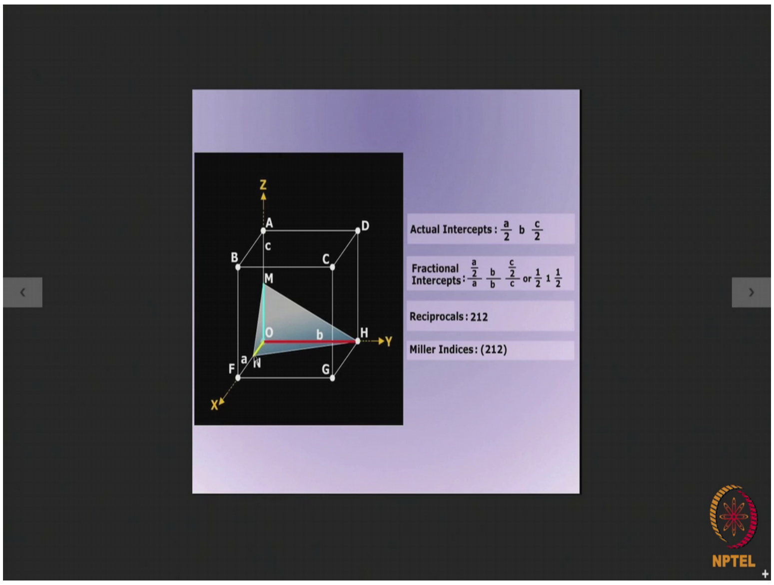

Actual Intercepts : $\frac{a}{2}$ b $\frac{c}{2}$

Fractional Intercepts : $\frac{\frac{a}{2}}{a}$ $\frac{b}{b}$ $\frac{\frac{c}{2}}{c}$ or $\frac{1}{2}$ 1 $\frac{1}{2}$

Reciprocals : 212

Miller Indices : (212)

Now, what about this plane over here N and H in the cubic unit cell with lattice parameters a b and c? Now you see that this plane is such that it makes an intercept O N which is half of a on the X axis it makes an intercept O b I am sorry O H which is equal to the b and it makes an intercept O M which is equal to half of c. So, the intercepts wait by the plane M and H on X Y and Z are a by 2, b and c by 2 respectively.

Next step is to find out the fractional intercepts. So, the fractional intercepts are a by 2 by a, b by b, c by 2 by c or half one and half. What have the reciprocals the next step? The reciprocals are 212. So, if we put this number within a first bracket then it becomes the Miller Indices of the plane M N H. Sometimes we may face some problem in determining the Miller Indices.

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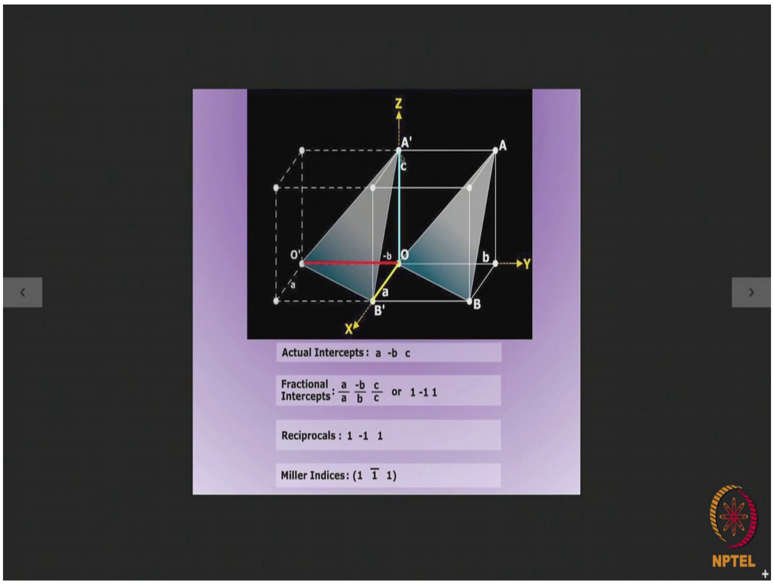

Actual Intercepts : a -b c

Fractional Intercepts : $\frac{a}{a}$ $\frac{-b}{b}$ $\frac{c}{c}$ or 1 -1 1

Reciprocals : 1 -1 1

Miller Indices : $(1\ \bar{1}\ 1)$

Say for example, in this particular unit cell we have a plane A O B, now this particular plane is such that it passes through the origin at O now how to name this atomic plane. It becomes difficult because it passes through the origin O then what we do; we take a plane parallel to the given plane A O B in the adjacent unit cell. So, this is the adjacent unit cell and we draw a plane which is parallel this plane is A dash, O dash, B dash and which is parallel to the plane A O B. Now if we look at this plane this plane intercepts the X axis at a distance a, it intercepts the Y axis at a distance minus b, this is plus b on this side this minus b and it intercepts the Z axis at a distance of c.

So, what are the actual intercepts for the plane A dash, O dash, B dash? This a minus b c. So, in order to get the fractional intercepts we divide these numbers by the corresponding lattice parameters and we get the value 1, minus 1, 1. So, the reciprocals of these numbers are again 1, minus 1, 1. So, the Miller Indices are written by writing these numbers within first bracket normally the minus sign is written on top of the number. So, it becomes 1 bar 1 1. So, this plane has got the Miller Indices 1 bar 1 1, but remember this plane is parallel to this plane. So, all planes parallel to this plane will have the same Miller Indices.

Then we come to naming a plane in the hexagonal system.

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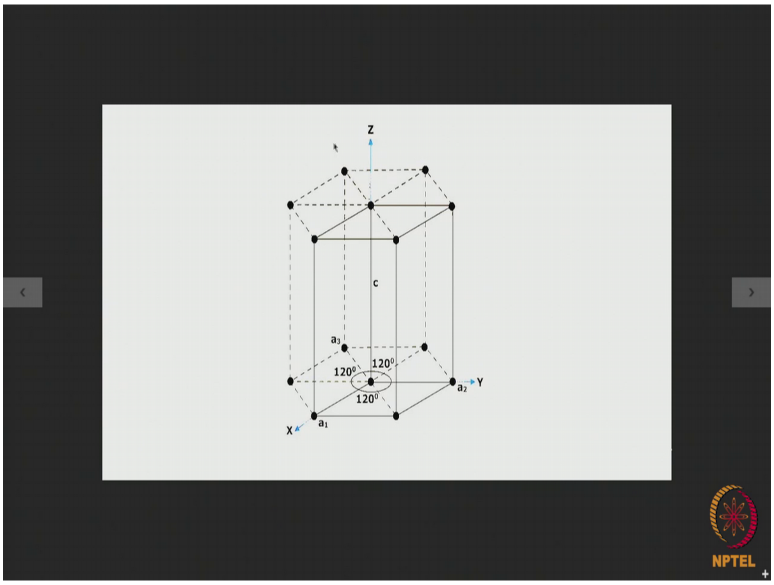

Now, as we can see here this is a hexagonal unit cell, as I mentioned earlier also it is also possible to take one-third of the unit cell as a unit cell of the hexagonal system. So, either we can take the intact hexagonal figure of unit cell or take one-third of it as the unit cell.

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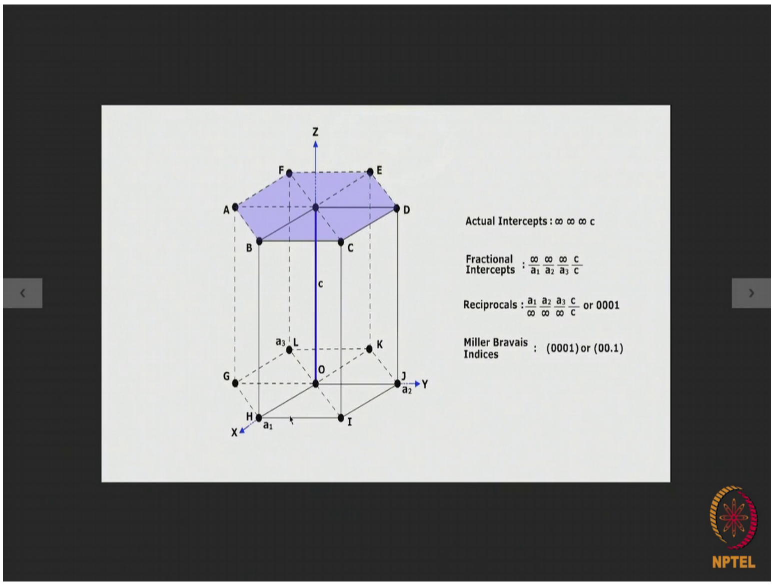

Actual Intercepts : $\infty\ \infty\ \infty\ c$

Fractional Intercepts : $\frac{\infty}{a_1}\ \frac{\infty}{a_2}\ \frac{\infty}{a_3}\ \frac{c}{c}$

Reciprocals : $\frac{a_1}{\infty}\ \frac{a_2}{\infty}\ \frac{a_3}{\infty}\ \frac{c}{c}$ or 0001

Miller Bravais Indices : (0001) or (00.1)

Say we want to name the top plane which has been shown by the blue color say this is the plane A B C D E F. Now in the hexagonal system we have a four coordinate system you see here for example, in this plane the lattice parameters are a 1, a 2 and a 3 and then we have the c parameter perpendicular to this given plane. So, our job is to find out what are the Miller Indices of the top plane. So, what are the actual intercepts made by this plane on these four axis. As it is this particular plane will never intersect along this axis along that axis or along that axis since this is parallel to the basal plane, and it intercepts the c axis at a distance see the you know or rather the Z axis at a distance c.

So, the actual intercepts made by this plane on the four axis are infinity, infinity, infinity and c. So, the fractional intercepts will be infinity by a 1, infinity by a 2, infinity by a 3, c by c. Reciprocals will be a 1 by infinity, a 2 by infinity, a 3 by infinity c by c or 0001. So, we can put this number within first bracket 0001 which are known as the Miller Bravais Indices in case of a hexagonal system. This can also be written in this form 00.1.

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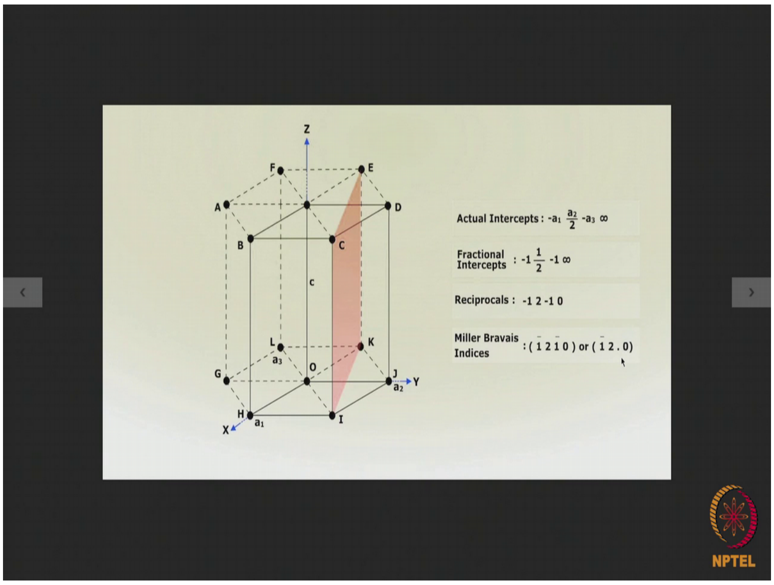

Actual Intercepts : $-a_1$ $\frac{a_2}{2}$ $-a_3$ $\infty$

Fractional Intercepts : $-1$ $\frac{1}{2}$ $-1$ $\infty$

Reciprocals : -1 2 -1 0

Miller Bravais Indices : $(\bar{1}\,2\,\bar{1}\,0)$ or $(\bar{1}\,2\,.\,0)$

In a similar manner in the hexagonal unit cell if we have a plane given by I K E C we can easily find out the intercepts the fractional intercepts and the reciprocals and the Miller Bravais Indices you know the Miller Indices in case of hexagonal systems are known as Miller Bravais Indices are bar 1 2 bar 2 0 or it can also be written as bar 1 2 dot 0.

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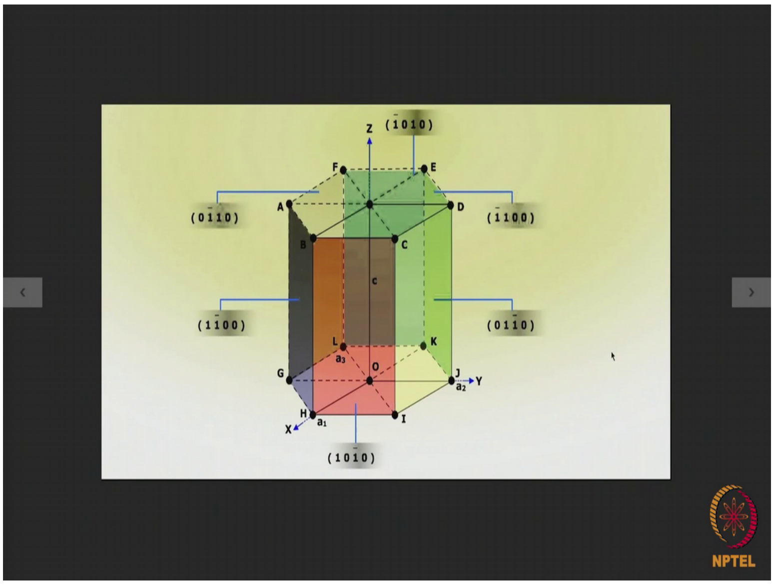

Following the same procedure it is possible to name different planes belonging to the hexagonal system. Now, will go to naming a crystallographic direction. In a unit cell we can see that there can be many directions.

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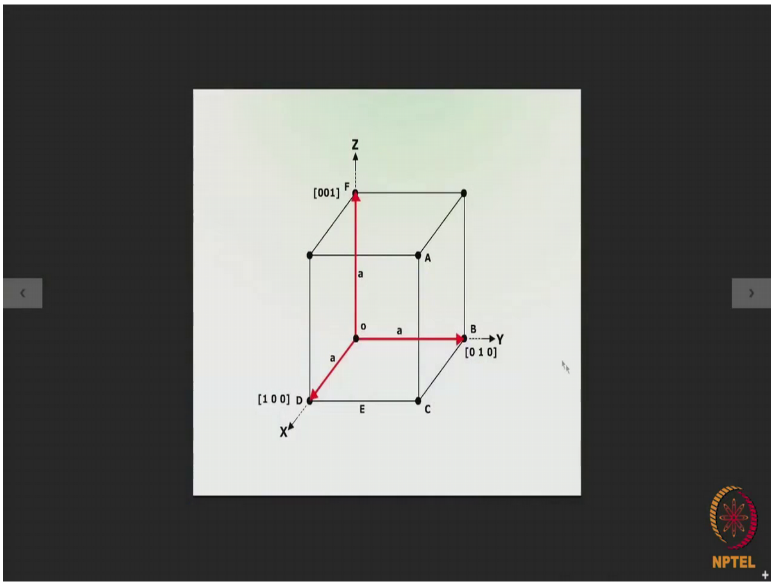

For example say if this is a cubic unit cell this is a direction this is another direction and this is a third direction. Now how we are going to name this direction? Say this particular direction. So, here what we are doing really we are starting from the origin and going towards this particular point. So, how much we move from here to here? We move a distance a along X axis and then do not move at all along Y or along Z. So, the numbers are 100 put it in a third bracket and that indicates this particular direction.

Now, what about this particular direction here? So, we move from the origin to the point b along this direction. So, how we do that? We do not move at all along X axis. So, the total movement along X is 0, then remove unit lattice parameter along the Y axis. So, we put 1 and do not move along the Z axis at all, so again 0. So, this is the 0 1 0 direction, similarly this direction will be the 0 0 1 direction.

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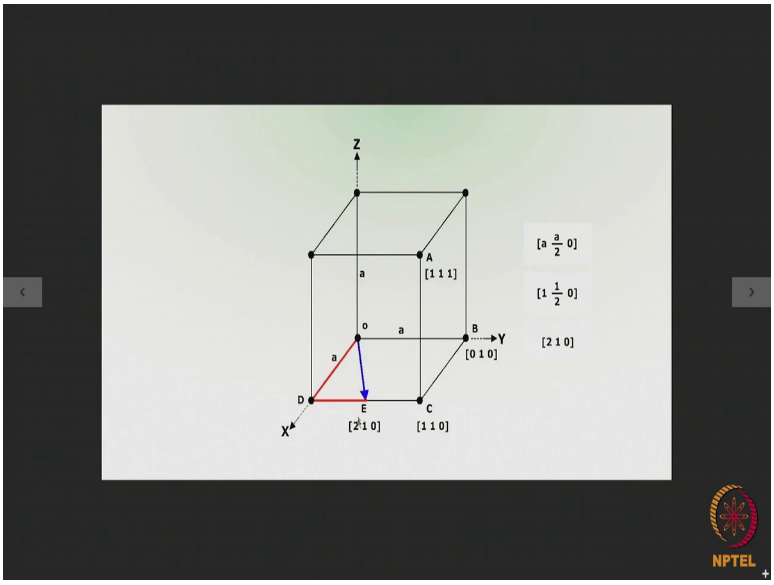

Now, say we want to find out this particular direction here given by the blue arrow. So, what should be the direction? Again the principle is very simple. Whenever you want to find out a direction you have to move along the X Y and Z directions only in order to reach that particular point. So, our movement will be in a direction parallel to the X direction or and the direction parallel to the Y direction and a direction parallel to Z direction. So, who how we reach from this point to this point, well as you can see here we have to first move along the X axis. So, we move a unit lattice parameter a along this direction and then or simply yes and then how much you move along the Y direction half the lattice parameter here. So, if we move by distance a along this we move a direction distance a by 2 along this direction and do not move at all in the Z direction. So, we move by a a by 2 0 along the three directions. So, it becomes 1 1 by 2 and 0 and it becomes you know in you can multiply by 2 to make it 2 1 0. So, when you put it in a third bracket that is the 2 1 0 direction. So, this is normally the procedure we follow.

So, whenever we want to find out any direction we figure out what is the starting point and what is the end point and then start moving along the direction parallel to X parallel to Y and parallel to Z in order to reach that point and that will give us the direction of the given the Indices of the directions Miller Indices of the direction. Sometimes it becomes difficult to find out a direction the unit cell.

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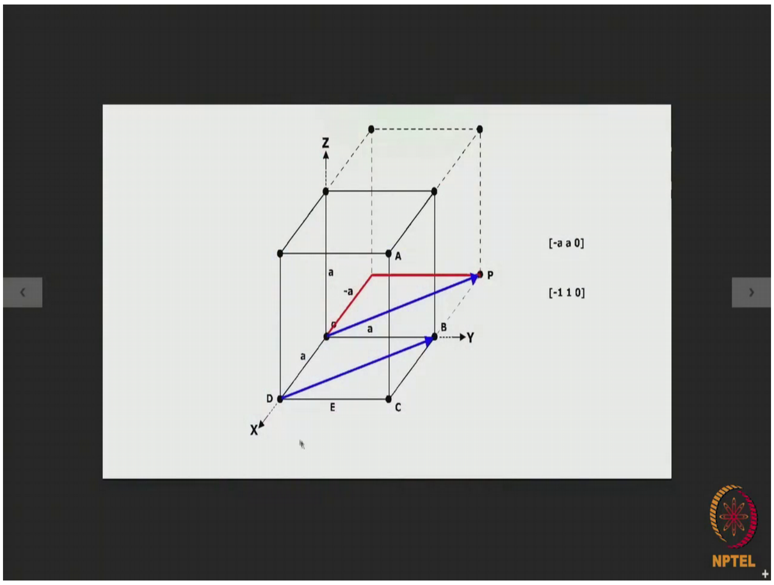

[-a a 0]

[-1 1 0]

Say for example, we want to find out this particular direction here. Now this direction belongs to this front unit cell given over here. So, this is the direction we want to find out; that means, we want to we are moving strong the point D to B, but you see the problem is the way we find out the direction is we start from the origin.

So, here we are not at the origin, but it really does not matter, you see in a lattice since all the points are having identical surroundings any point in the lattice can be taken as the origin. Say for example, let us talk about the unit cell at the back of the given unit cell given by the dotted line. So, this can be considered as the origin for that unit cell. So, we draw a line parallel to the given line. So, O P is the line which is parallel to the given line O B. So, if we can find out what this direction is it will be the same as that on the given direction. So, what is the direction of O P? How we reach the point P from the point O how it is possible? Now you see if we want to do that from the origin we move a distance minus a along X. So, the first movement will be minus a along X, then how much we move? We move a distance a along Y and do not move at all along z. So, the indices are actually minus 1, 1, 0 put it in third bracket. So, minus 1, 1, 0 it can also be written as bar 1, 1, 0. So, this is the direction given by O B in the diagram.

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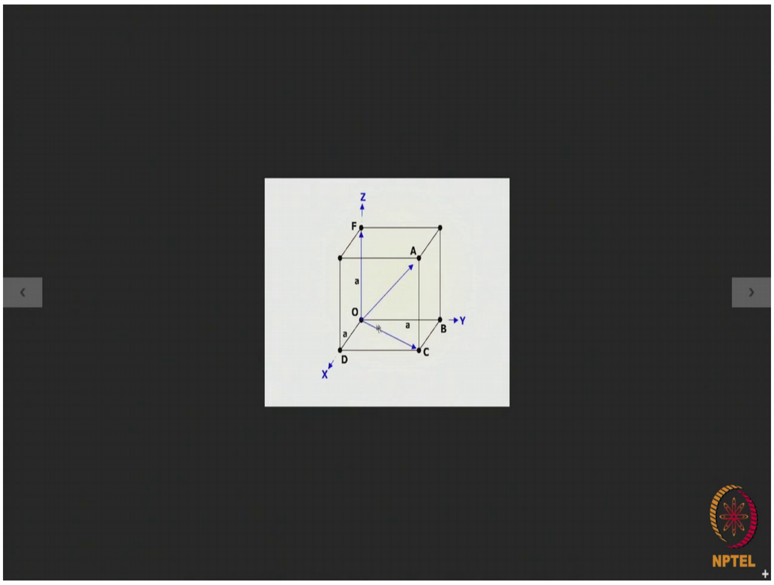

Now, in a similar manner it is quite possible to find out this direction or this direction for example, if I want to find out this particular direction along O C we know that we move unit lattice parameter along X axis, unit lattice parameter on Y axis and no movement along Z, so it is a 1 1 0 direction and what about this particular direction. Well again following the same procedure from the origin we move unit lattice parameter along this direction along X unit lattice parameter along Y and unit lattice parameter along Z to reach this point. So, this direction will be 1 1 1.

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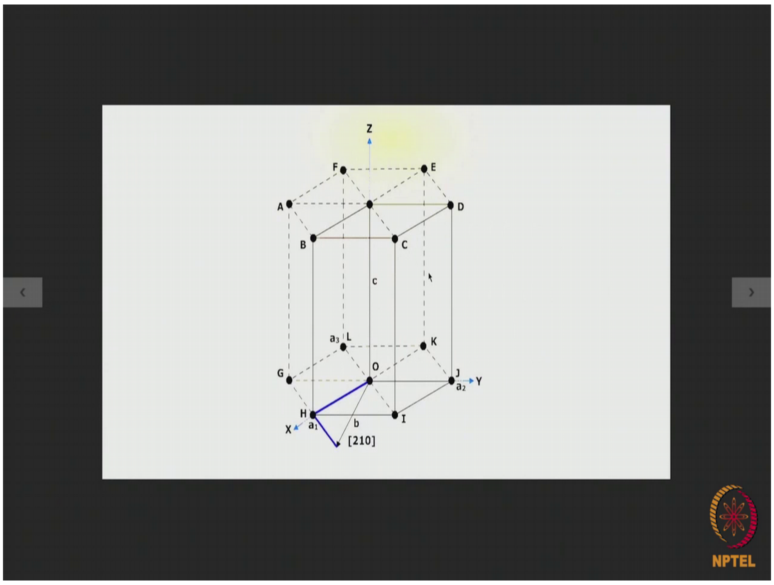

When it comes to the hexagonal system as I already told you, you will find we can find out the direction with respect to the entire hexagonal unit cell or the one third of it which can be taken as unit cell. Say we want to find out this particular direction as given in the diagram. So, how we reach this point from the origin? Now we move along X a full one unit in the lattice parameter, then half a lattice parameter along the other axis here this is one axis this is one axis and this is the third axis and we do not move along the Z direction at all. So, in this particular case we will have a situation it will be 1, half and 0. So, make the whole number, so it will be 2 1 0 direction. So, in this way it is also possible to find out any direction in the hexagonal system.

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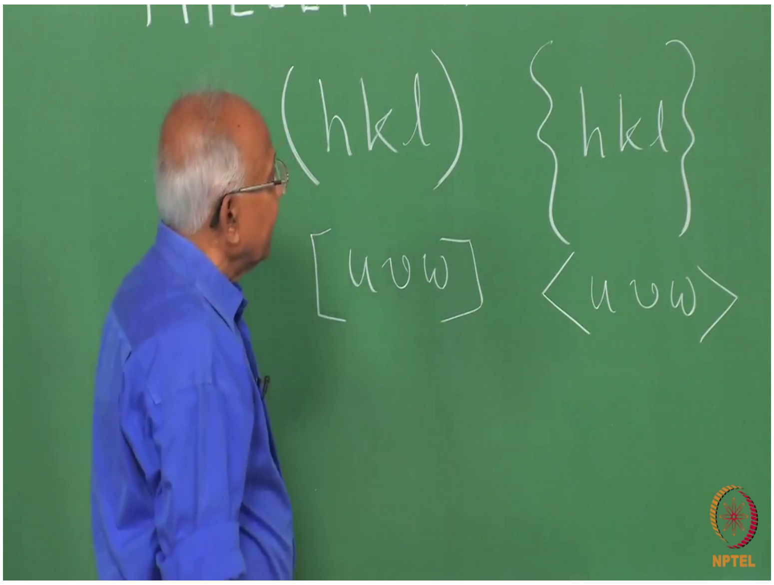

Now, if we write a number h k l within first bracket that indicates a particular plane h k l along integers. Now, as we have already seen in a cube there are 6 similar faces you know in the unit cell the front plane, back plane, right hand side plane, left hand side plane, top plane, bottom plane all out of the same time. So, in order to indicate similar planes are based on the same topic we write h k l in this type of a bracket. So, this is the Miller Indices of a single plane this indicates Miller Indices of planes which are all similar similarly if we write a number u v w in the third bracket that indicates a direction. Now there can similar directions in unit cell at the same time. So, if we write u v w in this type of a bracket indicates all the directions of the same type.

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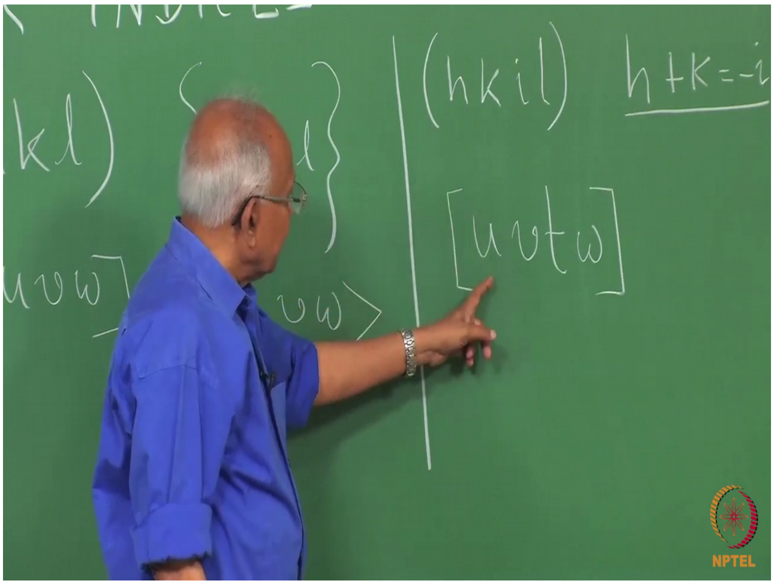

Now, in case of hexagonal materials considering four axis the plane a particular plane is written as h k i l, in case of other systems this is a three digit theory, it case of an hexagonal there are four because there are four axis. Now it can be proved that h plus k is equal to minus i. So, when you find out the indices we must make sure that h plus should be equal to minus i, it can be proved mathematically. The other thing to remember is when it comes to a direction in a hexagonal system we write it as u v t w and in fact, we follow the same procedure as in case of naming a plane. So, u plus v must be equal to minus t. So, when you name it direction we must make sure that it follows that kind of procedure.

Now let us go to the different types of crystals that we normally come across.

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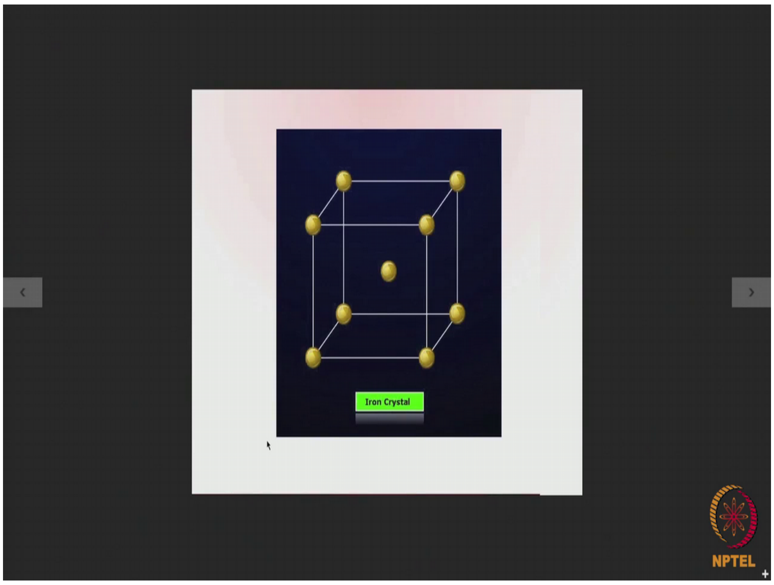

So, look at an iron crystal. In an iron crystal it is a BCC unit cell. So, we have iron atoms at all the 8 corners and 1 at the body center position.

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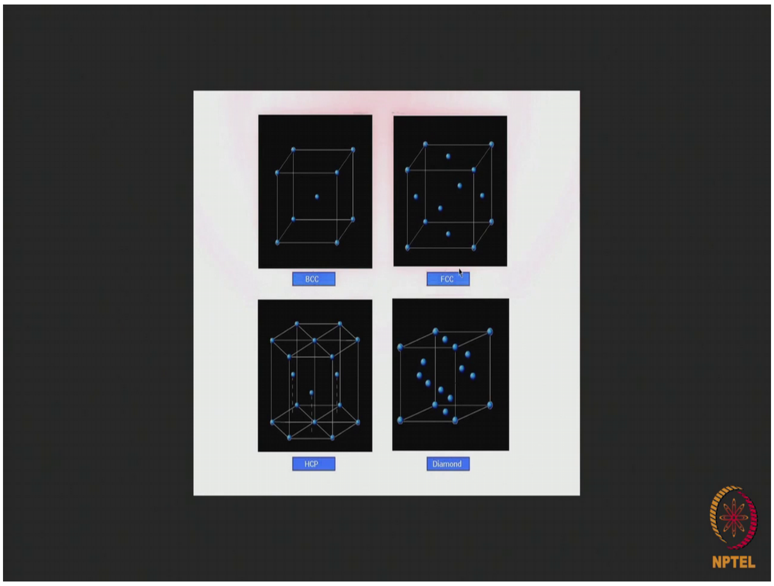

Now, we know that this is a BCC unit cell since we have along with the 8 corner atoms 1 at the center; this is an FCC unit cell where we have got the 8 corner atoms and 6 atoms at the center of the 6 faces. Now this is the unit cell of a material which has hexagonal closed packed structure, you see if it were a simple hexagonal structure then there are these atoms on the top plane as shown and on the bottom plane, but the moment we put three more atoms inside this becomes hexagonal close packed. The position of these atoms I will show later on. Now this is a diamond crystal. So, basically again you have a an FCC kind of a structure in fact, a diamond unit cell has got 8 atoms per unit cell which I will come to later I will explain, right.

Now how the atoms are packed in the different systems?

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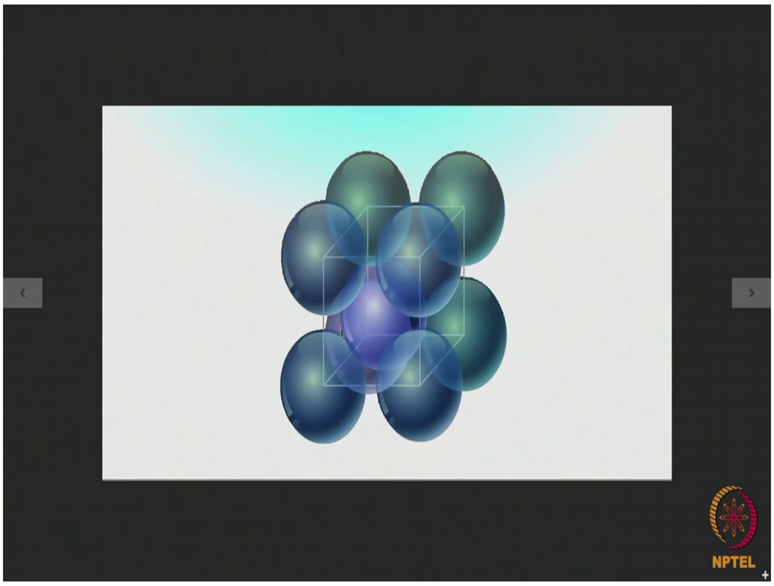

Say if we talk about a BCC unit cell, in a BCC unit cell we have got the atoms at the 8 corners. So, 8 atoms or the 8 corners and there is a central atom, since atoms are the same material atoms are of the same size if you try to pack you know these atoms in this manner you will find that all these 4 plus 4 8 corner atoms each one of them will be touching the central atom, but between them they do not touch one another. So, in a BCC structure we find that the centre body centered atom is touched by all the 8 corner atoms, but the corner atoms between themselves they do not touch one another.

Now, when it comes to the FCC crystal structure, this is at FCC crystal structure and I have shown here the atoms on the 1 1 1 plane or an FCC unit cell.

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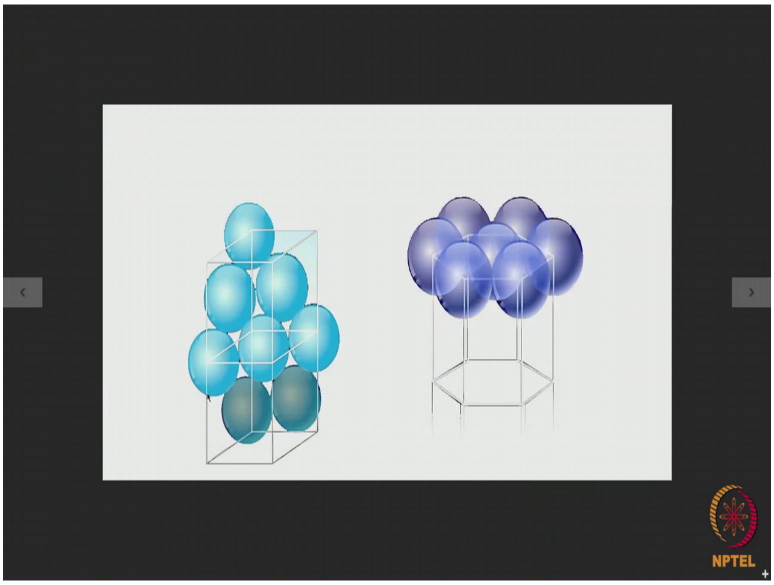

Now if you look at the way these atoms are arranged you see they are very very closely most closely packed; that means, atoms are touching one another in this manner you know they cannot become more close is the closest possible approach of these atoms here. Similar thing happens if we consider the 0 0 0 1 plane of an hexagonal unit cell, in the hexagonal unit cell also this on this face a 0 0 0 1 face you have a central atom which is touched by the 6 surrounding atoms. So, these are the closest kind of packing that is possible. So, in FCC material if we look at the 1 1 1 planes the atoms are most closely packed you cannot make them any closer, similarly in the hexagonal system if you look at the 0 0 0 1 plane the atoms are most closely packed

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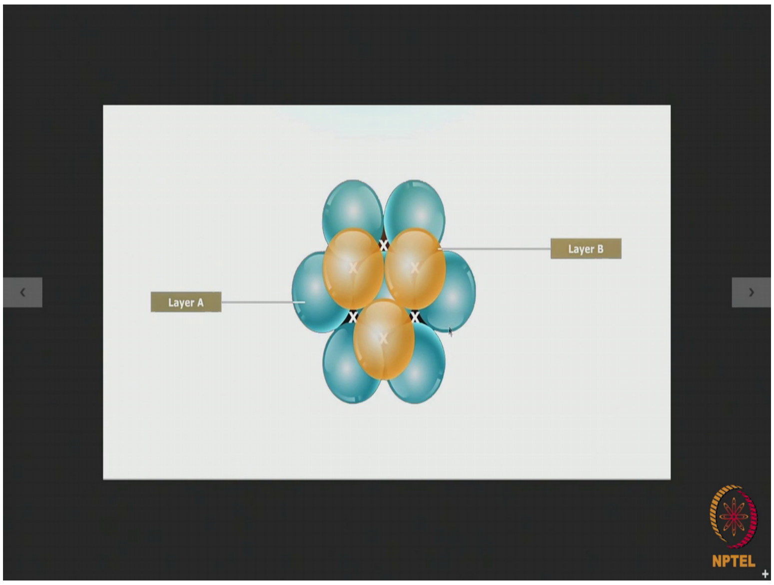

In fact, if we put you know in there containing 6 atoms which touch one another and also touch a central atom here than in order to build up the structure we can put other atoms in this gap regions this is one such region this is another, this is the third, this is the fourth, this is the fifth, this is the sixth position. So, now, we are trying to show how an FCC structure can be built up layer by layer and how an HCP structure can also be can all built up layer by layer.

Say for example, if we take a single layer as shown by the blue color atoms they are most closely packed. So, this is a first layer we have the central blue color atom surrounded by 6 neighbors and this is the closest possible approach that can be made as in the 0 0 0 1 plane of an hexagonal crystal. Now how we build up the next layer? Either we put atoms here, here or here this is one possibility, the other possibility is we can put atoms here, here and here. You see we cannot put atoms at all these 6 provisions because there is not enough space the 6 atoms cannot be squeezed in to those positions. So, once you fill up this position, this position and this position and go on adding more and more atoms in that layer you can build up a second layer. So, once we do that this second layer you know we can call it the layer b. So, the blue colored atoms at the bottom they fall the layer A and this for the layer B. Now when we look at and hexagonal closed pack structure as we already found out.

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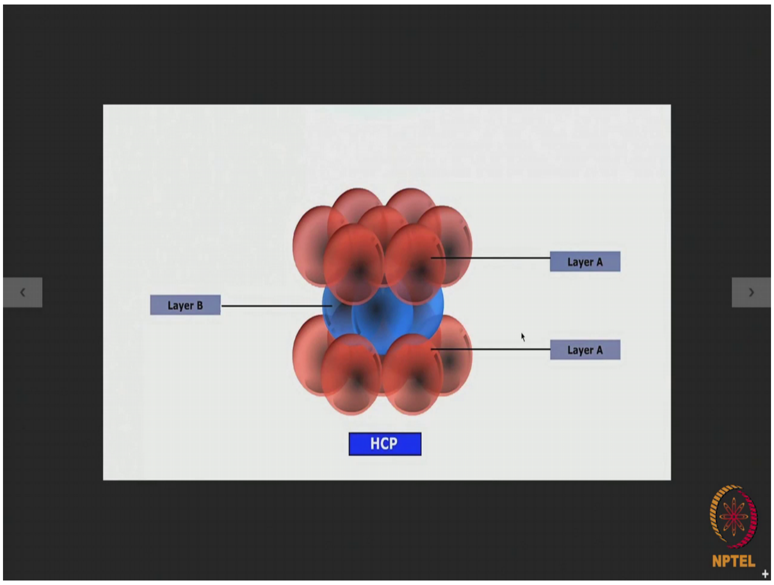

This can be built up by putting a layer A on top of that a layer B, on top of that again a layer A on top of that again a layer B on top of that again a layer A. So, this continues A B A B sequence. So, this is, this gives us an HCP crystal structure.

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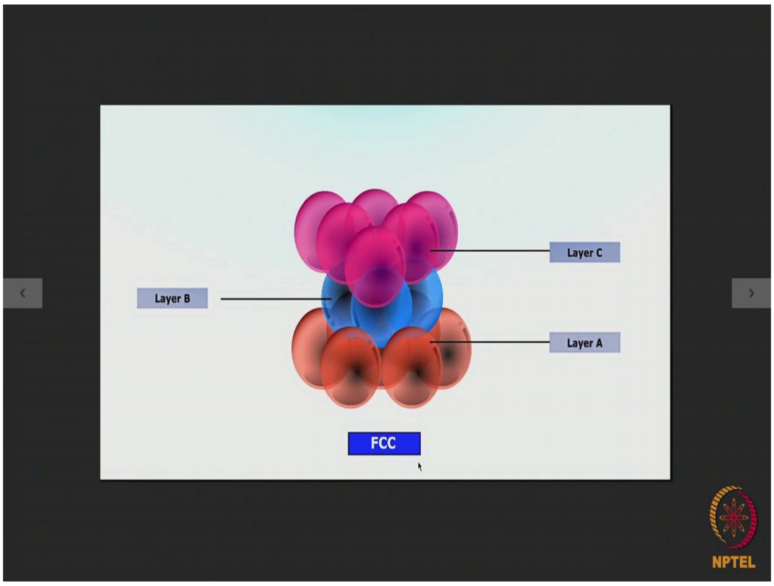

On the other hand if we have the first layer A layer then we have got the B layer and then on top of that you remember that yes if we have instead of having atoms at this positions if we have atoms in this, this and this position that will constitute what is known as the C layer.

So, if we do it in this way that we put it A layer on top of that we put a B layer on top of that we put a C layer then that is the situation in FCC materials. So, the stacking of atoms in HCP will be A B A B this type whereas, in case of FCC materials this tacking will be layer A layer B layer C again layer A layer B layer C like that. One thing we must remember that the way we build up the FCC or HCP stacking the atoms are packed most closely that is the reason why they we say that the FCC or HCP unit cells these are very closely packed and HCP and FCC structures are known as the most closely packed structures. On the other hand the BCC structure is not the most closely packed there are quite a bit of space remaining within the unit cell. So, this is a more open kind of a structure.

Now we come to compound, crystals say for example, if we have a crystal of sodium chloride we have got two different types of atoms over there - sodium atoms and chlorine atoms or sodium ions and chlorine ions. Up till now we have been talking about atoms of the same kind only, but now we are talking about compound crystals where we have got say two different types of atoms. So, while packing those atoms together in the unit cell certain rules are followed, and what are those rules?

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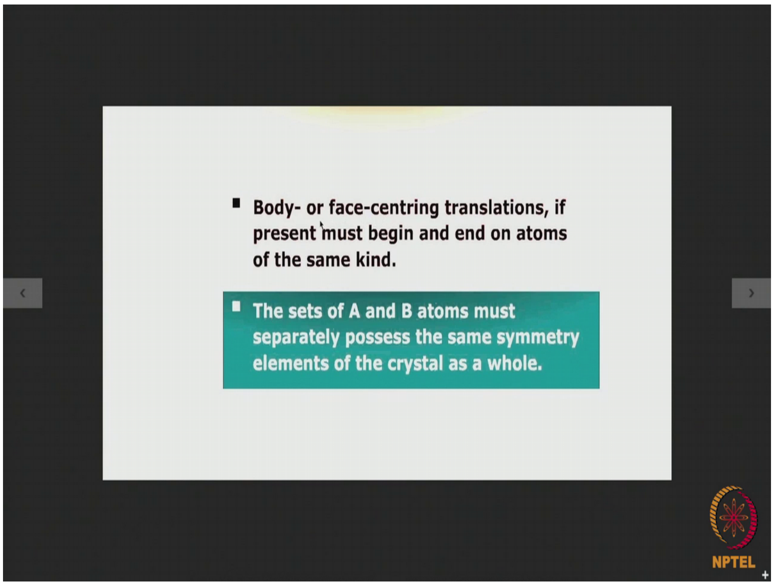

- Body- or face-centring translations, if present must begin and end on atoms of the same kind.
- The sets of A and B atoms must separately possess the same symmetry elements of the crystal as a whole.

The body or face centering translations if present must begin and end on atoms of the same kind, now I will tell you what it really means.

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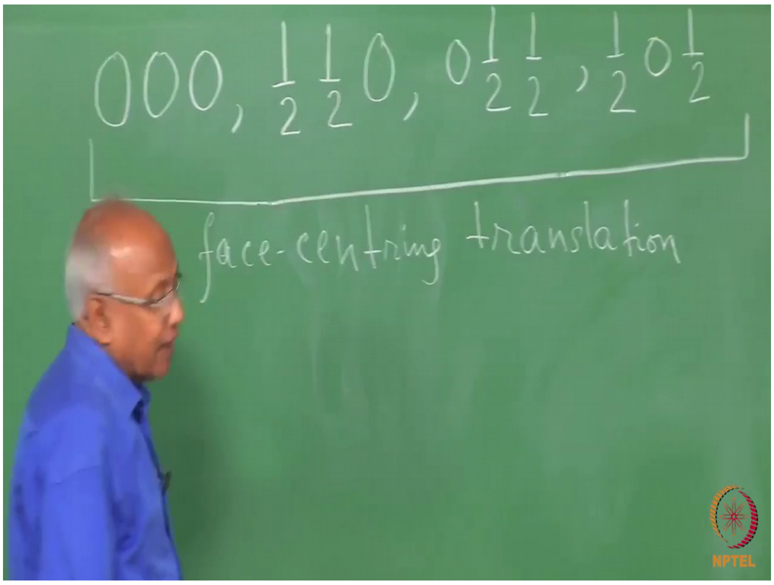

As we have already seen in case of an FCC unit cell there are four atoms per unit cell located at these four points. So, these are the fractional indices of the four atoms in a unit cell of FCC material. Now this goes by the name of face centering translation, face centering translations. So, what it says - body or face centering translation, so in case of FCC. Now, in case of a BCC material we know that that there are two atoms per unit cell and their fractional indices are 0 0 0 and half half half and these go by the name of body centering translation.

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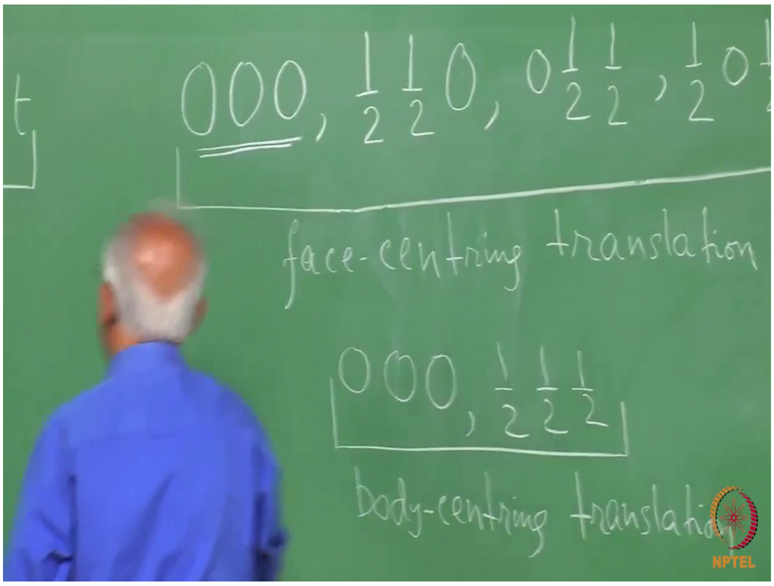

So, the first rule is for a compound crystal body of face centering translations if present must begin and end on atoms of the same kind, I will show you while illustration. The second rule is the sets of A and B atoms must separately possess the same symmetry elements of the crystal as a whole; that means, say if we take a sodium chloride crystal as you rarely see that there are four sodium atoms or four sodium ions rather and four chlorine ions per unit cell of sodium chloride. So, there are two types of atoms you know sodium and chlorine or A and B. So, the second rule says the sets of A and B atoms must separately possess the same symmetry elements of the crystal as a whole; that means, if you look at only the sodium atoms or only the chlorine atoms in the unit cell of sodium chloride individually they must show the same kind of symmetry as the crystal as a whole.

Now, we will see that you know what really means.

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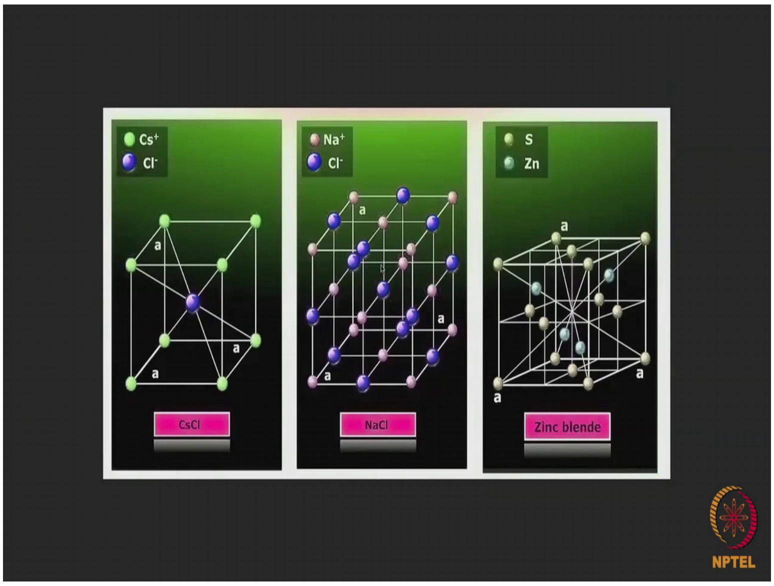

So, there are some examples of compound crystals here it is cesium chloride. So, the chlorine ion is at the center and cesium ions are at the corners of a cubic unit cell. Now this is a sodium chloride crystal, the locations of sodium and chlorine are shown here this is a zinc blende system or zinc sulfide, the sulphur and zinc atom the positions are given here, now I will show it a little bit more detail now.

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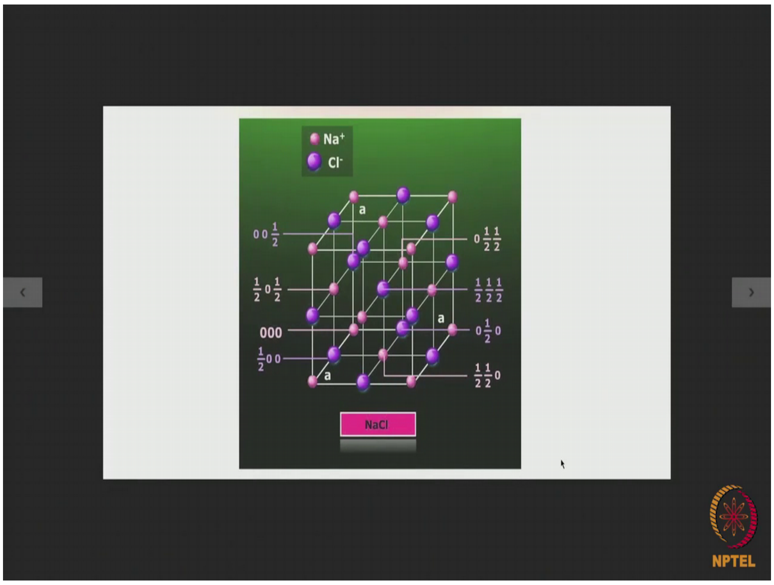

Say this is sodium chloride. So, you see here the smaller atoms are the sodium atoms or ions of the sodium and the bigger ions are the chlorine as shown over here. So, if you look at only the sodium ions you know for example, here this is a sodium ion this, this, this and this again here this, this, this, this again here you can see this. So, looking at the sodium ions what we find that they have the locations as in an FCC unit cell. So, their locations are given by 0 0 0 half of 0 0 half half and half 0 half.

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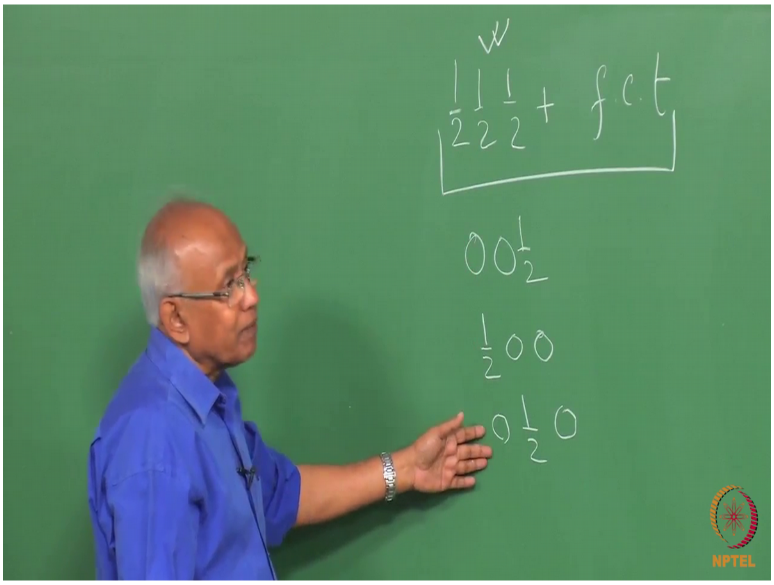

Now, what about the chlorine atoms? The chlorine atoms have the locations given by half half half plus what is known as the face centering translation. For the chlorine atoms one atom is at half half half position and others can be found out by the face centering translation; that means, the locations of the chlorine atoms will be similar to that of the sodium atoms they have the same kind of symmetry. So, what is the face centering translation? For sodium atoms if one atom is at 0 0 0 location, the other three are obtained by adding half half 0 to it 0 half half to it and half 0 half to it.

In a similar manner if we look at the location of the chlorine atoms or chlorine ion rather it is half half half and then we add up these to find out the locations, but you see if you simply add up then the locations will go outside the unit cell the fractional coordinates you know will become such that they will be away from the particular unit cell we are talking about.

So, face generate translations can be positive also can be negative also. So, what we do these numbers we subtract from half half half the central. So, chlorine atom and what are indices, what are the fractional indices we get if we subtract half half 0 - then it becomes 0 0 half if we subtract 0 half half, from this it becomes half 0 0, if we subtract half 0 half then it becomes 0 half 0. So, you see that in a sodium chloride unit cell there are four sodium ions at these four locations and what about the locations of the chlorine ions? These are the four locations of the chlorine ions. So, the total number of ions per unit cell of sodium chloride will be 8 the sodium atoms or ions are located at these positions whereas the chlorine ions or atoms are located at these positions.

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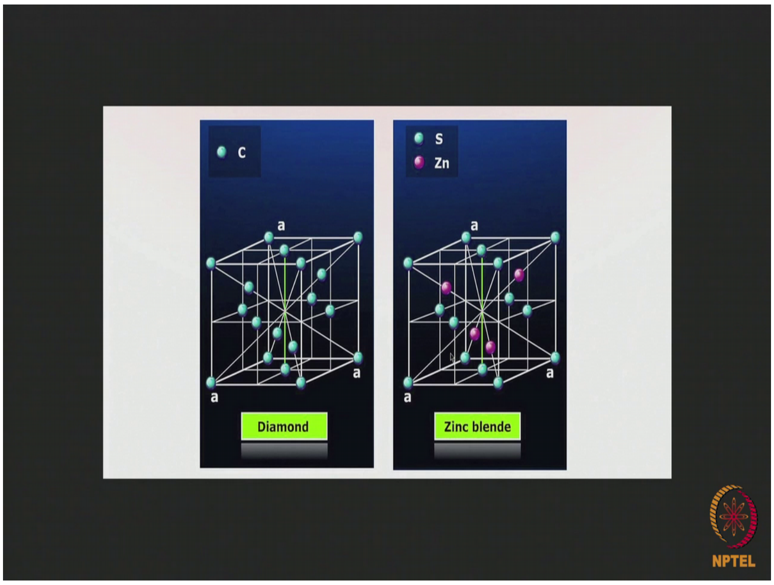

Now when it comes to diamond and zinc blende zinc blende is zinc sulfide. So far as the arrangement of the atoms in the unit cell are concerned in diamond there are 8 atoms per unit cell, 8 carbon atoms per unit cell and again in zinc blende also there are 8 atoms per unit cell - four of them are of sulphur and four of them are of zinc as shown over here. What about the locations of those? Now if we look at the diamond structure there are a total of 8 carbon atoms per unit cell and I will write down the locations of those atoms within the unit cell.

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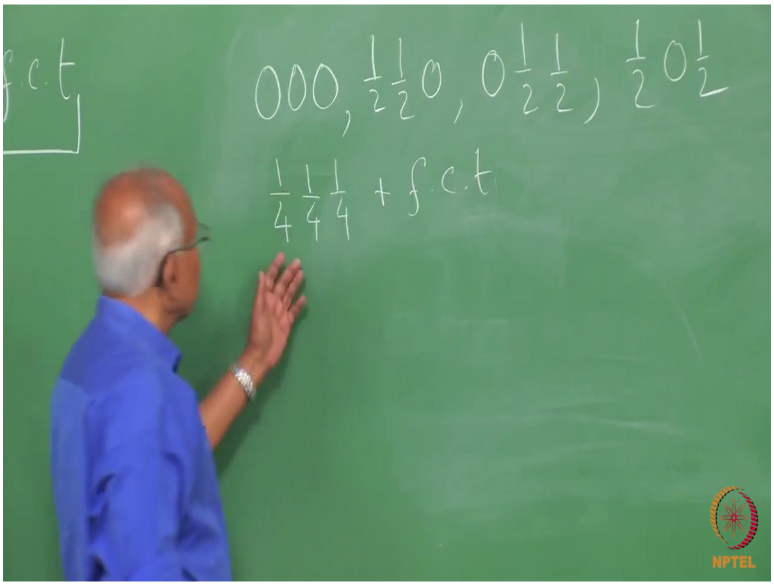

So, in diamond there are four carbon atoms at 0 0 0, half half 0, 0 half half and half 0 half as in case of an FCC unit cell, and what about the others? The others are at the locations one-fourth, one-fourth, one-fourth plus the face centering translation.

So, what we do add up these numbers to that one by one and you get the locations of the all four atoms the extra four atoms in diamond. So, there are 4 plus 4 8 atoms carbon atoms per unit cell of diamond, these are the locations of the 4 and other 4 are located at this plus the face centering translation.

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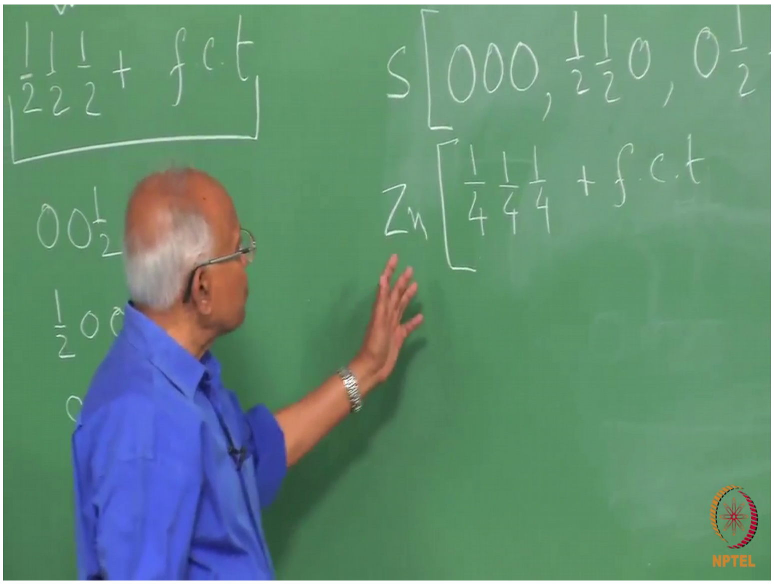

Now when it comes to zinc sulfide again these sulphur atoms are at this locations and what about the zinc? They have got this particular location and I have already shown you how to find out the locations by using the face centering translation. So, in both diamond and in zinc blende we find that there are 8 atoms per unit cell, in diamond all 8 atoms are carbon atoms; in case of zinc blende - four are sulphur, four are zinc atoms and the locations have been given over here.