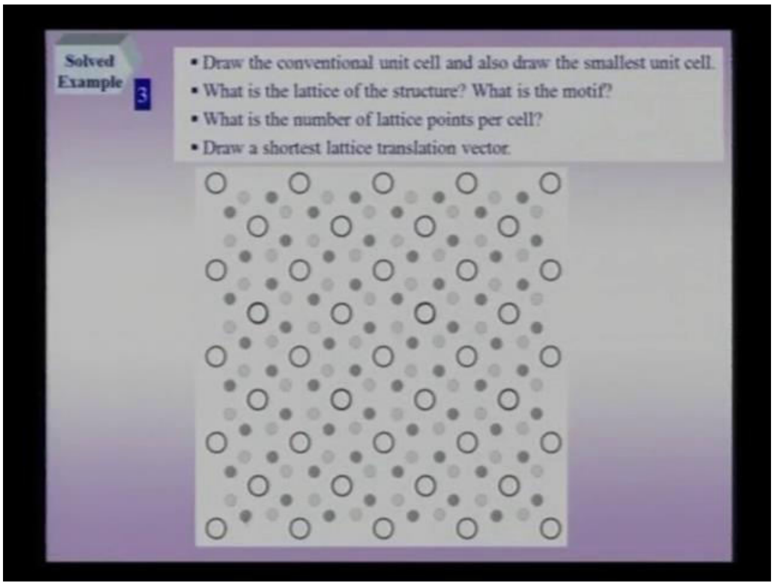
Structure of Materials
Prof. Anandh Subramaniam
Department of Materials Science and Engineering
Indian Institute of Technology, Kanpur

Lecture - 07
Chapter-02
Geometry of Crystals: Symmetry, Lattices

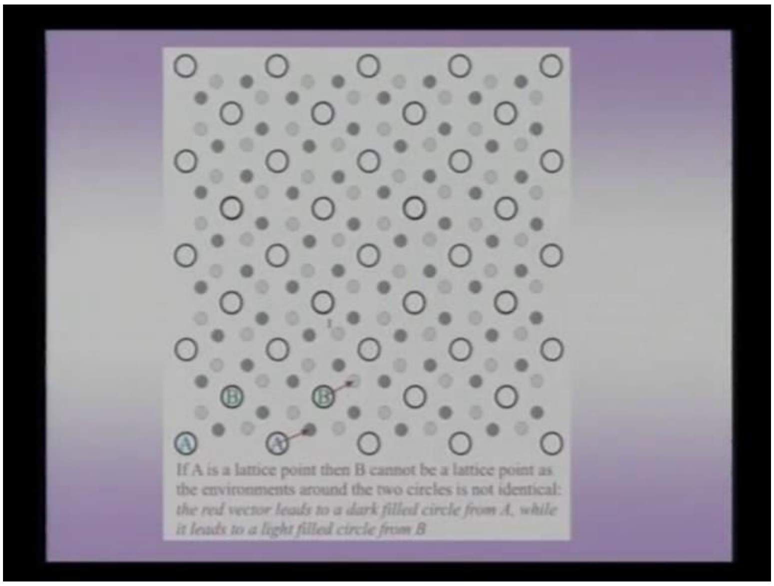
Let us consider another example to clarify some of the basic concepts, which we have been considering on this chapter. For instance, there is a structure shown to you on the screen.

(Refer Slide Time: 00:37)



Let us draw the conventional unit cell and also the smallest unit cell for the structure, what is the lattice parameter for the structure and what is the motif. We should also try to calculate the number of lattice points per cell and also draw the shortest lattice translation vector. As you can look at the structure, it is got 2 large circles, which are white colored, there are 2 grey colored circles, one of them dark grey, the other one light grey and they form a pattern, which looks very beautiful in two dimensions.

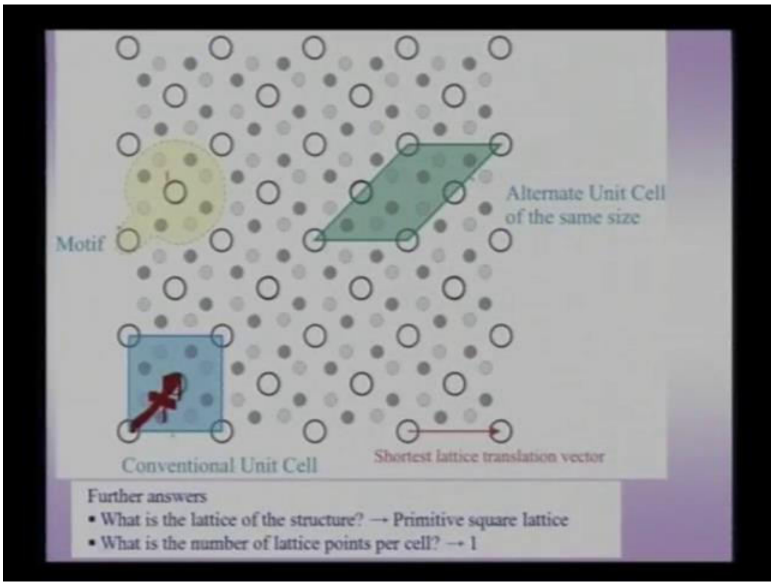
(Refer Slide Time: 01:12)



Now, I need to identify the lattice points, before I can start to draw lattice translation vectors or the unit cell. Let us look at two circles, which look identical at least in form but, we will try to identify, if they both qualify to be lattice points or not. So, let us consider A and B as the two circles, if I look at A then, at a certain distance of course, by going along x and in coming along y direction, I land up at a dark grey circle. If I do the same translation operation as shown by this red vector, I land up on a light grey circle, this implies A and B do not have identical surrounding.

That means, A and B both cannot be simultaneously lattice points so now, for my choice, let me go ahead in choose A as a lattice point that means, all the A's would form a lattice these point, (Refer Slide Time: 02:14) this point, this point. Equivalently, I could choose B as the origin and the set of B's would also form a lattice point but, the point to be noted is that, A and B both simultaneously cannot be lattice points because, of the environments being different.

(Refer Slide Time: 02:30)



Now, let us overlay the unit cells, the shortest lattice translation vector and the motif, which will go on to generate this crystal. Now, as you can see, if I join the 4 corners made of A kind of circles then, I can get a blue unit cell, which is also happens to be the smallest unit cell. However, I can go and choose an alternate unit cell, as shown by the green colored outline, which also happens to be the smallest size unit cell. How do we know it is a smallest size unit cell of course, I can calculate the area and find out that, both of them have the same area.

There is another possibility, let me calculate the number of lattice points in this blue cell, each one of these corners contribute one fourth and therefore, the net contribution to this is 1 lattice point per cell. Similarly, since these two circles do not belong to lattice points, which are of the B type, only the corners contribute and the net contribution from these corners to the green unit cell is again 1, which tells you that it is the primitive unit cell. So, if you choose at the conventional unit cell, you would actually go and choose the blue unit cell.

Now, what is the shortest lattice translation vector, the shortest lattice translation vector in this case is, the one which connects the A position to another A position, as shown by the red colored translation vector. Of course, I would have also chosen the equivalent one, which is the one connecting A position along the y direction to another A position so, both of them will be the shortest lattice translation vectors. This obviously, the vector connecting this A atom to the B atom, is not a lattice translation vector, that point has to be noted.

Mister Deaiptosh has a question for us.

Student: What is the difference between conventional and shortest unit cell?

You mean, that smallest shortest unit cell so, question of Mister Deaptosh is, what is the difference between a conventional and the smallest unit cell. This point we are considered in somewhat detail before that, we used to 3 criteria when we go ahead and make a choice of an unit cell. Number 1 being the symmetry so, we choose a unit cell, which has symmetry common cell with that of lattice and the highest possible symmetry.

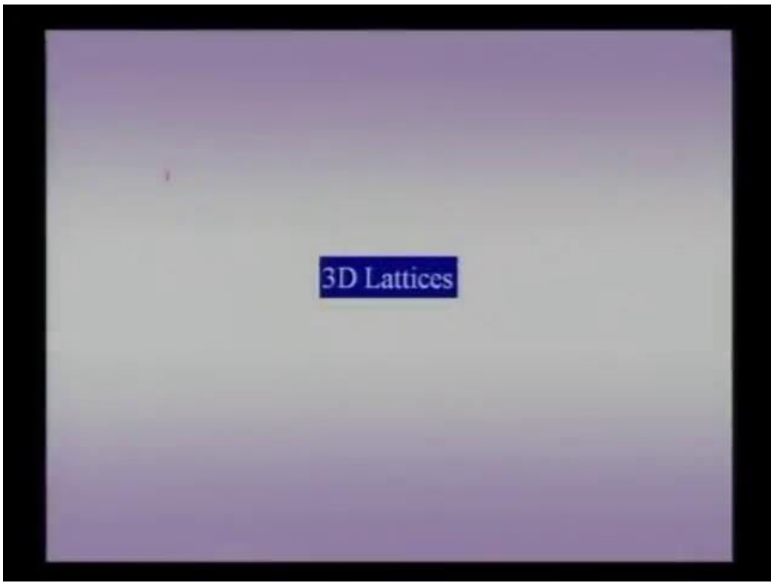
Number 2, if there are 2 unit cells having the same symmetry then, I would choose a unit cell which has the smaller size. But, if both of these fails to resolve the issue then, I would choose an unit cell, which is guided by some kind of a convention. May be, there we will considering example later on, in which we will see that, even this convention is not without some kind of a common sense logic.

Now, in this case, the blue versus the green is choice, which we are trying to make, it is clear of course, again to reattribute important fact, we are not talking about just the symmetry of the lattice, we are independently considering the symmetry of the unit cell also. So, the symmetry of the obviously, the square unit cell is higher, compared to the symmetry of the parallelogram saved unit cell. Because, this square unit cell will have 4 fold symmetry in the centre, it additionally will have those mirrors, which we have seen.

And therefore, my preferred unit cell for this, which solves for the conventional unit cell is the square unit cell. So now, let us me find out, what is the motif for this structure, which I need to put at each lattice point so that, I can generate entire structure. The motif happens to be consists of 2 open circles, the A and the B circles, as I labeled them before, it consists of 4 dark grey circles, which are filled are gray and 4 light grey circles, which I have been put within this red dotted line and shaded yellow for metastabiility.

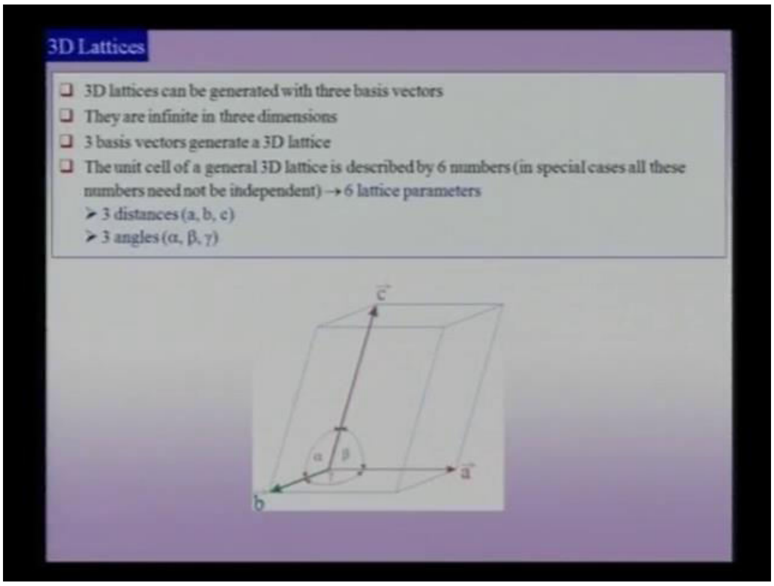
So, this is my motif, which goes and sits at each lattice point to generate this crystal structure, which is shown in the figure. Now, what is the lattice of this structure, it is primitive square lattice and what is the number of lattice points per cell, since it is a primitive lattice, it is got 1 lattice point per cell. So, this example again brings out the importance of the lattice and also the motif, and the ways we can choose a unit cell and also the shortest lattice translation vector.

(Refer Slide Time: 06:52)



Now, it is time for us to go and consider 3 D lattices so far, we have been dealing with one dimensional and two dimensional lattices. Now, let us consider some three dimensional lattices and we shall try to study their properties as well. Now, to generate a lattice in three dimensions, I need 3 non coplanar vectors.

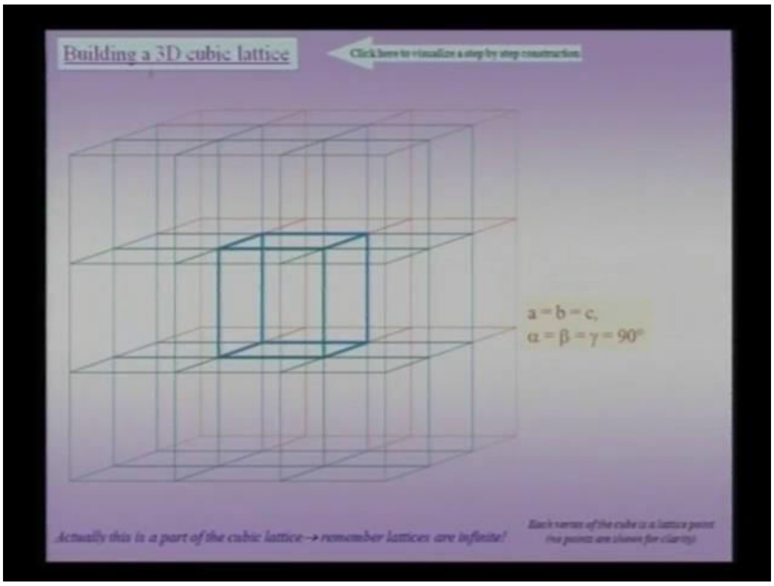
(Refer Slide Time: 07:12)



For instance, in this figure you can see, these non coplanar vectors marked as A, B and C, there are 3 angles which can be considered. The angle between the A and the B, which is given by the gamma, angle which is actually opposite the C vector, it is the face which is opposite to the C vector. Similarly, you have the beta angle and the alpha angle, which go on to define a general parallelepipedon, a parallelepiped in three dimensions.

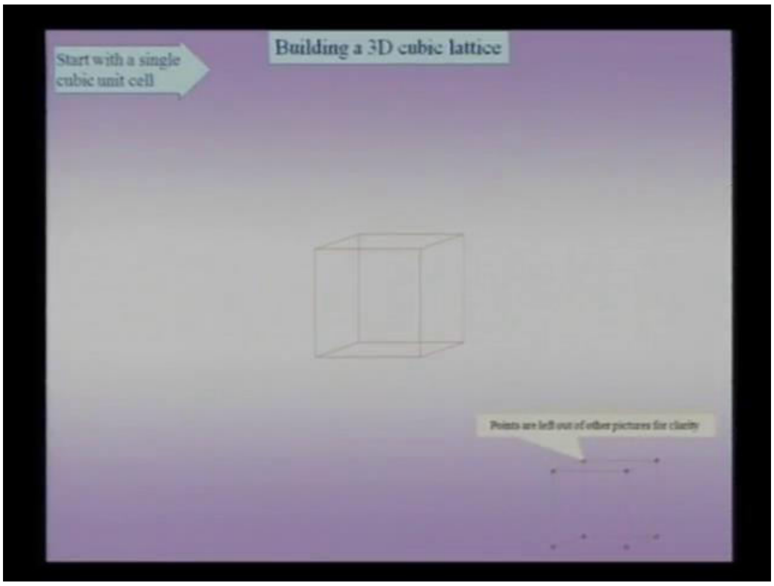
Now, these lattices are infinite in three dimensions and we can, as usual choose a unit cell, which can be used to describe these lattices in three dimensions. These as shown in this figure, we have 6 lattice parameters to describe a general lattice in three dimensions, these are 3 distances a, b and c, and there are 3 angles the alpha, the beta and the gamma. Now, as you go along studying these lattices, we will see as we deal two dimensions, there will be always be special cases wherein, some of the distances like a or b or c maybe equal to each other and there maybe some of the angles, which have some special values.

(Refer Slide Time: 08:21)

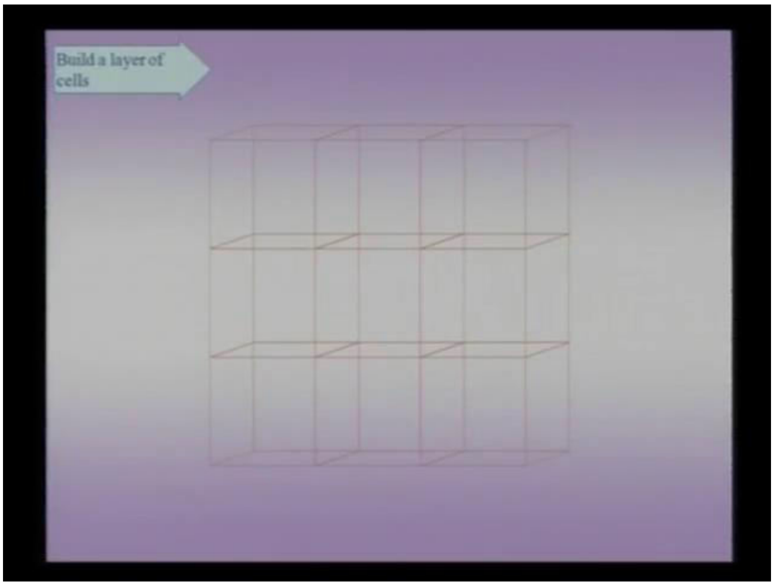


Now so, this is for instance, shown that you can actually have a three dimensional cube, which is a space filling cube. To visualize the step by step construction, let us launch a small video.

(Refer Slide Time: 08:35)

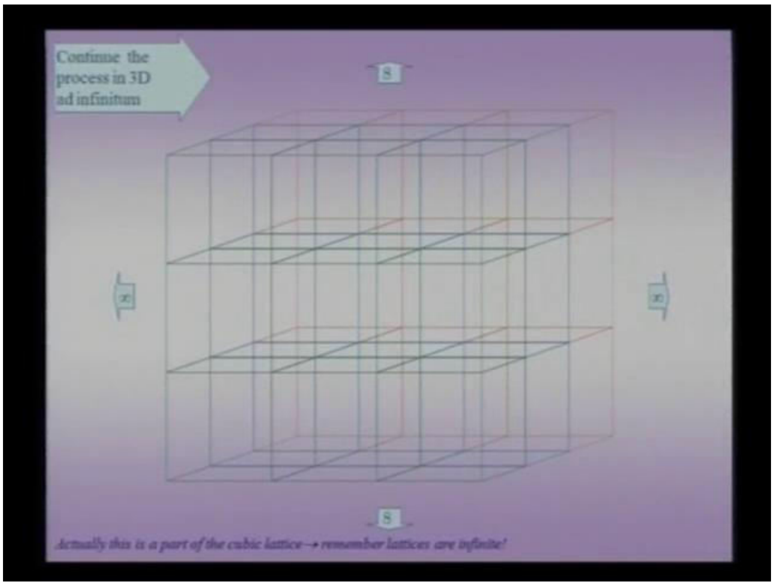


(Refer Slide Time: 08:44)



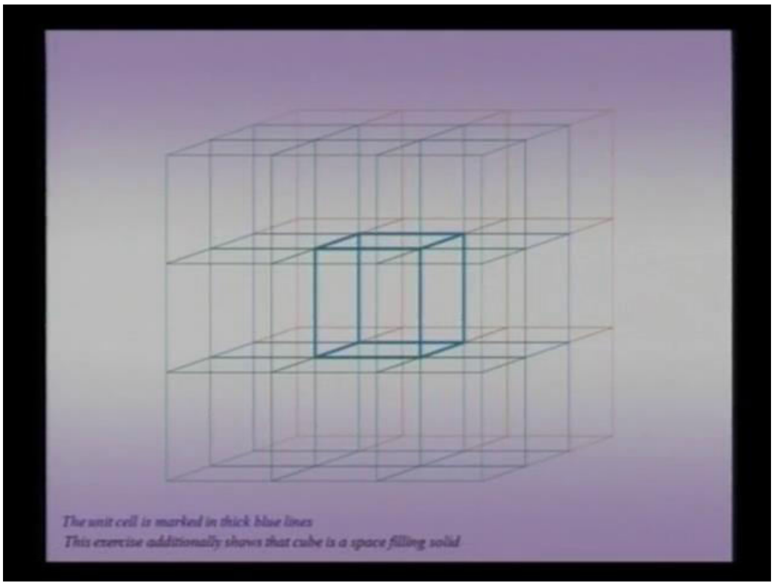
So, let us start with the single cube and then, go on to make a cubic lattice, the lattice points are at the vertices of the cube and have been left out from the construction for the sake of clarity.

(Refer Slide Time: 08:50)



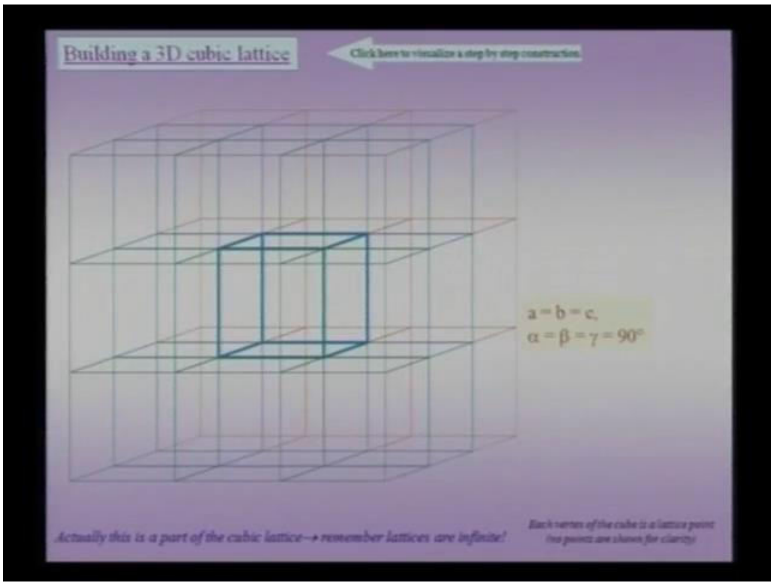
So, first starting with the cube by make a layer of cells of course, this layer has to extend to infinity, along two dimensions and then, I make the second layer. And on top of that, I can make a third layer and going for to infinity in the direction, which I am considering.

(Refer Slide Time: 09:06)



You can clearly center of this figure, which is been darken by the blue line, this exercise additionally shows the important point that, cube is a space filling solid.

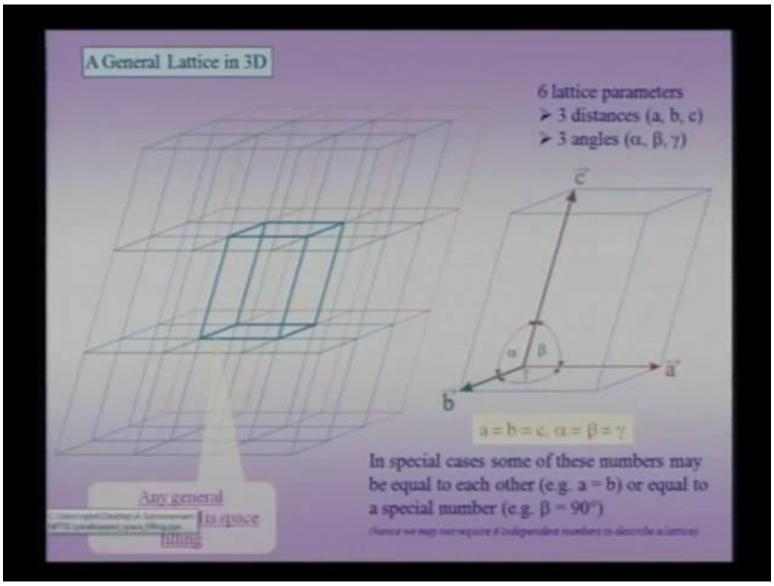
(Refer Slide Time: 09:22)



So, if I have such a lattice, which is a cubic lattice then, the lattice parameters of the unit cell, which goes on to describe this lattice will be a equal to b equal to c, and alpha is equal to beta is equal to gamma is 90 degrees. Again to emphasis, this actually a lattice that means, that it only conserve array of points at the corners of these or the vertices of this cube. And these lines are just for visualization and they have no physical meaning as far as the structure goes.

And we have to also remember that, these lattices would be infinite along the 3 directions, the x direction, the y direction and the zee direction.

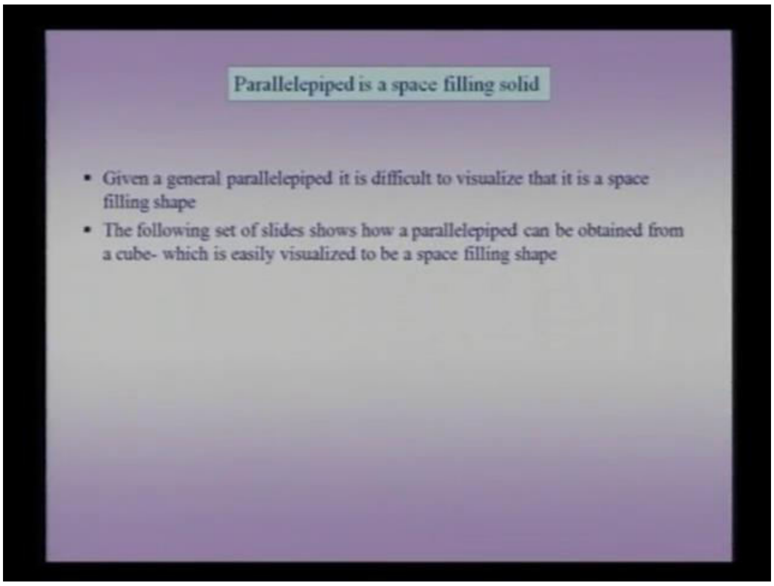
(Refer Slide Time: 09:58)



Now, this was a very special case of a 3 D lattice, which I started off with let me now, switch to the other extreme case wherein, we have the most general possible 3 D lattice wherein, I have no constraints on the alpha or the beta or the gamma. And a, b and c also have to be independent parameters, which contains values depending on the kind of lattice I am considering, the size of the lattice I am considering.

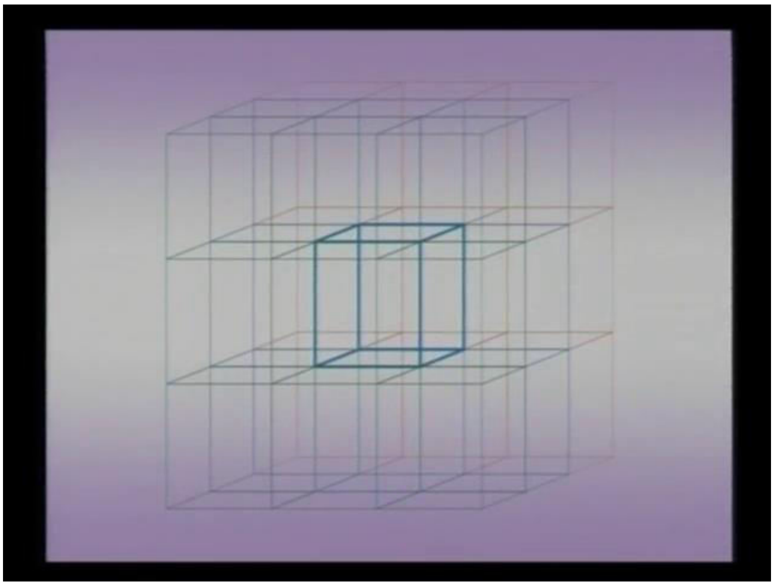
Now, let us try to visualize, how this lattice can be constructed starting with the cubic lattice, which I saw before. And additionally, this will show us, this excise will show us that, any general parallelepiped in three dimensions is actually a space filling parallelepiped. This might seem obvious after the construction of from the figure, which is drawn for you here but, unless this exercise is taken up at least for once.

(Refer Slide Time: 10:54)



It is sometimes is confusing, when you see some general kind of parallelepiped and it makes you wonder, are they really space filling.

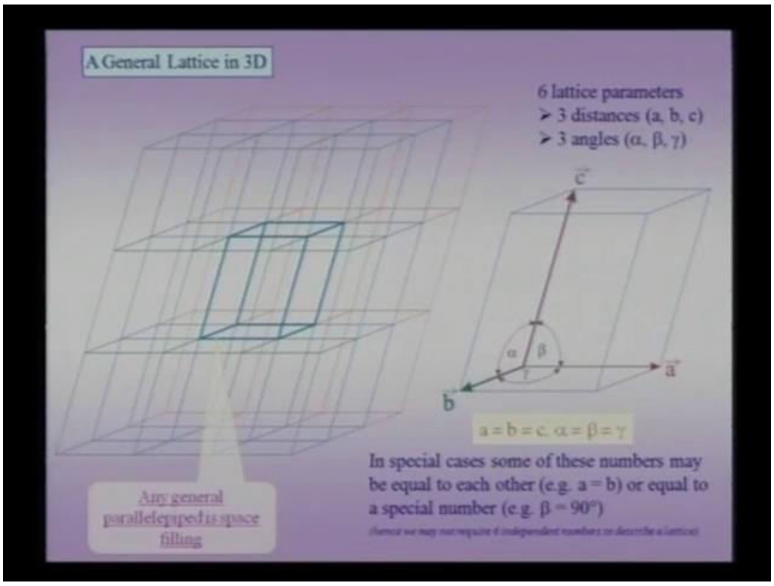
(Refer Slide Time: 11:04)



So, let us start with the original cube, which I had construct before, this is the cubic lattice with the cubic unit cell overlaid on the central one. I have the 3 directions, first I start by dilating along the zee direction, I pull this lattice along the zee direction. So that, now the C lattice parameter becomes different from the other two lattice parameters. Further to this, I can perform additional operations like I contract the lattice along the other direction, which is so that now, I am have a squeezing operation, which is taking place.

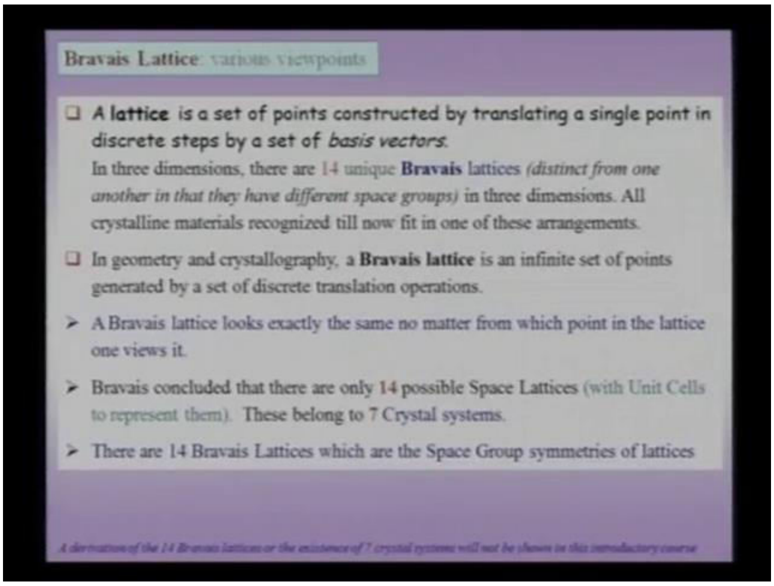
I do not want to stop here so, I done a dilation operation then, squeezing operation, I again go ahead and do a shear operation on this kind of a lattice. The shear operation is shown by the two shear vectors and the top and the bottom.

(Refer Slide Time: 11:30)



And you can see that, this a finishing lattice has been completely distorted with respect to the starting lattice and none of the original directions or distances are equal and also the angles have been distorted. So, this is now, a general parallelepiped and it happens to be a space filling parallelepiped. So, we have now considered the important fact that, any general parallelepiped can be a unit cell for a lattice in three dimensions and that is space filling solid as well.

(Refer Slide Time: 12:22)



Now, the lattices in three dimensions are called the bravais lattices and there are 14 of this so, let us try to read the matter written in the slide to understand, what are these bravais lattices. As usual, a lattice is set of points constructed by a translating a single point in discrete sets by a set of basis vectors. So, there are 3 basis vectors in three dimensions and we land up with 14 unique bravais lattices distinct from each other, have different space groups.

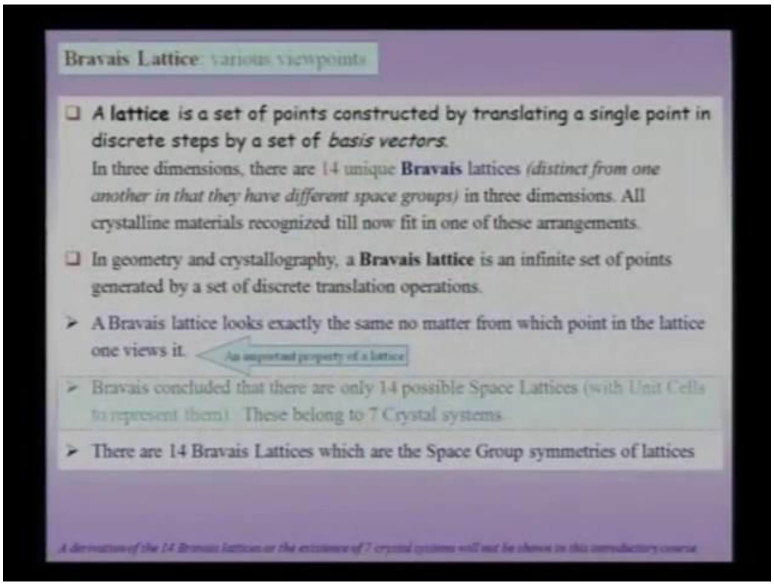
We have not constructed this conceptual space groups in detail but, in this slide we try to have a broad overview, eventhough some of the concepts are beyond this elementary course. All crystalline materials recognized still now, fit in one of these arrangements made by this 14 bravais lattices. In geometry in crystallography, a bravais lattice is a infinite set of points generated by a discrete set of translation operation.

Like before, translation is the key operation, when it comes to distinguishing lattices and important property of the bravais lattice is, a bravais lattice looks exactly the same, no matter from which point in the lattice one using so, that is an important property of lattices. And we will have few more things to say about this important property of having identical surroundings and the view from any lattice point. Bravais had concluded that, there are only 14 such possible lattices and we introduce some conventional units as to represent these lattices as before and an important point to be noted, that these 14 bravais lattices belong to the 7 crystal systems.

Of course, we will have much more to say that, how we go from lattices to crystals and then, how we classify these lattices into the 7 crystal systems, what do I mean when I say a crystal system, all these aspects we will consider in considerable detail when we actually start to build lot of crystals using these lattices. An important point, which might be noted is that, there are 14 bravais lattices, which are space group symmetries of the lattices.

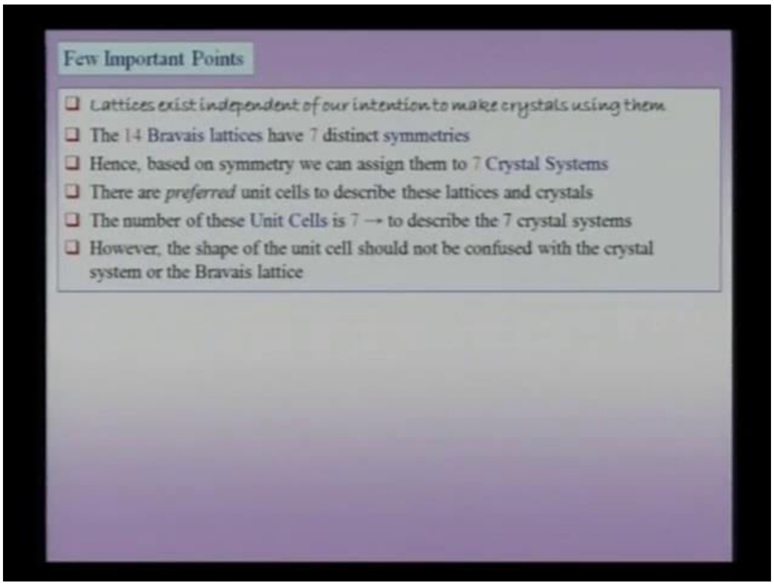
So, this again is the advance concept but, just for the passing, it is worth wide to note this statement, which is written in the end. So, we are not showing the derivation of either these 14 bravais lattices or we do not prove the existence of 7 crystals in this elementary course, but it is worth wide to note these important numbers, which will form the basis for quite a bit of the treatments, we will be did in this course. Once again, I have highlighted the important property of lattices.

(Refer Slide Time: 14:50)



And also, the existence of 7 crystal systems and the 14 bravais lattices.

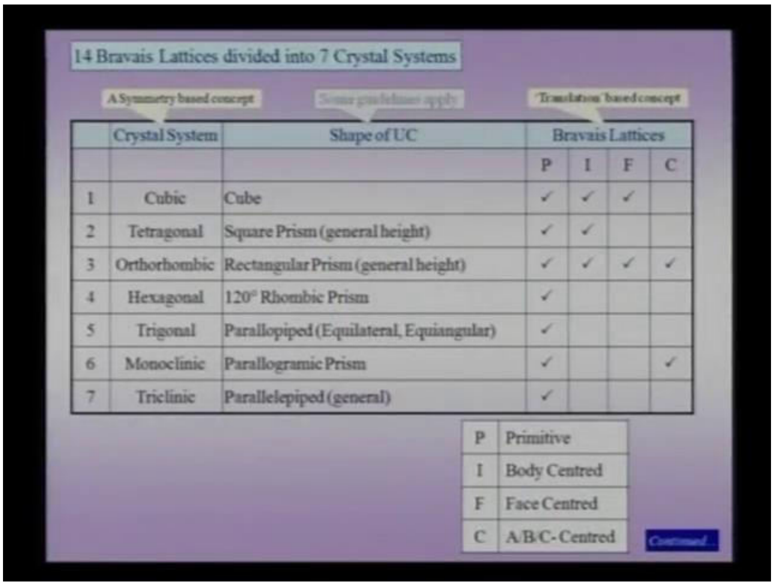
(Refer Slide Time: 14:55)



Further, let us consider few more important points, before we actually take the three dimensional lattices one by one, lattices exist independent of our intentions to make crystals using them. So, this is has to be understood clearly, yes in crystallography, our idea is to use these lattices from making crystals but, their existence is a mathematical fact and they do so without our intention to make crystals using them. The 14 bravais lattices are 7 distinct symmetries and this aspect that, based on symmetry we can assign these 14 bravais lattices to the 7 crystal systems.

So, there is a logical reason, why do we have 7 crystal systems and that is the symmetries of the 14 bravais lattices, there are preferred unit cell to describe these lattices and crystals. The number of such unite cells is 7, which we used to describe the 7 crystal systems however, we should again note that, the shape of the unit cells should not be constitute confused with the crystal system or the lattice. So, this is an important point, will again return to it in various forms to understand this varying point so, what are the 14 bravais lattices.

(Refer Slide Time: 16:05)



I have a question from Mister Patel.

Student: Sir, here the which lattice and crystal systems, they are 14 and 7, they are fixed number or we can vary.

Very very good question I have got from Mister Patel again here, first thing the s is slightly silent in bravais. So, it has to be pronounced as bravais lattices, in English we often have lot of words, in which the last alphabet is silent like p a p e r is paper and not paper, the r has to be little silent. So, this is bravais lattice and address to the specific question, are these numbers fixed, yes mathematically speaking, these 14 bravais lattices exist independent of anything else, that is a mathematical construct.

So, as long as you impose requirement, that you have translation as a symmetry and every point has identical surroundings then, you will land up 14 bravais lattices. If you look at the symmetry of these bravais lattices, you will see that there are 7 distinct symmetries. Now, would they still an independent question, would you want to call the 7 symmetries as 7 crystal systems or would I want to play some games further to it.

We had seen in two dimensions that, the crystals with three fold symmetry of course, we will come to this topic little more detail later also. But, we had briefly considered this aspect that, crystals with three fold symmetry and crystals with six fold symmetry both are put under the same umbrella and they come under the 120 degree parallelogram crystal or the 120 degree rhombus crystal.

Now, if you do not want you 7 boxes to put and call 7 different crystal names, with some people do, some of the people actually put crystals in the hexagonal class and the trigonal class, which we will construct of course, very soon. That means, crystals having only one three fold axes or having one six fold axes under the same group that means, they do not want classify them as separate classes. So, in that, if you do such a kind of a classification, you land up with only six crystal systems but, the preferred system is a 7 crystal system.

Because, as you can logically see because, they come from the 14 bravais lattices, which exist independently and if you look at the symmetries of these 14 bravais lattices, there are only 7 distinct types, which form the 7 crystal systems. So, let us try to divide this 14 bravais lattices into the 7 crystal systems and also study some important properties of them. So, we have an idea on the second column, which is a symmetry based concept, which is a crystal system.

On the second, third column, we got the shape of the unit cell, which is wherein, as we saw certain guidelines of here, apply when we try to choose the shape of the unit cell. On the right hand side, we have the bravais lattices, which is purely a translation based concept. So, what are the bravais lattices and how to be divide them into the 7 crystal systems. So, the 7 crystal systems are the cubic, the tetragonal, the orthorhombic, the hexagonal, the trigonal, the monoclinic and the triclinic crystal systems.

Now, sometimes a word crystal class is also used to describe the 32 point groups and that terminology is confusing with, when you talk about crystal systems and therefore, toward crystal classes, is to be typically avoided when describing crystal structures. Now of course, we just not very important at this stage but, just to for instance, list the some of the shapes of these typical unit cells, a cubic crystal is described by typically a cubic unit cell, a tetragonal crystal is described by a square prism of a general height, the orthogonal again which is of the general height.

That means, the height has to be different from any one of the other two lattice parameters in the plane. The hexagonal crystal is described by 120 degree rhombic prism, the trigonal crystal is described by a parallelepiped, a special kind of parallelepiped which is equilateral and equiangular which means, every face is identical and every angle is identical.

And we might also briefly see, how we can go from trigonal cubic crystal to a trigonal unit cell, the monoclinic crystal is described by a parallelogramic prism. And a triclinic crystal is described by an unit cell, which is of the most general kind of a parallelepiped wherein, there are no special constrains either on the sides or on the angles. On the right hand side, are the bravais lattices we shall of course, take up each one of these bravais lattices point by point, there are 4 types of bravais lattices, which are possible.

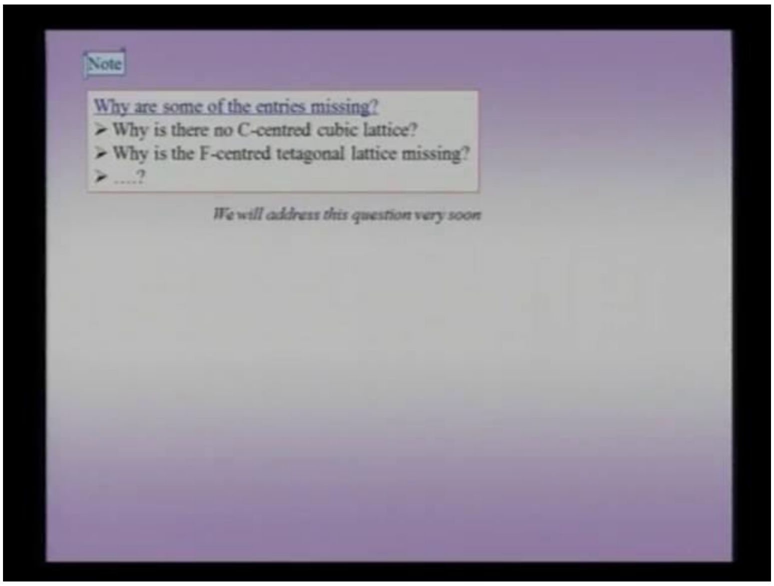
The P which stands for the primitive, I which stands for the (Refer Slide Time: 20:50) in German, which is the body centred. So, please remember, this is not from the English word therefore, I stands for body centred, F stands for face centred and the alphabet C is used sometime as a side centred or the base centred or sometimes it is also called the C centred lattice.

How could the C centred need not be along, only the c axes you could have A centring or the B centring but as a class, they form the C centred lattices. So, if you look at this table, let us see that, what kind of cubic lattices are possible, you can have the primitive cubic lattice, the body centred cubic lattice and the face centred cubic lattice but, there is no C centred cubic lattice possible. Similarly, you can see in tetragonal class, you can have the primitive, the body centred but, there is no face centred or C centred cubic lattices in the list.

In the hexagonal class, again you have certain things missing, in the trigonal class the same I, F and C are missing, the monoclinic class as you can see from the list, is the orthorhombic case wherein, you have the primitive, the body centred, the face centred and the C centred lattice possible. So, let us take up these 14 bravais lattices, as they are divided into the 7 crystal systems, we will return into this concept of a crystal system in little more detail.

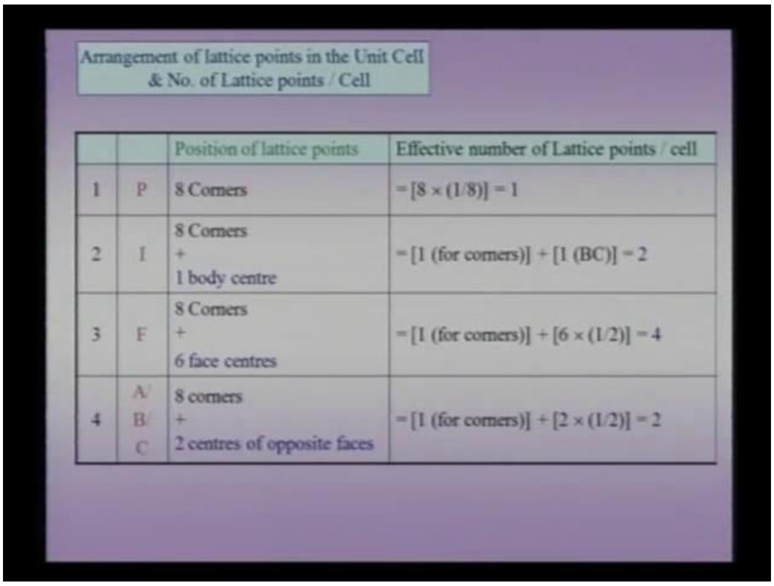
Therefore, if any confusion exist, would be clarified at later point so now, we are basically trying to understand the lattices. One important question, which comes to our mind when we consider these lattices is that, why are some of the entries missing. It was very clear when you looked at this list for instance, the hexagonal lattice there was only one the primitive, all others was missing.

(Refer Slide Time: 22:37)



So, in the list there are many of these lattices, which were missing and like in the case of two dimensional lattices, we can ask this question, why some of these lattices are missing for instance specifically, why there is no C centred cubic lattice. Why the F centred tetragonal lattices missing, we will soon return to this question and answer with a few examples, why some of these lattices gone missing.

(Refer Slide Time: 23:02)

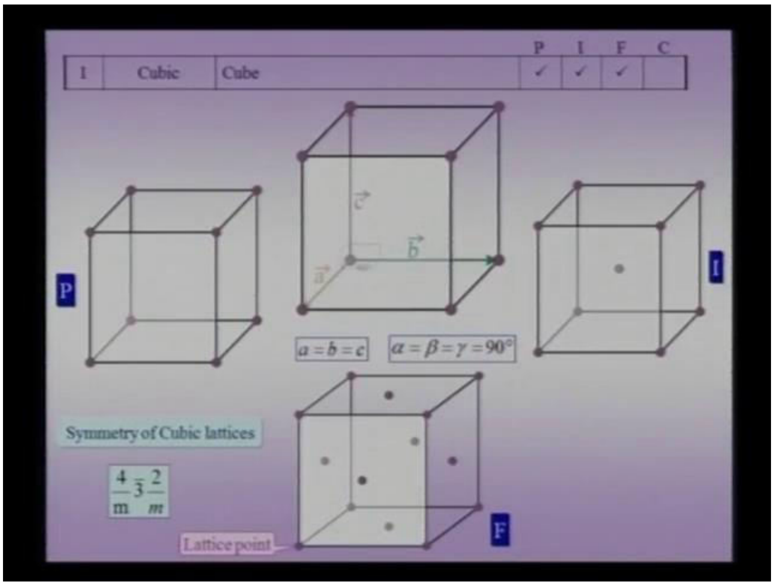


So now, since there are 4 types of lattices possible, the primitive, the body centred, the F centred or the face centred and the C centred lattice possible now, let us look at the contribution each lattice point makes to or unit set. Now, in a primitive lattice, each lattice point at the corner contributes only a average of one eight of course, depending upon the shape of the lattice, this contributions may or may not be equal, as we have seen before.

But typically, you have 8 of them contributing a total of one eighth on an average, giving rise to 1 lattice contribution, in the case of a primitive unit cell therefore, primitive automatically implies 1 lattice point per cell. In the case of the body centered lattice, the 8, as before give a contribution of 1, at the which once located at the vertices of the lattice or the lattice of unit cell, they give a contribution of 1. There is one, which completely included within the unit cell, which is giving a contribution of 1 therefore, all body centred lattices have to contribution of 2 lattice points per cell.

For the face centred, you have we will see that, there are lattice points at the corners and in addition, there are lattice points at the centre of each face of course, you will see examples to make this matter very clear. But, there are lattice points at the centres of each face, each face is shade between 2 unit cells and therefore, they have contribution of half. Since there are 6 faces, we have contribution of 3 from the faces, 1 from the corner making it a total of 4 lattice points per cell. In the case of the C centred lattice, there are 1 contribution as usual coming from the corners in addition, there is 2 half contributions coming from the opposite set of faces, making contribution of 2 to the unit cell. That means, they are effectively 2 lattice points per cell, in the case of a C centred or A centred or B centred lattice.

(Refer Slide Time: 25:12)



So, now, let us try to take these lattices one by one in three dimensions and try to understand a additional using model, that how can we understand lattices. So, let us start with the cubic lattice, as we saw in the cubic lattice we can, the shape of the unit cell is a cube as shown you in the centre. There are 3 kinds of centrings or additional lattice points possible, only two of them are present one is missing so, you have the primitive, the body centred and the face centred, no C centring is possible.

And you also additionally, can ask the question why is the C centring not possible now, whenever we are showing such a figure, I will have the general figure in the middle, which show the basis vector and the relationship between the angles of these basis vectors. We will also show this relationship, interrelationship between the lattice parameters explicitly at the bottom in addition, we will also show the three lattices possible.

An important point to note in these figures would be the symmetry, which is on shown in the blue colored box. Now, this is the very important point to note because, we said that this 14 bravais lattices only 7 distinct kind of symmetries. That implies automatically, that let it be a P lattice or a P cubic lattice or the body centred cubic or the face centred cubic, the symmetry of all of those kind of lattices will be the same, which will be along according to the Harmon MoGwan symbol, 4 by m 3 bar 2 by m.

So, what I will do now is that, let me show this is a cube on the left hand side image only, lattice points are present along the vertices. Like I told you in the body centred case, we have lattice points in the corner and in addition, there is a lattice point at the centre of the cell. And if you want to track the vertices of that or coordinates of that lattice point, it will be half half half and such a lattice point will be, line along the body diagonal of the cube.

So, it will be half the distance of the body diagonal of the cube now, in the case of the face centred cubic lattice, you obviously, have the lattice points at the corners and in addition, you have lattice points at the centres of each face. So, there are 6 faces and percent of each one of these faces, we have a lattice point. (Refer Slide Time: 27:38) and as we are pointed out in the previous slide, each one of these can only contribute half to the unit cell.

Because, each unit such unit cell will be shared between two neighbors and therefore, this is lattice point make a contribution of half to this unit cell. Before I take up the case of tetragonal lattices, let me try to illustrate what we have seen so far, for the cubic lattice using some other models I have got right with me here. And before I go to the model, Mister Patel has got a question.

Student: Sir, how can I determine the symmetry independently, (Refer Slide Time: 28:14)

Very good, so this symmetry representation though, we have dealt with an a little bit or in a brief manner in the very first chapter maybe, we can return to it later in the course. But, this is basically, what is called the Harmon MoGwan symbol and we saw that a cube actually has a symmetry. So, may be using a model, I briefly show how the symmetry elements are possible but, as you might remember, we have consider this in the early chapter on symmetry cut (Refer Slide Time: 28:47).

So, to answer Mister patel’s question, I got a model here of a cube and using this, I will show the symmetries of this cube and for now, I will assume to the points, which are relevant of these lattice points at the corners, which are in red color. So, you can see the red colored points and I wish to show the symmetries of this cube obviously, this cube has a four fold symmetry, which goes from the centre of one face to the centre of the other face. This is my four fold axis and as if you look at the Harmon MoGwan symbol, I have got the symmetry of the cube as 4 by m, which I can write on the board.

(Refer Slide Time: 29:27)

Now, the symbol 4 by m tells me that, there is a mirror perpendicular to this four fold axis and actually, the seat of the mirror is exactly half way between the top face and the bottom face. Similarly, the cube would have a four fold axis along any one of these directions, joining the centre of the opposite faces and there would be a mirror, which bisects these edges so, that is the 4 by m symmetry, which is the cube having.

It has an additional symmetry, the 3 bar symmetry which you can see, a 3 bar symmetry implies a three fold roto inversion axis, which is actually an higher order operator as compared to the three fold axis. Yes, a cube also has a three fold symmetry along the body diagonal, as you can see, this is my body diagonal of the cube and there is a threefold symmetry.

But, whenever I have a higher order symmetry then, I use that symmetry to describe the object and not the lower order symmetry to give an example, let me consider a hexagon on the board. So for now, will have to assume this is a regular hexagon and this hexagon would have a six fold symmetry at the centre. Needless to say, this hexagon also have a two fold symmetry and a threefold symmetry but, these symmetries are lower order symmetries as compared to the six fold symmetry.

And therefore, whenever a question is asked, what is the symmetry of this hexagon, I will report the symmetry of this hexagon is six fold and I will not use lower order symmetries, which happened to be sub group of these six fold symmetries. Similarly, even though the cubic lattice of the shape of a cube has a three fold axis along the body diagonal, I will report the symmetry to a 3 bar symmetry and not merely a three fold symmetry.

Now, as you will see very soon, the very characteristic symmetry of a cubic crystal is this existence of this three fold along the body diagonal and not the existence of the four fold. The last symmetry, which I need to consider in the symbol is the 2 by m symmetry, the two fold axis is exist at the line joining the opposite edges. So, the opposite edges are joined by line and that line is the direction of the two fold axis, you take any pair of edges say, the this edge and this edge, and you have a two fold symmetry.

How do I now got a two fold symmetry, I can rotate it by 180 degrees and the cube will look exactly identical. It is similar to the existence of a three fold symmetry along the body diagonal, in which case I would rotate by 120 degrees to leave the shape invariant. Now, apart from this two fold, there is a mirror perpendicular to two fold so, my two fold direction is this, to joins the opposite ends to the body diagonal and the mirror bisects this two opposite faces as a diagonal.

So, I have a plane, which passes through like this, the mirror plane which actually bisects this line joining the two opposite edges. So, I have a 2 by m symmetry and therefore, as a combined symmetry, I can write the symmetry of this object as 4 by m 3 bar 2 by m, which is the characteristic symmetry of all cubic lattices. As we were discussing cubic lattices, I have it means some models here, which I am going to use to explain the lattices, which we just known so on the computer.

In between, I have a question from Mister Ravi.

Student: Sir, is there any 4 bar symmetry in cubic crystal?

A good question again, can be a 4 bar symmetry into the crystals but yes, there can be 4 bar symmetry in cubic crystals and we were actually consider some examples of those crystals wherein, 4 bar symmetry exist. But, the higher symmetry in this case happens to be the four fold and therefore, we consider the higher symmetry to describe these lattices. And then, we make crystals out of this we will see that, those crystals can actually have lower symmetry and along those possible symmetries is the 4 bar symmetry.

So, now, let us focus on these 3 models I have got with me here, in this case you will have to assume that, these are actually not large blue spheres but, actually points. Because, now we are considering lattices and therefore, lattice consists only of points so, these for my consideration, are points. Later on, I will use a same models to describe crystals, at that point of time, you will have to assume they are motifs but for now, they are lattice points.

So, I have a model of the simple cube on the left hand side, I have a model of the body centred cubic structure on the right hand side here and behind those two models, I have got the structure of a face centred cubic unit cell. So, let take up one of them in hand the simple cubic unit cell, as I can clearly see that, this has got 8 points at it is vertices, each one of these points is now shared between 8 such cubes. one cube of course, is this one there will be cube to it is right, which also share this lattice point, there will be a cube above it, which will share a lattice point, there will cube on this quadrant, which is also share this lattice point.

And correspondingly, there will be 4 cubes behind it 1, 2, 3 and 4, which will share this lattice point effectively, this sphere has been shared by the one eighth of region of this lattices and therefore, effectively the contribution to this lattice is just 1. So, this is my simple cubic unit cell, which is the unit cell of the cubic lattices now, let me pick up the body centred cubic lattice, again I have to assume that these are not spheres and these are merely points.

Now, if I look at the unit cell now, the unit cell is a cube as before because, all the edges of the cube are marked in red. These additional points have to be ignored because, these additional lines or strands have to be ignored because, they are just merely there in place to hold the central position in place and they are not meant us to be any descriptors of this unit cell so, unit cell itself is made of these red strands. Now, as you can clearly see, these 8 points contribute one eighth to the cell, totally making a 1 lattice point.

In addition, there is 1 in the centre, which is completely contained within the unit cell and that has a contribution of 1 to this unit cell and therefore, it has a contribution of total

2 lattice points per cell. Now, as I pointed out well I mentioned in the videos, that this lattice point bisects the body diagonal. What is the body diagonal of the cube, the body diagonal of the cube is the one, which is the connecting this bottom sphere to the top sphere, which is along the three fold axes of the cube or before if we use the correct terminology 3 bar axes of the cube and this body diagonal is bisected by this point in the middle.

Now, how many of such body diagonals are there in this cube, it is obvious from this, there are 1, 2, 3, 4 body diagonals within this cube and each one of those four body diagonals is bisected by the central point, which is the position half half half in the cube. Now, let us take up the next model, the model of the face centred cubic lattice now as usual, we have points in the corners the 8 points in addition, every face centre has a point in the middle.

As before, I should only focus as far as unit cell goes on the red strands and not on these other metallic strands because, those are there just to hold the balls in place and not to describe the unit cell or the structure. Now, the contribution as I pointed out from these opposite face falls is just half the unit cell, as you can see only half of this slides in the unit cell, other half is on the unit cell in the right. And therefore, have the contribution of 3, these opposite back contributes 1 and there are 6 such pairs therefore, you got the contribution of 3, one from the corner, 4 lattice points per cell.

Now, this lattice point bisects the face diagonal, which is the 1 1 0 direction of the cube and therefore, all the face diagonals are bisected by this lattice point. Now, an important point to note, either for this kind of lattice or for the body centred cubic lattice is the existence of identical surroundings. When we say existence of identical surroundings, I mean if I am a sitting at this lattice point or I am sitting at this lattice point, space should look exactly identical to me.

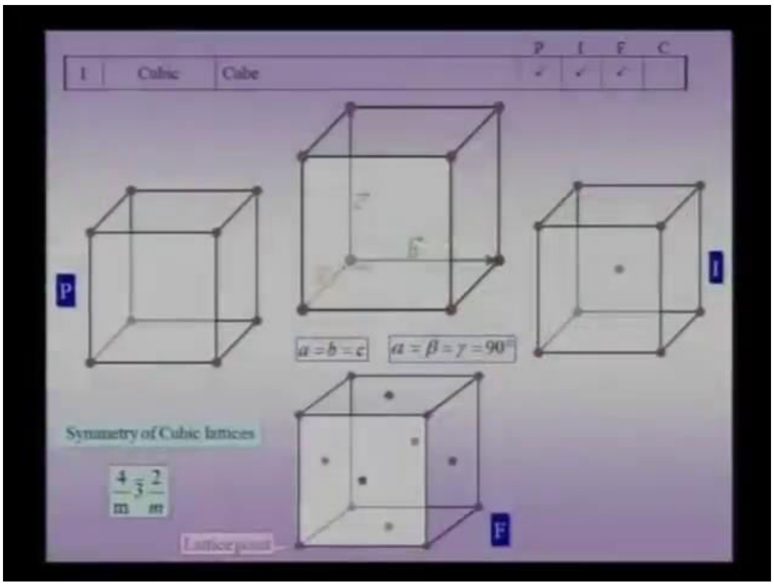
If I am sitting at this lattice point, I travels along the x direction by a distance half, travels my x direction along half, z direction half, I would come to the lattice point. If I do the same exercise half half half, I land up on another lattice point, and which clearly shows that, every lattice point has an identical surrounding. The same visualization sometimes is little more difficult for the cubic lattice but, we should nevertheless try to do the same.

And in this case, what is my shortest lattice translation vector, my shortest lattice translation vector in this case is not a cubic, it is actually this vector, which joins the 0 0 0 position to the half half 0 position. So, this is my shortest lattice translation vector, which I can show by this red arrow here so, this my shortest lattice translation vector and if I use miller indices to describe this vector, it appear half half 0 vector or the half 1 0 vector, as it is conventionally written.

Now, as responding out, each lattices has an identical surrounding that means, if I start from for instance, this point travel along the x direction half, travel the y direction half, I land up at a lattice point. Let me do the same exercise and let me see what happens so, I travel half half and land up at a lattice point. Similarly, I can locate longer and longer translations to locate different kind of suppose, I want to land up at this lattice point, I can go x half, y half, z 1, if I do the same operation again, I will land up at the lattice point.

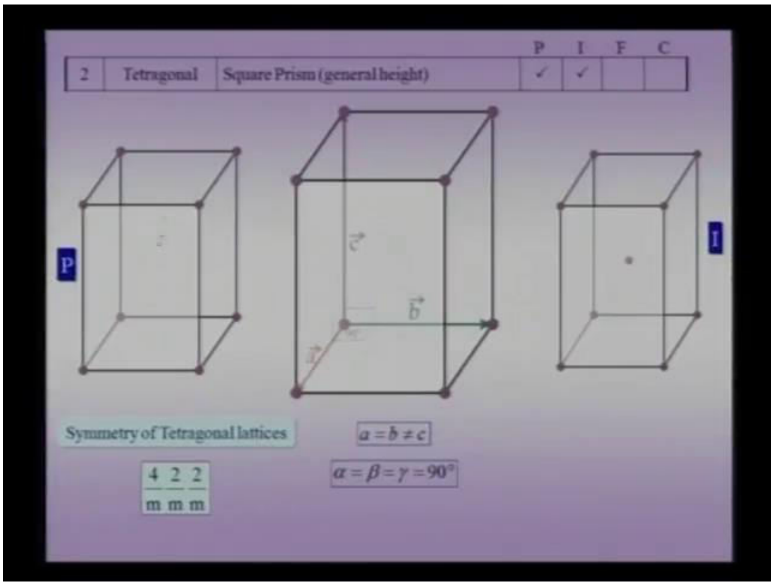
So, even though, when at the way I am representing this cube, the way this cube has been drawn it seems to me that, these lattice points are somehow looking different from these lattice point. It is not the case, every lattice point is exactly identical, I could have chosen the origin here and the unit cell will look like this. I could have chosen the origin at this half half 0 point and origin again would look exactly identical.

(Refer Slide Time: 40:13)



So, we have seen, that there are 3 distinct cubic lattices the primitive, the body centred and the face centred.

(Refer Slide Time: 40:18)

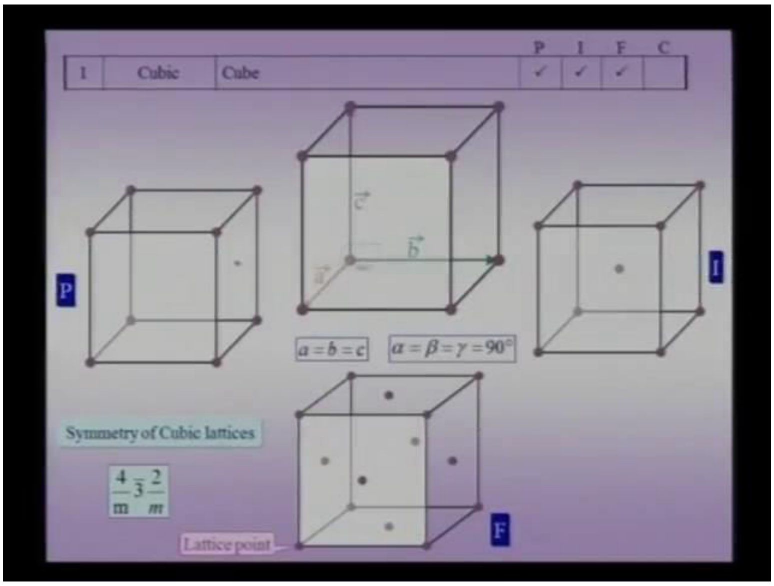


Now, let us go down to certain lattices, which slightly lower symmetry like the tetragonal lattice. The typical unit cell as you can see, which is used to describe these tetragonal lattice is a squared prism that means, there is a base which is square and it is a prism in the zee direction. If I want to write down the lattice parameters for such a unit cell, it will be a equal to b, which is not equal to c and alpha is equal to beta is equal to gamma is equal to 90 degrees.

Therefore, is an orthogonal system, if you look at the lattices which are possible for the tetragonal system, they are the primitive lattice and the body centred tetragonal lattice, the face centred and the C centred lattices are not there in the listing. As before, the primitive lattice means there are only lattice points at the corners of the cell and I mean, I am talking about a body centred tetragonal lattice, there is one point at a distance half half half, which is the body centring position.

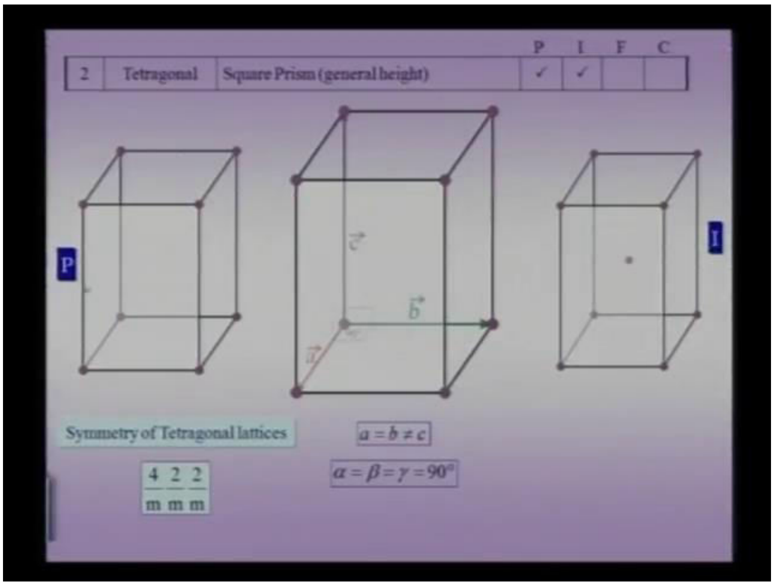
As before to qualify for a lattice, every lattice point should have a identical surrounding which is what, is true for this kind of a body centred lattice aspect. Now, the symmetry of these tetragonal lattices happens to be 4 by m 2 by m 2 by m. Now, all the tetragonal lattices that means, both the once shown here, the primitive and the body centred tetragonal lattice should have the symmetry 4 by m 2 by m 2 by m symmetry. Now, you can clearly see that, the 3 in the second place is missing and that is important to note. Additionally, we saw in the case of a cubic lattice, that the 3 face, 3 orthogonal faces you put along the x, y, z direction, you would actually have a four fold axis like here.

(Refer Slide Time: 42:14)



I could draw four fold axis starting from this and going upward, the fourfold axis which connects the centers of these two opposite faces and one along the y direction.

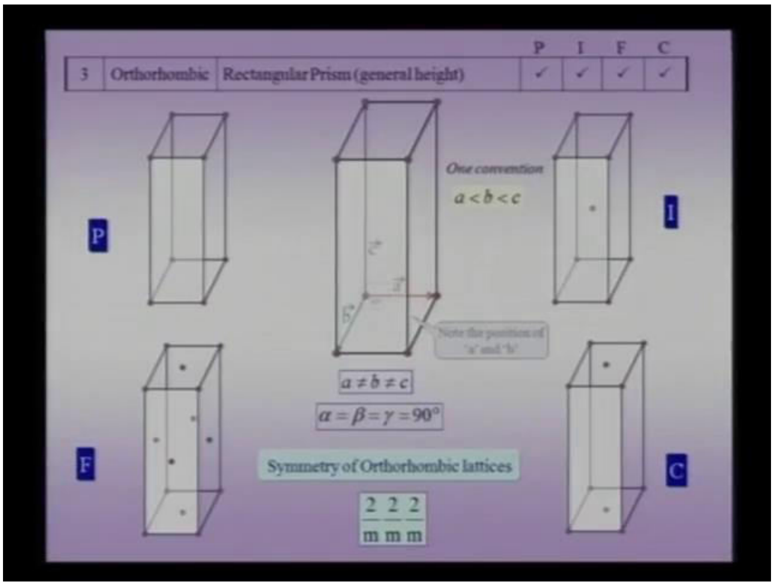
(Refer Slide Time: 42:23)



You can clearly see, there is only one four fold axis in the case of the tetragonal lattice and that fourfold axes happens to be along the C direction. You can draw the four fold directions starting from the centre of this face to the centre of the top face. So, the symmetry of all these tetragonal lattices is 4 by m 2 by m 2 by m so, where are these mirrors, the mirrors are the ones as before, bisecting the body into two. So for instance, four fold would be along this direction and the mirror would be bisecting this face.

Now, corresponding to the mirror, which is this mirror you can have a two fold axis, which goes in the this, what we might call the y direction, which is along the b direction. So, the b direction is a direction of two fold, the a direction is the direction of two fold and only the c direction has four fold symmetry in the case of the lattice or there are mirror itself, which is been shown here.

(Refer Slide Time: 43:27)



We can now consider even lower symmetry crystals or lattices and in this case, the third lower in the list is the orthorhombic lattice. The unit cell you used to describe such a lattice is the rectangular prism and this rectangular prism means, you got a rectangle, which is been allow to grow in the third dimension and therefore, grows to be a orthorhombic unit cell. The one typical convention used when you describe these kind of a unit cells is that, a is chosen to be smaller than b, which is showed in to be smaller than c.

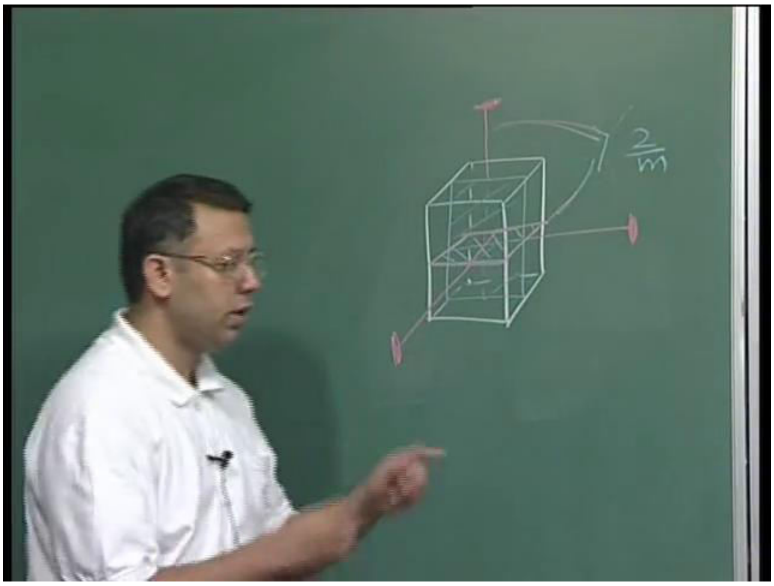
But, there are other convention which are also possible but, there is no great sanctity as for the symmetry or of the lattice in this choice of the order of the lattice parameters at lengths. But however, certain conventions obvious help in communication across crystallographers and medical scientists working in the area. What are the kind of lattices possible in the orthorhombic case, all possible lattices are there the primitive, the body centred, the face centred and the C centred lattices are possible.

And as you can see from the figure, there is no relation between the A, B and the C lattice parameter however, all the angles have been constrained to be 90 degrees. As in the case of the cubic lattice, the primitive lattice has only points in the corners, the body centred orthorhombic lattice has one additional point in the centre, the face centred orthorhombic lattice has points in all the corners and additionally, at the centre of each face.

As before, these lattice points make a contribution of half to the unit cell, while the ones in the corner make a contribution of one eighth to the unit cell. There is an additional lattice possible for the orthorhombic case, which is the C centred lattice and there could be cases where, instead of the centring b along the c direction, you can choose a centring along the b direction or the a direction and this additional lattice points only contribute half to the unit cell.

So, this is the C centred orthorhombic lattice, which is an addition to the previous list as far as, the cubic and the tetragonal lattices go. In the tetragonal lattice we saw that, the lattice has got a four fold symmetry and therefore, we have a symmetry of 4 by m because, you can see clearly, this is these 4 points are related by a four fold symmetry. Now, these 4 points are not related by four fold symmetry and therefore, you got a symmetry of the orthorhombic lattices, as being 2 by m 2 by m 2 by m. That means, each one of these directions would be a two fold axis and the mirror is perpendicular to it. So, let me go down to the board and draw such a lattice just for the sake of convenience and see, how they can get the 2 by m symmetry.

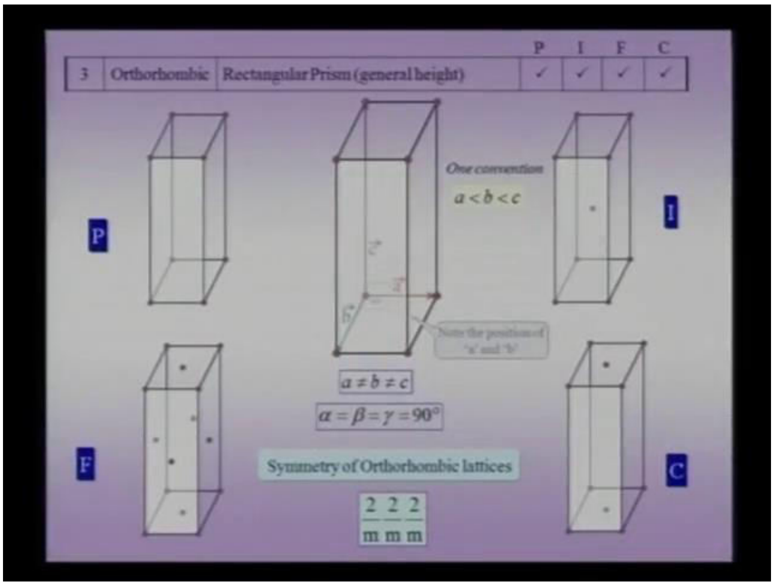
(Refer Slide Time: 46:21)



So, this is my for instance, a general orthorhombic unit cell suppose, I am not considering the a's and b's as shown in the diagram but, I just considering a random orthorhombic lattice. So now, this is my directional the two fold for instance, which I show by the symbol, which connects the opposite faces. Now, the mirror plane in this case scales as before so, to combine symmetry of these two operators, I write as two by m symmetry.

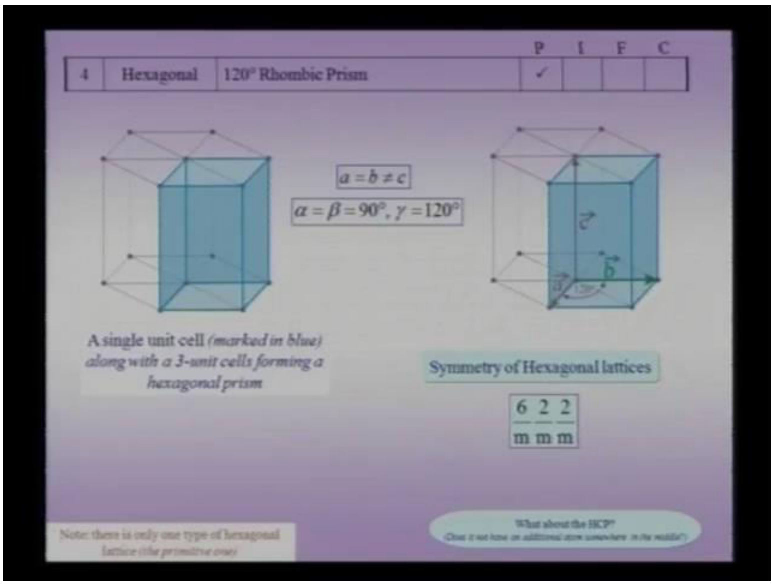
Now similarly, this direction is also a direction of two fold and there a direction also has two fold. Correspondingly, there are mirrors, which connect these faces as well and to avoid drawing too many mirrors, I just draw two of them you can see that, there are mirrors which are perpendicular to these 3 two fold directions. Therefore, I got two fold axis and the mirror perpendicular to it, this two fold axis has this mirror perpendicular to it, I just outline this mirror in red direction so that, I know that this is the one, which is perpendicular to the two fold so, I got 3 2 by m symmetry.

(Refer Slide Time: 48:02)



So, let me return to the slides so now, orthorhombic lattices have 2 by m 2 by m symmetry. And as we shall see later that, some of the crystals, which belong to the orthorhombic crystal class could can have a lower symmetry.

(Refer Slide Time: 48:12)



The next lattice we consider is the hexagonal lattice and as the name suggests, the hexagonal lattice has got a six fold symmetry. Now, the only kind of a hexagonal lattice possible is the primitive hexagonal lattice, the body centred, the face centred and the C centred hexagonal lattices are not possible. If you look at the unit cell of a hexagonal lattice, it is actually 120 degree rhombic prism, it is the prism which is drawn in the blue color.

Now, often you would see representations in text books wherein, you would have actually see an hexagonal cell is being drawn. It is to be absolutely clear, this is actually a combination of 3 cells, it is a composite of 3 cells and not a single unit cell for the hexagonal system. Now, the reason for drawing 3 unit cells is obvious it is show that, we can actually visualize the hexagonal symmetry, which is present in these lattices.

The basis vectors for such a unit cell are a, b and c, the angle between a and b is constrained to be 120 degrees, if it not constrained then, this lattice would not have this hexagonal symmetry. The angle between a and c and similarly, the angle between b and c is 90 degrees so, we can have that, the relationship between among the lattice parameters as a equal to b is not equal to c. Alpha is equal to beta is equal to 90 degrees, the alpha and beta are in the angles between a and c, and the b and c axis and the gamma, which is the angle between a and b is equal to 120 degrees.

The hexagonal lattices have a symmetry of 6 by m 2 by m 2 by m symmetry now, what we shall do before we go to deep into this hexagonal lattices. We would like to actually see a model of this hexagonal lattice and try to understand, this lattice in a little more detail. And the model we have got here, is again a combination of 3 unit cells and we again, will deal in a single unit cell within these 3 unit cells.

To understand the concepts we were just talking about, the existence of an hexagonal lattice, I have model here infront of me, which I will use to illustrate the hexagonal lattice and also the unit cell of the hexagonal lattice. But before that, I have a question from Mister Patel.

Student: Yes, we know that, here I, F and C points are absence but, we are determined to know, what will be the symmetry points if we locate some points.

Very good question so, Mister Patel has asking I know for sure, that given the fact that I can listed only a simple hexagonal lattice. What happens if I actually enforce by putting centrings for instance, I can put a C centring, I can put a centre at each one of these faces a lattice point and I can have an F centring or I can do a body centring to this kind of a lattice, what would happen.

This is precisely the kind of questions we will ask in coming slides and we will answer that, how these lattices, all these other possibilities are not available. So, we will precisely take up this very question, we will do the hypothetical experiment, which have precisely suggesting in the coming slides and we will answer that such other additional lattices do not exists so, very good question and we will been taking it very soon.

So, let us look at this lattice and ask before, you will have to assume that these are merely points and this is a lattice therefore, there is no motif to decorate this lattice. The typical unit cell is the one, which is shown in red color you can see here and if you look from the top, you can clearly see that, this unit cell has got this structure, has got hexagonal symmetry the six fold symmetry.

As before, I think there is one additional red which hss been marked here but, please ignore this two red's of the top and the bottom because, they are not part of the unit cell. The only red's, which need to be consider are the ones, which are this rhombus shape and one at the bottom, which are rhombus shape. Therefore, this is a composite of 3 unit cells and this unit cell cannot be taken to this unit cell, which would be another rhombus by merely a translation.

And therefore, I would reduce our composite and not a alternate unit cell or a parallel unit cell so, if I use this unit cell to describe this lattice then, I cannot use this unit cell or this unit cell to describe this lattice. However, this unit cell is related to this unit cell by a rotational symmetry of the hexagonal lattice. Now, let me take up this model in my hand and try to understand it from various perspectives.

So, we saw that, this is got the six fold symmetry, which is obvious along the c direction now, it is also got a mirror perpendicular to the c direction, which is the mirror which passes through the centre of this body along the c direction. So, I can put a plane, which is a mirror which is going exactly between the top and the bottom planes. Now, in some terminology, this is sometime called the basal plane, these planes are called the basal planes and these are called the prism planes and some inclined planes are called the pyramidal planes.

Now, the other symmetry, which is worthwhile to note is the two fold symmetry and you can notice, that this structure between it is opposite edges has got a two fold symmetry and therefore, if I rotated it by 180 degrees, you have a two fold rotation axis. And additionally, I can pass the mirror, which is perpendicular to this two fold and the mirror would pass, as you can see from this side, would pass like this. So, if I have a sheet of paper then, I can show you and Mister Ravi will help me with a sheet of paper, will show you where is that plane.

So, took a sheet of paper here then, you can see that the plane, which passing through this central plane is actually the mirror plane. And this sheet shows you, that this mirror plane is perpendicular to this two fold axis therefore, this structure has quarter 6 by m 2 by m 2 by m symmetry. One question we can ask is that, how was this hexagonal structure related to some common crystal, which we come across the hexagonal close packed crystal and this we shall answer in due course of time.

So, again to repeat, the important salient feature regarding the hexagonal lattice, this whole hexagonal structure is not the unit cell, though it could still classify as a cell for a structure. The conventional cell is this one marked in this red which is nothing but, a rhombic prism.