Structure of Materials

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Lecture - 4
Geometry of Crystals: Symmetry, Lattices

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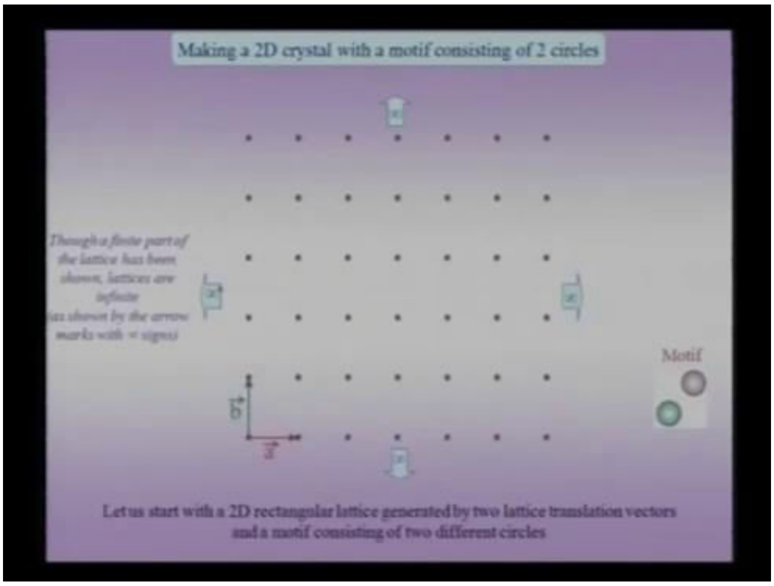

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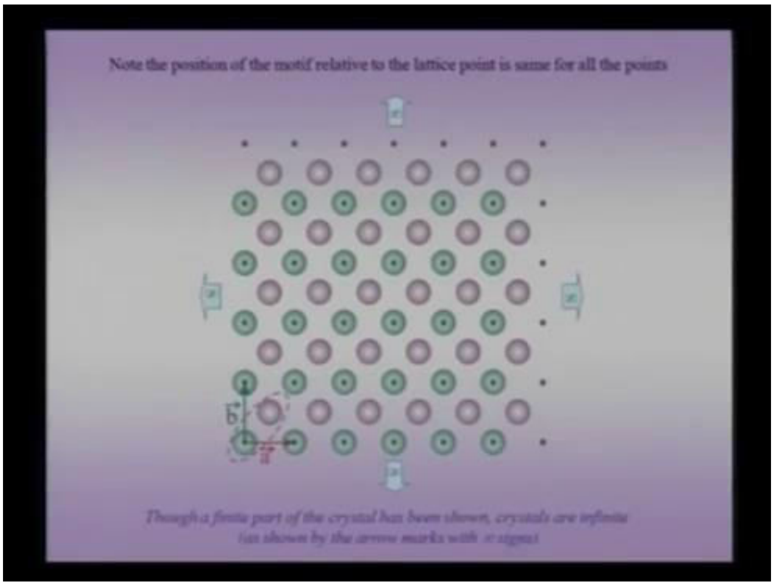

Let us construct a 2D crystal by showing this video example. So, here we have a 2D crystal which is infinite along the two directions, which has been generated by two basis vectors a and b.

And the motive is a two circle motive, so let us see how this crystal is constructed, so first we impose the lattice translation vector along the x direction this is done infinitely along the x direction. Then we impose the lattice translation vector along this row of these two spheres along the y direction, it is to be noted that the position of the motive relative to the lattice point is exactly identical as we go from one lattice point to the other.

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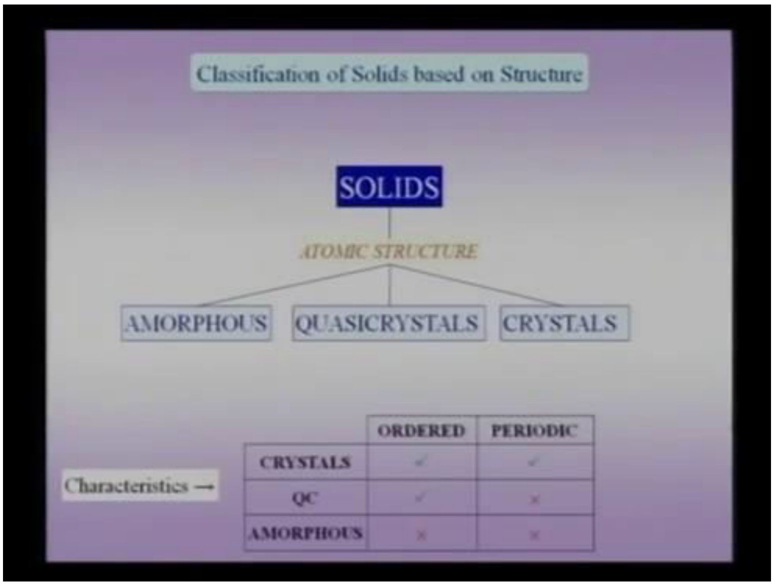

Let us revise somehow of the aspects we have considered, so far especially with regards to crystals. We have seen solids based on atomic structure can be amorphous, quasi crystalline or crystalline, and in this current topic we will extensively deal with crystalline structures.

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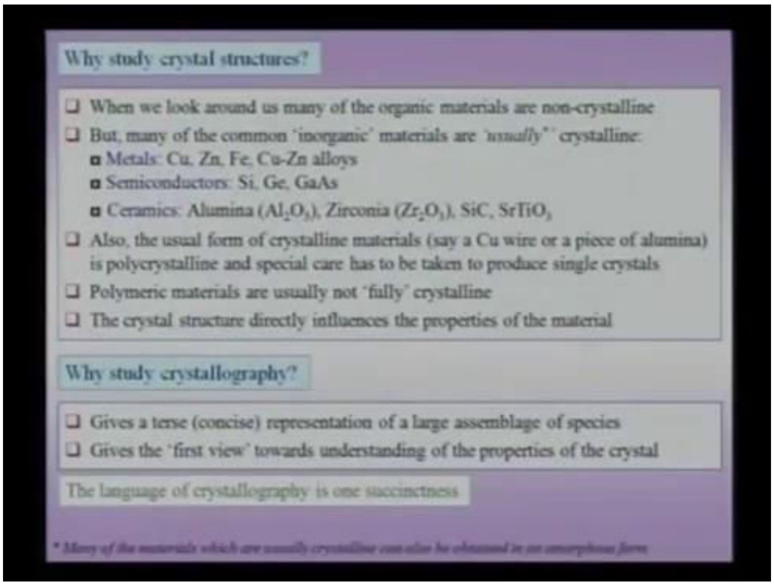

We are considered the motivation for studying crystalline structures, as we see that many of the important engineering materials, like metals, semiconductors and ceramics are crystalline in nature in their usual form. We had also seen that some of these can also be obtained in non crystalline forms, we are also talked about the language of the crystallography, language which is used to describe crystalline structures.

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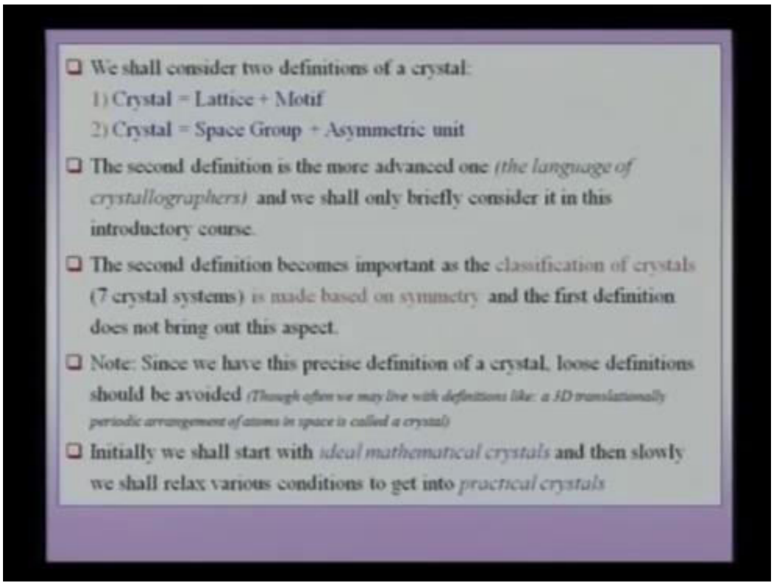

And we had seen that it is a language of succinctness, it is a language of terseness, where in we try to represent an infinite crystal in a very finite form in as little as information as possible. So, let us try to track the key words which we dealt with, and the first definition we had given the important definition was that a crystal is a lattice plus a motif. So, there are two key words here, and let me write them down on the board for a continuous reference. ((Refer Time: 02:40)) We had mentioned that this is synonym for a motif which is called a basis, and we had further mentioned that we will try to avoid this terminology, but as it can lead to a confusion with the term basis vectors.

And, so we will use the terminology motif whenever we are trying to represent something, which is going on to decorate a lattice which will finally, give as a crystal. The second definition which we are briefly mentioned and perhaps we will not go in to lot of detail in this course is the definition of the crystal, where in invoke the concept of a space group and a symmetric unit.

So, the crystal according to the second definition is a space group plus an asymmetric unit. The second definition which is based on symmetry becomes important especially when we are trying to classify crystals, and one of these classifications we will considered that there will be seven types of a crystal systems. And once we define a crystal in a regress form the way we had said here, we should typically avoid, glues and improper definitions of a crystal as this can lead to lot of confusion.

And important point we have said was that initially we would start with dealing with ideal mathematical crystals. And later on in various ways we will relax a conditions which are imposed by this ideal mathematical crystal, and try to develop what we may call real or a practical crystals. It is very clear that any crystal found in nature is; obviously, not a mathematical crystal, a mathematical crystal is a construct of our mind and as we see, one of the conditions in straighter way which cannot be met when we are talking about a crystal is the infiniteness, no crystals can be infinite.

But, we see there are other conditions we will relax as well, and go from a ideal mathematical crystal which we are going to learn first. And then we will construct the more practical crystals, and that will be our goal in future lectures.

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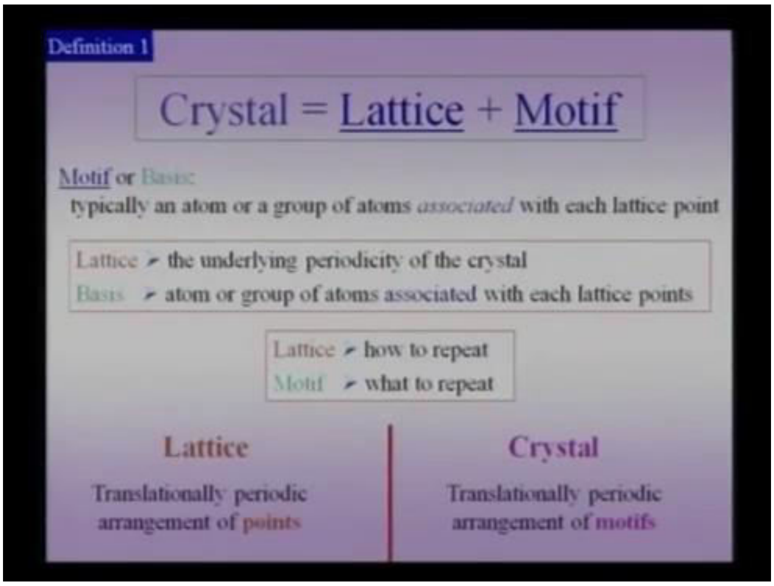

So, let us look the definition of a crystal lattice plus motif that is what we have done, we have said that lattice tells us how to repeat and the motif tells us what to repeat, this what get considered. And we had gone in to considerable depth to understanding what kind of motif’s are possible, which can go and decorate a lattice. We had made a additional point that the motif is nearly associated with a crystal a lattice point, and not actually need not actually position on the lattice point. So, this is a settle point, but never the less important in understanding the crystals.

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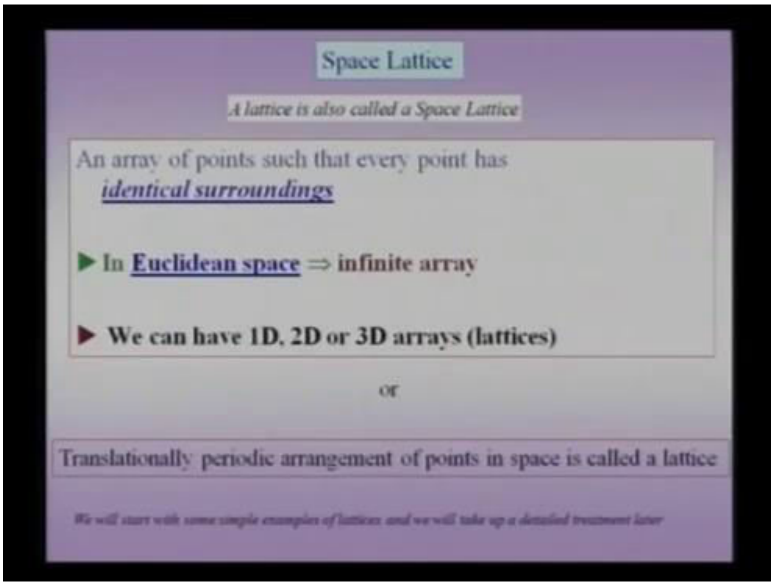

So, among the two keyword we have listed on the board the lattice and motif, so we need to understand the word lattice first. Typically lattice is also called a space lattices, and an array of points and space such that every point has a identical surrounding we define as a lattice. And we also said that in Euclidean space that is flat space, and such an array would be infinite, often we may also see a definition of a lattice as a translation ally periodic arrangements of points and space which we call a lattice.

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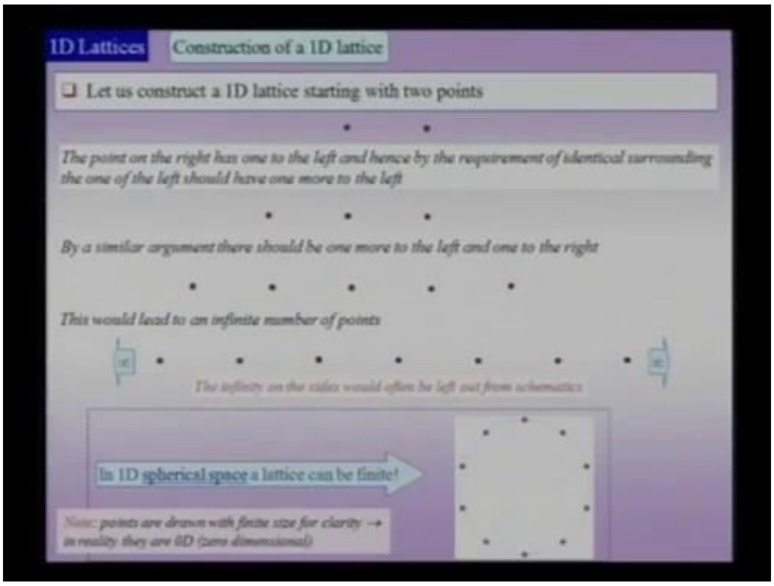

We had also constructed a 1D lattice, which is perhaps a simplest lattice and we saw that it is infinite in one dimensions. We have seen that how actually we can construct a 1D lattice starting with two points, where in we impose the condition that every point has to have identical surroundings. So, the criteria that every point has to have identical surroundings, automatically lives us to an infinite lattice in one dimension.

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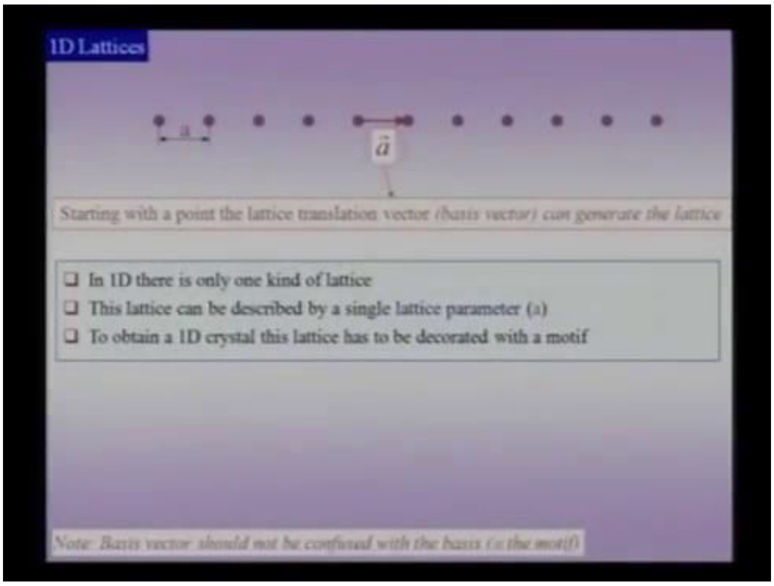

And we also saw that such a lattice a one dimensional lattice is described by a single lattice parameter, a single lattice translation vector which can be a the vector or if you are taking about the lattice parameter, the modulus of a which is the a without the vector sign. So, a lattice in one dimension needs just one parameter to describe it completely.

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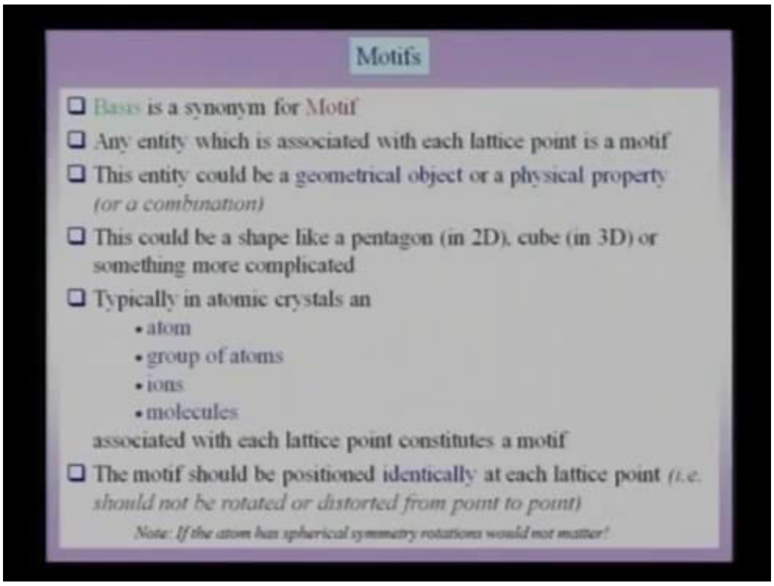

Then the second key word in the definition of a crystal is the motif and we wanted to understand what can constitute a motif. So, an important point we had made, though we did not take up in detailed consideration, so for was that any entity associated with the lattice point is called a motif. Such a entity could be a geometrical object, and we consider some examples as we see in the next slide or as a physical property or it could be a combination of geometrical object and a physical property.

The geometrical objects we could be a pentagon or any irregular object as well, but we also made a point. The typically atomic crystals which is as we see in future lectures is of considerably importance to this course could be an atom it could be a group of atoms, it could be ions, it could be a molecules, these molecules could be small molecules or could be a large molecules or in some cases we may consider some examples, it could be an entire virus which is could be an living organism.

So, a living organism like a virus could be crystalline and therefore, it could be as an large object as a virus. An important point about this positioning of the motif with respective to the lattice points, we considered was that it has to be positioned identically with respective to each lattice point. We are not allowed to rotate distort or any way tamper with the motif placing at each lattice point of course, if the object has a kind of symmetry those symmetrical rotations would be irrelevant.

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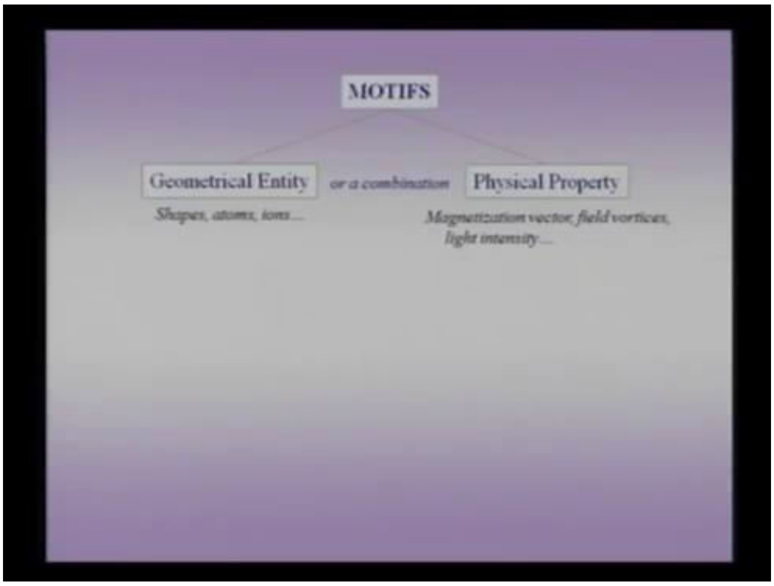

So, to summaries the importance point of the motif it could be a geometrical entity or a physical property. And a typical physical property could be magnetization vector, and you could have a cases where in motif is actually a combination of the geometrical entity and a physical property.

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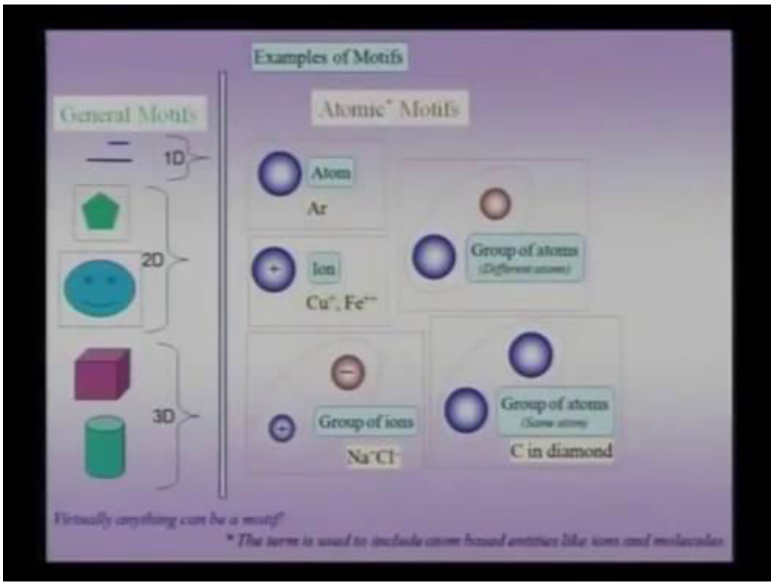

So, some of the examples of motif’s we considered where, on the left hand side are some geometrical motif’s and we saw only possibility in one dimension was a lance segment. In two dimensions you could have various shapes, regular or irregular some examples of regular shapes could be a pentagon, a square, a hexagon, a heptagon, in three dimensions you could have various shapes and this could be a cube or a cylinder or a sphere or any one of these.

It is also important for us to consider atomic motif’s as listed on the right hand side, and we saw that they could be a single atom, like an organ atom, there could be an single ion, they could be a group of ions or a group of an atoms. And their goo group of ions an example which of course, we will consider in detail later is example of a sodium and a chorine ion, sodium atom ion being positively be charged and chlorine atom is negatively charged.

So, we see that there is a considerable variety when it comes to the various kind of motif’s which are possible we also constructed someone dimensional crystals.

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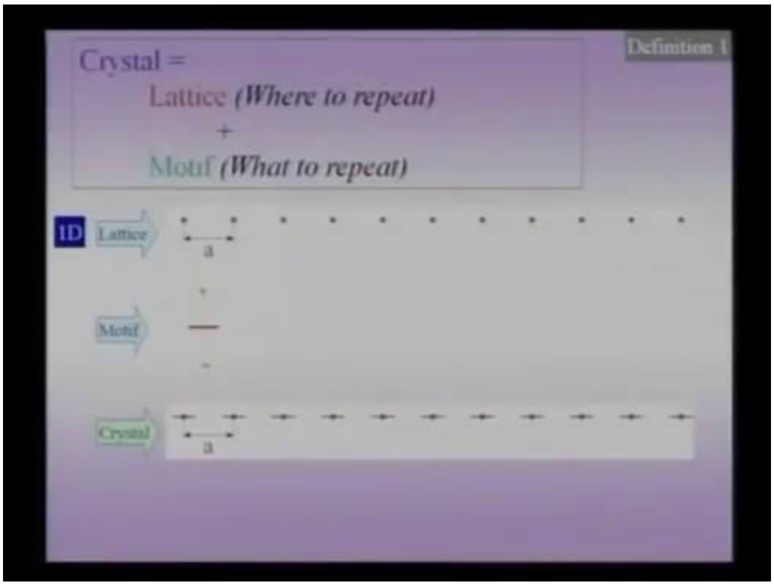

And an example shown here, where in we start with the line segment which we used to decorate a one dimensional lattice. And a crystal obtained is a one dimensional crystal, so the only variation we have in terms of the motif here is the length of the motif here which is one dimensional. And the only variation which is possible in terms of the lattice is the lattice parameter, so these two possibilities with regard to the lattice and motif can give you a variety of crystals all in one dimension.

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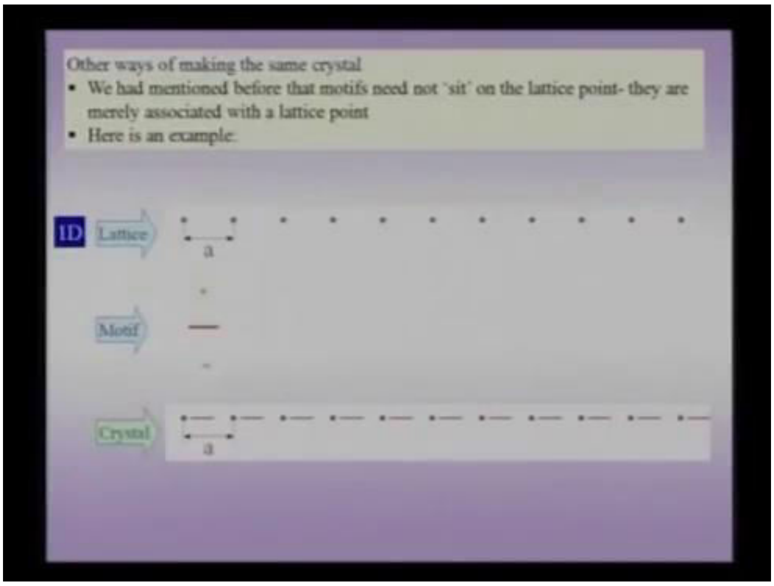

We emphasize the fact that a motif actually need not to be physically positioned on the lattice, we considered the fact that we could actually move the motif with respective to the lattice by a certain shape, which is seen here and position it with respect the lattice. The crystal in any sense not changed from the previous crystal it is description would be exactly identical as the precious crystal, they the only difference is that the way we have put the motif relative to the lattice point.

And this is a just a convenience we may use it for certain reasons, but never the less the crystal we have obtain is a exactly identical to the crystal we had previously obtained where in we had placed the motif directly on top of the lattice point.

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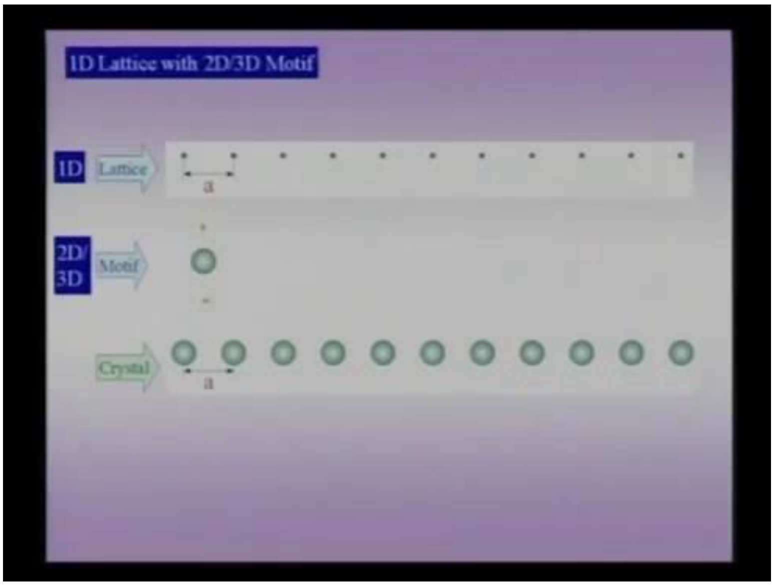

We said that we could actually relax the condition of the strict one dimensional motif that means we could have two dimensional motif and three dimensional motifs which we can use to decorate a one dimensional lattice and we are doing, so to have a better understanding of a crystals here at this point of time. And an example here was a circle which we reduce which could be a two dimensional motif or it could be a sphere, which is a three dimensional motif which could go on and decorate to our lattice with lattice parameter a.

So, the crystal of obtain is shown in the bottom and truly speaking it is a two dimensional or a three dimensional crystal, as the motif's of a higher dimension then the one dimensional lattice we started off with then we went on to understand a slightly more complicated motif.

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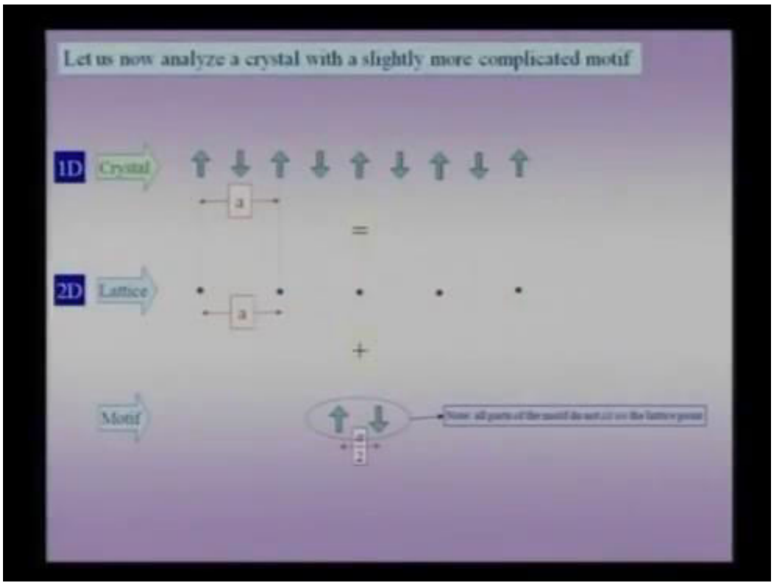

And we will consider this motif again and again in various context to understand various kinds of important concepts, which comes in to crystallography. And this was the example where in we had a up arrow and a down arrow decorating a lattice with a lattice parameter a. We had said that the motif in this case is an up arrow and down arrow with a spacing between their components of the motif being a by 2. An important point which came here was the point we had mentioned slightly before that some parts of the motifs or the entire motif actually need not set on the lattice point.

In this case the down arrow do not sit on the lattice point, it is only the up arrows visit sit on the lattice point, which brings us to the important consideration that not all centers of these entities are lattice points. Only the up arrows centers are lattice point of course, we could also do an alternative, then we could choose the centers of the down arrow lattice points, but having chosen either the up arrow center or the down arrow center, we can use only one of the two as the point for the lattice of course, we can choose the lattice point somewhere in between the two also.

But, for simplicity we will assume that here that the center of the up arrow is lattice point, which automatically implies center of the down arrow is not a lattice point. So, we shall revisit this kind of a crystal to understand more concepts later.

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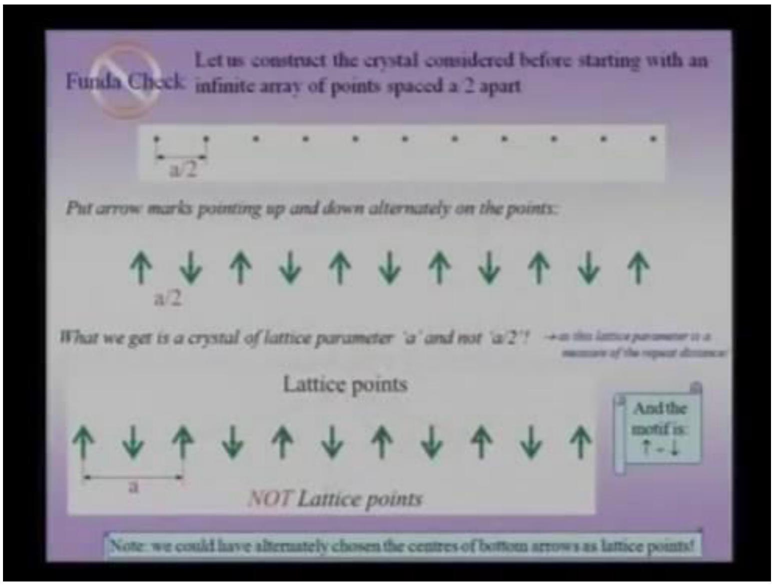

So, we had also gone head and sort of cleared our fundamentals on this very problem of an up arrow and a down arrow by stating that not all points which were originally suppose if we had started with an array of points just a by 2. Then after the crystal has been constructed then not all centers are lattice point, and that is what we had simplified using the figure at the bottom. Then we went on to create 2D crystals and we had done, so to understand more concepts which could not be clarified in the case of an 1D crystal.

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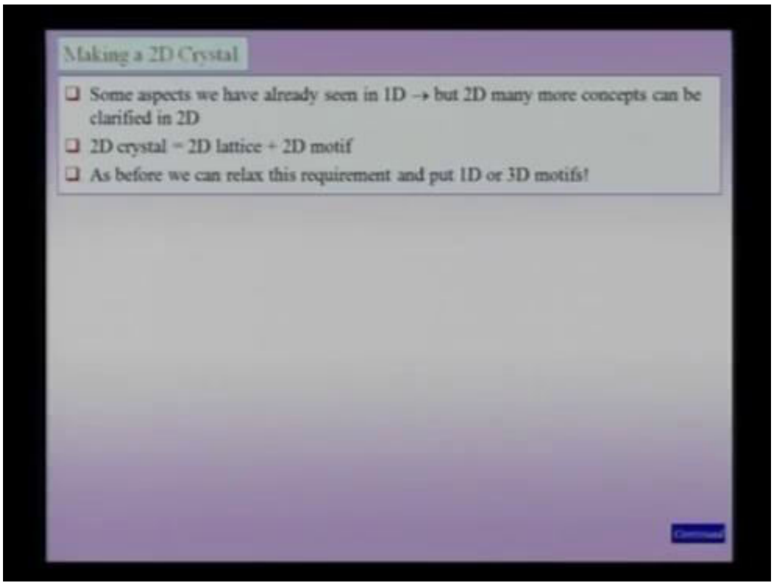

So, we said one set 2D crystal would be a combination of a 2D lattice and a 2D motif of course, like as we have done for the 1D crystal we can relax the conditions, and try to put three dimensional motif's on a two dimensional lattice to create a crystal.

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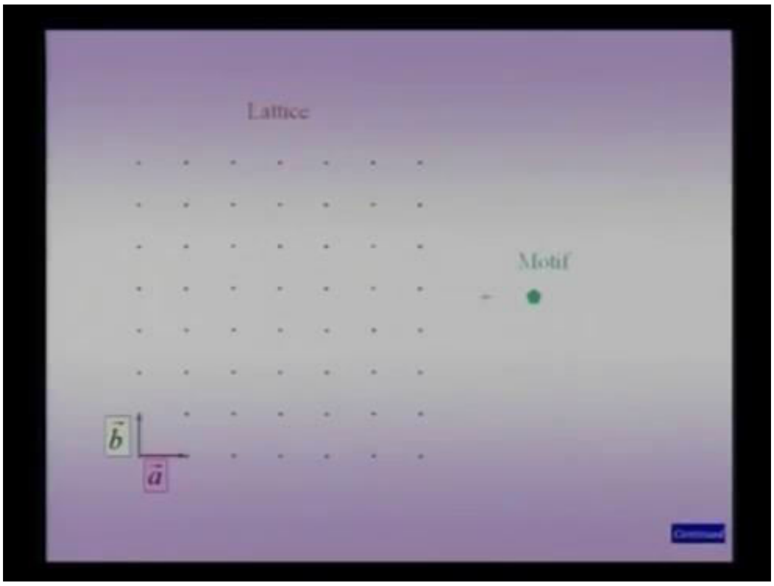

So, the first example we consider of a two dimensional lattice is as shown in the left, we had seen that there are two vectors we need which are not collinear to generate the lattice. These vectors are a and b, the a vector along the x direction and the b vector along the y direction, and this lattice though it has not been shown here, it is infinite in two dimensions and only a part of the lattice is shown here or as because, we cannot put doggy entire lattice on a screen.

So, there are two basis vectors and in the current example the angle between the two basis vectors is 90 degrees. But, as we shall see soon this angle can be any arbitrary angle for a general lattice, the motif we had considered was a two dimensional motif which is the shape of the green pentagon. As we have seen any other two dimensional shape regular or irregular ((Refer Time: 16:03)) in understanding or in the process of making a two dimensional crystal.

So, starting with the two dimensional lattice which has been generated with two bases vector which are not collinear, and motif is in the shape of a pentagon we went ahead and created a two dimensional crystal.

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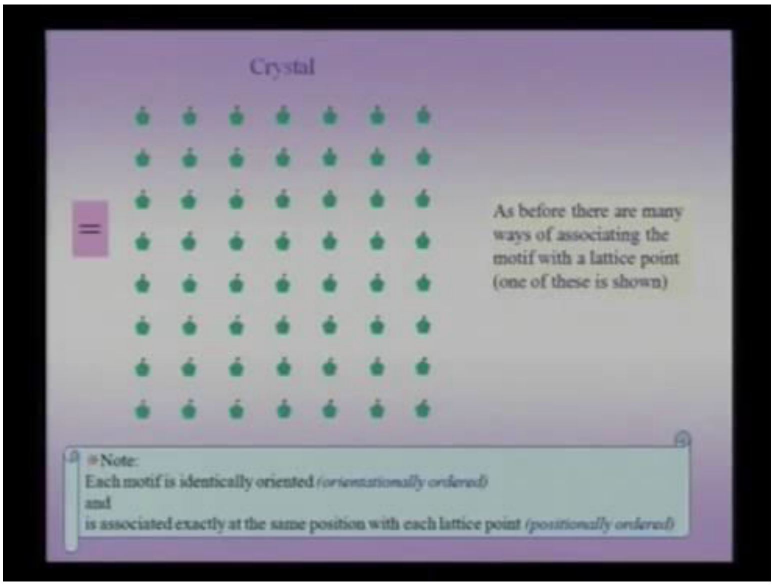

And like in the case of the one dimensional lattice and the one dimensional motif there are many ways of associating this motif or over laying this motif on the lattice point, and one of them has been chosen here where in the tip of a pentagon is a point, which is co insides with the lattice point. One point which is very, very clear while we did this just to reiterate that we are not allow to rotate or distort the pentagon, as we go from one lattice point to the other.

And once the crystal has been created as the lattice is finite in two dimensions, the crystal is also automatically infinite in two dimensions. Now, important point which comes out when we look at this crystal is that it has got two kind importance order, one is that it has got positional order which is clear from the fact that each of the motif is sitting identically on the lattice point. And it has additionally got a orientational order.

The reason for us to consider this positional order and a orientational order is that, when we goes from these mathematical crystals to real crystals we may call something a crystal. Even when some of these criteria relaxed that is we want to go from ideal mathematical crystals to real crystals, then some of this criteria would be relaxed. That means we would may consider either one of the two, we may only consider a orientational order or we may only consider the positional order in the definition of a crystal.

So, the important property here was orientational order the positional order of the crystal, we had seen that these crystals are infinites. Therefore, we need a method to succinctly represent the crystal and the method we had suggested was to choose a unit cell.

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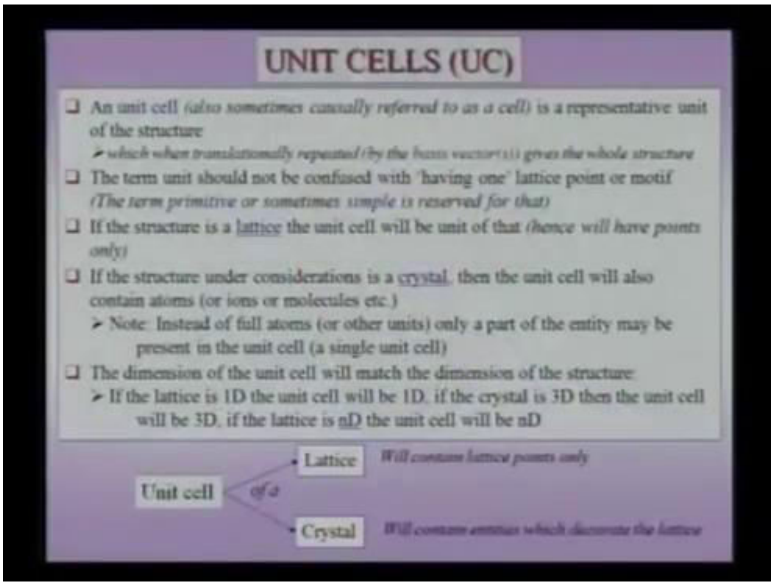

We have an unit cell and we have a basis vectors, so unit cell is nothing, but a part of the infinite lattice or part of the finite crystal. So, unit cells in represent a lattice or they can represent a crystal, and when had a super imposed on them the repeated translation vectors, one in one dimensions two in two dimensions we would get a crystal or a lattice depending on the unit cell you start off with. We had said that the word unit should never be confused with the fact that there is one lattice per cell per one motif per cell the whenever you have one lattice per cell such a unit cell is called a primitive unit cell.

And the word unit nearly represents a fact that it is an unit of the entity structure, so it is like a building a brick of the wall, starting with the brick you can construct a wall. Similarly, starting with the unit cell you can construct the entire lattice or the entire crystal and therefore, it is called a unit cell and not because, it has only one lattice point per cell. Another important point which we consider was that, in a typical unit cell we may have the entities broken into pieces, and we will see that in the examples or we had seen that examples which we had considered before.

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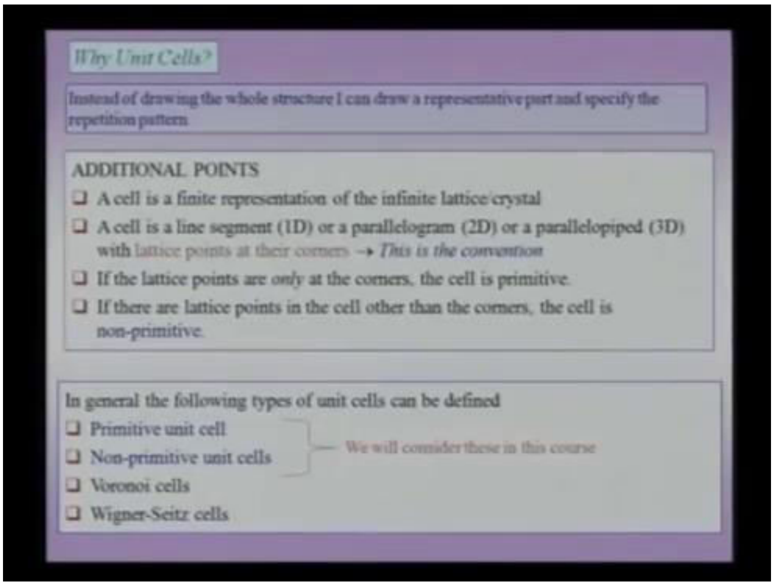

Some of the points we had considered when considering unit cells is a fact that, that in a typical unit cell you have only lattice points at the corners, if you have one dimensional cell at the end of the unit cell segments you would have lattice points. And this is a convention and later we had also considered some examples of unit cells, where in their lattice point do not sit at the vertices. If the lattice point only at the corners of the unit cell, we call it a primitive unit cell.

And other wise if there are more than one lattice point per cell we called it a non primitive unit cell. We also pointed out there other kind of unit cells or cells which we people consider which have moraines cells and ((Refer Time: 20:05)) cells and we will not typically deal with this in this elementary course.

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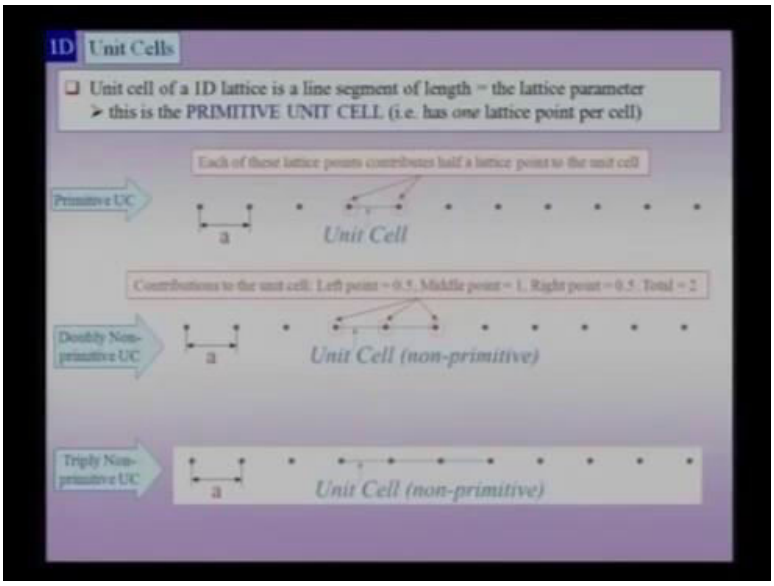

So, we con further went on to take up the example of a one dimensional lattice, and we tried to understand primitive unit cell, the doubly non primitive cells, and the triply non primitive unit cell. As you can see in the primitive unit cell we pointed out that the lattice point per cell is one, half coming from the left hand lattice point half coming from the right hand lattice point totaling up to one lattice point per cell.

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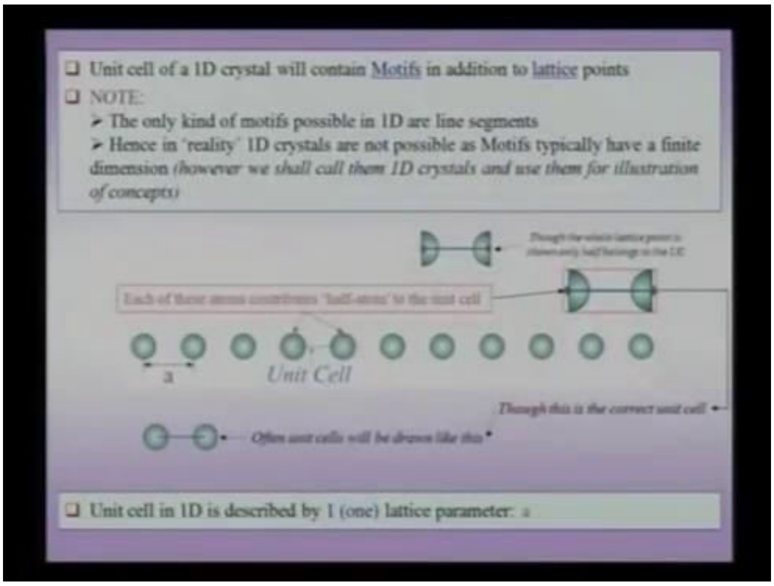

In the double primitive non primitive unit cell, the entire contribution of the central lattice point to the cell exists one on the left and one the right contribute half each contributing a total of two to the unit cell. A triply non primitive unit cell similarly would have a contribution of three lattice points per cell.

We had also said since there are only kind of motif possible in 1D line segment if real crystals are made even on one dimensions, they would actually be having a three dimension motif typically on the one dimension lattice. So, let us consider at this point of force it might be worthwhile just as I to mention then it has prove that one dimensional crystals are not theoretically possible.

So, let us consider the example of one dimensional crystal as shown here, and we wanted to see the actually in the unit cell we have only half the circle or the sphere coming inside the blue line, which is the unit cell. And the right hand side again it was half put to gather to these half's, you have one circle per unit cell and also correspondingly one lattice per unit cell.

A point again at this stage is that typically sometimes we draw unit cells the way it has been shown here, where in you draw the complete circles keep of course, understanding at the back of our mind is that, that is just a simplified representation and the real unit cell should be look like the one shown here.

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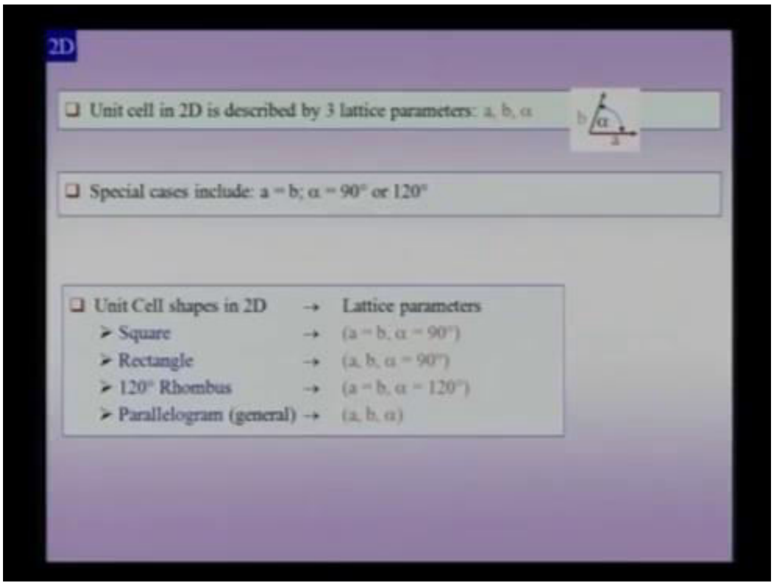

We also considered to their two dimensional unit cells, and we said we require three lattice parameter to describe a two dimensional unit cell, the two lens case a and b and an include an angle between them alpha. We also said that there are typical cases or special cases where in you have special constraints on the distance lattice parameter or a special constraints on the angles. The special constraints on the angles could be 90 degrees or 120 degrees, while in special cases a could be equal to b.

There are four types of unit cell which are observed in two dimensions, these are the square, the rectangle the 120 degree rhombus and the parallogram. In the square unit cell a equal to b and alpha a equal to 90 degrees, in the rectangle unit cell a and b are arbitrary numbers which are not equal to each other, and alpha still equal to 90 degrees. In the 120 degree rhombus a is equal to b, but the alpha as a special constraint on it that it should be equal to 120 degrees.

The parallelogram unit cell is the most general unit cell possible, where in a b and alpha are three parameters which have no constraints placed on them. So, as we have listing key words on the board, let us go down the board and right down special key word, the word unit cell. ((Refer Time: 23:38)) Let us consider a two dimensional lattice as printed on this sheet of a paper, we will try to generate a two dimensional crystal as we have done on the computer before, for this sake I have got a pile of three disks.

And for now you should assume that these three disks are of the same color therefore, we will assume that there is no difference in color. And therefore they can constitute an ideal motif which is something like a two dimensional motif, and I decorate this two dimensional motif on this lattice, as you can see to generate a two dimensional crystal. As this motif is got circular symmetry it is not matter if I rotate to the motif with respect to the one motif with respect another motif.

But, suppose this fare of a different shape like the shape shown here, then I am not allow to rotate this motif from one lattice point to other, in that case I will have to identically place the motif and I cannot rotate the motif as I go from one lattice point to an other. But, for now I would continue making this crystal with these set of disks, which I have got with me here, so as we had seen the problem before that such a crystal would be infinite, and all I can do best here is to only take a finite representation of this crystal to generate this two dimensional crystal.

As you can already see the generating an ideal mathematical crystal on a sheet of a paper can be tricky, and there could be impractical certain distortions, which would allow the practical crystal to be slightly different then the ideal mathematical crystal, which we have describing on a computer. As we are running out of disk I will stop here, and not try to fill the hole of this two dimension sheet of paper it is clear that the unit cell for such a two dimensional lattice would be this one square, which is here is this square which I tried to shade here.

After considering this two dimension crystal, let me try to focus little bit of attention on the unit cell which we have chosen for the two dimensional lattices, and the two dimensional crystals. So, I got some models here with me this model as you can see consists of balls, and magnets, and this clearly is an example of a square unit cell or a unit cell of a square lattice. So, in such a unit cell is repeated you would actually get a two dimensional crystal.

If you want to go from a square unit cell and actually consider a rectangle unit cell, this is exemplified by the rectangle shown here of course, this is a very special rectangle where in length is a certain faction of the, but in general a rectangle unit cell could be of any arbiter shape, the only constraint being is that a should not be equal to b. In both cases you can clearly see, the included angle between a and b is 90 degrees I can further perform a simple experiment of trying distort this unit cell.

So, once distort this unit cell clearly now this unit cell as transform into a parallogram unit cell. This included angle can any angle depending on the kind of distortion imposing on this, and even after the distortion you can clearly see that the two opposite sides are parallel. And therefore, this is a parallogram unit cell of the most general type, where in there is no constraints either a or b or on the included angle.

Now, suppose I take this square unit cell, but now perform a very special kind of a distortion, where in I will try to match in distortion and try to create a rhombus out of that square, when I try to create rhombus; obviously, since the distortion is not going to change the length of the four sides it will remain as such. But, the distortion I will carry forward, till the included angle between the two sides become 120 degrees and that is what I have done here on the right hand side.

Clearly see, this is a unit cell of an 120 degree rhombus, and after making the distortion I have put in the plastic which is shown here. To actually show that the constraint 120 degree and therefore, you have a 120 degree rhombus unit cell starting with square unit cell nearly by a distortion of it such the included angle becomes 120 degree after considering some simple practical models, we will return to our discursion of 2Dunit cells.

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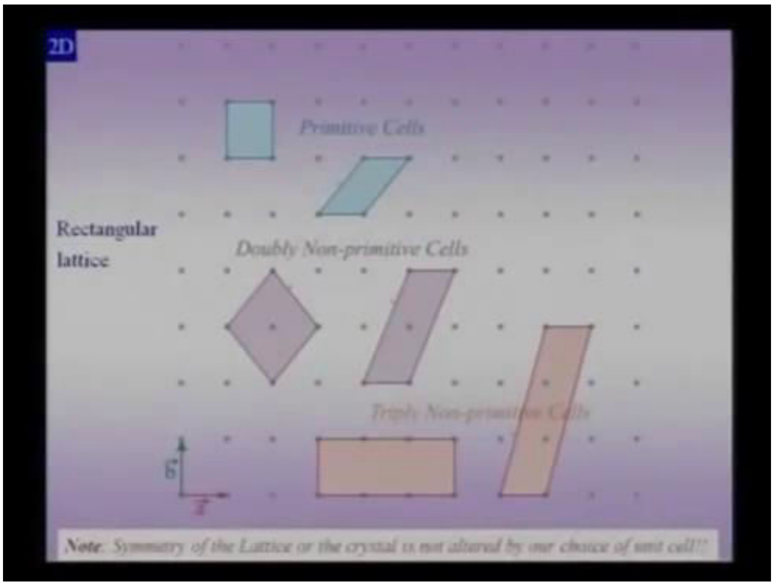

We are seen that there are primitive unit cells, doubly primitive cells and higher order primitive unit cells, when we talk about lattices. In the case shown in the figure we have a two dimensional rectangular lattice, where in the blue unit cells are primitive unit cells and the brown shaded once are doubly non primitive and the orange shaded one are triply non primitive unit cells. An important point which we make here, and perhaps we return to it again and again was a fact that our choice of the unit cell, either for a lattice or for a crystal is not going to alter anything about the structure we are considering.

Just because, I use a unit cell on the blue color shown in the right hand side, which is of the shape of parallogram our unit cell or our structure is not going to change in any way. And it would be equally well to represent ate in any other of the unit cell, irrespective of its primitive or non primitive, so all possible shapes of unit cells are possible, but there are other kind unit cell which are we call preferred unit cell, which will we will use of am.

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So, let emphasize perhaps obvious, but important point symmetry of the or a kind of a lattice or the crystal is not altered by our choice of the unit cell, so this is simple, but very important point.

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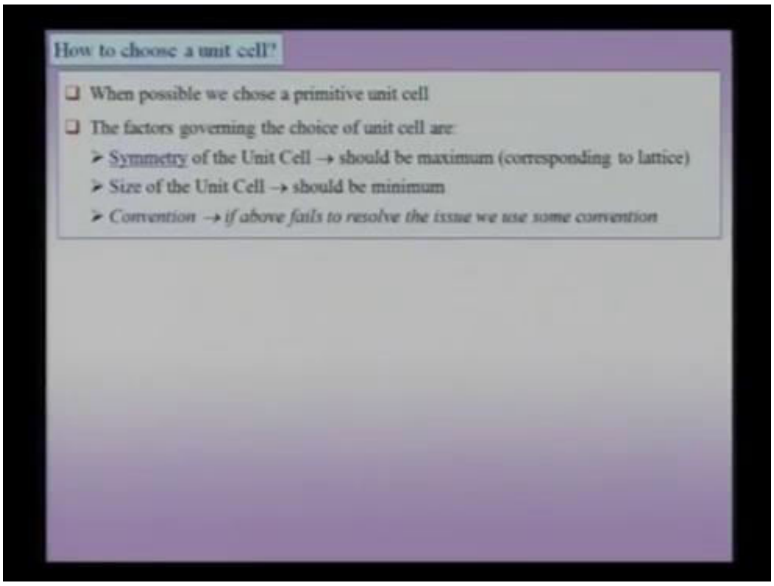

Now, how do we go about choosing the unit cells or as we pointed out there are infinite ways of choosing unit cell even for a very simple structure like a two dimensional lattice. But, there are certain guidelines which helps us in choosing a unit cells, so that what we may call a convention, so that when we communicate with each other we have a standard unit cell which we can refer to. So, the first criteria which typically is use is the criteria of symmetry, we try to choose a unit cell which has a maximum symmetry.

And typically the symmetry of the unit cell would be same as symmetry of the lattice or the crystal we are considering. The second criteria we impose is the size of the unit cell, we will try to keep it a minimum, and if both of this criteria fail then we try to settle down on convention where in we resolve the issue by choosing unit cell which we call the standard unit cell for a particular kind of a structure.

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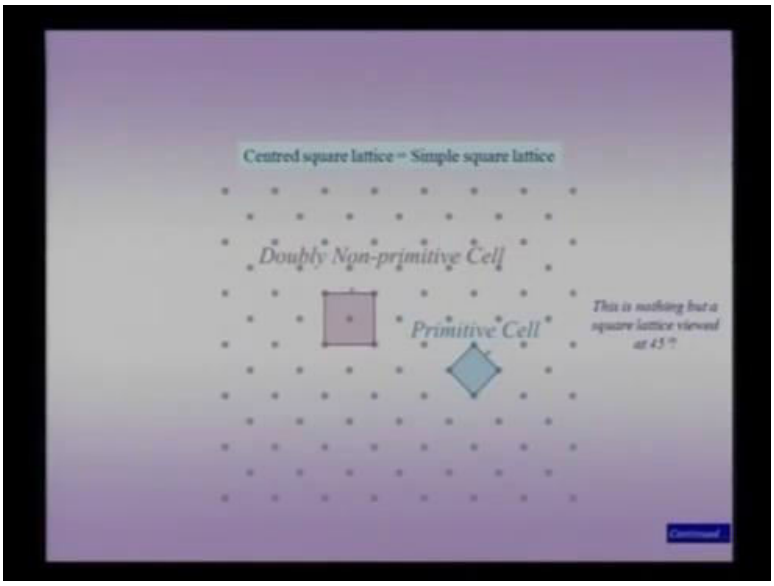

So, the three factors are symmetry size and convention, so suppose have a lattice here as shown here. We have something which looks like a centered square lattice, we can choose a doubly non primitive unit cell or the blue unit cell which is the primitive unit cell. In this case the symmetry of both the unit cell is exactly identical, as we can see both of them got a fourfold access in the center, the mirror planes and other symmetries are also identical for the two unit cells.

And now when we are talking about symmetry of the unit cell, it should not be confused with the symmetry of the lattice or the symmetry of the crystal, we are describing the lattice it is merely the symmetry of the unit cell we are talking here. Since, the symmetry of these two cells are identical we would go ahead and choose the one, which is one the right hand side, which is the blue unit cell which is the smaller unit cell, yes you would have notices all we have done in this case actually draw a square lattice at an angle of 45 degrees, which makes it look like a centered square lattice.

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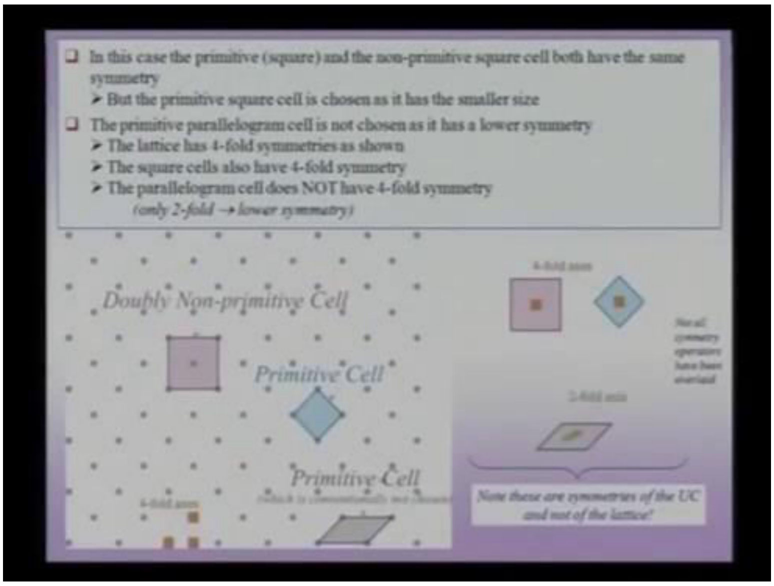

In the same case of the square lattice we could have chosen certain other kind of non primitive unit cell as shown in the figure below in this case this is a parallogram unit cell. Clearly this is not a preferred choice, as this parallogram unit cell only have a tow fold accessory center, while the other two unit cells have four fold access at center. Therefore, we would definitely not go ahead and make a choice of the wrong the parallogram unit cell, even though it has a size which is identical size in this case implying area, which is identical to the primitive unit cell.

For the sake of understanding I have also drown some of the four fold access of the lattice on the same figure.

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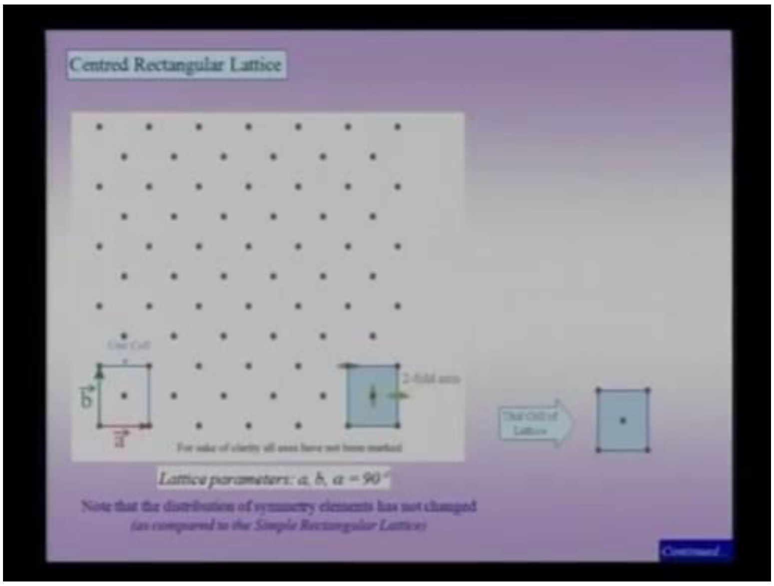

Now, suppose I have a centered rectangular lattice which generated by a two basis vectors a and b. Therefore, this lattice is only two fold access, and there are no fourfold access in this, and the lattice parameter are a and b which are not equal, and the included angle is 90 degrees. The unit cell which we choose for this case is a centered rectangular unit cell and even though we have a smaller unit cell ((Refer Time: 33:46)) which is the primitive unit cell which is of the shape rhombus.

We typically choose the rectangular unit cell, we will have a little more to say about this later. Because, in this case as it happens both the unit cell have the same symmetry, the primitive rhombus unit cell and the rectangular unit cell, but we do not go for a smaller unit cell we actually use the convention that we will actually use the bigger unit cell which has a shape of a rectangle. So, in this case actually convention which comes to the fore because, the rhombus shape unit cell and the rectangle shape unit cell both have a twofold symmetry for instance at the center of the unit cell.

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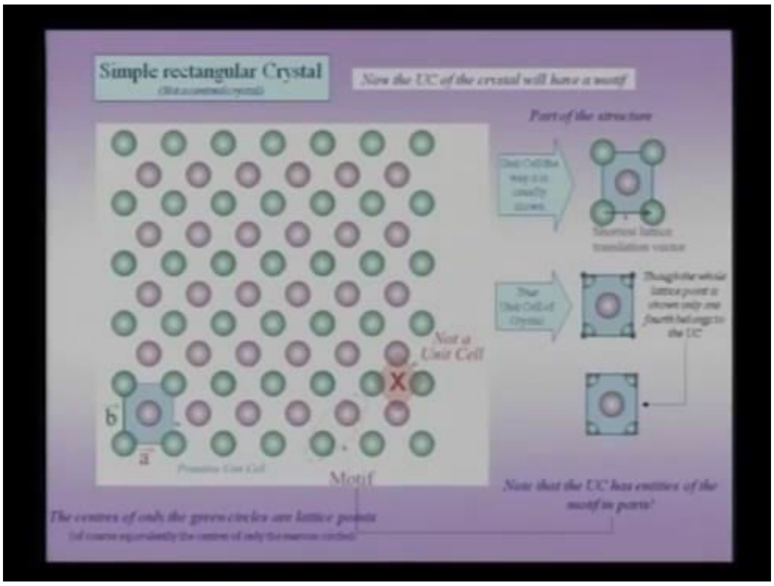

Now, let us consider how to choose unit cell for a crystal, so we have a simple rectangular lattice as shown in the figure on the left. And we want to generate a crystal by putting a motif which consists of a green circle and a brown circle, so by putting this we are now obtained a infinite two dimensional crystal. The unit cell can be chosen in many ways as before, but one choice is clearly not true which is one which is shown in the right hand side here.

You cannot chose the unit cell as the corners of this rhombus are not lattice point, if we choose the center of the green circle of the lattice point, than the center of the brown circle cannot be a lattice point. And therefore, we had stated that in conventional typical unit cell, all the vertices has to a lattice points, this cannot be a unit cell, this unit cell is not a centered unit cell. But, a primitive unit cell again because, a center point is not a lattice point, and this such a unit cell has only one lattice point for this blue cell.

And we had also noticed that in this unit cell you can define the shortest translation vector as the one, which is shown here by the brown line. We will return to the concept of a shortest lattice translation vector, when we deal with this locations especially, we have shown in this example that the b vector is actually longer in length as compared to the a vector.

And this is the way we typically show this unit cell, and we are clearly mentioned that the preferred or the more correct way to show this unit cell would be a the way that is shown in the bottom down diagram, where in the circles have been cut in to four parts and placed at the four corners of the unit cell. The contribution of the green and brown circles to the unit cell has not changed, all merely changed is the representation. So, this is also tells us an important example that the unit cell may have it is the entity is going on to decorate the lattice in parts.

And therefore, we should be little care full in understanding the unit cell if it is drown in the way it is shown here. It does not mean that the atom has actually if suppose to decorating entity was an atom, it does not mean that their cutting of an atom and placing in four parts it is merely a representation of the unit cell.

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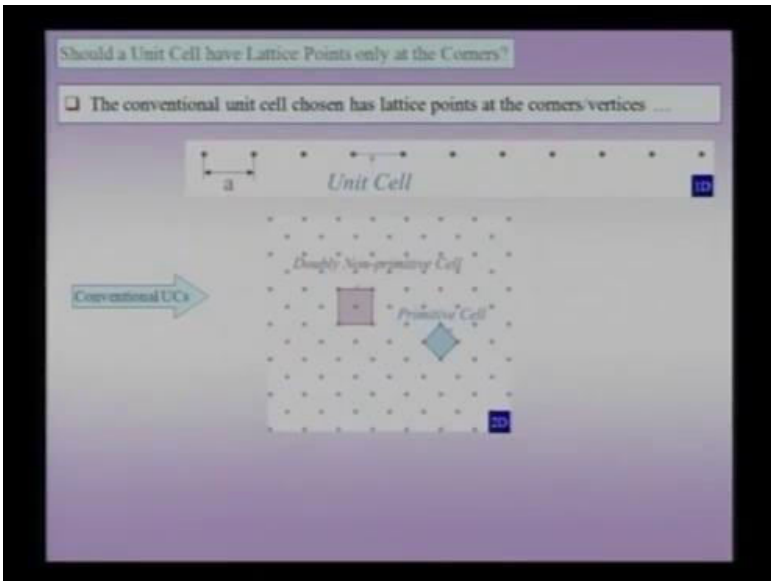

We had asked another question in the previous lecture that should a unit cell have a lattice point only at the corners. We said that in a typical conventional case we only keep lattice points at the corners, but for special reasons we may want to choose unit cells where in lattice point are not just present at the corners.

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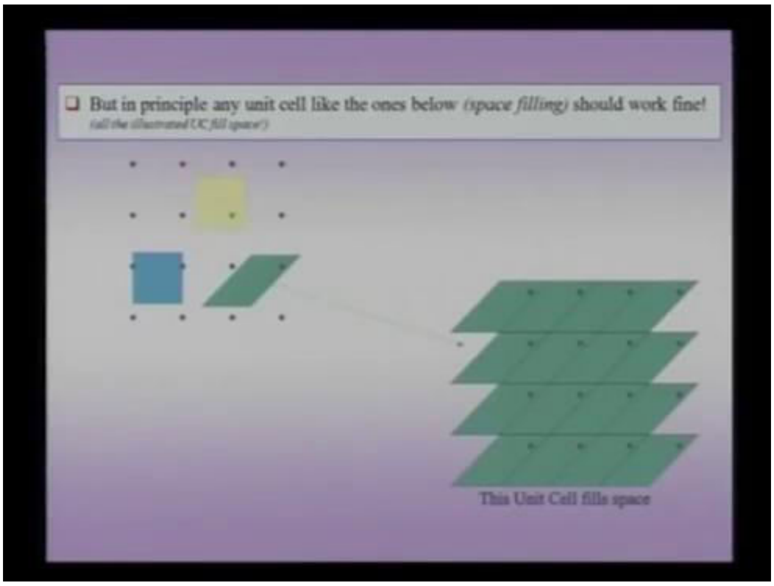

But, there alternatives possible as shown here, so there are three alternatives which are shown here, one is the yellow colored unit cell, one is the blue colored unit cell, one one is the green colored unit cell, all three are possible space filling geometrical entities in this case there are two dimensional entities. And the only requirement that the cell can perform the role of unit cell is that it has to be space fully; that means, the structure after putting this unit cell with along x and y direction lattice point translation vector, we should not be left with any gaps in the structure.

So, we can clearly see for instance in the example shown that the green unit cell is a space filling unit cell. But, it is also clear that the four corners of the unit cell do not contain lattice points, nice way of understanding this is that the one nice thing that comes out in understanding unit cells like this, it is clear from this that these unit cells are primitive.

Because, clearly there is one included lattice point inside the unit cell there is one included lattice point inside the yellow unit cell, there is one included lattice point inside the green unit cell. In the case of blue unit cell there are two half's contributing to the one lattice point per cell.

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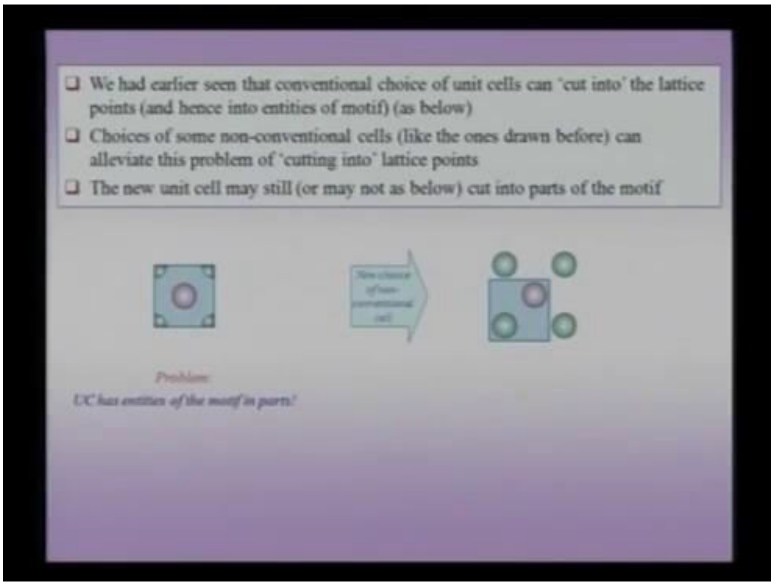

And we had said that suppose you are not interested in cutting of the entities in representation of the unit cell. Then such a choice of a unit cell one on the left hand side as shown entities in cut from the one on the right hand side shows that the unit cell has one green circle, and one brown circle which is what we understand from the fact that it is the primitive unit cell. Let us now consider a space lattices in little more detail before we actually go down and start understanding the three dimensional structures, which are the typical crystal structures which are of importance to us.

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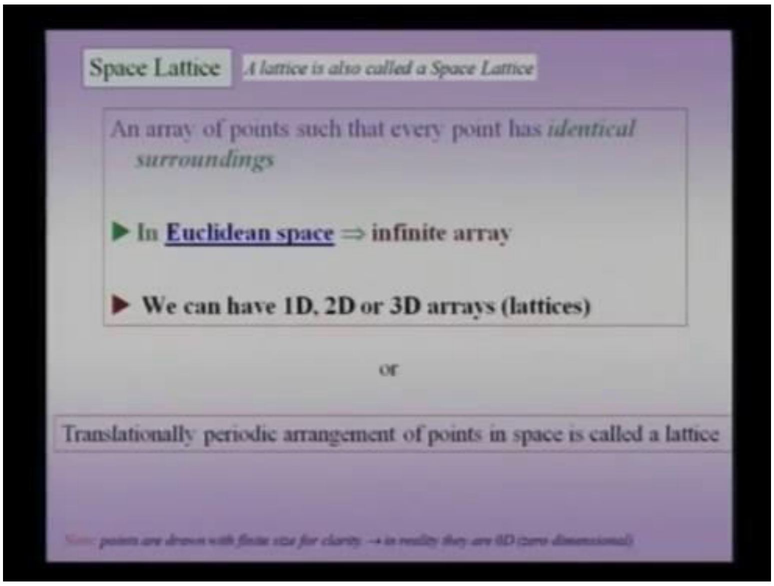

This definition of a space lattice we have already considered and I will merely re state that a space lattice and a array of point such that every point has a identical surrounding it also consider some one dimensional lattices as shown in the figure.

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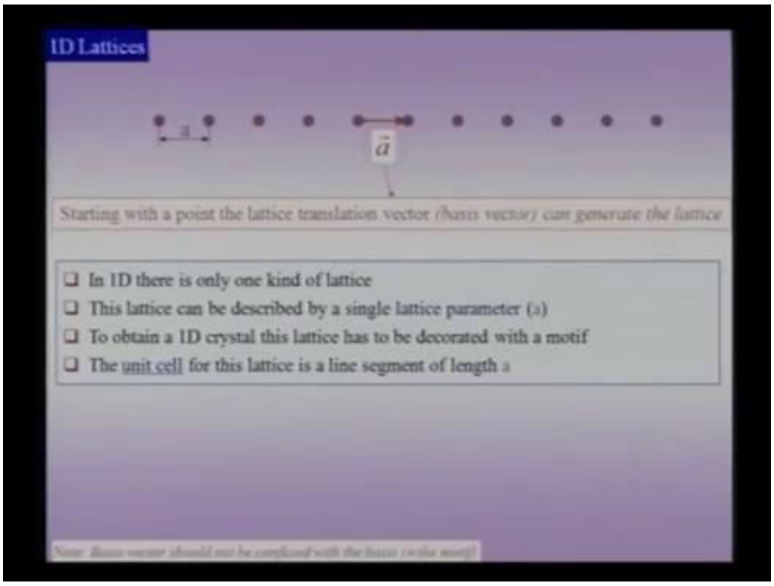

And we are stated that the unit cell has a lattice parameter just given by a, we had also considered some two dimensional lattices.

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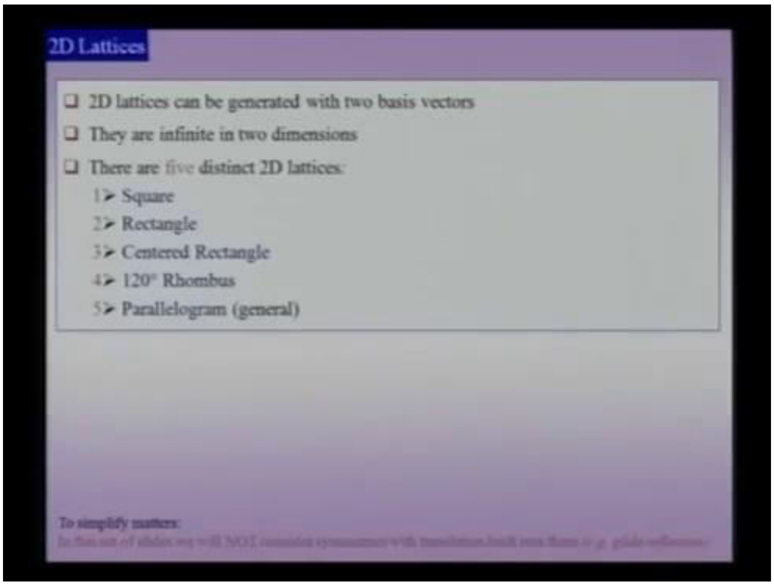

And we had said that there are five distinct two dimensional lattices, so this is the new point we are considering here, that the two dimensional lattices which can be constructed two basis vectors. And which are infinite in two dimensions, there are five different two dimensional lattices which are distinct from one another, these five two dimensional lattices are the square lattice, the rectangle lattice, the centered rectangle lattice, the 120 degree rhombus lattice, and the general parallelogram lattice.

And important point which is to noted here is that, we are previously used some of these terms like the square or the rectangle in the context of the unit cells. At no point of time there should be any confusion between the shape of a unit cell and the kind of a lattice we are considering, often there this is being the course the reason that some the important understanding is the secured by the use of the same term for two different kind of a object, one in this case being a unit cell whose shape is being described, the other being a lattice.

And we had clearly stated that the lattice will remain un effected by our mere choice of unit cell of one type or the other. So, to reiterate there are five types of lattices in two dimensions, these are the square the rectangle the centered rectangle, the 120 degree rhombus and the general parallogram lattice. In the some of these slides we will see that we will not consider all the symmetries over laid on the lattice, but typically for instance we will omit glide reflection, and other kind of complicated operators which involves for translation.

But, typically we will only super impose, mirrors and rotational symmetries which will be sufficed for us to clarify the point we need to make. So, before I leave this slide let me reiterate this point again that this common terminology between lattices, and the shapes of a unit cell can be cost for a considerably confusion and it is that every point of time clear that even though this word use square is also used for an unit cell, there should be no confusion that square lattice is a different kind of entity as compared to a square unit cell.

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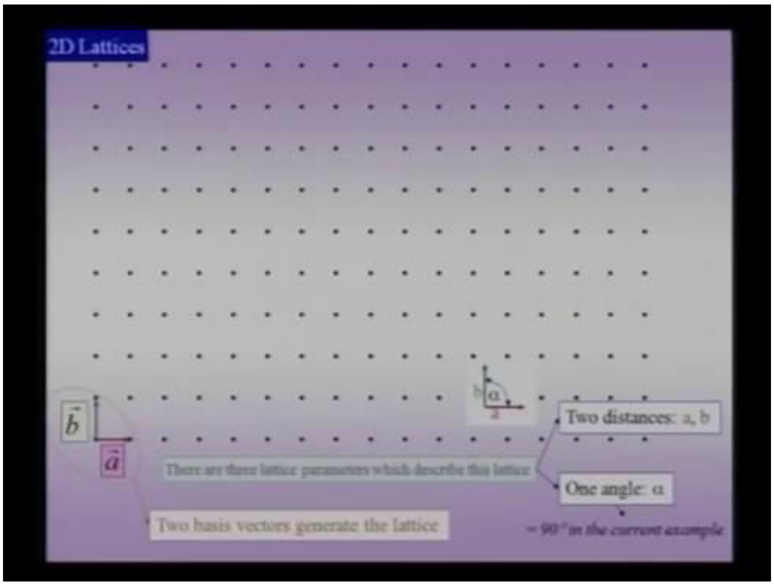

So, we had already said that two dimension lattice generated by two bases vector with an included angle, and in the example shown in the slide this include angle alpha happens to be 90 degrees.

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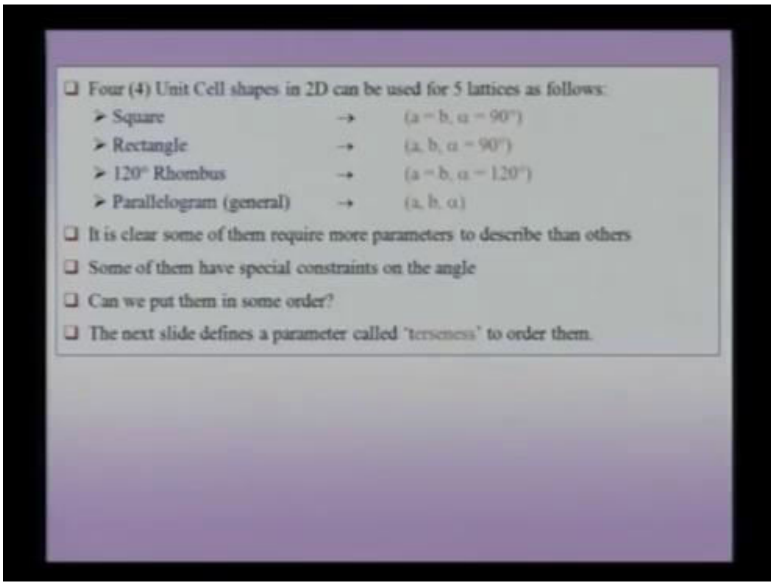

We had also seen that four unit cell shapes are typically used to describe these two dimensional lattices. We will have a few more thing to say now before we go ahead and actually take up the five different two dimensional lattices in detail, that we have this five two dimensional unit cells it is clear that some of them we have expenditure of more lattice point parameters as compared to some of the others, and some of them have a certain constraints on the angle.

So, we want to put some of these unit cells in certain order, and the parameter we choose to defining this order is a parameter we called courteousness. So, that we can order this unit cells and clearly this order where help us understand that some of them are somehow more symmetric, then the others or some of them are have a lesser expenditure or parameters.

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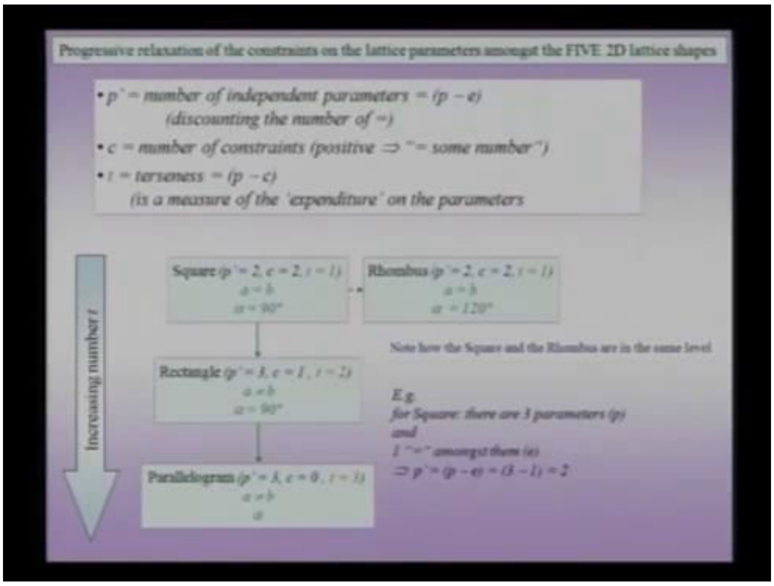

So, we will define some parameters to understand the terseness, we will define something known as p prime which tells you the number of independent parameters required. Which is nothing, but the number of parameter, but n number of equations which connects some of these parameters, in other words if there are equal to signs anywhere in the parameter, then that will go into the contribution of e, c will be the number of constraints.

And if there is a some positive constraints, then we will the numbers will increase, we will define terseness as the difference between p and c which is the number of parameters minus the number of constraints. So, terseness tells us that what is the measure of the expenditure on the parameters, more the expenditure on the parameters then lower will be it is place in terms of the lattice parameter tree.

So, let us concentrate the square lattice where in the number of in all of these cases, the number of independent parameters 3, which is just a b and alpha. And we have one two equations which connect them, as you can see, so the number of constraints is 2, so 3 minus 2 is 1 which is the terseness value for the square lattice. If you consider the rhombus lattice, the number of variables is 3, the number of constraints one of them being a equal to b the other constraint being on the angle, which is 120 degrees.

Therefore, the distance between 3 minus 2 is 1 and therefore, the terseness value for the rhombus lattice is also 1, which is why the square lattice and the rhombus lattice have been placed on the same level. Now, if you look at the rectangle lattice there are three variables, and the number of constraints post in these variables is that a is not equal to b that means, it will remain general while the alpha angle has been constrained to be 90 degrees.

Therefore 3 minus 1 is 2 the terseness value is 2; that means, we are having more expenditure in this case of a rectangle as compared to the square on the parameters and therefore it comes down as compared to the square or a rhombus in terms of the lattice parameter expenditure. If you look at the parallogram lattice the a b and alpha are all general; that means, number of constraints is 0 therefore 3 minus 0 is equal to 2, the terseness value is 3. And therefore the parallogram lattice falls at the lower level as for of the expenditure on the lattice parameter goes.

So, this slide basically tries to tell you that we have a certain expenditure on the lattice parameters. And therefore, more the expenditure lower will that unit cell be in the tree, and based on the expenditure the square and the rhombus are at the top of this tree.

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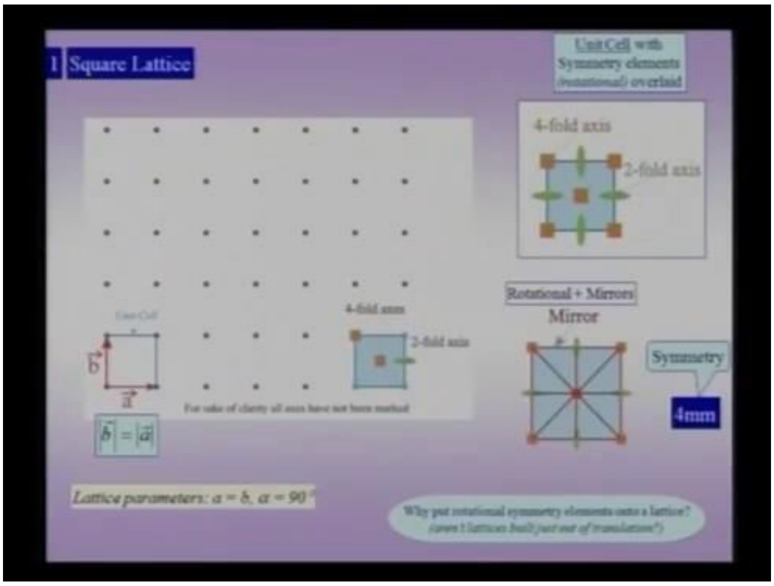

So, let us now consider the 5 two dimensional lattices one by one, so shown in this example is a square lattice. In the case of the square lattice there are two vector which go on to generate a lattice, but the important thing is that, the modules of a vector is the same as the modulus of b vector. In other words a is equal to b the included angle alpha is 90 degrees, and this is the characteristic of the two dimensional square lattice, if you look at the square of the unit lattice as shown in the blue color here, we can over lay on symmetry operators.

And what we have done is that we have not over laid all the possible symmetry operators on the square lattice this is, so that there is some clarity in thought. But, given the fact that if there is a symmetry operators sitting here, and there is a lattice transition vector a; that means, there has to be another equal ant symmetry operator which is a 4 fold which has to sit here.

Similarly, if you have a green colored 2 fold access sitting here, and if you have the a lattice translation vector in this case I would consider a minus a then automatically there has to be a green two fold access which has to sit here and correspondingly here, correspondingly here correspondingly here. In other word if I can locate one symmetry operator anywhere in the lattice, then this symmetry operator would also go ahead and completely fill up these two dimensional lattice or a space, given these two lattice translation vectors.

So, there will be 4 fold here there would be another 4 fold here, there will be another 4 fold here and, so forth. This 4 fold is not actually sitting on a lattice point, but is the center of the unit cell, so if I now impose the a translation vector, the minus a in this case I will have one more 4 folded this position. And if I translate it by b I have one more here, this is nothing, but stating the fact that whatever is contained within a unit cell has to be repeated.

In the previous cases what we considered was motif which was contained in the unit cell, and which was repeated by the lattice translation vectors. In this case it is not the motif, but the symmetry operators of the lattice clearly again to re emphasis, we are now considering the symmetry operators of the lattice and not the symmetry operators of the unit cell or other unit of the symmetry of the unit cell. And therefore, the unit cell will just repeat all the symmetry operators which are contained within it or across the entire two dimensional lattice.

For sake of clarity I have shown here, the two dimensional unit cell here, along with the over laid symmetry operators with rotational symmetry operators. So, you can seen that all 4 corners at and the center contain 4 fold rotational access, the center or the edges contain a 2 fold rotation access. Further if I want to over lay the mirror planes on top of this unit cell, then we can consider unit cell which is been shown below, as before 4 fold access continue to be at their original positions or the 2 fold axis which continued to be originally positions as in the unit cell before.

But, additionally we got these mirror planes which are shown by this red lines, so the edges of the cell are also a mirror planes, apart from the ones which are shown by these red lines which goes pass the center of the unit cell. There are two distinct mirror planes, the one which is vertical and the one which is inclined at an angle of 45 degrees, we do not have to consider the horizontal or the other diagonal.

Because, if I consider the vertical mirror plane, then the 4 fold access will take the vertical mirror plane to the horizontal mirror plane. Similarly, the one diagonal mirror plane will be taken by the 4 fold to the other diagonal mirror plane, the short hand notation of describing this kind of a symmetry combination is shown in the blue rectangle, which is nothing, but 4 m m, the 4 standing for the 4 fold access 2 m m standing for the m 1 which is a vertical mirror and the m 2 which is a diagonal mirror.

A question which; obviously, comes to mind is that, why do we put rotational symmetry elements on to a lattice or n lattice suppose to be constructed only of translational elements. This is an important question, it is true with that lattices are built out of translations, as in this case it is a and b lattice translation vector, but once a lattice has been generated we will notice that the lattice will have certain symmetries, and this is very, very important for us to observe these symmetries.

And note them because, our classification of crystals is typically based on these symmetry operators. So, to re emphasize the point I will ask mu self this question again, why do we put in rotational symmetry elements on to a lattice, and in addition of force I could put mirror and other symmetry operators on lattice. The question we are asking is that why do we put these kind of symmetry operators on to a lattice, while the only kind of a symmetry which was required to generate the lattice was the translation.

The answer of this question is that, it is very important that we actually over lay these symmetry operators on the lattice. Because, when we try to classify these the crystals made out of these symmetry operators, symmetry is of paramount importance more, so then even the translation which originally created. So, in all future considerations of a lattices we will typically try to over lay these symmetry elements on the lattice, and we will try to understand it later how these symmetry elements are come in very handy in classifying lattices and crystals based on that.

What while point may be at this stage which we will re visit in of course, in detail later, which is again related to the fact of the symmetry of the lattice and the symmetry of the crystal.

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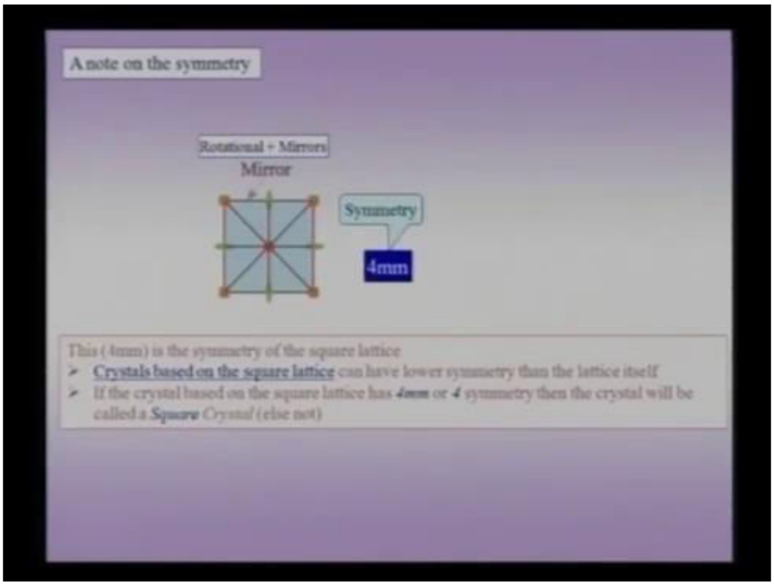

The symmetry of the lattice is what we considered before is nothing, but the 4 m m symmetry. Now, the lattice will always the square lattice that is will always have the 4 m m symmetry irrespective of what motif I used to decorate on the lattice, so the underlying lattice have 4 m m symmetry. But; however, the crystal based on this lattice can have a symmetry lower than that of the lattice, this is a very, very important point.

So, I will re repeat the sentence crystal based for instance in this example on the square lattice can have a symmetry, which is lower than the symmetry of the lattice. For instance I could place motif on the lattice such that the crystal has either a 4 m m symmetry or a symmetry which is just a 4 fold. Then the crystal which are generate I will call it as square crystal otherwise I will not call it as a square crystal, we will of course, return to this point detail in later.

So, at this point all I need you to understand that there are more considerations than just symmetry of the lattice or the shape of the unit cell of the lattice, which go into define crystals. And if I play some motif of lower symmetry then the symmetry of the lattice is then that motif in alter the symmetry of the crystal I have generate, and the original symmetry of the lattice may be lower or may even be completely destroyed.

So, to re emphasis based on the symmetry of the motif which I put on the lattice point these symmetry of the crystal which I generate from the lattice may be lower with respect to the may first of all of course, remain same as the symmetry of the lattice, it may be lower or in extreme example may be completely destroyed.

And when I talking about completely destroyed I am talking about these mirror planes and rotational symmetries, and not the translation symmetry of course, if I had no translation symmetry in the final crystal which I have created such a structure is called a morphs structure, and not a crystal.

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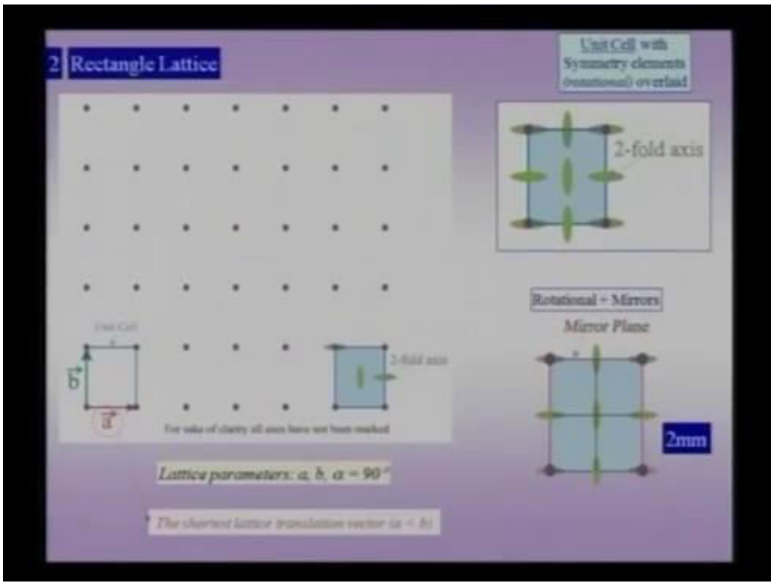

The second in the list of lattices is the rectangular lattice, the rectangular lattice is generated by two basis vector a and b, which are at an angle of 90 degrees. The rectangular lattice has no 4 fold access it has only 2 fold access, and with respective to the lattice point as you can see there is the 2 fold access at the lattice point there is a 2 fold lattice between two lattice points. And there is a 4 fold access which is between 4 lattice points, which forms the corners of the blue unit cell as shown.

In the case of this rectangular lattice a or b one of the two may be the shorter one which we shall call the shortest lattice translation vector, for this lattice. Any other lattice translation vector will be longer for instance suppose I consider a lattice translation vector connecting the diagonal of this unit cell. This is going to be longer then a and b; obviously, there are lattice translation vectors which are even longer like the one shown here or the lattice translation vector which can connect these lens.

But, the shortest lattice translation vector will continue to remain a as modulus of a is less than the modulus of b. On the figure on the right hand side I have shown on a unit cell of this rectangular lattice, all the 2 fold access over lay, thus you can see here there are various 2 fold operators. And apart from the lattice points there also present at the centers or the edges, and also defender of the entire unit cell, and as I have told you before that I am for sake of clarity I am not drawing all the lattices all the symmetry operators on the entire lattice.

But, once you obtain a unit cell, than that unit cell is translated to get the entire lattice with all the symmetry operators over laid on the lattice. As before apart from these rotation operators I can also consider mirrors, and that is shown in the figure below you can clearly see that the edges of the unit cell are also mirrors as shown by this red lines. There are two other mirrors, the one vertical mirror and one horizontal mirror and an important point to note as compared to the square lattices that as there is no 4 fold access at the center, these two mirrors are not equivalent.

The vertical mirror cannot become the horizontal mirror by any rotation of any symmetry access. And therefore it is a two independent mirrors, and the short hand notation to describe the symmetry operation is 2 m m and if you want little more to be explicit I will call the vertical mirror as m 1, and the horizontal mirror as m 2. And therefore, have a combination of a 2 fold and two mirror planes which is the short hand notation for all the symmetry of this lattice, make the point clear this is the symmetry of the lattice, and not nearly the symmetry of the unit cell which I have chosen.

But, it also happens to be the symmetry of the unit cell as shown in this figure because, I have chosen a unit cell in this case which has a symmetry, which completely commensurate with the symmetry of the lattice, the third lattice which I consider is the centered rectangle lattice.

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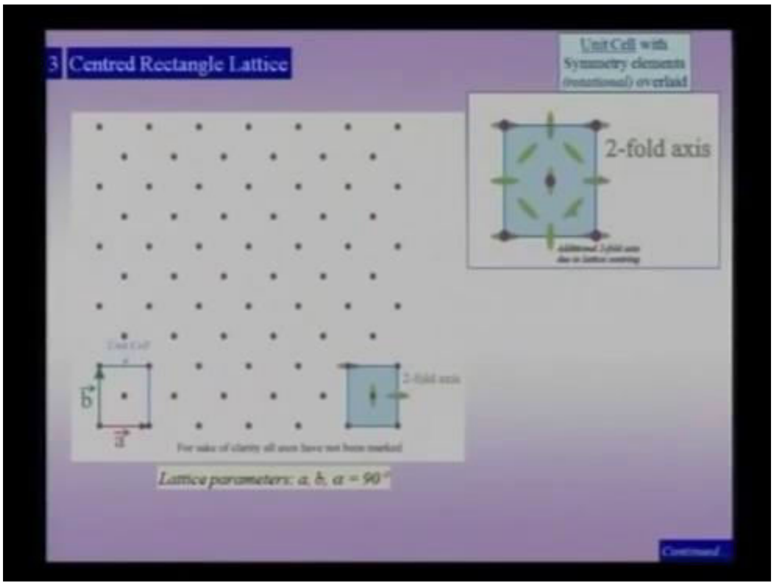


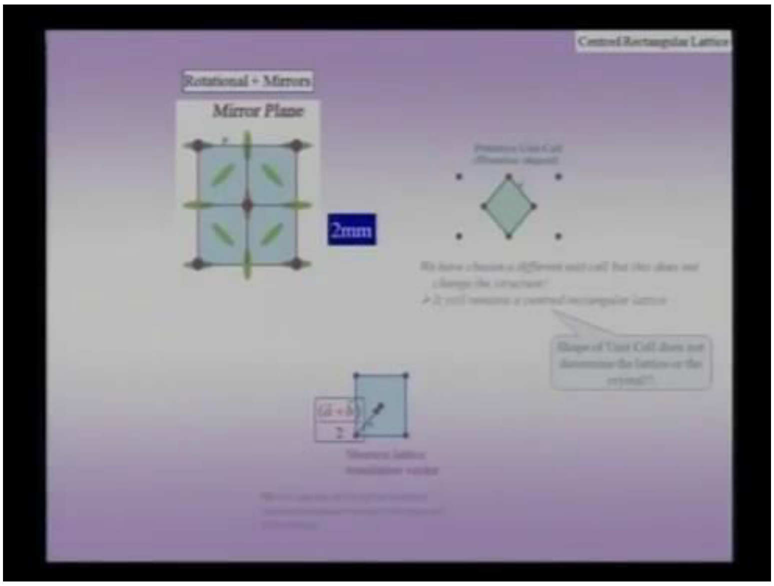
It is clear the centered rectangle lattice as the name suggests has a centering point apart from the 4 lattice points of the corner. Of course, the word centering you have to understand clearly is with respect to the previous unit cell, we consider a previous cell for the normal rectangle lattice. And this is centered with respect to that normal rectangle lattice, and not by alternate choice of unit cell where in the alternate choice of unit cell as we can see can be primitive unit cell, in which case that unit cell will not be centered.

The lattice parameter as previously for this lattice are a b which are independent, an alpha which is a constraint of 90 degrees. The shortest lattice translation vector as the previous case happens to be a, the important thing to note here is in terms of the symmetry of this lattice, which is shown here in the right hand side for detail. Here apart from the corners, which are originally had 2 fold access in the case of the normal rectangle lattice.

And the side edges which also had a 2 fold access at the center and 2 fold access at the center entire unit cell, their additional 2 fold operators ((Refer Time: 59:14)) mid way between the two lattice points. So, suppose I take a diagonal and I take half the diagonal, then there is a 2 fold operator located exactly at the middle of the diagonal or in other words at one fourth distance along the diagonal of the rectangle. So, their additional symmetry operators which come in to play, when we are describing the centered rectangle lattice.

And these additional symmetry operators are important, when actually try to decorate this lattice with a motif which we lead us formation of crystal.

(Refer Slide Time: 59:57)



So, let us consider this centered rectangular lattice in little more detail what we had considered before in the previous figure has been shown here, which has over laid on it rotation and mirror symmetry operators. And we had stated that it has got symmetry which is 2 m m, we could alternately choose an primitive unit cell as shown on the right hand side, which is rhombus shape.

And we had earlier pointed out that by convention we actually choose the non primitive unit cell, which is in the color blue for the case of the rectangle lattices. Both the centered rectangle lattices, and the normal rectangle lattice we actually choose a rectangle unit cell. While we had a choice of making a green unit cell which is in the shape of a rhombus, which we should have been a which should have had a smaller size which should have been a primitive unit cell, we shall continue our discussion of the two dimensional lattices in a next lecture.