Structure of Materials
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Lecture - 3
Geometry of Crystals: Symmetry, Lattices

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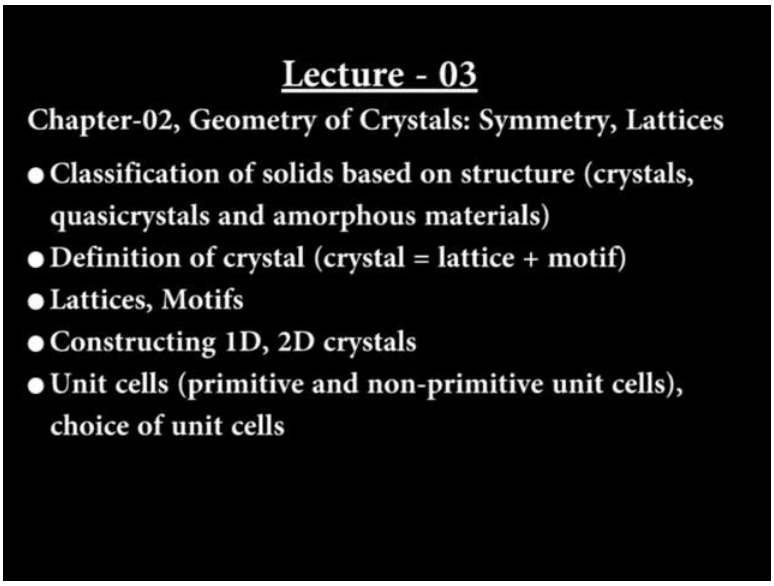

In today's lecture we will cover the topic on geometry of crystals, the basic topics in this sub topics would be space lattices, motifs and crystal systems. The course basically we cover a elementary material on geometry of crystals. But students who are interested in learning more can consult advance text like elementary crystallography by M J Buerger and also the structure of materials by MIT professors like Samuel M Allen and Edwin L Thomas. What is that we are trying to learn in this chapter?

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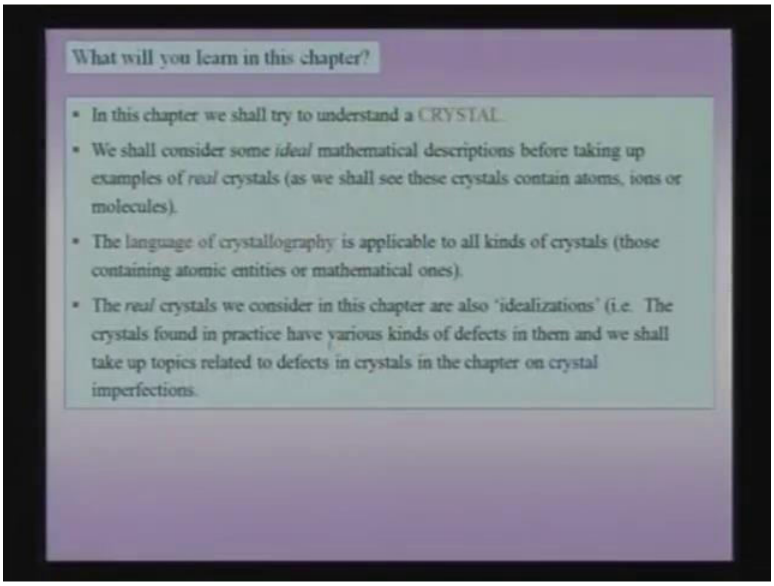

We will try to understand what is a crystal, we will consider for some ideal mathematical descriptions of crystals before taking up what are real crystals and as we know real crystals actually consists of atoms, ions or molecules. In the language of crystallography, crystals are described in a very formal way and we will take these kinds of a formal crystal and real crystals in this chapter are also idealizations. Real crystals are actually have defects and various other imperfections and those topics will be taken on in later chapters.

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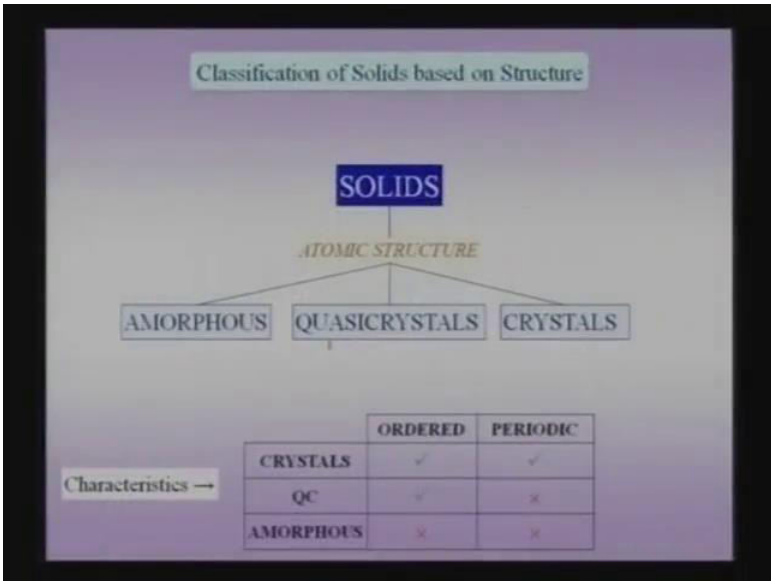

We have already briefly considered the classifications of solids based on structure, based on, and the structure we are talking about here is the atomic structure. Based on atomic structure we can have amorphous materials, quasi crystalline materials and crystals. The basic characteristics of these three classes of materials are crystals are ordered and periodic quasi crystals are ordered, but they are not periodic and amorphous materials are neither ordered nor periodic. In this chapter as we see, we will only consider crystals and amorphous and quasi crystalline materials may be constructed briefly in the later chapters.

The first question of course, we have to ask ourselves is that why do we need to study crystals structures? This is an important question because, when you look around us we see that most of the materials we see are actually not crystalline. The wood which this material is made of, the plastic around us typically, the cement and all these are typically non-crystalline materials. The human body for instance is typically not a crystal.

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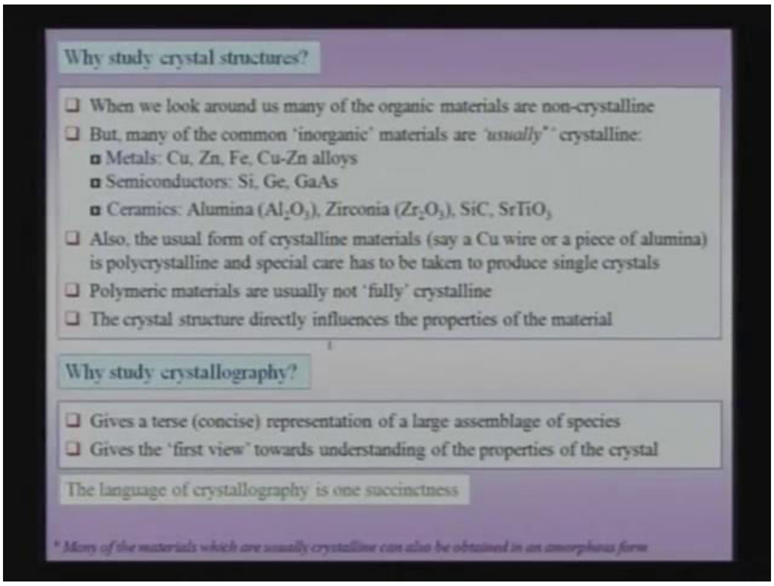

But then we do with not of con, engineering important engineering materials like metals, semiconductors and also ceramics which are actually crystalline. Examples of metal would be copper zinc, pure metals or alloys of these which can be crystalline. Semiconductors like gallium arsenide, silicon or germanium are also typically crystalline. Examples of crystalline ceramics are alumina, zirconium, silicon carbide, strontium titanate and the list is actually very very long. If one important thing to note of course is that, single crystals are actually very very rare typically when you take, for instance a copper wire or a metallic vessel.

For instance, stainless steel vessel actually it is poly crystalline and later, in later chapters we actually formally define what is a poly crystal, but for now we need to know that, the entire structure is not a single crystal. And polemic materials also typically never get fully crystalline and therefore, we should not be confused by looking at the world around us that most materials are actually non-crystalline. But most of the industrial important application materials are of crystalline materials and important reason we need to consider a crystal is because, crystalline materials the properties are directly influenced by the fact that the material is crystalline.

And that is an important reason for us to study crystal structures, the language of describing of crystal structures is a language of crystallography. And why do we need to study crystallography, which is what we are going to start this chapter with is, it gives us a concise or a very succinct representation of a large assemblage of species. What are these species etcetera, we will consider in very detail very soon. And as usual see the language of cryptography is one of succinctness. We had usually said that many of the usually industrial important materials are crystalline like metals and semiconductors.

We should also note that many of these materials can also be obtained in amorphous sounds as well and this we will see in later chapters. In this chapter for instance, we will consider two important definition of crystal.

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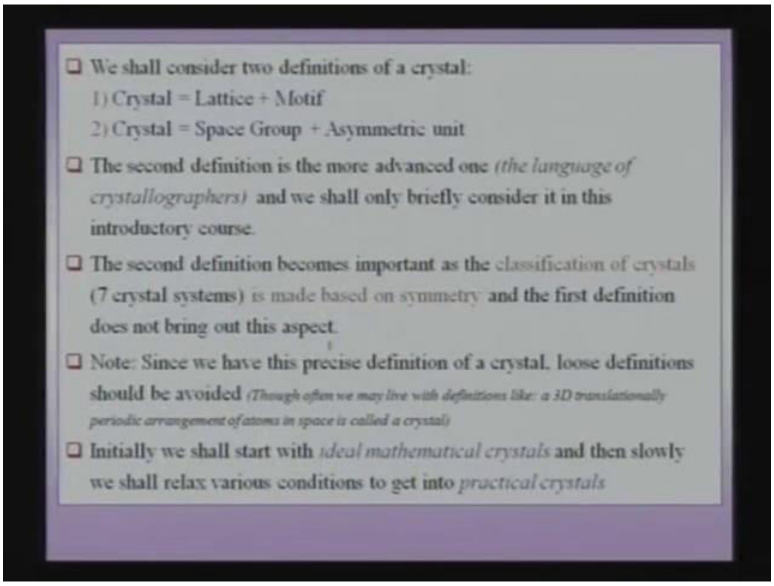

The first definition which is the simpler one, which we shall explore in detail and the later definition, the second one we will only consider briefly in this elementary course, but is an important definition as well. The brief definition of crystal the elementary one is that a crystal is a lattice plus motif. So, there are two components to a crystal lattice and motif, the second definition is the definition of the language of the crystallographers. And though it is very important and especially its important comes to the fort, when we consider a classification of crystals. In classification of crystals, it is typically based major on symmetry and therefore we have to invoke the concept of a space group, which has embedded in a concept of symmetry.

And once we have defined a formal way of dealing with crystal, we should avoid loose definitions of the crystal and this is very important. And though in Persian language some we may often deal with definition of a crystal as a 3D transnationally periodic arrangement of atoms in space. But now that we have a formal definition of a crystal as a lattice plus a motif or alternately as a crystal, being a space group plus asymmetric unit we should not deal use language which is not precise. As we had pointed out before, initially we start with ideal arithmetical crystals and then, slowly we will progress to real crystals, which are really the practical crystals we deal with real day life by relaxing various criteria. And one of the criteria we will do is actually introduced defects in the crystal.

So, let us look at the formal definition of crystal in a lot more detail, a crystal being a lattice plus motif. So, we have two important terms here one being a lattice, another being a motif. So, we will try to understand these two terms in lot of detail, there is a synonym of a motif which is often used by crystallographers and that is a basis. Though we will try to avoid this kind of a use of basis because, the word basis can often be confused with a basis vector. Therefore so, we will stick to the word motive when we are trying to define a crystal.

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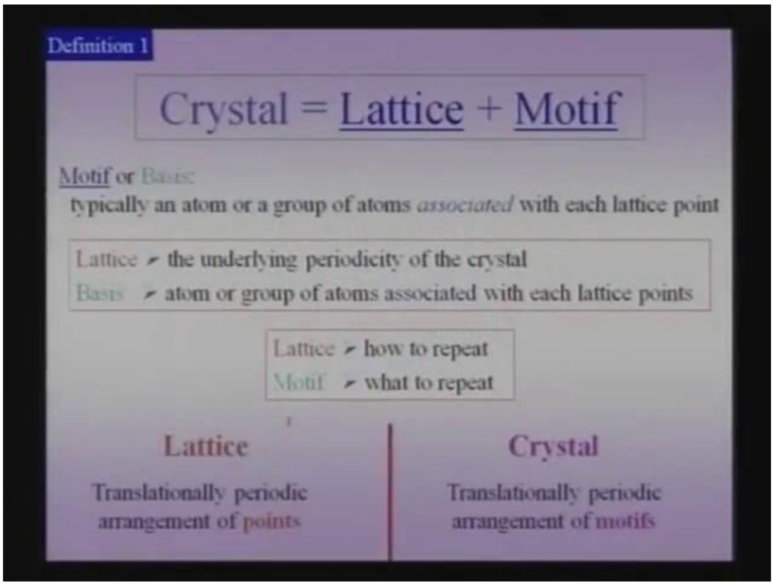

So, what is a lattice? At the first look we can understand the lattice to be the underlying periodicity in a crystal. So, a lattice actually captures underline periodicity of a crystal, a basis actually is any entity typically as we shall see, it consists of an atom or a group of an atoms associated with each lattice point. We will take up examples these to clarify the points, but the key word when we are talking about basis, the word associated which been highlighted.

So, a lattice tells us how to repeat and a motif tells us what is that which has to be repeated and a lattice picks up the translation periodic arrangements of points and a crystal is a transnationally periodic arrangements of motifs. So, it has to be absolutely clear at this point of time that, a lattice and a crystal are different things and when you put a motif on a lattice only then we can get a crystal.

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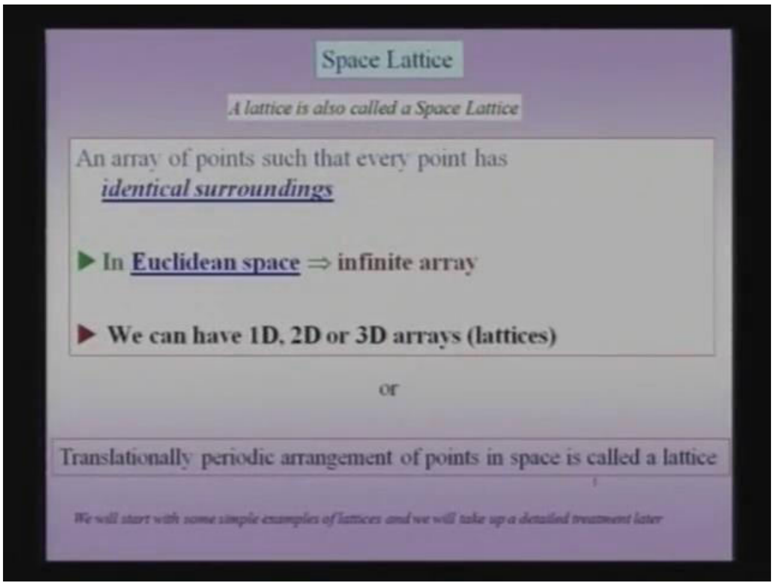

So, the first thing we need to understand in the definition of crystal is lattice which is commonly referred to a space lattice. The simplest and a nice definition of a lattice as we shall see is that, it is an array of points in space such that each point has identical surroundings. So, the key word is that every point in the lattice has identical surroundings, as we shall see by considering examples that is in Euclidean space which is nothing but the flat space such an arrangement of points leads to an infinite array of points. In other words in Euclidean space lattices are infinite, lattices can exist in one dimension that means, we have only one dimensional reputation of atoms.

They can be two dimensions or they can be in three dimensions of course, as a mathematical concept you can have a lattice in n dimensions and n here can be 7 dimensions, 10 dimensions or any other kind of dimension, you wish to consider. A more commonly referred to definition of a lattice, which you might come across in text books is that a lattice is a transnationally periodic arrangement of points in space. We will of course, start with some simple examples of lattices, before we take up a detail description of lattice. So, to summaries this line a lattes is an array of point such that each point has identical surrounding.

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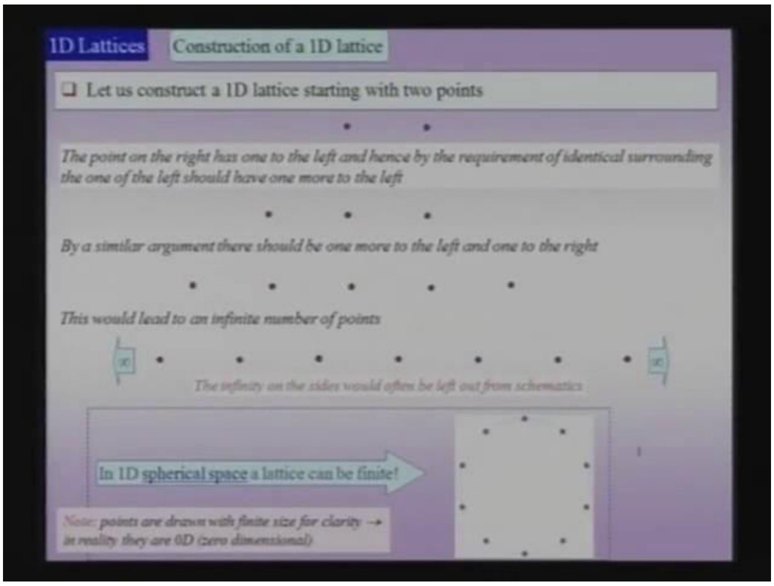

Now let us consider a construct a one dimensional lattice. So, let us start with two points separated in space say by a distance a, we can clearly see the point on a left has a point to its right and the point on the right has a point to its left. And this is ((Refer time: 10:01)) situation as for a, as creation of a lattice goes as each point needs to have an identical surrounding. That means, the point on the left needs to have one point to its left at distance a. Similarly, the point to the right needs to have one more point to its right at a distance a.

So, if we repeat this process we see that in this one dimensional space, actually we will get an infinite set of points. So, the distance between each point would be a and this lattice would be infinite in one dimension. As a curious example, we can consider a set of points, an array of points in spherical one dimensional space that is on a circle and we can see that, it can be finite in a circle, but this is not the typical kind of lattices we consider.

Typically we consider crystals in 1, 2, or 3 dimensions, but typically in Euclidian space and therefore lattices are infinite for, as far as our normal consideration goes. Another point to be noted is that many of our drawings will actually shows these point as finite circles, but it should never be mistaken that these are actually geometrical points and therefore they are really 0 dimensional in ((Refer time: 11:17)).

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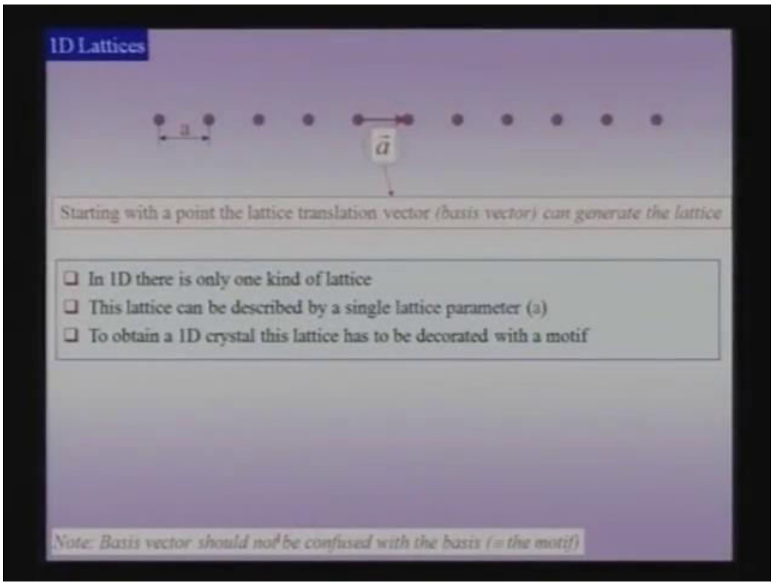

So, let us look at the lattice we have one dimensional lattice we have constructed, we can clearly see that the fundamental lattice translation vector, which can generate this lattice is a vector joining two lattice points, the point one here, the point here. And the fundamental lattice translation vector is a, also it can be clearly seen that there is just one kind of a lattice in one dimension. And this kind of a lattice is described by a lattice parameter a and once we decorate this one dimensional lattice with a motif, we would get a crystal in one dimension.

Of course, this lattice parameter can be changed and therefore we would have different one dimensional crystals or one dimensional lattices, which are different from each other only by this lattice parameter a. And as I pointed out before, that we should never confuse the basis vector with the basis which is a synonym of the motif. So, the second important entity which we need to consider when we want to define a crystal, is the motif. So, the question we are asking is that what can constitute a motif, what kind of motifs exist in practice and how do we understand these motif in relation to these lattice points we have generated.

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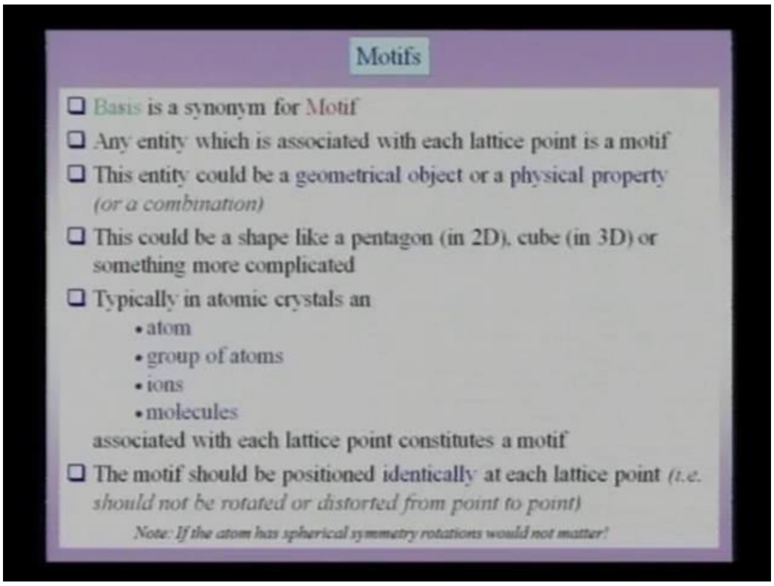

As it pointed out the basis is a synonym for the motif. An entity which can be associated with each lattice point is a motif, as associated see this is a very broad definition and the kind of the entity could be a geometrical object or it can even be a physical property. Or it can be a combination of geometrical object and a physical property, though in this course typically we will see that under normal circumstances we would typically put a geometrical object. And this geometrical object could be an atom or a group of an atoms, which will go on to decorate lattice point to create a crystal.

In two dimensions for instance, a motif could be at pentagon or a cube or in three dimensions it could be cube or it could be something more complicated geometrical object. But as is told you in typical atomic crystals, this could be a group of an atom, ions or even molecules which are associated with each lattice point. One important point while decorating a lattice with a motif which needs to be noted is that, you should put the motif identically at each lattice point. You should not rotate, distort or any way mangle the motif when you go to one lattice point to another, this is an important point.

And as we shall see if you do any of these then, those will become a different kind of a consideration, which we will take up examples of these as well as we go long. One this of course it is obvious that, if suppose I am putting a spherical atom in a lattice point then, since it has spherical symmetry, rotations do not matter as far as these spherical atom goes. In other words from one lattice point to another, I can rotate motif and put it and it would make no difference to the way the motif is decorating the lattice point.

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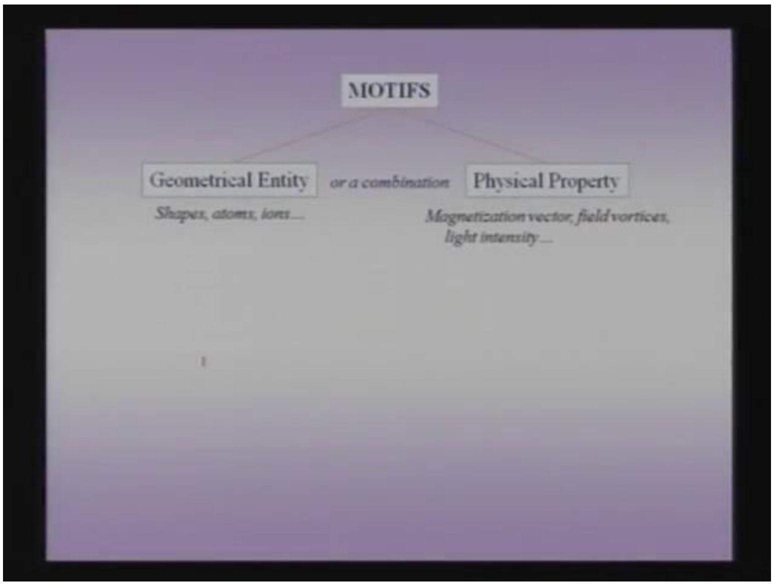

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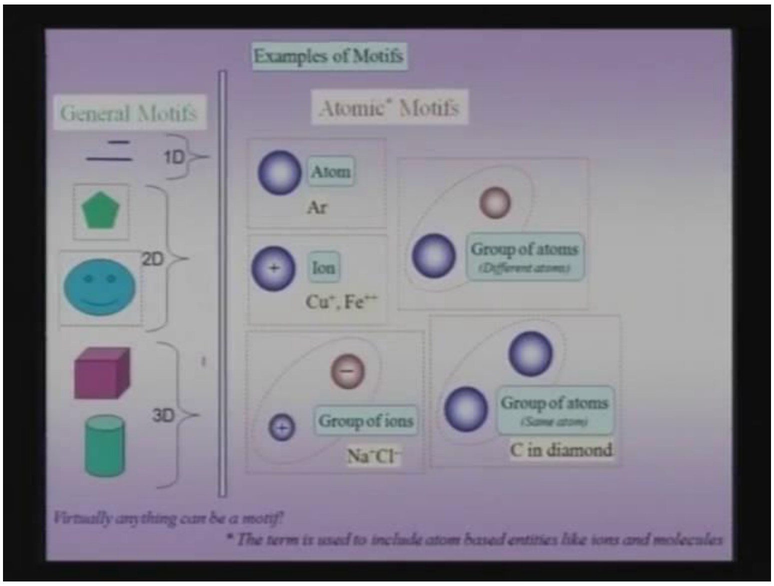

Just to summarize and highlight the important point as far as motif goes, motifs can be a geometrical entity a physical property like magnetization vector, field vortices, light intensity etcetera or it can be a combination of physical property along with a geometrical entity. And as I pointed out before, we will focus on geometrical entities first and later on may we consider some examples of a physical property decorating a lattice point.

So here are some examples of motifs on the left hand side we have geometrical general motifs, which are shapes and in right hand side we have atomic kind of motives, which can go on to decorate a lattice point. And I say below, virtually anything can be a motif so the one dimensional motif typically is the line segment and the only variable what here is the length of the line segment and therefore there is no other kind of one dimensional motif. Two dimensional motifs can be like a pentagon or a square or any other complicated two dimensional shape.

Three dimensional shapes are those like a cube or a ((Refer time: 15:31)) or a cylinder or any one of those. Atomic motifs could be a single atom motive like an argon atom as in the example above, they can be as ion like copper ion decorative a lattice or an ion decorating a lattice. They could be a group of an atoms which are of different kinds, they could be one or two atoms constituting the groups or they could be many more or they could be a group of ions which can go on to decorate a lattice. Often it is found, we will see that atoms of the same type also go on to decorate the motif like, we will consider an example later where in carbon atoms, two of them go and decorate FCC lattice.

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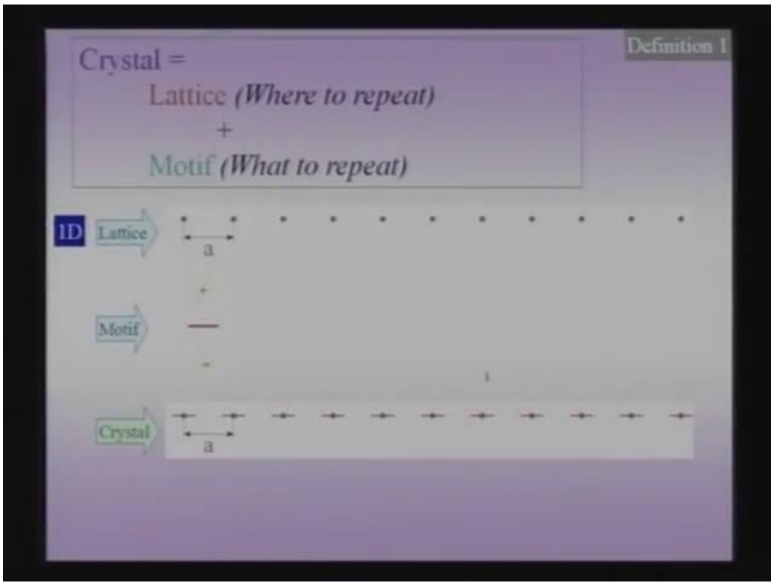

So, let us construct a one dimensional crystal by starting with the one dimensional lattice and here we are dealing with the simpler definition of crystal where, in a crystal is a lattice plus a motif. So, let us consider the one dimensional lattice of lattice parameter a and the motif possible in one dimension is the line segment and let the, let the line segment be b and I can form a crystal by putting this motif at each lattice point, as it has been done in the figure below. And here therefore, obtain the one dimensional crystal of lattice parameter a.

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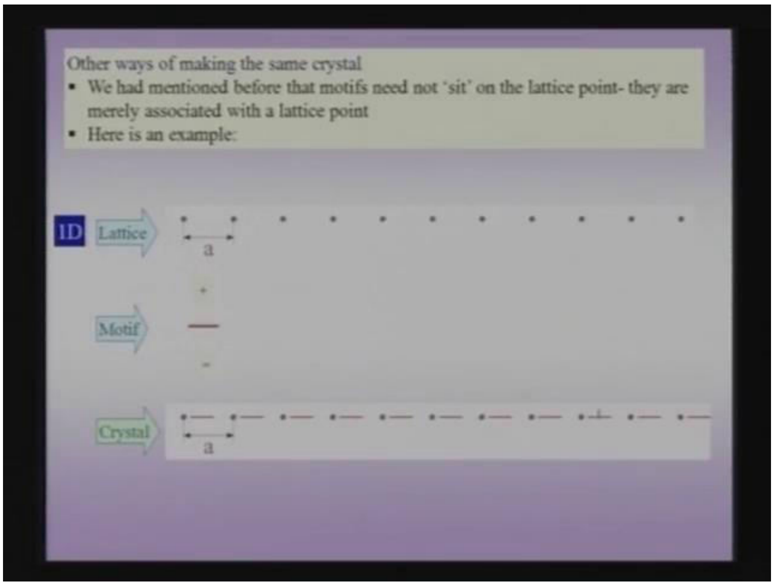

Now, we will consider some important points before we progress to other kind of motifs, we can look at the same crystal in a different way. We start with the same one dimensional lattice, which is one dimensional lattice of lattice parameter a and put the same motif at each lattice point. But now, we will try to highlight the fact that we did not actually make the lattice, the motif sit on each lattice point. But we need to merely associate motif with a lattice point, which is being done in the case crystal constructed below. As you can see clearly that, none of the motifs actually sit on the lattice point, but they are at a final distance away from the lattice point.

This is obviously a very simple and easy to understand point, but often you will see in real crystals an example will be pull ring for instance, which will consider later that atoms actually do not even sit on the lattice point. We can do a small relaxation of the condition that, we need to put a strict one dimensional motive on a one dimensional lattice. And actually start putting two dimensional or three dimensional motifs on a one dimensional lattice and the reason we would like to do so is of course, to understand crystals in a elementary one dimensional way before we go on to more realistic crystals, which are actually three dimension.

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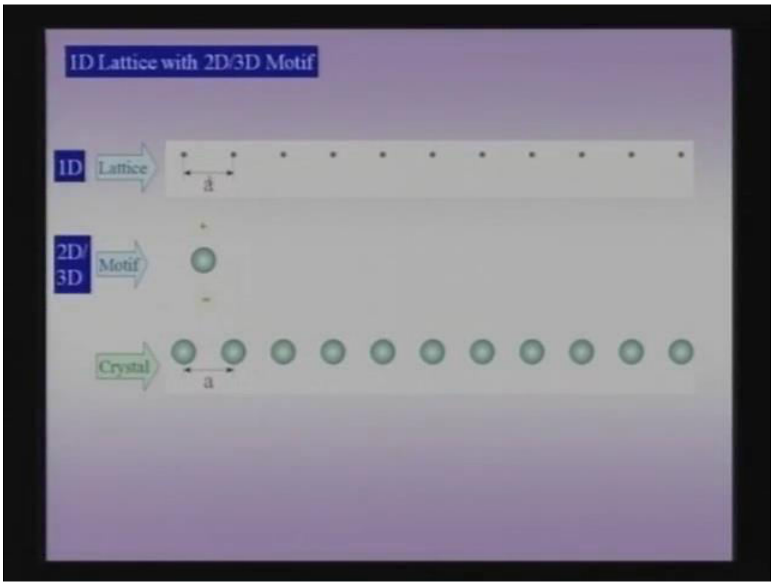

So, let us start with the lattice which are one dimensional lattice before with a lattice parameter a. Of course, I can put a spear or a circle as a motif in each lattice point and therefore, I can get a crystal as in a figure below, which consists of a periodic arrangement of circles as spears on a one dimensional lattice.

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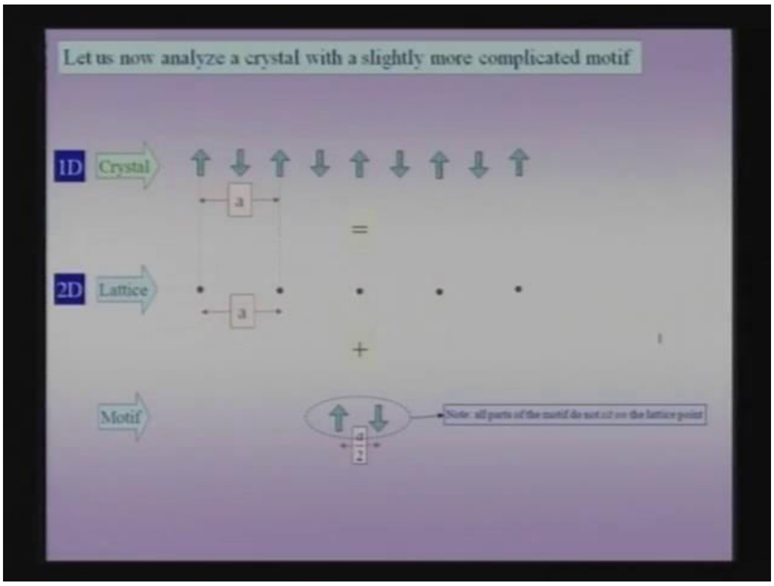

Now we can also consider more complicated motifs, which can go on to decorate a lattice. An example here is the one which is shown, which consists of an up arrow and the down arrow, which repeats itself in a one dimensional space. And here we will do the inverse process, we will first start with the crystal and then we will try to analyze this crystal in terms of the language of the crystallography, which is a lattice plus motif. So, we have one dimensional crystal here where in, there is a up arrow down arrow and up arrow and down arrow repeating itself in one dimensional space. It is also clear that the motif is actually not a strictly dimensional motif, but it is a two dimensional motif and the purpose here is to understand that how we can understand this crystal, in terms of a lattice and a motif.

So, we will see that the lattice underlying lattice has a spacing a, in other word the centers of all the up arrows alone constitute a lattice and the down arrow centers are not lattice points. Alternately, we could only consider the centers of the down arrow as this lattice points and not take up arrows as a lattice points. So, let us consider first case where in the centers all in the up arrows are lattice points therefore, the lattice point parameter of the crystal was a, the lattice parameter of the crystal lattice is a. And the motif now, is a combination of up arrow and down arrow and separation between the two being a distance a by 2.

Therefore the motif consists of two parts, an up arrow and down arrow which is separated by a distance a by 2 and when I put this at each lattice point, I get the crystal which is a crystal consisting of up arrows and down arrows. And also this also highlights the point which we considered in the previous line, that all parts of the motifs here actually do not sit on the lattice point. For instance, the up arrow actually is the center around the lattice point, while the down arrow sits at a distance a by 2 from the lattice point.

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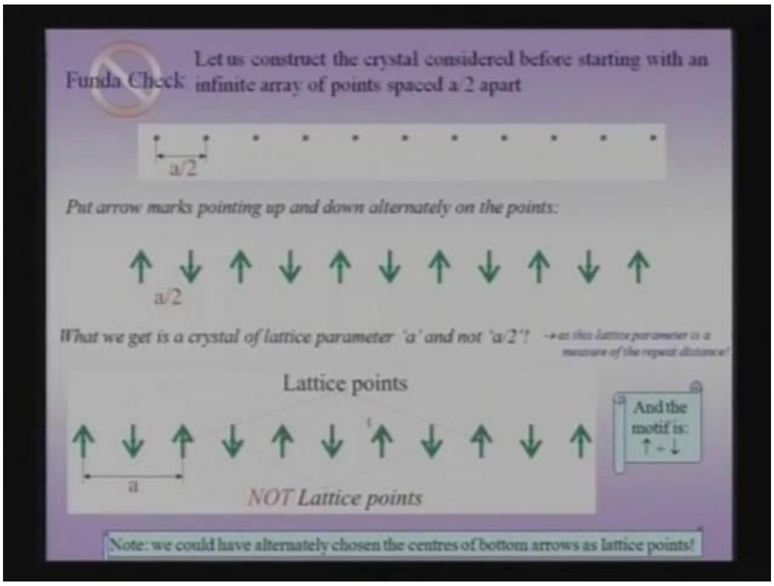

So, we will revise the same crystal once again by doing the inverse process, that is actually constructing the crystals starting with a lattice. Of course, we could start with the lattice, we is an array of point which is based a distance a by 2. As you look at this lattice in isolation, what is the lattice parameter of this lattice? It is a by 2, it is very clear. Now, suppose I put my combination up arrows and down arrows and what I do is that, at the first point I put an up arrow, the second point I put a down arrow ,the third point I put an up arrow, in fourth point I put an down arrow and so forth and doing and doing. So, I have generated a one dimensional crystal.

Now, let us look at the crystal a little more carefully, when I look at the crystal it is very clear that the repeat distance is actually a and not a by 2. Therefore, the center of each arrow is not a lattice point and only the centers of the up arrows are actually lattice points. Therefore, the lattices now has a, once a crystal has been constructed now the lattice parameter of the crystal is a and not a by 2 and therefore only the centers of the up arrow are lattice points. Of course, I said pointed out before we could have alternatively chosen the centers of down arrows, I see at these points and we could have made the same crystals once more. And it is clear motive now consists of an up arrow and down arrow which are separated by a distance a by 2.

Now we will proceed to two dimensions and we will try to make a two dimensional crystal. The two dimension is slightly more complicated than one dimension, but it also serves to illustrate more concepts when we consider actually a two dimensional crystal.

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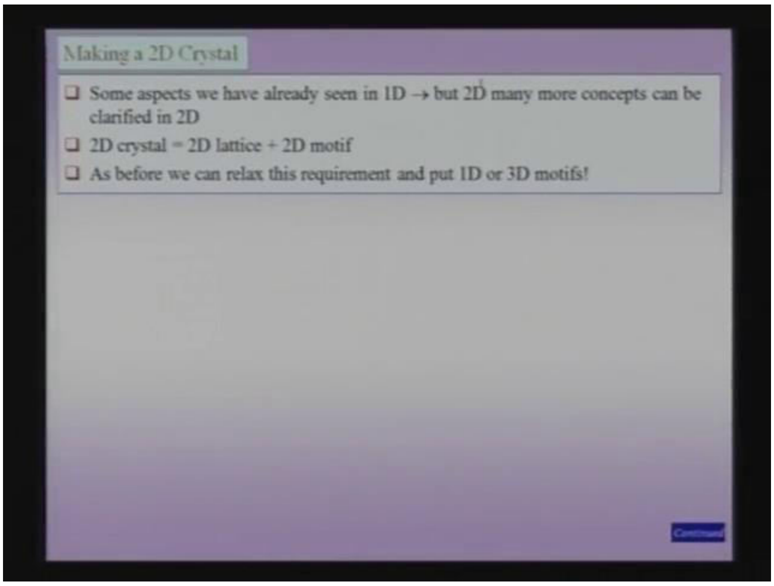

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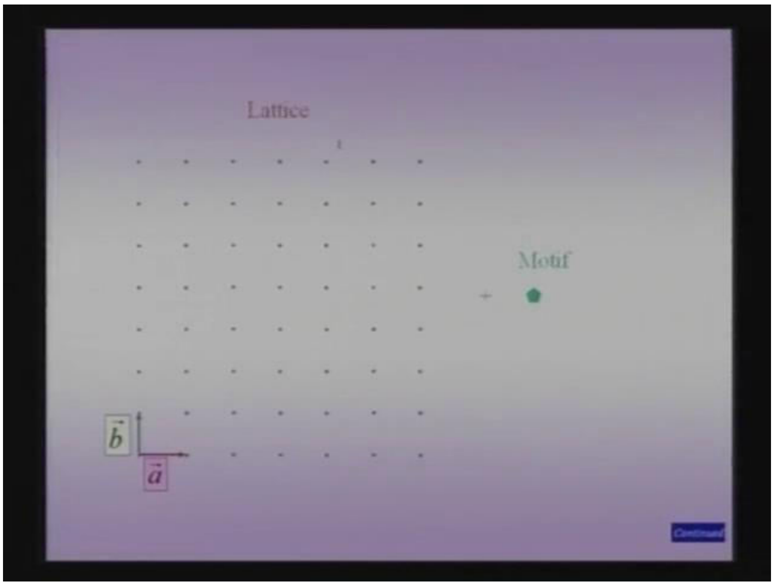

As in the case of one dimensional crystal, a two dimensional crystal is nothing but a two dimensional lattice, which has been decorated with a two dimensional motif. And as before we can actually relax this requirement, by putting one dimensional or three dimensional motifs on to a two dimensional lattice, to generate a crystal which is not actually truly two dimensional, but has a dimensionality between that of a lattice and motif.

So, let us start by constructing a two dimensional lattice and progress to make a two dimensional crystal. So, on the left hand side of the figure we can see a two dimensional lattice, as before because of the requirement of identical surrounding, we will see that if this point has a point above it at a distance b, this point has a distance a to its right another point. Then identical surrounding would mean that, this point as well needs to have a point at its right at a distance a and a point above at a distance b. This would automatically mean lattice is infinite, but as we are limited by our space of our screen, what we will consider here are finite representations of the infinite lattice. But we should never forget that, actually lattices in Euclidean spaces are infinite.

Another point we can clearly see is that, we could make a two dimensional, one dimensional lattice with a single lattice translation vector, but we need two translation vector for generate two dimensional lattice. And here it has been shown in this example, the two lattice translation vectors have been labeled a and b, it is also clear that these two lattice translation vectors cannot be collinear. They need to be co planer that means, they cannot, they have to generate two dimensions. Now, in practice a could be equal to b and therefore or the angle between a and b could be any arbitrary angle, unlike that angle shown in the example where it is 90 degrees.

The motive shown here is a general motive which is a pentagon, as we have considered before any of the two dimensional shapes would constitute a two dimensional motive. So, we started the lattice which is two dimensional and a finite part of the lattice issue known here for clarity and we will have a motif, which is go on to decorate this two dimensional lattice. And as we have seen there are two bases vectors we generate the lattice, a and b and there is an included angle between the two bases vectors.

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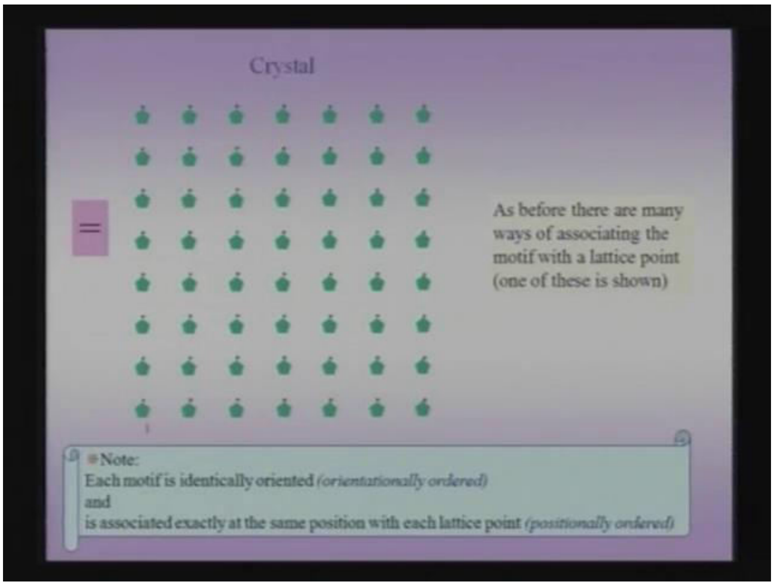

So, the crystal we have obtained is the one which is shown in this figure and as before we see that, each lattice point has been identically associated with a shape pentagon. There has been no rotation or no shift from as we go from one lattice point to another, as we go on to decorate the lattice with this motif. As before there are many ways of associating with this pentagon with this lattice and therefore, we could have many representations of the same crystal in terms of the same lattice and the same motif. An important point which comes to forth when we consider this example is a fact that, each motif is identically oriented.

In other words crustal like these are orientationally ordered and each point is exactly positioned with respect with the lattice point as each other motif. And therefore these crystals are positionally ordered therefore, one key factor which goes on to describe crystals, if they are orientationally and positionally ordered. As we shall see later that some of these conditions may be relaxed and still we may go on to consider crystals, which are may be partially oriented ordered. But still we will call them crystals but, at this point of time we are considering ideal mathematical crystals which are perfectly orientationally ordered and perfectly positionally ordered.

We have seen that when we want to describe a crystal, we need to consider infinite lattice. Needless to say this is impractical proposition and also needless to say when we want to document such a crystal, it is going to be a tedious task, the way to ((Refer time:

26:57)) this problem is to consider a finite representation of an infinite lattice and the way to do it is, by considering something knows as a unit cell.

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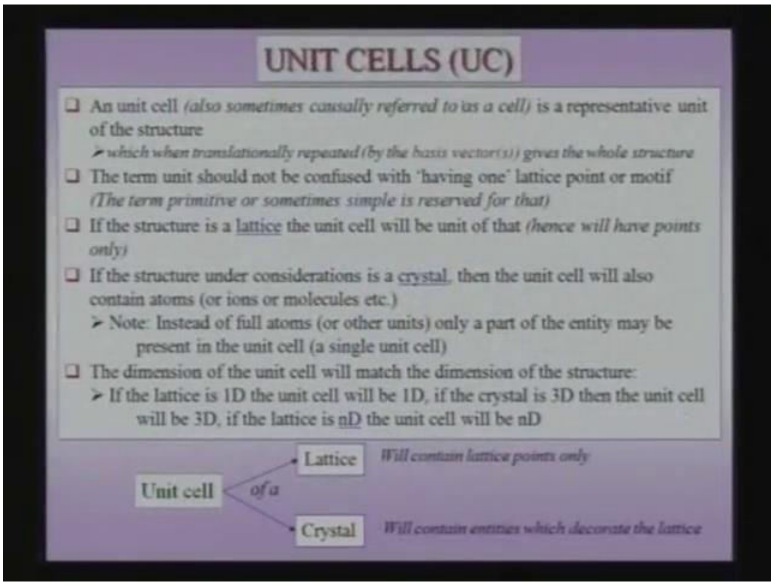

Unit cell is also, sometimes referred to as a cell in common literature and is the representative unit of the structure. Now, when this unit is transnationally repeated obviously by the bases vectors we get the whole structure, which is the crystal structure in our case. Of course as we shall see that look at referring to the figure at the bottom, that unit cell can be for a lattice or can be of a crystal and when the unit cell has only lattice points, then the crystal will also be that considering only of the lattice. When we are actually considering unit cell of a crystal then the unit cell will also contain parts of the motif, when we are talking about a unit cell of a crystal.

An important point to note when we are describing unit cells is a fact that, the word unit should not be confused with the fact of the actually the crystal or the lattice having only one lattice point per cell. That term used to describe a single lattice point per cell is called a primitive or sometimes a simple unit cell. If the structure under consideration is a crystal then, the unit cell will have typically atoms and molecules as we have seen, but another important point to be noted at this stage is at inside the unit cell, there may not be full atoms only parts of the entity may actually be present inside a single unit cell.

And we will consider this by actually sighting examples, it is also obvious that dimension of the unit cell will match the dimension of the structure. For instance, suppose I am talking about the unit cell of a one dimensional crystal then, the unit cell will be a one dimensional unit, which is nothing but a line segment. For a two dimensional structure, we will have a two dimensional unit cell. Similarly, for an n dimensional structure unit cell will actually have n dimensions and therefore n fundamental arteries translations vector.

So, to summaries the slide an unit cell can be for lattice or can be for a crystal, if it an unit cell of a lattice, then it will consists of only points, geometrical points. If it is a unit cell of a crystal then, in addition to lattice points it will also consists of motifs.

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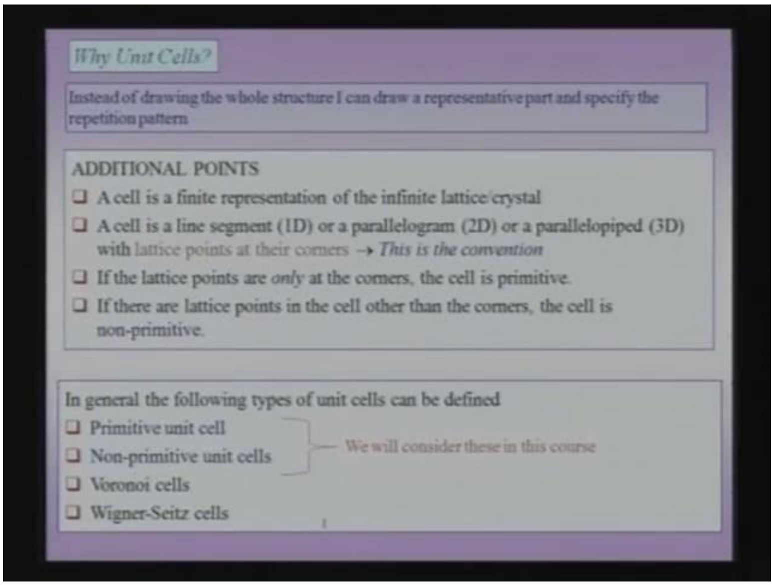

We have already considered the basic motivation of the need for considering unit cells and to emphasize again, the idea is to actually have a finite representation to describe an infinite repeating pattern. Therefore we are conceive in our description of the crystal structure, a few you additional point are noteworthy at this stage when you are talking about unit cells that, typically the lattice points are present only at the corner. So, the unit cell and but this is only a convention and we will take up examples of cells, in which we need not to put lattice points only at the corners of the unit cell. But typically the remainder of the course we will follow only the convention that is, we will put lattice point only at the corners of the unit cell.

In addition there are no other points any other point in the unit cell then, such a cell is considered primitive and we will consider examples of primitive and non-primitive cells in 1, 2 and 3 dimensions. There are other terminology which you would come across when you are studying text books and these other kind of cells possible are Voronoi cells Wigner Seitz cells. But in this elementary course we will only consider examples of primitive unit cells and non-primitive unit cells.

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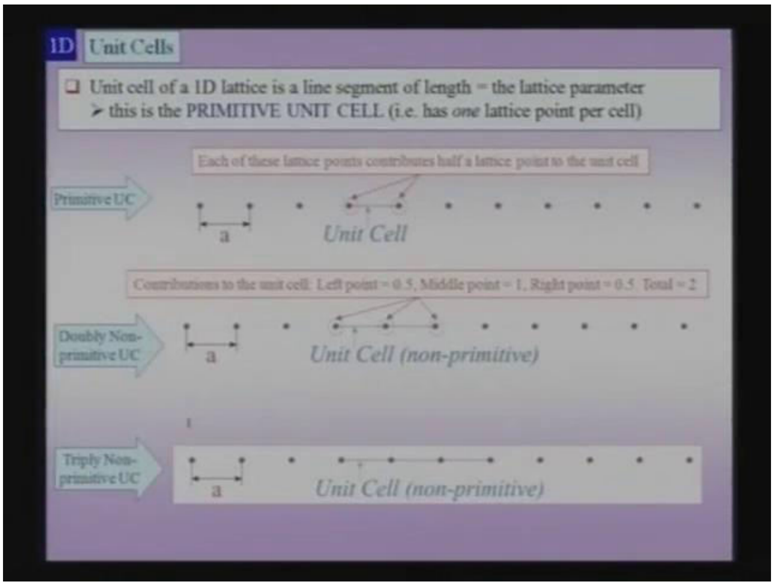

So, let us find out what is the unit cell of some of the structures we have already described and let us start with the one dimensional crystal. So, before you go to the one dimensional structure let us consider the primitive unit cell of a one dimensional lattice. So, the primitive unit cell is nothing but a line segment which extends from half of a lattice point to the center of the next lattice point. So, let us see how what are the contributions to these unit cell from the lattice points, it is clear that the lattice point on the left only contributes half to the unit cell.

Lattice point to the right contributes only half to the unit cell and on the whole the unit cell contribution is one lattice point per cell. And since this has only one lattice point per cell it is called a primitive unit cell and if there are more than one lattice point per cell, then we will call it a non-primitive unit cell. The example shown in the second figure below shows a non-primitive cell, which is a doubly not primitive cell and in this case we can consider a unit cell as shown by the blue line. So, let us find out what are the contributions of the lattice points to this blue line. The central point is fully with in the unit cell and therefore has a contribution one.

The lattice point to the left contributes half to this unit cell, while the lattice point on the right contributes another half to this unit cell and therefore, the total contribution to this unit cell from this lattice is two. And therefore we call it as a doubly non-primitive unit cell ((Refer time: 32:15)) we can go and consider triply non-primitive unit cells and higher non-primitive unit cells. The example on the bottom of the slide shows a triply non-primitive unit cell. In this case the contribution from the point on the left most is half right most is half making one and there are two additional points making full contributions to the unit cell.

Therefore, we have total contribution to the unit cell being 3 and there for being unit cell is called a triply non-primitive unit cell. Let us look at this same concept of a primitive non-primitive unit cell from the point of a crystal.

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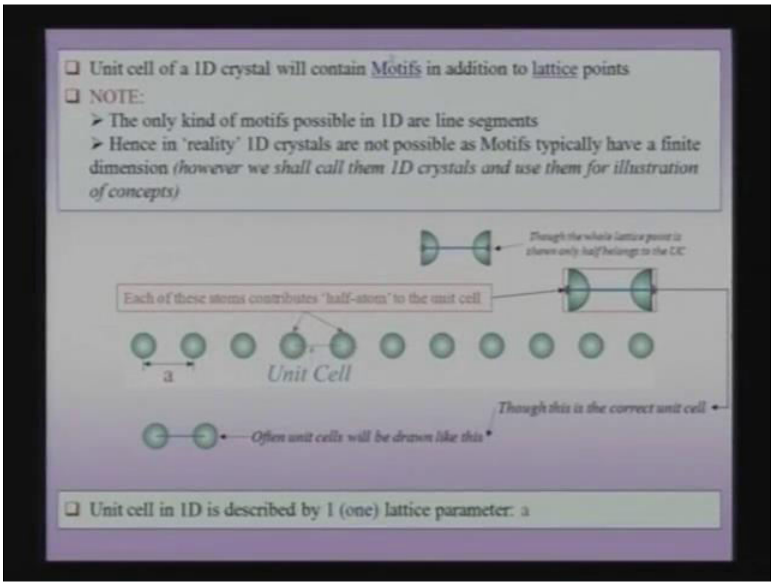

If we are talking about a crystal unit cell will addition to the lattice point will also contain motifs. The only kind of motifs we construct before in one dimensions was the lice segment, but in reality we know therefore that we cannot have just line segments in one and real crystals therefore are not possible. But we shall use these kind of one dimensional crystals for the purpose of illustration. So, let us consider the crystal wherein we have put a circle or a sphere as among the one dimensional lattice and we will consider what is the contribution of the units here inside the unit cell.

So, the typical conventional representation the way typically this unit cell would be shown is that, there is a sphere on the left or the circle on the left and a circle on the right at the ends of an unit cells. But this is clearly unsatisfactory and a more correct description would be where in here and half the motif is sitting to the left. And similarly, half the lattice point is contributed the unit cell form here and half the lattice point is contributed from this lattice point to this unit cell. And therefore, the complete unit cell would actually be something like this, which has a certain extent on the two dimension second dimension.

So, the point to be noted here is that often you would draw diagrams which shows a unit cell having a complete atoms, but the thing to be noted is that only a part of actually entity may actually belong to the unit cell. So, this kind of a representation is just for simplicity and the real representation is the one that is shown in the figure above here. Also that is clear that, such a one dimensional crystal is described by one lattice parameter which is a.

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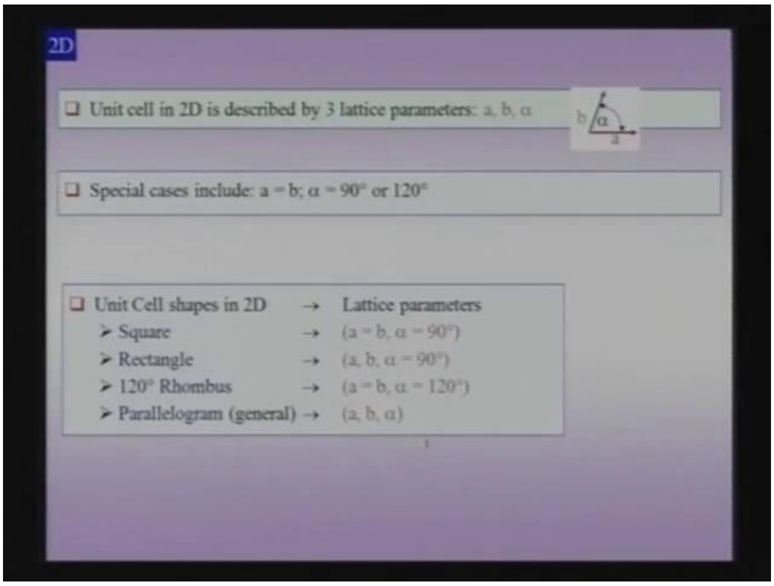

Now let us proceed to two dimensional unit cell in, two dimensions is described by three lattice parameters. These are two distances a, b and there is an angle included which is alpha. There are special cases which are possible, cases in which the lattice parameter a and b are identical, the lattice parameter alpha is 90 degrees or the angle alpha can be

120 degrees. Unit cell shapes in two dimensions, can be a square, rectangle, a 120 degree rhombus or a parallelogram and the parallelogram being a general parallelogram.

The lattice parameter restriction for some of these are, for a square you can have a equal to b and alpha a equal to 90 degree. In a rectangle lattice a and b are not equal, but alpha is still 90 degrees. In a 120 degree rhombus a and b are identical, but alpha is 120 degrees and a general parallelogram a b and alpha have no restrictions placed on them. In this elementary set of lectures we are only describing or pointing of the existing lattices, we will take up little more detail later on, when we will describe some examples of these square rhombus unit cells and crystals based on these.

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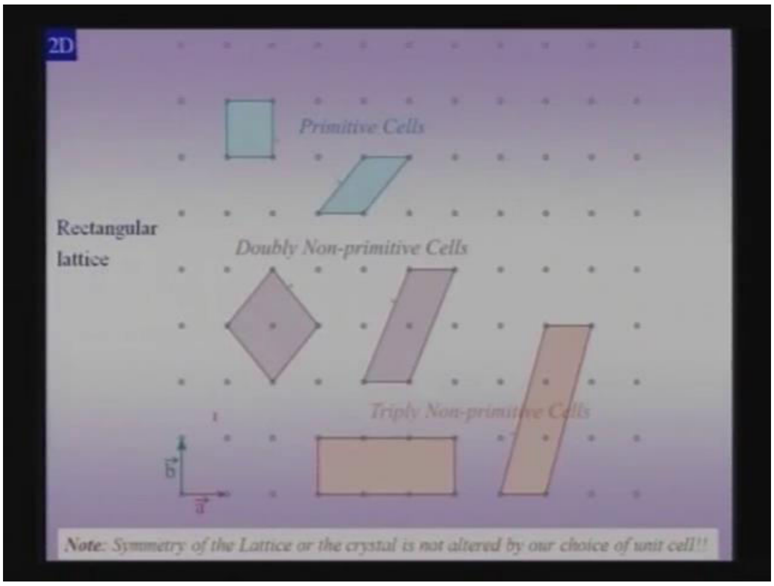

So, let us go back and consider two dimensional lattice which we have constructed before, which was generated by two lattice translations vectors a and b. So, this is the two dimensional lattice and as before this is nothing but a finite representation of the infinite lattice. This is a rectangle lattice because, a and b are identical, not equal to each other and the included angle is 90 degrees. So, let us try to construct primitive, doubly non-primitive, triply non-primitive unit cell for the case of this rectangular lattice. It is clear that the blue cells are both primitive unit cells because, the contribution of the lattice to the unit cell is 1.

In the case of the rectangular unit cell, it is clear contribution of each one of these lattice point is 1 4 and there are four lattice points at the corners and therefore, the net contribution is 1 to the each lattice point, at each unit cell. In the case of the parallelogram of the unit cell it is clear that the contribution of the each lattice point cell is not equal, but net contribution to the unit cell is 1. And therefore, these unit this kind of a unit cell is also a primitive unit cell. There are two examples of doubly non-primitive cell given below, both of these unit cell actually consist of 2 lattice points per cell.

There is one in the center of each one of these cells and there are four at lattice points of the corners, together contributing 1. Therefore the lattice point count for each one of the unit cells is 2, one from the corners and one from the centers of the unit cell. So, is the case on the right hand side where they combine the lattice contribution from the four, lattice points in the corner point is one and one in the center adding one more giving a doubly non-primitive unit cell. The ones in orange are the triply non-primitive unit cells where in, each lattice point or each unit cell is contributed by multiple set of points, those in the corner of unit cells and those which are also present on the edges in this case and those present with in the unit cell in this case.

So, let us do count for one on the left, the four lattice point on the corners contribute one four to the each unit cell and therefore making the net contribution of one lattice point to this unit cell. Though once these two shares half the lattice point of the unit cell similarly, these two and these four together make contribution of 2. And therefore the total contribution to this unit cell is 3. Similarly, the orange one at right also has three lattice points with in the unit cell 1, 2 and the one-fourth the total 4 1 totally being contributed from once in the corners.

Therefore we have now consider primitive and non-primitive unit cells in one dimensions and also two dimensions and point out again the word unit should not be considered with primitive unit cell. The word and we will consider examples unit cells of different types as we go along.

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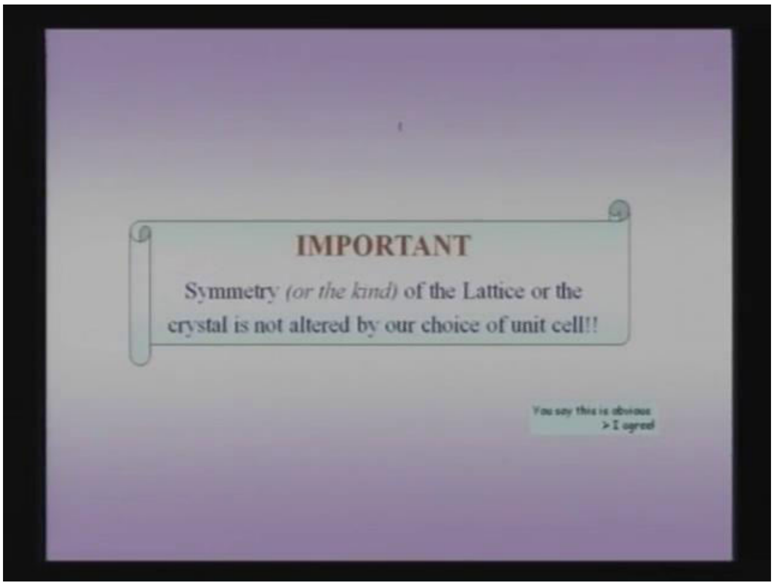

Another point which is perhaps obvious is that, the symmetry or the kind of the lattice or the crystal is not altered by the choice our choice of unit cell. This might seem like a trivial point initially, but this is a very important point that I can make a multiple choice of unit cell for the given crystal or the given lattice. And some of the examples are like in this slide before, but any of my choices is a legitimate choice and would all constitute valid unit cells, but the structure remains unaltered irrespective of the kind of the unit cell I choose.

It is also obvious that the symmetry of some the unit cells are lower than the symmetry of the lattice, but still nevertheless we can use those kind of a unit cells. And those unit cells would go on and describe the structure equally well as any other kind of the unit cells. And there are reasons as we shall see later that, we would want to actually choose some of the non-primitive unit cells for a better description of the crystal structure or of the lattice. So, to reiterate this important point, the symmetry or the kind of the lattice or the crystal is not altered by our choice of the unit cell.

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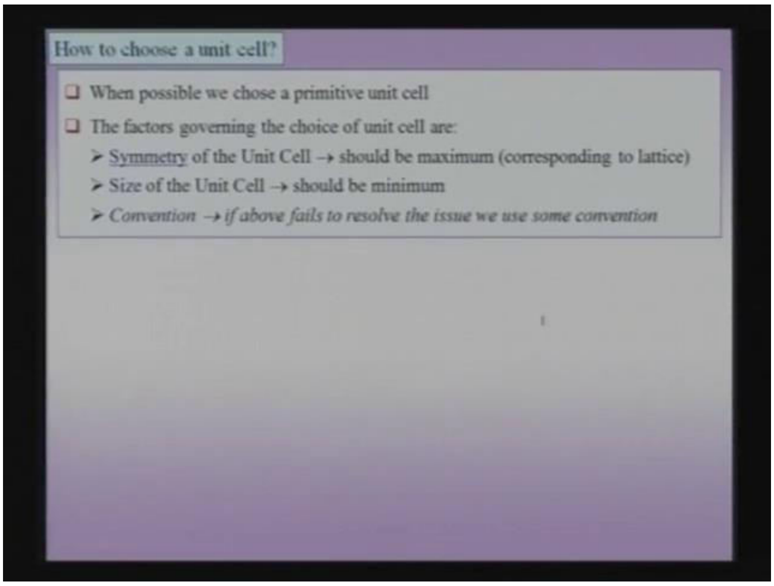

That brings us to the next question, how do I choose a unit cell? As you have seen that we can actually make a primitive choice or a singly doubly non-primitive choice or a triply non-primitive choice. So, the question arises how do I go ahead and make a choice of an unit cell. So, there are some guidelines which helps us making a choice of unit cell and as to emphasis the word, the key word is guidelines. These guidelines are we try to use a unit cell, which has a maximum symmetry preferably which matches the symmetry of the crystal lattice being described.

Second haven taking care of the symmetry aspect, the size of the unit cell should be a minimum possible. If both this criteria fails then, we stick to some convention which we shall always use in describing the crystals of a type. So, to summaries this slide and to emphasis the points again, when we want to make a choice of a unit cell a Merida, a variety of choices exist at our disposer. But then we have certain guidelines which would guide us in making a choice of a unit cell, which is in a some sense can serve a universal representation of the crystal structure.

So, the what are these guidelines, the first guideline being the symmetry of the unit cell that ((Refer time: 41:54)) to choose the unit cell which has the maximum symmetry, typically commensurate with the symmetry of the structure. You will try to keep the size of the unit cell to a minimum possible and there are special cases where in, both these criteria would not be sufficient or would not uniquely resolve the issue. And therefore we would stick, we would generate a convention which should be use uniquely, use a single kind of a unit cell for the class of structures. So, let us consider examples to actually clarify this point of how we use a symmetry or the size in choosing unit cells.

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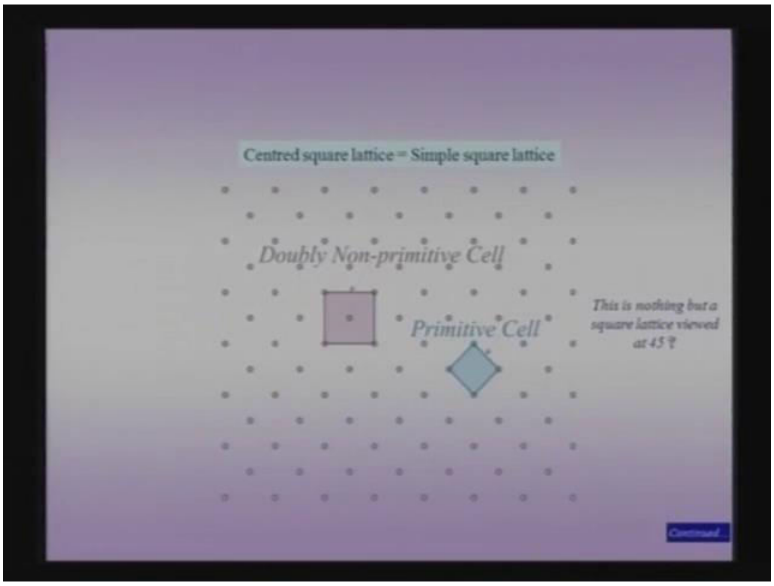

So, let us consider a square lattice and in this case of course what I am doing? I am moving the square lattice at an angle of 45 degree rotation. So, there are two possible choices of unit cell as shown in this, a doubly non-primitive unit cell and a primitive unit cell as shown by the blue color. Before both are valid and legitimate choice of unit cell and, but the one which is preferred is the blue unit cell for two reasons because.

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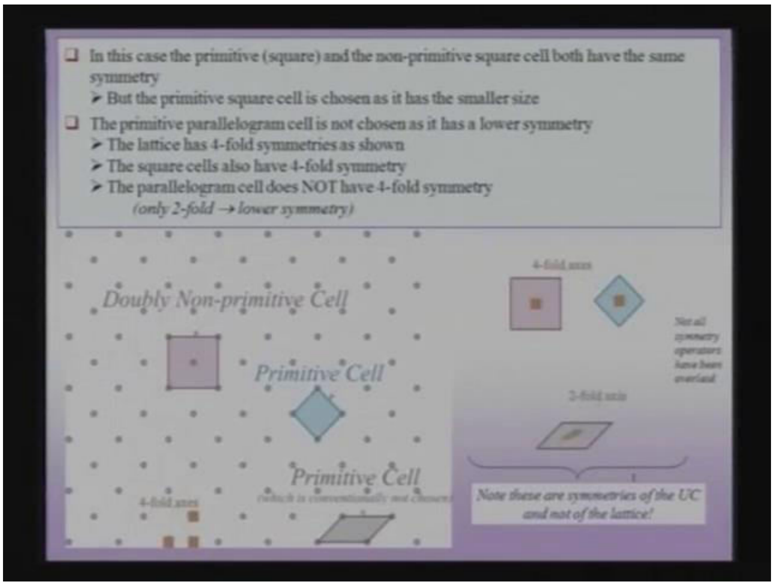

Number one, if you look at the decimeter of the unit cell of the blue and of the other colored unit cell, we seal that both of them have a fourfold access in the center of them. Therefore the symmetry of the unit cell is same and therefore we could have made a choice between the, based on the first criteria it is no unique resolution between the two unit cells. But now let us look at the size obviously, the second, doubly non-primitive unit cell is twice the size of the blue unit cell and therefore the preferred unit cell for this case is the blue unit cells, which has the same symmetry as that of the lattice. As we can see in the figure that, the lattice has a distribution of four fold access, at various points lattice points.

And the sum between the two lattice points and the unit cell also has the fourfold access and hence based on symmetry I would choose a square unit cell and based on size I would choose square unit cell of the smaller size, which is nothing but the blue unit cell. So, to review this example I have got here a square lattice which is shown rotated 45 degrees. In another words the viewed along with this direction, I would see the square lattice the normal way it is shown. There are multiple choice of unit cell possible for this lattice, I can choose the one like the one in blue.

I can choose the one shown in this brownish color, which is a doubly non-primitive unit cell or I can choose triply non-unit primitive cell or unit cells of various other shapes. Clearly those other shapes unit cells have a low per symmetry than the unit cells which are shown here in the figure. Now what is the symmetry we are comparing, we are comparing the symmetry of the unit cell with the symmetry of the lattice and what is the symmetry of the lattice? Though we have not shown all the symmetry apparatus overlaid on the lattice, but we can clearly see that the lattice has fourfold symmetry.

Now both the unit cell shown in the figure have fourfold symmetry, but based on the second criteria the size criteria I would go on to choose the color unit cell as a preferred unit cell for describing this two dimensional square lattice. Another possible primitive cell is shown in the figure which is in the shape of parallelogram, but clearly this would not be a preferred choice of a unit cell. Because, you can see that this unit cell has only a twofold access at its center and not a fourfold access, again to reiterate the fact which we had stated in the couple of slides before, let me go down to the slides which we have shown before.

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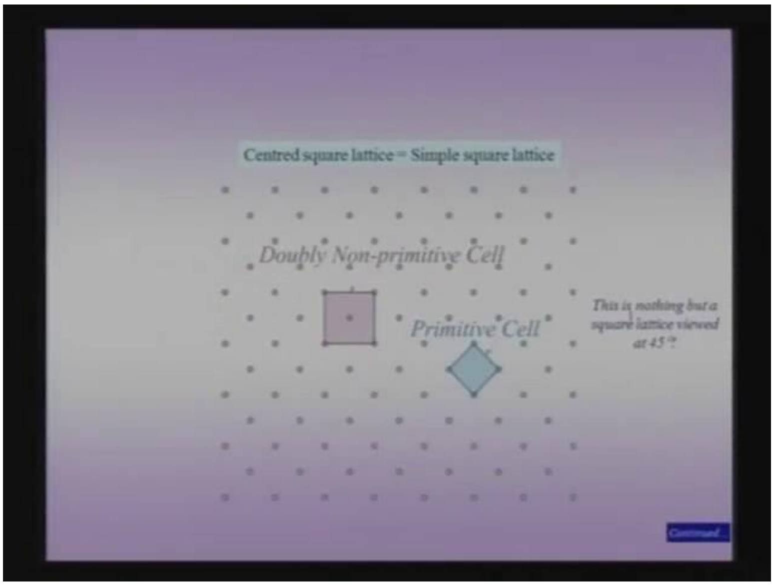

My choice of unit cell is left to me and any of these choices is a valid choice and my choice of an unit cell is not going any way to alter the symmetry of the structure, which I am describing. Therefore, even this unit cell is a valid unit cells though not a preferred unit cell. In the previous example wherein, we had considered a square lattice we had seeing that a primitive unit cell was the preferred unit cell, based both on symmetry and size. Now we will consider a set of centered rectangular lattice where in, at the preferred unit cell is not a primitive unit cell and in fact it is a doubly non-primitive unit cell.

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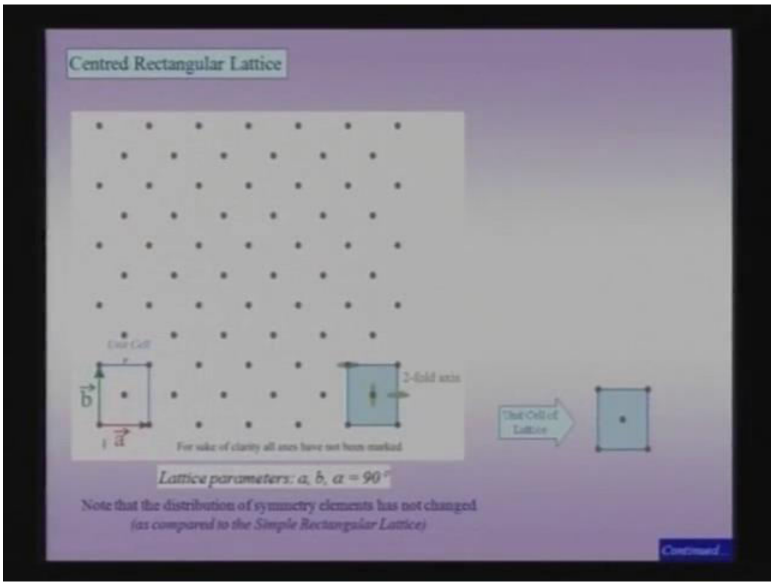

So, this is the centered rectangular lattice and this is been generated by two basis vectors a and b for a rectangular lattice, the included angle being 90 degrees. So, let us consider a primitive unit cell which is in the shape of a rhombus. Now clearly if you look at this symmetry of this unit cell, it is got the symmetry which is two old compared to a square. In the example we considered before we had a square lattice and the preferred unit cell was a square unit cell, which was a primitive square unit cell. In this example we will see that, we will actually have a non-primitive unit cell which is the unit cell, which is normally considered to describe centered rectangular lattice. Centered rectangular lattice it is generated by two bases factors a and b which are 90 degrees apart.

Now, if we can also we can consider a primitive unit cell as shown in the green color, which is rhombus shaped. As before, the contribution from the four points at the corners of the unit cell is 1 totally 1. We can have an alternative unite cell which is blue colored, which is in the shape of the rectangle and which is contribution of one-fourth from the four lattice point that is corner and one from the center. Therefore, having two from the total unit cell therefore, this is doubly non-primitive unit cell. In this case, the symmetry of both unit cells is the identical, but still we prefer the unit cell which has 90 degrees separation between the basis vectors.

So, in this case even though the based on size and symmetry the green unit cell is the preferred unit cell. Here, we go by convention and actually choose the blue unit cell as the conventional unit cell to describe the centered rectangular lattice. We will have to say few more things about this later, but currently we will assume that based on convention we are actually going for a doubly primitive unit cell, which also seems reasonable looking at the shapes of the two unit cells. And again as before, the distribution of symmetry elements is not changed as compared to the simple rectangular lattice, which we are considered before.

So, the unite cell of this lattice is just been conventionally chosen is a one on the right, which is lattice point at its corner and one at the center of lattice unit cell.

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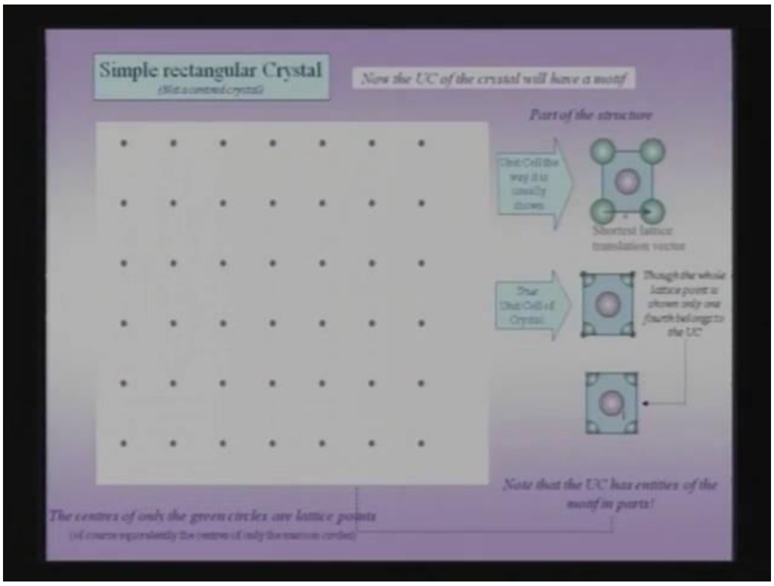

Now, let us make a simple rectangular crystal and also try to understand how to construct a unit cell for this simple rectangular crystal. In addition to the lattice points, obviously the crystal will have a motif and in this case, the motif consists of two kind of entities a green sphere and brown colored sphere. So, let us start with this simple rectangular lattice and over lay the motif on top of it to get a rectangular crystal, which has been done as shown. The basis vectors remain unchanged which are a and b and we can have an unit cell as shown before which is in the color blue.

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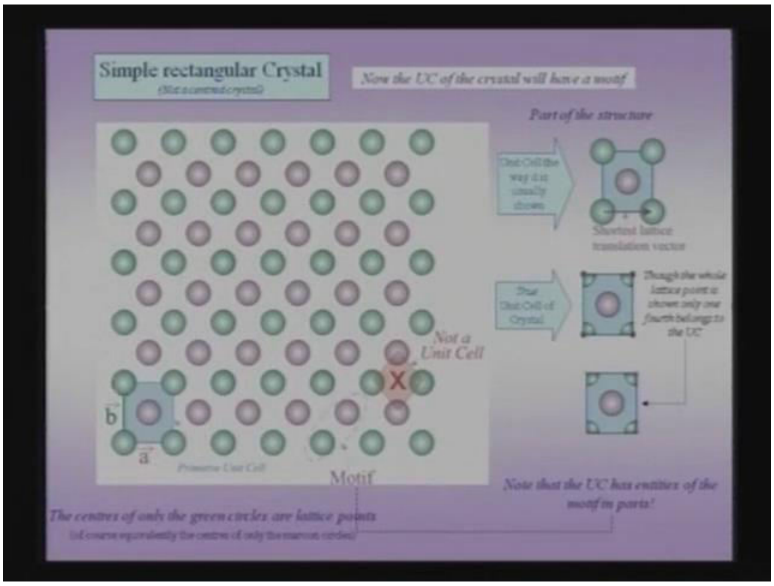

Now the shortest lattice translation in this vector crystal is the one a and the lattice factor b is longer in length. And if I consider now part of the structure which is shown here, we can clearly see the true belonging or the true region of the unit cell does not contain the entire green sphere. But it is containing screen sphere in four parts, which are associated with a four corners of the unit cell. Similarly, the lattice point is also broken in to four parts and are at the four corners of the unit cell. The point to be made here or to be noted here is that in normal representation you will see a unit cell as a figure at the top, where in you will see the whole circle instead of the one-fourth of the circle which is being placed in the structure.

Now the motif clearly which decorates the each lattice point is a green sphere and a brown sphere and therefore at each lattice point you place a green sphere and a brown sphere, to generate the crystal from the lattice. A thing to be noted here clearly is that, the one which is not a unit cell is this rhombus shaped structure here, which was the unit cell in the case which was considered previously.

So, in this centered rectangular lattice this could serve as a unit cell, but in the case of the crystal clearly this is not a unit cell as the four corners are of different kind of spheres. On the other, there are two different kind of spheres on this corner and this corner we have green here and at the top and bottom corner we have a brown sphere and therefore, this is not a valid unit cell of the structure.

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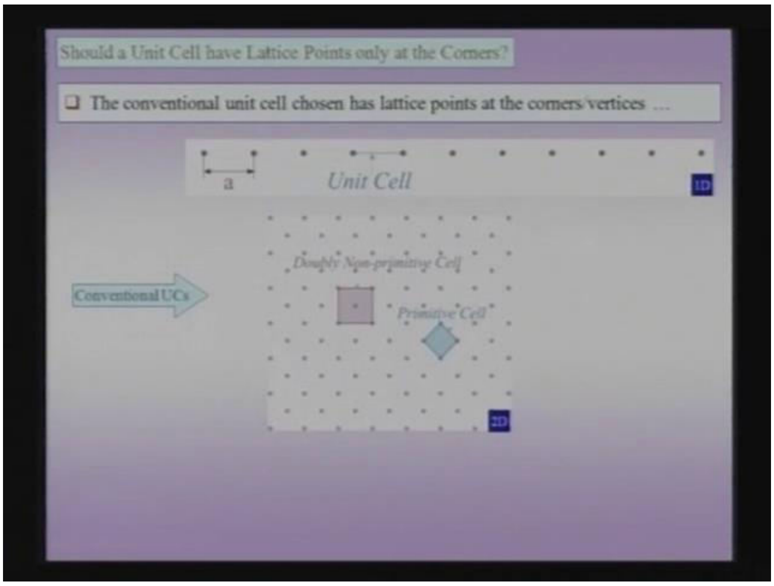

Now let us address an important question, which we had alluded to before that should a unit cell have lattice point only at its corners. Clearly it is only a convention that, we put lattice point at the corners of a unit cell and in some cases it might be constructive to actually not do so to understand the structure better.

So, for instance the unit cells we have considered before in one dimensional and two dimensions with the unit cells are shown here. For instance, the one dimensional unit cell had points at the corners of the one dimensional line segment, which is unit cell. Similarly, in the conventional unit cell chosen for the square lattice, we had this blue and the doubly non-primitive brown unit cell, but in both cases we had lattice point at the corners of the unit cell

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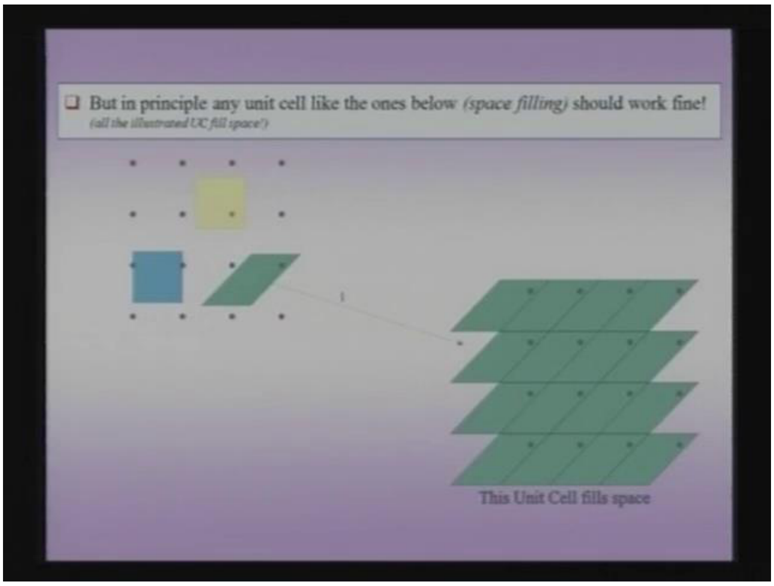

Now, let us consider some cases where in we do not want to put lattice point of the corners of the unit cell, but they could also cons, be construed as cells which can make up a structure. And some examples the yellow one, the blue one and the green one and as we can see from the example, this green unit cell when transnationally repeated along two directions can actually give the whole structure. Therefore, this is also valid cell though which is not conventionally chosen. So, to reiterate the, an important point we have seen that conventional unit cells have a lattice point of their corners, but we could always choose cells which do not have lattice point of their corners.

Three examples of this square lattice point have been shown in the figure. One is the yellow one, second one is a blue one and the third one is a green one. The important requirements for all these cells obviously, have to be that this cell has to be space fully. In other words if you are talking about one dimensional structure, the unit cell has to be a space filling one dimensional line segment. In two dimensions the shape chosen should be space filling in two dimensions. Similarly, in three dimensions the shape chosen should be space filling in three dimensions and starting from a unit cell or a cell we generate the space filling structure, by imposing the three lattices translation vectors in three dimensions the two lattice translation in two dimensions.

And in one dimension, just the single lattice translation vector and the best illustration of this, the fact that the green cell also works as a cell for the structure is by actually considering the, importing the lattice translation vectors to see that actually, the space is that filled by the green cell as well. Similarly, the yellow cell and the blue cell will also serve as valid unit cells or valid cells to the structure though conventionally we do not consider such kind of cells in description of crystal structures of lattices.

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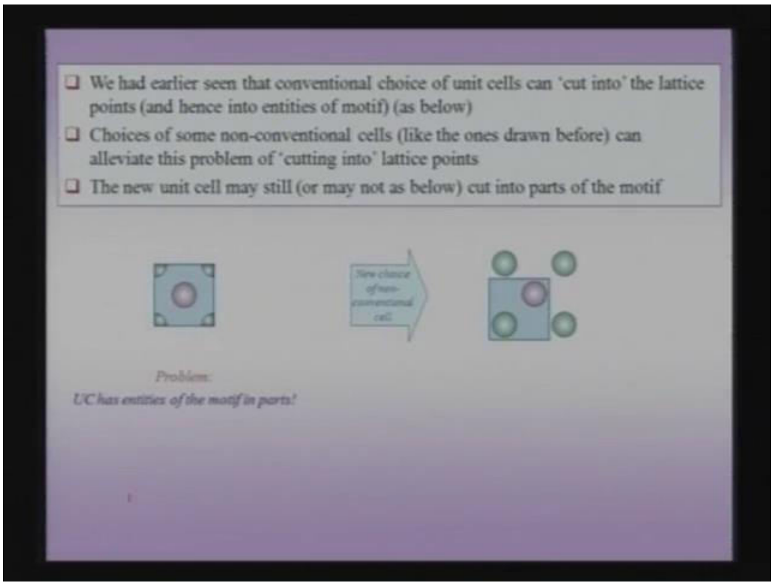

One place where in choice such unit cells could be instructive is in understanding that, when we had actually constructed some of the crystal structures we saw that, the unit cell actually cuts the parts of the motifs in to many pieces. And this can be to a little confusing actually we are making counting of the unit cell or the contribution of the atoms or the lattice points to the unit cell and such problem can be alleviated by construct moving the lattice cells. In other words considering the unit cells of this kind we have seen in the previous slide which is this slide. Where in, this unit cell, the yellow unit cell and blue unit cell are of the same size, but have been translated with respect to the origin a little bit.

So, if have unit cell in parts as shown in the figure below we can make a new choice of a unit cell, which is obviously a non-conventional representation of the unit cell. Where in I have translated the blue unit cell a little bit therefore now, the unit cell consists of one green entity and one brown entity with the unit cell and none of the parts of the unit cell have been cut in to parts. So, when I making a counting it is very simple here, left hand side have to make one-fourth in to 4 to get one and one green sphere or a one green circle and one brown circle sitting at the center.

In this case clearly it is one green and one brown which contribute to the unit cell. So, you have seen that when we want to choose unit cell, there is a conventional way of doing so, but certain non-conventional way is can help us in understanding the structure, which we are dealing with presently.