Structure of Materials
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Lecture - 02
Geometry of Crystals: Symmetry, Lattices

I have got in front of me certain geometrical shapes, for instance this is called a cube this is the octahedron, this is the tetrahedron, this is the dodecahedron, and this is the icosahedrons.

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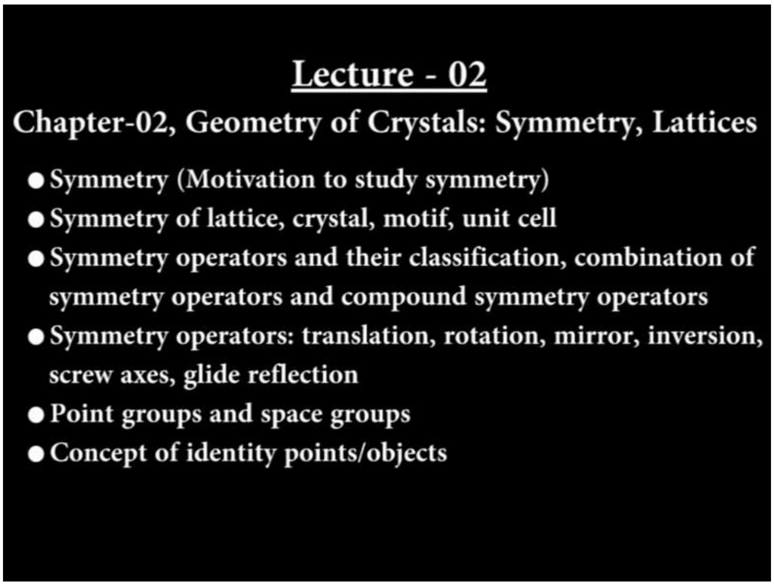

One thing which might be obvious looking at these shapes is that these are not irregular shapes, there is a certain regularity to them for instance every phase of this solid is triangular. At every vertex of this solid you find there are 5 triangles, which come together, if you look at this solid for instance you find that every face is actually pentagonal and at every vertex you have 3 of these pentagons coming together.

So, there is some inherent beauty in these solids, in fact this shape the dodecahedron was considered the crowning glory of Greek civilization, and therefore it up these kind of solids appeal to the human mind. So, what is that we have in common in all these solids, and how can we understand these solids from a language, which is the language of symmetry is what we are going to consider in this chapter.

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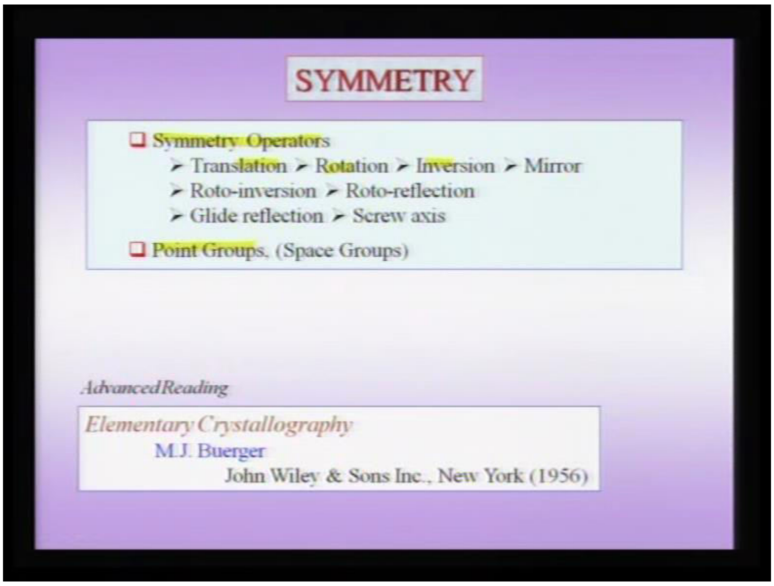

So, we will take up the concept of what is known as symmetry operators, we will talk about symmetry operations like translation rotation inversion etcetera, and we will briefly introduce the concept of point groups. For students interested in more detailed and advanced reading, the classic text by M. J. Buerger on elementary crystallography is worthwhile reading.

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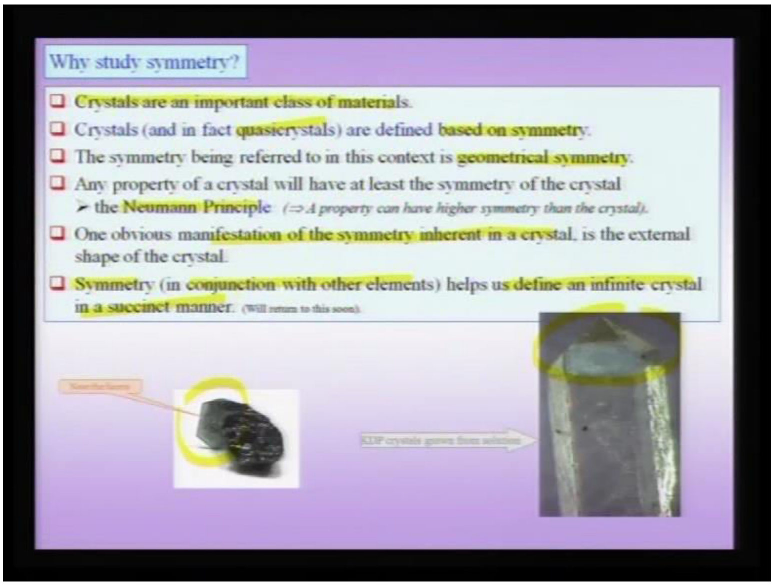

The first question of course, we should ask ourselves is why study symmetry, now suppose I look at a crystal what we call a well grown crystal, and on the bottom there are

2 crystals, which are shown here. One on the left-hand side, and one on the right hand side, the one on the right hand side is a potassium di phosphate crystal grown from solution. And you are immediately you notice the beautiful symmetry of the external faces which are forming, and this is one of the important characteristics of well grown crystals.

That they have an external symmetry or an external shape or a form which is well-defined, and crystals form an important class of materials. And therefore, the language with which you describe crystals is, in fact the language of symmetry, and additionally it will be worthwhile noting even quasi crystals are defined and described based on the language of symmetry.

Of course, the in the current context the symmetry we are talking about is what is known as the geometrical symmetry, and of course, there are generalized versions of symmetry in physics, which we shall not be dealing in these set of lectures. An important point another motivation why we need to study the symmetry of a crystal is because, any given property of the crystal it could be a refractive index.

It could be any other property like conductivity is has a cemetery which is at least the symmetry of the crystal, typically it could have a symmetry higher than that of the symmetry of the crystal, but it at least has the symmetry of that of the crystal. And this is known as the Neumann principle, and as you have seen from example of the crystal, which is shown below that one of the obvious manifestation of the symmetry inherent in a crystal is the external shape of the crystal

And that is why when we want to describe crystal, the best language is the language of symmetry, and which is the crux or the core of the language of crystallography. Symmetry in conjunction with other elements help us define an infinite crystal in a very succinct or terse manner, and that is one of the reasons why we take up crystallography which is centered around the concept of symmetry.

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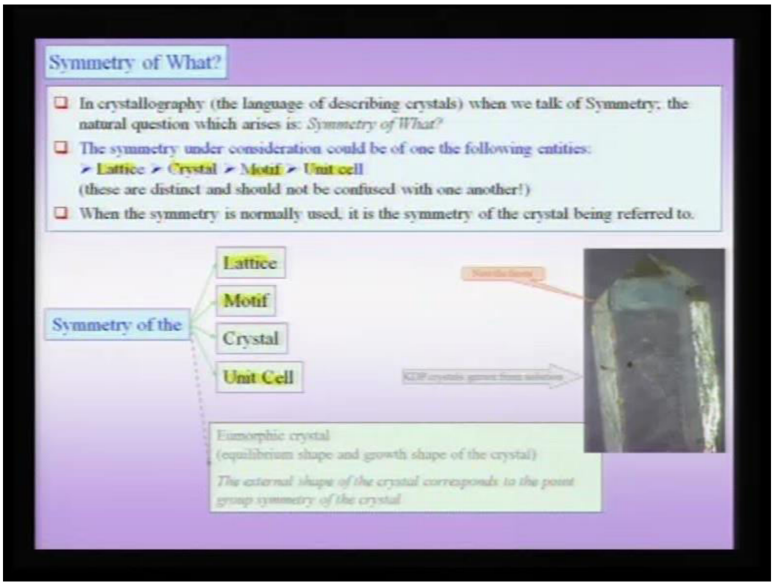

Now, there are a lot of concepts we will be introducing during the course of this set of lectures, those concepts involve concepts lattices, motifs, unit cell etcetera, but before even we introduce those concepts. We should note that when we are talking about symmetry it could be the symmetry of any one of these entities, which could be under consideration.

So, suppose I could be talking about symmetry of the crystal which is what is primarily important, but in certain specific contexts for instance we could be talking about symmetry of the lattice, or the symmetry of the motif, or the symmetry of the unit cell. And that is why when description of symmetry is being made it is very, very important to note under what context, what is the central focus of the description which is being kept in mind. Additionally, we could also be talking about the symmetry of the growth of an external shape, which we considered this crystal has a certain symmetry, and we could be describing the growth form of the crystal which also would be coming under the class of symmetry descriptions.

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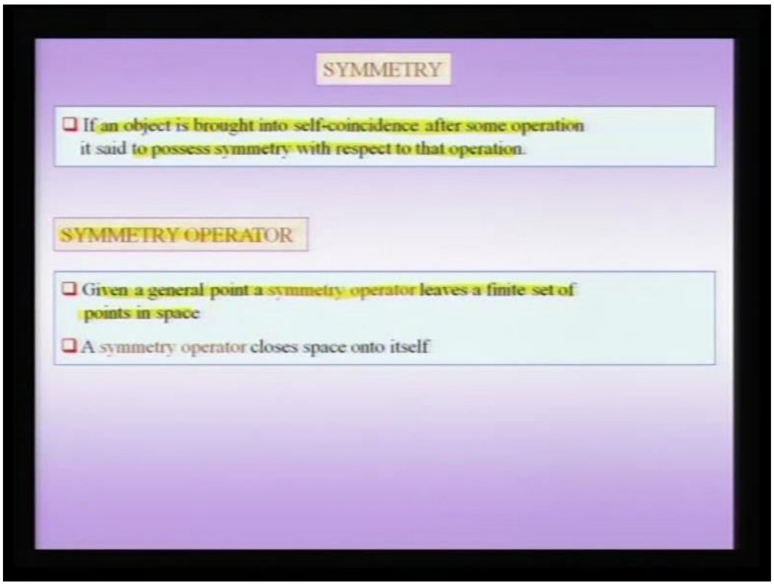

An object is supposed to possess symmetry, when if it is brought into self coincidence after some operation, then it is said to possess symmetry with respect to that operation. Now, for instance the obvious symmetry which we are all accustomed to for instance is the human face or the human body, externally it has got an approximate mirror symmetry that is if you place a mirror in the centre of the body.

Then you will see the left hand side reflects the right-hand side or equivalent lead the right-hand side reflects the left-hand side, of course this is an approximate external symmetry that we have got. And additionally, the human mind is well tuned to appreciate symmetry in any body and as the ancient Greeks had done, they had, in fact come across these solids, which are known as the platonic solid, which I had described.

Sometime, back the cube, the dodecahedron, the icosahedron and the tetrahedron, and therefore this a natural ability of the human mind to appreciate symmetry, but in this context we will take up symmetry in a more formal way. A way which is ideally suited for describing crystals, and the other entities we have talked about in the previous slide like unit cell lattice etcetera. So, if an object is brought into self coincidence after some operation, it is said to possess symmetry with respect to that operation.

So, naturally question is that what is a symmetry operator, given a general point a symmetry operator leaves us a finite set of points in space, that is if I have a symmetry operator and I have a general point in space. Then at the end of the symmetry operations it you end up with a finite set of points, and in other words you can describe the symmetry operator as that, which closes space into itself.

Later on, we will be talking about symmetry operators which involve translation, and in that case we will have to assume that it leaves a finite set of points within the unit cell, which is another concept we will be dealing with later. But, essentially as you start with a point then the symmetry operator acts on that point, creates a finite set of points, and typically this finite set of points we're referring to is within the unit cell.

Of course, the question we sort of allude at to we can ask more formally, then why do I need to talk about symmetry and symmetry operators. If an object for instance a crystal or it could be another general object, which is under consideration has some symmetry then we need not go and describe the whole of the object.

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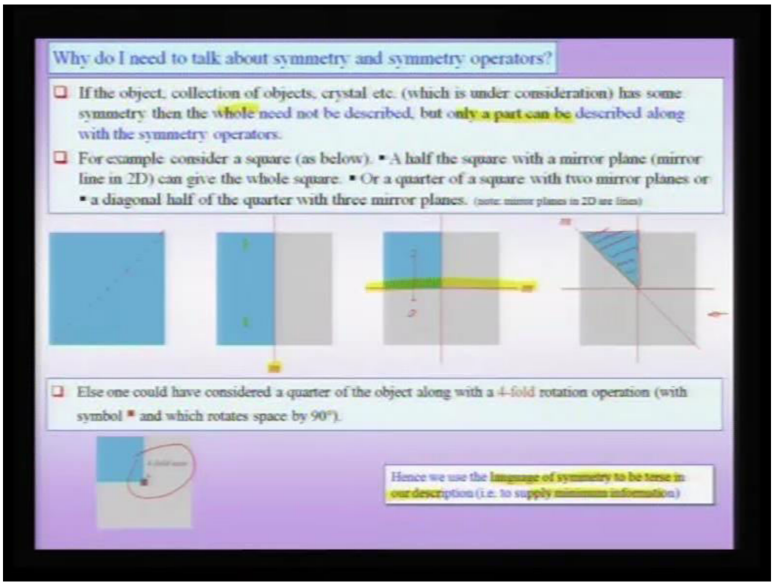

We can just describe a part of the object in conjunction with the symmetry operators, and I will get the whole object. In other words I am conserving my information or conserving my labor in describing only part of the object in conjunction with symmetry, that the object is got, therefore I will get an entire object without having to describe a lot or prescribe or a lot of information.

For instance, I have got a square in my example, and the square has a mirror symmetry, we will formally de look what is a mirror symmetry, but we all know from our commonsense experience, we know what is a mirror. So, the mirror for instance would reflect the left-hand side of the blue rectangle into the right-hand side, and therefore create the entire square. Additionally, we can also imagine horizontal mirror which is present, which means that this horizontal mirror can actually reflect top part of the blue rectangle to the bottom part, which I will describe here.

So, this part is reflected to the part below, and therefore I will get my entire blue rectangle, in other words instead of working with the entire square. I can work with half the square or quarter the square, and these 2 mirrors will produce all the 4 quadrants of the original square, additionally if I notice this object additionally has a mirror which is the diagonal mirror which is shown in the figure in the right-hand side.

So, if further I do not have to describe the entire what do we call one fourth of the square, I can actually describe one triangle in conjunction with this mirror, which will produce this square. In other words what I have done is that all I need to prescribe is this one triangle, in this triangle in conjunction with these 3 mirrors, one diagonal mirror, one vertical mirror, and one horizontal mirror will give the entire blue square back to me.

Therefore, I conserved my information or I have described my object into the least part conjunction with the symmetry operators, symmetry present in the object, and therefore I get my entire original square. Yes, we shall see soon there are other symmetry operators which could we could invoke for instance, what is something known as the fourfold axis, which could also generate my original square, from one quadrant of the square.

In other words the language of symmetry to be in physio, so that we can be very terse in our description, so that we can supply minimum information and generate the maximum amount of knowledge possible. This is very, very useful, because typically crystals are infinite and many, many crystals we will be talking about have very, very many number of atoms inside them or for instance there could be irons present in crystals. And I do not want to be prescribing the position, and the type of iron present for hundreds of them, so I can actually conserve my effort by putting the minimum required information along with the symmetry present in the system.

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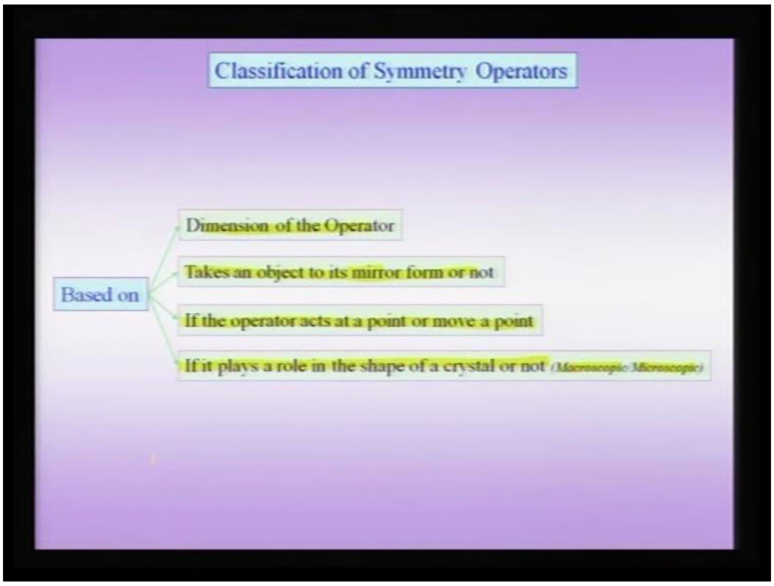

How can I classify my symmetry operators, and what kind of symmetry operators exist is the next question we will try to address, so based on dimensional of the operator, based on if the symmetry operator takes the object to its mirror form or not. Based on the fact that if the operator acts at a point or moves a point, or if it plays a role in the shape of the crystal or not, for instance is it microscopic or is it macroscopic.

So, I have multiple ways of classifying symmetry operators, and therefore coming to know of the very many different kinds of symmetry operators, which are present which are especially relevant to crystal. So, to summarize once again this slide, so I can classify symmetry operators based on the dimension, based on if it takes an object to its mirror form or not, based on the fact that if it leaves a an object around the point or moves it from place to place, or if it has any role to play in the external shape of the crystal or not.

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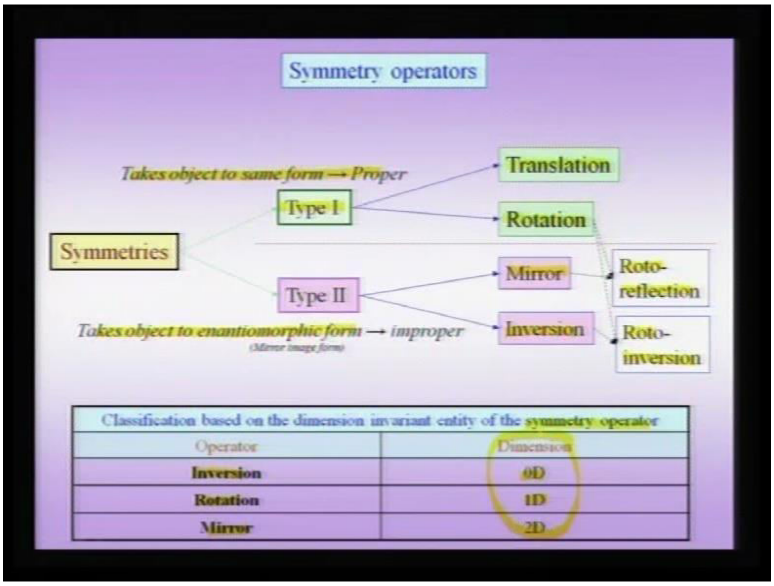

So, we have certain symmetry operators, which whose names are on the right hand side here, for instance the translation, the rotation, the mirror, and the inversion. And further we will see that there are other symmetry operators like roto-reflection, and roto-inversion we shall be taking up some of these very soon, but this is an attempt to give a broad overview and classification of all the possibilities.

So, there are type 1 symmetry operators, which take to an object to it is same form, and there are type 2 symmetry operators, which take an object to it is what is known as the mirror form or the enantiomorphic form. Now, it is to understand what is a mirror form, the best example we can consider is our hand the human hand. So, you got the left hand and the right hand, I can perform no rotation or translation operation to make my left hand coincide on top of the right hand, because my left hand and right hand are related by a mirror operation right in the middle of my 2 hands.

Therefore, there is no possible translation or rotation object which can take my right hand to my left hand, or equivalently my left hand to my right hand. These are 2 different kind of objects, and one is if you call the right hand one, the other one is the enantiomorphic form or the left-hand one. Therefore, there are symmetry operations like mirrors and inversion, which take an object to its mirror form or the enantiomorphic form, so do roto reflection and roto inversion, but a near translation for instance.

Suppose, I just move my hand by a certain distance such an operation will not take an object to its mirror form, so does, so does not rotations, so I rotate my hand I still land up with a left-hand and not a right hand. I can classify my symmetry operators based on the dimensional of the operator, from since inversion is a zero dimensional operator, rotation is a one dimensional operator, and mirror is a two-dimensional operator. And of course, this dimensional is assuming that our whole space in which we are working is the three-dimensional space, and not a lower dimensional space.

We shall these aspects shall become clear once we actually take up these operations, and see how his operations have an effect on space, and have a effect on points in space. So, we can classify symmetry operators based on if the symmetry operator takes an object to its mirror form or leaves, it in original form symmetry operators, can also be classified based on its effect on the external shape of the crystal.

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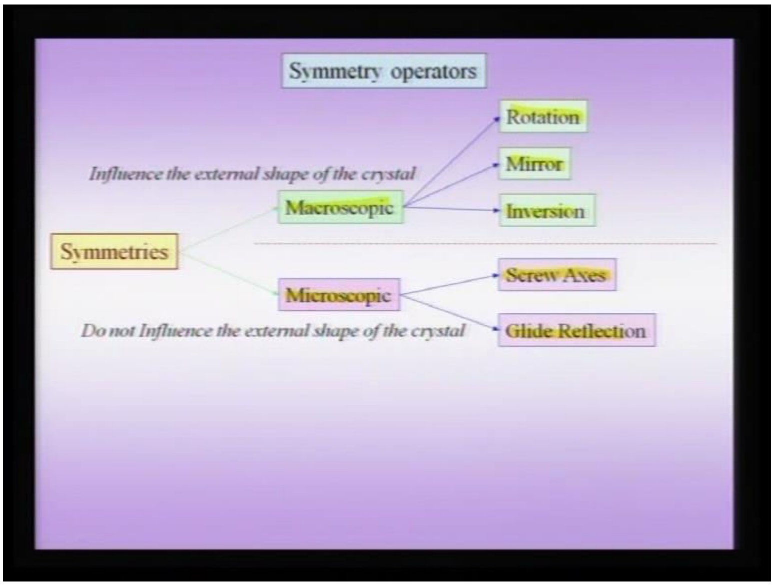

And therefore, we talk about macroscopic symmetry operators and microscopic symmetry operators, screw and glide reflection for instance which we will take up much later in the describing of symmetry. Do not have an external any effect on the external shape of the crystal, they are actually they involve translations the screw and glide reflection which are of atomic dimensions.

And therefore, or dimensions of the order of lattice parameters typically in crystals, and therefore they have no effect on the external shape. Well on the other hand rotation mirror and inversion, which has a 3 macroscopic symmetry operators, have an effect on the external growth shape of a or a for instance the external equilibrium shape of a crystal.

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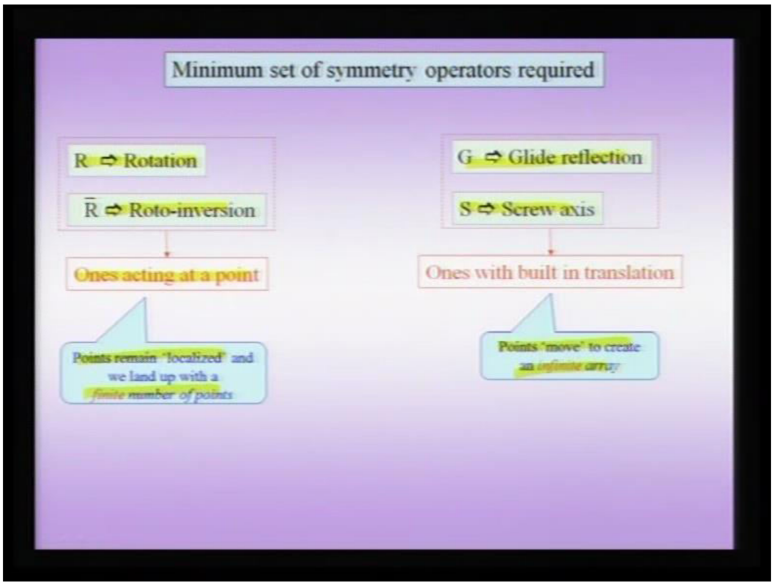

Additionally, we have to note that there are many symmetry operators available to us, but some of them are absolutely necessary to describe crystal, well some of them could be redundant. In other words I can get away by not using all the symmetry operators, which I had described, so far for instance, suppose I want to describe a crystal, I can work with rotation and mirror and not, in fact invoke inversion at all.

Otherwise, I can actually work with rotation and inversion, I cannot invoke mirror for instance, so there is a possibility that I can work with a lower set of symmetry operators, then actually available in the crystal. And this was also obvious from the example we considered before for example, this square, the blue square had 2 horizontal one horizontal mirror one vertical mirror and one diagonal mirror, but we saw that. Actually, it additionally has some other symmetry operator, which we call the fourfold axis, but I did not have to invoke the fourfold axis to create my full square.

Therefore, there are some additional redundant operations, which also might be present which I need not invoke, to if I want to generate all the symmetry acting at a point then the bare minimum I require is rotation and something known as the root inversion. And in this case of course, I am at a point I am not moving from one point to another in space and these points remain localized.

And we land up with a finite set of points at the end of what is known as a loud combination of operators, but on the other hand if you are talking about guide reflection screw. Then we end up actually moving the point and land up with an infinite array, but within an unit cell there will be only a finite number of points.

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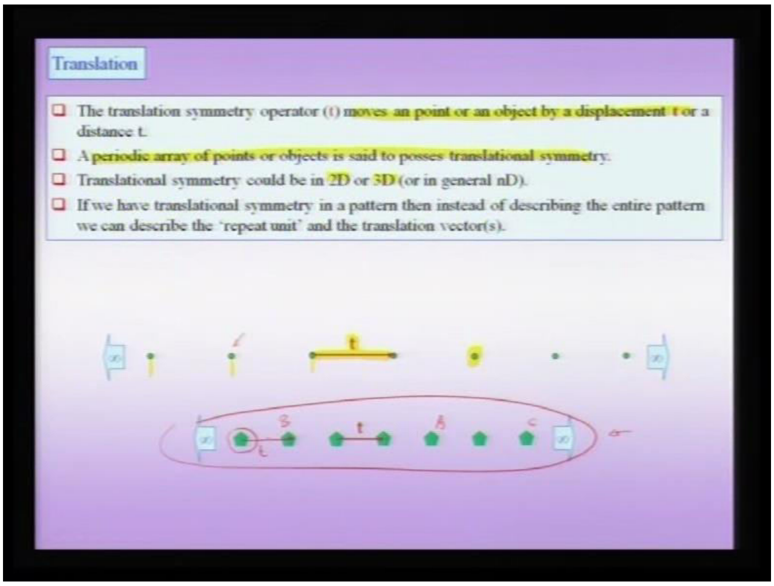

So, what is the first operation which we need to consider, which is very, very relevant to crystals because every crystal has at least guaranteed one minimum symmetry associated with it, which is the translation. And in fact, the very definition of lattices, which we will come across later is based on this operator, which is the translation operator. A translation operator just simply moves are point by a certain vector t, and in three-dimensional space, actually you could have 3 different components along with 3 basis vectors.

Here is an example below in the figure, in which I have an one dimensional crystal, in which I have the crystal beam created by one dimensional translation operator the t vector. Therefore, I have a lattice point, from this lattice point I generate another lattice point, and so forth, therefore if I have this translational symmetry, it does not matter to me, where in this array I am sitting. For instance, if I am sitting at this point the entire space would look exactly identical, as if I have had to sit in a different point to its left for instance at this point.

Similarly, if I have a crystal here and in this crystal which is now consisting of pentagon's, and which has got translation symmetry it does not matter if I am sitting at point A which is here, or at a point B which is here, or at a point C which is here. And entire space will look identical to me and that is why, it is this crystal is expected to possess or it is supposed to possess translation symmetry, and what does a translation symmetry do.

It actually produces a periodic array of point starting with a single point and if you start in an object, it will produce a periodic array of objects. And this translation could be in one dimension as the example below, it could be in two-dimensions or it could be in 3 dimensions. Therefore, if I have translation symmetry I do not have to describe the entire crystal, all I have to do is take up for instance an one unit of crystal for is in this pentagon. And in addition to this pentagon I can describe a translational vector t, and I will land up with the entire crystal. So, there is a certain advantage certain brevity certain succinctness, when I use symmetry operators to describe crystals.

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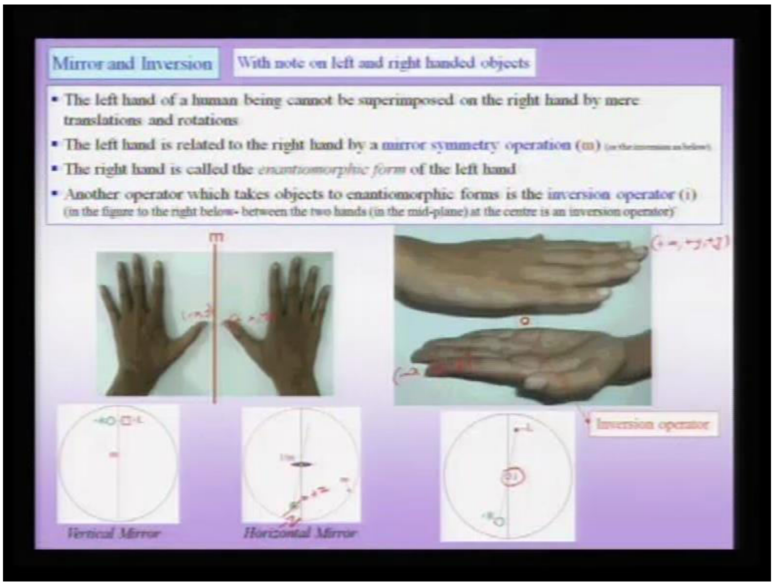

The next symmetry operator, we consider is the mirror and the inversion, the left-hand side shows a mirror operator which we had of course, briefly construed just now, and the right-hand side shows a inversion operator. Now, as I pointed out suppose I have my 2 hands, I can visualize a vertical mirror plane between 2 hands on the other hand. Suppose, I place my 2 hands like this that is my one hand is above, and then one hand is below, then I can think of an operation, which is an inversion operation right at the middle of between the 2 planes in which my 2 hands exist.

Therefore, both of these operators, my mirror operator and my inversion operator take an object to its enantiomorphic form or take an object to its mirror form. The mirror is a plane, therefore it is a two-dimensional operator, in three-dimensional space my mirror is actually a plane, which takes my left hand to my right-hand, while the inversion operation is actually a point.

So, inversion is zero dimensional mirror is a 2-dimensional operator, so this 0 dimensional inversion operator, again takes my left hand to a right hand, but as you can see that a point xyz becomes minus x minus y minus z, when an inversion operator acts on it. So, these are 2 ways of taking an object to an enantiomorphic form, but given the dimensionality it is clear that they are not identical.

And also given its effect on a general point how a mirror acts is that suppose, it had a point here which is at a plus x then the mirror operator takes it to minus x, but leaves it at the same distance y height. On the other hand an inversion operator takes an object which is at point at plus x, plus y plus z to a point which is right below here, which is minus x minus y minus z. So, if you take which is also shown in a diagram right here below, if I start with an vertical mirror here and a right-handed object, which is above the plane of a thin sheet.

Then the right-hand object is taken to its left handed object by the mirror plane, of course you could have an horizontal mirror as shown here. In which case you will start with a point which is say for instance a green right-handed object above the plane, is taken to a red square which is actually below the plane by an exact distance, which is if this were this were at a distance of plus z.

Then this red square would be attempt of minus z from the plane on the other hand a inversion operator, as I pointed out is a zero dimensional operator, which takes an right-handed object to the left-handed object, the right-handed object being above the plane and the left-handed object is below the plane as shown here.

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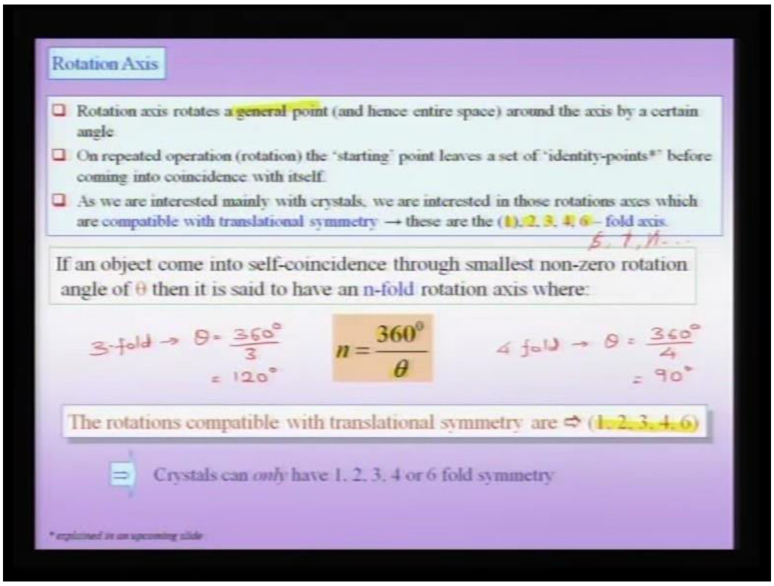

The next operation they consider here is known as the rotation axis, in the case of the rotation axis, we if we start with a general point and an axis which is known as the rotation axis. It rotates a point and leaves a finite set of points, now an what you call an n fold rotation axis is a rotation axis, which rotates a point by 360 degrees divided by theta. Therefore, if you have a fourfold axis, then the rotation angle theta would be for a fourfold axis on the other hand, suppose I am talking about a threefold axis, therefore there is a characteristic rotation associated with every axis which is an n fold axis.

In general of course, you would notice that I can actually start with the single point, and land up with an finite set of points if I have an axis of rotation. And this n code actually be any number starting from 1 2 3 all the way up to some higher numbers up to infinity, but then in the description of crystals. We are especially concerned with those rotations which are compatible or consistent with translational symmetry, or the basic inherence ability of crystals.

And when we are putting this restriction of course, I am not showing the proof here, you would note we will land up with certain only certain allowed rotational symmetries. So, in general an we could have a n fold rotation axis, which is having any value of n like 1 2 3 4 5 etcetera, but then when you are talking in crystallography. We want to consider only those rotation axis, which are compatible with translational symmetry, which is basics requirement of all crystals.

And in that case we will only consider for instance the one fold which is a very trivial rotational symmetry, the 2 fold the 3 fold the 4 fold and the 6 fold rotation axis. In other words I do not have to consider the entire set of rotation axis, which includes for instance there is no 5 fold involved here, there is no 7 fold here, there is no 11 fold etcetera, etcetera.

Therefore, there is only a small finite set of rotation axis I need to consider, then I am talking about symmetry, rotational symmetry, which is consistent with translational symmetry or that which is consistent with crystals. Therefore, future focus will be on those rotations, which are compatible translations, which are the 1 fold, the 2 fold, the 3 fold, and the 6 fold, rotation axis, so let us try to understand what this rotation axis is and what it does to a general point.

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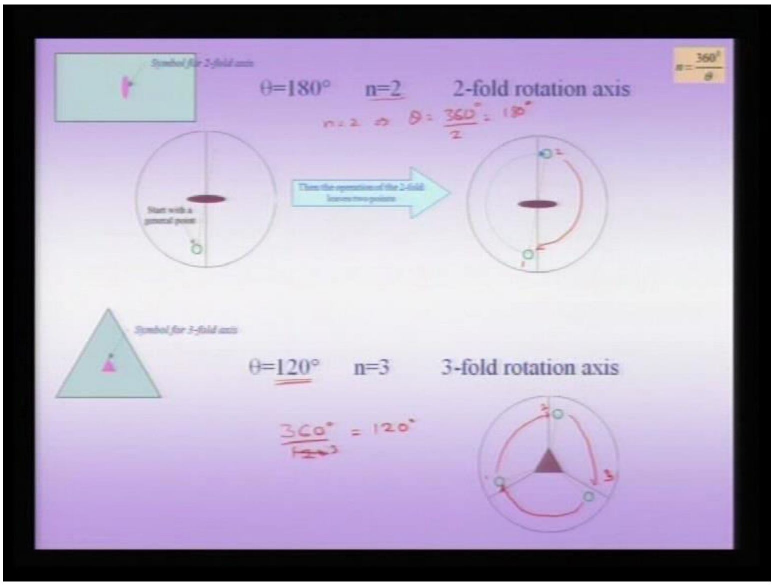

Now, a 2 fold rotation axis is an axis for instance, which is perpendicular to the plane of the figures shown here, for instance this is my circle, and a 2 fold rotation axis which has got as a symbol as shown here. It is caudal lens hype of a symbol and this rotation axis is perpendicular to the plane of the slide, this rotation axis therefore, is a one dimensional axis.

We have previously seen that the mirror is a 2-dimensional plane, the inversion is a zero dimensional point while rotation axis is an one dimensional line. And what does it do for instance a 2 fold axis due to a point for instance ring circle, which is above the plane of the slide, what it does we know that n is equal to 2 implies that the rotation is. Therefore, a twofold rotation axis rotates a point, and therefore the entire space for that matter by 180 degrees, therefore it rotates this point and takes it to this point.

So, I start with a 0.1 it produces 0.2 and a further action on that, finally closes space on itself and comes back to 1, therefore irrespective of how many times, this rotation axis operates it is going to leave only 2 points in space. This is an important point to be noted, similarly if you look at 3 fold axis would mean a rotation of 360 by 3, which we had seen before which is 120 degrees, and if you start with the general 0.1. Then a threefold rotation axis which is got a symbol of a filled triangle takes it to 0.2, which further takes it to a 0.3, and finally this 0.3 is closes close comes back to 0.1.

Therefore, irrespective of how many times this threefold rotation axis operates, you will have only 3 points, and to show this I have got a model here for instance, here I have got an axis which is threefold rotation axis and this threefold rotation axis is at a end of a triangle. So, now, I have a triangle, suppose I this assume is a threefold axis, it operates on this object then it is a triangle which is in distributable, with the triangle before, it operates again it produces a triangle in identical orientation.

So, just to make it clear here, so let me rotate it around, so that you can see the triangle better, so I have a threefold axis and I rotate by 120 degrees, I land up with a triangle pointing up wards, I rotate again by 120 degrees I land up with a pointing triangle pointing upwards. Therefore, a threefold axis is a triangle, as a triangle before and after its operation, similarly the other important crystallographically compatible rotation is the fourfold rotation axis, which produces a which is associated with a rotation of 90 degrees.

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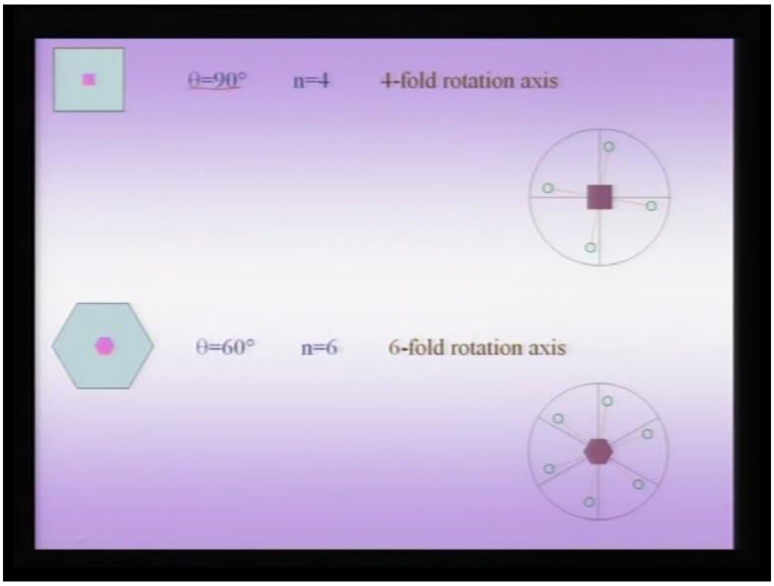

And, as before suppose I start with the general 0.1, then it rotates to a the point to 0.2 it rotates to the point to 0.3 comes back to 0.4, and finally the 0.4 is rotated to 0.1 which implies that space has closed on itself. And we have only 4 points starting with the general point, and a 6 fold rotation axis has a rotation of 60 degrees associated with it, and like before it leaves 6 distinct points in space starting with 1. I get 2, which is rotated to 3, which is rotated to 4, which is rotated to 5, which is rotated to 6, and this can be understood by taking an hexagon.

For instance you talk about hexagon, this hexagon it has got 6 fold rotational symmetry, I can rotate by 60 degree, it looks exactly identical. I rotate it by 60 degrees again, it looks exactly identical, I rotate it by 60 degrees again, and it looks exactly identical. Therefore, irrespective of many times I rotate it 60 degrees this entire hexagon will continue to look like an hexagon, so this brings us back to some of the geometrical objects we had considered before for instance.

For instance, we have a cube this cube has some beautiful symmetry that it has got a mirror plane, which is exactly splitting my cube into 2 parts, therefore if I only consider right-hand part of the cube along with the mirror, then I will get the left-hand part back. Similarly, you can also visualize a mirror which is the diagonal mirror, which is going vertically, so I can visualize a diagonal mirror going into this plain vertically like this.

And therefore, the right-hand part of the cube would reflect to the left and part of the cube, additionally you will notice that, suppose I look along the top of a cube then the top of the cube has a fourfold rotational symmetry. So, let me show it from this direction is it clear from this perspective, so the cube has got a fourfold operational symmetry, in other words suppose I rotate my cube by using this fourfold rotation axis, it will rotate and look exactly like before.

Similarly, the body diagonal of the cube has a threefold rotation axis, that means, if I rotate my cube, for instance this is a cube oriented like this and I rotate it along the body diagonal by an angle of 120 degrees, then it will look exactly identical. So, this rotation along this axis, for instance now I am holding the body diagonal horizontally and I rotate it by 120 degrees, the cube looks exactly as before and so forth.

Therefore, these geometrical figures have beautiful symmetries, and we will see later that some of the symmetries are compatible for instance with translation symmetry, like this is tetrahedron has got a threefold axis which is vertical. It is additionally got a mirror plane which is going through in the vertical fashion right here, on the other hand the symmetries with the icosahedrons, which is got a fivefold symmetry here or the dodecahedron, which is also got a fivefold symmetry here.

So, this pentagonal face has got a connecting the opposite face is got a 5 fold symmetry, but these 2 objects these 2 platonic solids are not compatible with translational symmetry. And therefore, you would not find crystals having these symmetries; however, there are quasi-crystals which have these kind of symmetries, so coming back to our rotational symmetries.

We summarize this slide by saying that in general of course, any fold rotational axis is possible, but we restrict ourselves to the one fold which means that basically you have a point which comes back to itself, which is a equivalent to a 360 degree rotation. A twofold equivalent to a 180 degree rotation, 3 fold which is 120 degree rotation, a fourfold which associated with 90 degree rotation, and a 6 fold associated with 60 degree rotation.

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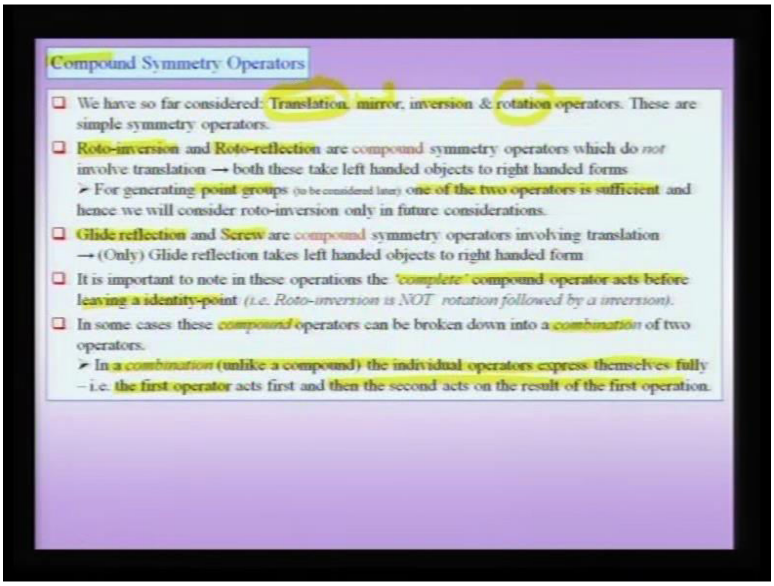

Therefore, we need to only consider these rotational symmetries, when I am talking about crystals, in addition to these simple or what you might call individual symmetry operators. There are other symmetry operators which are compound symmetry operators, and also there is a possibility of what is known as a combination of symmetry operators. We will try to distinguish these two, a compound symmetry operator is one which is a combination, but a fixed combination, in other words it is a compound of 2 symmetry operators like a rotation and an inversion.

And we have to notice here very carefully that this is not a rotation plus an inversion, but a roto inversion. And I will try to distinguish the difference between a rotation plus an inversion and a roto inversion or equivalently a rotation plus an reflection, as differentiated from a roto reflection compound symmetry operator. So, what are the simple symmetry operators we have talked about, so far it is the translation a mirror inversion and rotation, and now we are talking about compound symmetry operators like the roto inversion, and the roto reflection.

It is to be noted that these symmetry operators and entire symmetry operation acts before leaving a point, in other words a roto inversion is not a rotation plus an inversion. You cannot leave a point after rotation you'll have to start with a point perform the roto inversion, and then leave a point. Similarly, if I am talking about roto reflection I have to start with the general point I have to perform a roto reflection, and then leave the second point. While, if I was talking about a combination of a rotation and a reflection, which is a possibility then I can rotate.

For instance, suppose I am talking about a combination of 2 fold, and a mirror first I will rotate my 180 degrees, I will land up with 2 points, then I can perform the mirror operation, which will take these 2 points to further 2 more points, but in we will see what this roto reflection does by actually considering equivalent things. So, to summarize this initial part of this slide roto reflection and roto inversion are compound symmetry operators, we do not involve translation both these take left-handed objects to right handed forms.

So, these are operators of the second kind which we had considered, which take an object to it is enantiomorphic form, for generating point groups, which we will consider very soon. One of the operators, one of the 2 which is the roto reflection or the roto inversion is more than sufficient, and in general we will take up roto inversion in the further examples we take up.

Further, we can have compound symmetry operators which involve translation here, and a mirror for which is known as the glide reflection or we could have a translation in combination with a rotation, which is known as the screw symmetry operator. Therefore, we can have a glide reflection or a screw, and the important distinction between the 2 is that a glide reflection takes an object to its mirror form. While, screw takes an object to same form which means a left handed object in combination with screw will lead with a lead to an object, which is only left handed.

In some cases these compound symmetry operators which we have considered, for instance the roto inversion can be broken down into certain simple operations, but this does not mean that individual components are exactly identical to the components, which is giving rise to the compound operator. This will become waste when we perhaps consider an example, in other words in a combination like a compound the individual operators express themselves fully. That is the first operator acts first, and then the second operator results acts on the result of the first operation, that is what we call a combination while in a compound you have a combined operator acting all at once.

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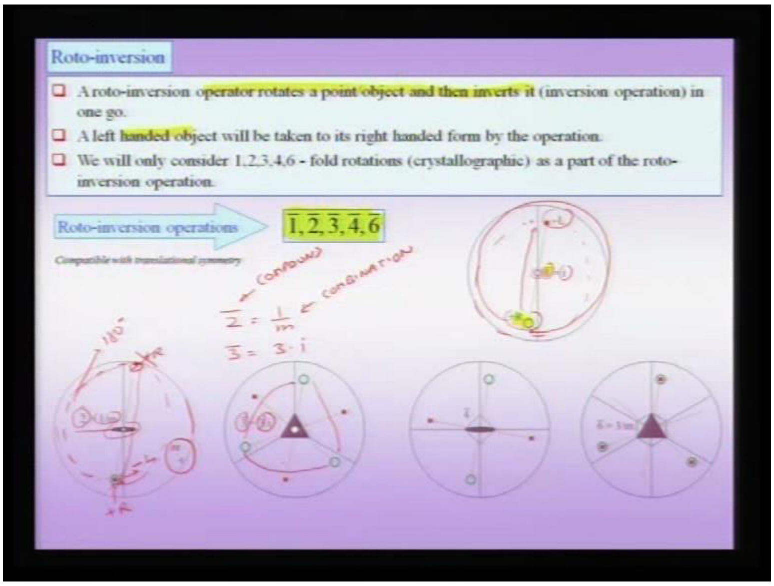

So, let us talk about one compound operator which is a roto inversion, which will clarify the position a roto inversion operate rotates a point and then inverts, it all in one goin other words it does not do in steps. And as I pointed out it will take a left hand object to its right handed form, and the roto inversion operations which are compatible with translational symmetry or the once which we had considered like in the case of simple rotation or the 1 bar, the 2 bar, the 3 bar, 4 bar, and the 6 bar.

In other words the symbol used to describe roto inversion is a number like the normal rotation with a bar on top, which tells us that it is actually a roto inversion operation and not merely a rotation . So, therefore, the roto inversion operations I need to consider are the ones, which are highlighted here which are the 1 bar, the 2 bar, 3 bar and 4 bar and the 6 bar, and let us see what how these operators act, when you start with the general point.

So, suppose I start with the right hand object above the plane, then the one bar operation implies that I rotate by 360 degrees; that means, the rotation is 360 degrees I come back here. But, I do not stop there, I do not leave a point there I invert immediately and when I do the inversion, I will land up with a left handed objects below the plane of the slide. So, and of course, what will happen further, if this roto inversion operates again I will start with this left hand point rotate by 360 degrees.

In other words I will go again 360 degrees and come back to the left handed object, but I will not leave a left handed object below the plane, of the board I will immediately invert and land up with a right handed object above the plane; that means, I have closed space on itself. Therefore, n inverse one bar operator, which is exactly equivalent to an inversion as we can compare it with an inversion operator, which also leaves to a points like this. One right-handed above the plane, one left-handed below the plane therefore, an one bar operator is exactly identical to the inversion.

And it leaves only 2 objects and not more not less and these 2 points would be one right-handed, and one left-handed. Similarly, I can talk about the 2 bar operator which will again involve a rotation and an inversion, but all in one go suppose I start with the right-handed green circle above the plane of the board. Then I can wrote what does a 2 bar imply that the rotation associate with the 2 bar is 180 degrees like in the case of a twofold, therefore I will rotate I will go all the way, but I will come back here, but I will not leave a point after the rotation.

So, I will come back right exactly above the green circle, but after that I will invert and so I made a mistake here. So, what I will do is I will start with the green circle I will go and rotate and come to a point which is 180 degree apart, and I will land up with a circle which is a green circle which is about the plane of the board.

So, I have performed my 180 degrees rotation, but I will not leave this point here, so this is not a point which is to be left here, but I will immediately invert, which will mean it will take this point to a point, which is below the plane of the board. And which is this red square which is minus n which is a left-handed object, therefore when I have 2 bar roto inversion operation. I start with a green circle rotate it do not leave a point invert it and come back right below the green circle, which completes my roto inversion operation.

If we will see that it is actually this 2 bar is equivalent to a one followed by a mirror, which is nothing but, an horizontal mirror. So, let us summarize the 2 bar operation, which we said is equivalent to 1 my m operation or a mirror horizontal mirror, therefore I start with the green circle above the plane of the slide. It rotates it by 180 degrees we landed here we do not leave a point, but invert right at the centre, and therefore I land with a red square, which is a left-handed object below the plane of the slide.

And a symbol as you can see for all these operators is the one bar is a one circle, the 2 bar has a symbol like a twofold, but with the circle in the centre, the 3 bar as you can see here is a triangle with the circle, in the centre the 4 bar operation is shown here, and similarly you can have a 6 bar. This slides also explain to you that actually the concept of the compound versus the combination. So, the 1 bar the 2 bar the 3 bar the 4 bar and the 6 bar are compound operators, but you have just now seen the 2 bar can be thought of as an horizontal mirror; that means, if I start with an green circle actually put horizontal mirror.

The mirror being this m which is marked here which is nothing but, the red circle on the plane, actually I will land up with these 2 points and irrespective of how many times this mirror acts. I will land up with only 2 points one left-handed, one right-handed the left-handed being above the plane of the slide and the left right-handed or the left handed being below the slide plane of the slide.

Therefore, I can break down this 2 bar operator, as a combination of one and an m, therefore this is my compound operator, and this is my combination of a one fold and a perpendicular mirror. Similarly, I can think of a 3 bar operator as a combination of a threefold and an inversion, therefore when I am talking about a combination, then each one can act independently.

From this I can start with a green circle, it can first act and leave a point here, then it can rotate and leave a point here, and finally this can rotate and come back to it is point. I am not performing the inversion like as 3 bar operator, and just performing the 3 which is mentioned here, further if I invert these then I land up with these 3 red squares, which are nothing but, left-handed objects below the plane of the slide.

Therefore, I can break down my 3 bar, which is a compound operator into a combination which is a 3 and an inversion combination, therefore there is a possibility in some cases of decomposing my compound operators into a combination operators. However, we should always remember that a compound operator leaves a point after performing it is complete duty which is for instance, in this case of a roto an inversion and then only you have a identity point.

You just try to understand for instance, this 3 bar roto inversion operation with respect to a cube for instance, where is a 3 bar roto inversion operation in a cube, and what do we see in a three-bar roto inversion operation there are 6 points which are created by this operation. So, I have a cube here, and originally I had pointed out that the body diagonal is has a threefold symmetry, but actually it has got a symmetry, which is higher than the threefold, because the threefold symmetry generates only 3 points.

While, we have just now seen that the 3 bar or the 3 bar roto inversion symmetry generates 6 points, therefore it is an operator having higher order as compared to a 3. So, the 3 bar operators and higher order as compared to the 3 fold rotation axis, now let us try to understand how where is a 3 bar operation and how we get to 6 points. So, if I consider my cube and my body diagonal which is passing as you can see here, so what does it do, if I start with the general point here which is one of the vertices of the cube.

So, I have totally 8 vertices for the cube, 2 of them I have taken away by putting my body diagonal line across that, and in addition to that I have 6 more vertices left. So, I can start with any one of those vertices for instance, and when a 3 bar rotation axis acts on this it is rotate it by 120 degree, which will take it here and invert it. So, as to produce an this vertex from that, so it will rotate by 120 degree giving me this and then it will invert it and produce this vertex from that. Therefore, when I start with this vertex, 120 degree rotation will take it to this vertex, and the inversion operation.

So, the inversion centre for this cube is the centre of the cube and that will take me to this point. Similarly, when I perform this roto inversion operation or the 3 bar operation again and again, I will obtain all the 6 vertices which are not contained in this body diagonal. Therefore, if you really want to describe the body diagonal symmetry of a cube, it is not just a threefold actually it is a 3 bar roto inversion symmetry operation. Another compound symmetry operator is the screw axis, which is a combination of rotation and translation, and as before you will perform a rotation and a translation and leave a point.

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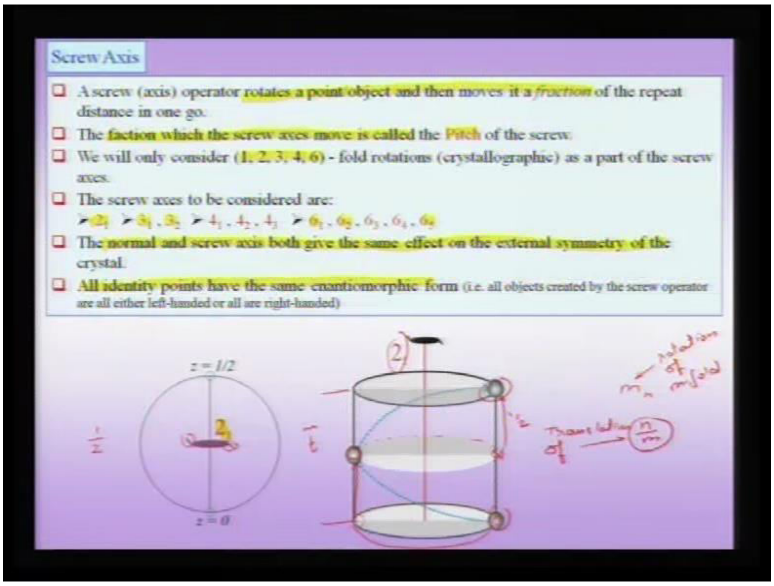

The screw axis operator rotates a point object and then moves it by a fraction of the repeat distance in 1 go, so this fraction of the repeat distance is the fraction of the translational symmetry which we talked about. So, all pixels have translational symmetry which we shall later on be correlated to the lattice parameter, therefore this fraction would be a fraction of the lattice parameter, which we are talking about. And since, typical crystals, for instance the copper crystal or for instance the magnesium crystal all have translational symmetries of the order of angstroms.

This fraction which of the screw axis the translational fraction is actually a fraction of that lattice parameter which again is order of angstroms. Therefore, this there is no external effect of this screw axis, on the external symmetry or the growth form of the crystal, therefore you cannot observe a screw axis looking at the external shape of the crystal.

The fraction by which the screw axis move called the pitch of the screw, and again like before we only consider the 1, 2 and 3 4 and the 6, which are the translationally compatible rotational symmetries, when you are talking about screw axis. This screw axis which we need to consider are the 2 subscript 1, the 3 subscript one the 3 subscript 2 and so forth as listed here, going up to 6 subscript 1, 6 subscript 2 to see 6 subscript 5.

And in this notation which we are seeing here for instance this figure below shows a 2 subscript 1 the 2 is the usual 2 fold rotation, which is implied and the 1 is implies that the translational fraction is 1 by 2. So, suppose I have an screw operator, which gives us m subscript n, which implies a rotation of m fold and a translational component, which is n by m, so this is my translational component involved in a screw axis.

So, let us see the effect of what a screw axis can do for instance a 2 1 screw axis, so a 2 1 screw axis is associated with twofold symmetry, and the 2 subscript one implies the translational component is half the repeat distance or the translational periodicity. So, I start with the general point here, so it will perform a 180 degree rotation from here to here and, but as I told you this is the compound operator, and therefore I will leave no point here, but I will translate by distance half my repeat unit.

So, this is my repeat unit and I will only translate by half the repeat unit and leave a point here, I will progress with this set of 2 one operations, which means that again I will rotate it. And come here by 180 degrees, but again I will not leave a point here, but translate it by a fraction of half, therefore when I start with a point here I will land up with a point exactly above the original point.

Now, this symmetry operator connecting this point to this point to this point is the 2 1 screw axis, which is shown by a symbol as it is a lens with certain amount of tail on both sides. So, this is an extended symbol it has got, so this is a the effect of a 2 one screw operator, later on we will also talk about the other kind of screw operators talked about here like the 3 1, 3 2, 4 1, 4 2, 4 3 etcetera.

But, we have to remember that all these screw operators move an identity point to its same form it will not take a mirror form; that means, if I start with the left hand objects, it screw operator will only leave left-handed objects. As, it goes along performing its rotations and translations, and as I pointed out, since the small fractional translations is not seen in the external growth shape of a crystal, the normal and the screw axis have the same effect on the external symmetry of a crystal or the growth form of a crystal.

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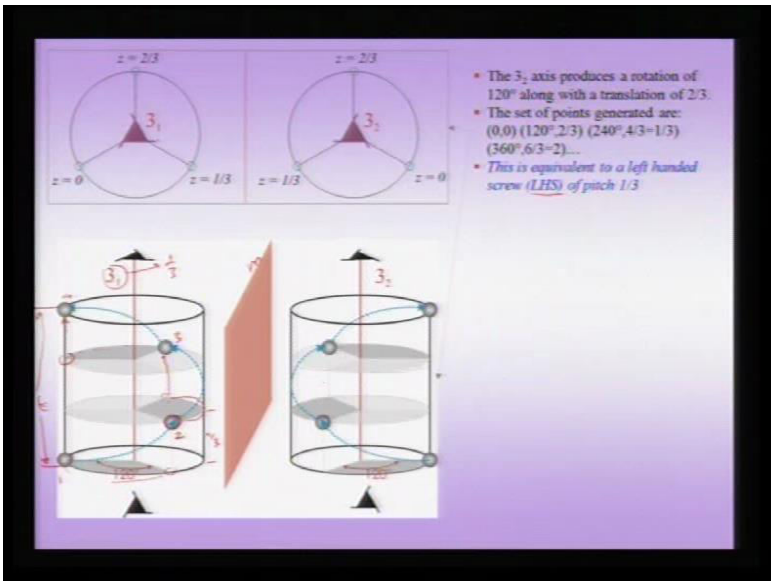

So, let us see how a 3 1 screw operator for instance acts, a 3 1 screw operator you start with a point it will rotate by 120 degrees, but it will not leave a point there, and it will translate by 1 by 3. Therefore, it will translate by 1 third, so this is my one third of the translational repeat distance, which is the total height t. Therefore, it will translate by one third and from starting with this 0.1, rotation by 120 degrees and followed by a translation of one third I will land up with this 0.2.

Further again this operator will act it will rotate by one third, which will take it to this point here, but it will not leave a point there translate by one third which will land up with 0.3. This will again rotate by 120 degrees and it will come here, but it will not leave a point there, it will translate by this one third and leave a 0.4 finally, which is exactly translationally related to 0.1 along the z direction.

Now, a 3 2 screw axis rotates by a certain rotation, which is 120 into 2, but actually if you want to compare a 3 1 rotation axis with a 3 2 rotation axis. You will notice that you can perform the operations of the 3 2 axis, but you will land up with the points, which are exactly related by a mirror operation m on the 3 1 screw axis. So, you can see that the symbol of the 3 1 axis is radiations like this, the 3 2 axis is exactly the mirror symmetry symbol, and so are the effects on the points left out by a 3 1 or a 3 2 screw axis.

So, a 3 1 axis leaves these set of points, while a 3 2 axis is exactly like a 3 1 axis, but if you consider 3 1 as a right-handed screw, then 3 2 is a left-handed screw, which again leaves 2 set of points like 1 2 is that. You start with 0.1, you rotate by the amount given by the rotational symmetry, which is written as the main part of the symbol, then you translate by a fraction which is a fraction of the repeat unit.

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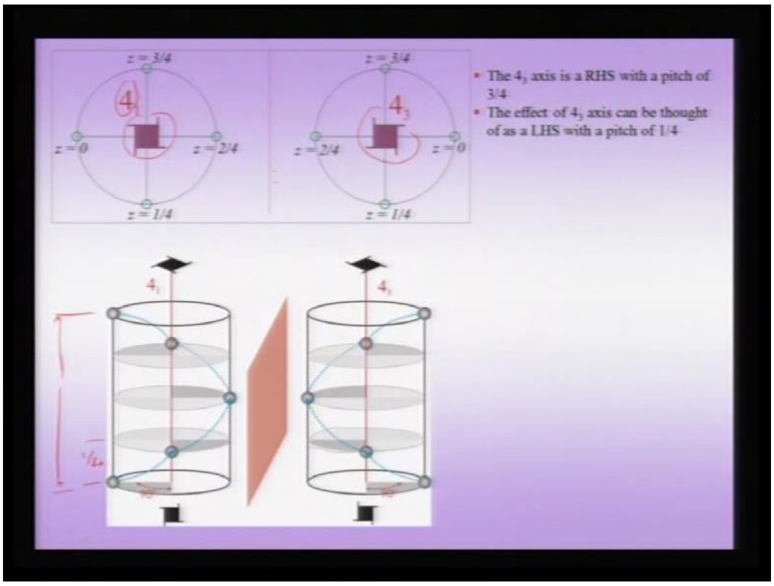

So, in the case of the 4 1 square axis for instance, you will rotate by 90 degrees and the translational component will be one fourth of the total translational symmetry, which is one unit along that z direction. So, and similarly like before the 4 1 rotation axis is related to the 4 3 by a mirror plane, and the symbols are also related by a mirror plane as shown here in the above view graph.

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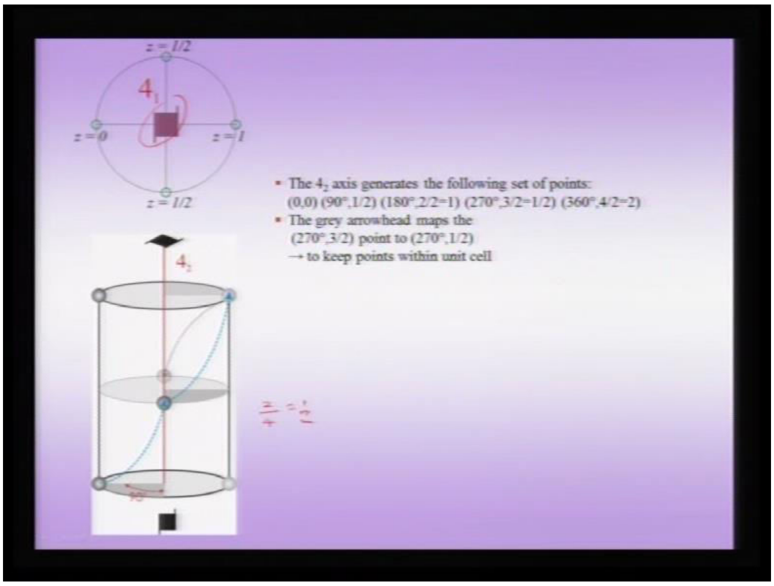

Similarly, we have a 4 2 axis which has got a symbol here, and you can see that in the 4 2 axis you have and 90 degrees rotation, and a translational component which is 2 by 4 which is half.

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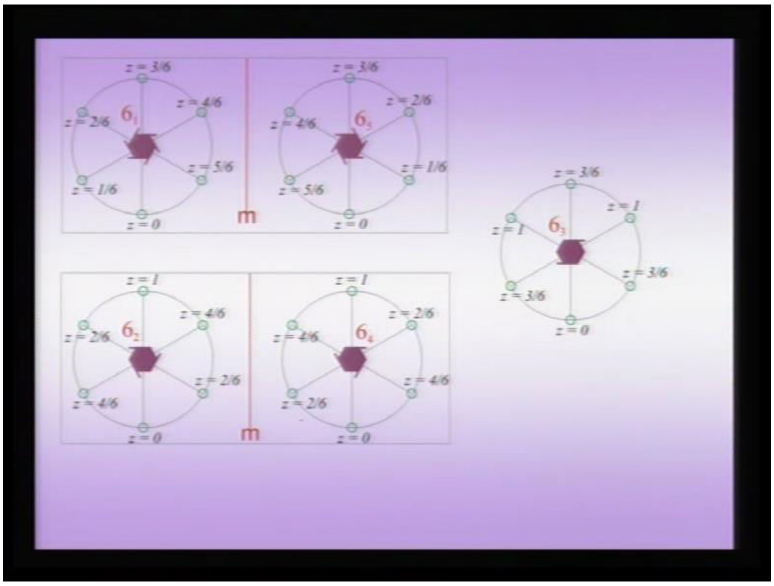

So, in effect all these rotation axis are very similar in their effect, and we need to consider them when we are talking about symmetries of crystals. And one of the some we will return to this concept later for instance the 6 3 screw axis is at the heart of for instance the hexagonal close pack crystal to be called hexagonal close pack crystal. So, some of these concepts we will return to later, but once we have understood one screw operator all the others are very, very similar in their effect, in leaving a set of points which are all either left-handed or all are right-handed operations.

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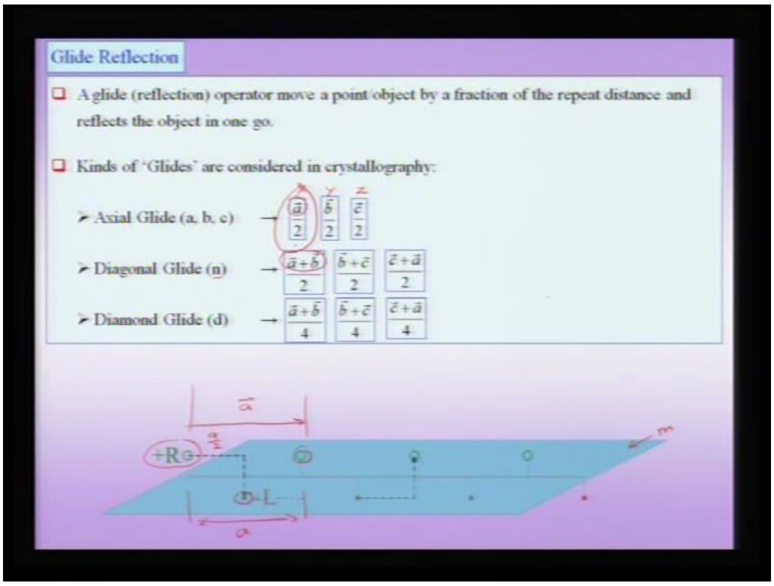

Another, we talked about a compound operation which is the glide reflection operator, and in the glide reflection operator you start with the point there is a translational compound which is a fraction of the translation. For instance, it could be a fraction of the translation along for instance the x-axis, and you reflect for instance suppose my translational component along a certain component is this. This is my translational periodicity, say for instance a then my glide reflection operator is a combination of a translation and a reflection.

So, the at the heart of a glide reflection operator is a mirror, so this is my mirror plane and what does a glide reflection operator do you start with a point, which is for instance a right-handed object above the plane of the mirror plane. It translates by a fraction of the periodicity now for instance, this is my periodicity along this direction is a then my translation component is a by 2.

Therefore, this is called a by 2 glide, therefore you translate by half and reflect, therefore you land up with a mirrors form of this object which is a left handed form and below the plane. Further, if this glide reflection operator acts again then you will move this point and reflect, and you will and up with the point exactly like the right-handed object above the plane, but now move by a point by lattice parameter a.

Now, this implies that if I have a glide reflection operator, then it will leave half its points as left-handed objects, and half the points would be right-handed, and not only that as the like in the case of the screw operator. When the glide reflection repeatedly operates it moves a point in space, and therefore it fills up along one direction in infinite set creates an infinite set of points as it repeatedly acts.

But, as you can notice the number of points within this unit cell or the repeat distance, now my this is my repeat distance is only 2, there is one here, and there is one here, one is a right-handed object, one is a left-handed object. In other words even though the screw and which we can go back, and see now for instance the screw if it keeps on acting would create a infinite number of points, but the number of points within this repeat distance t is only 2 1 here, and one here.

And similarly, for the glide reflection operator the number of points within the repeat distance is only a finite number, though if it these glide reflection operators act they keep on acting repeatedly and create an infinite set. The number I need to worry about is the number, which is a single repeat unit or the single unit cell as we will see later, so but there are many, many possible type of glides which are listed here.

Though, we will not be going into detail it is worthwhile to know that these kind of glides exist, for instance you could have a glide with the translation component along the one direction. You could have translation component for in this is along for instance the x direction, this could be a translation component along y direction or you could have a glide operator, which has a translation component along the z direction. We could also have what are known as diagonal glides which are given a symbol n, in which case the translational component is again half, but it has an average of the translation along x and y direction both.

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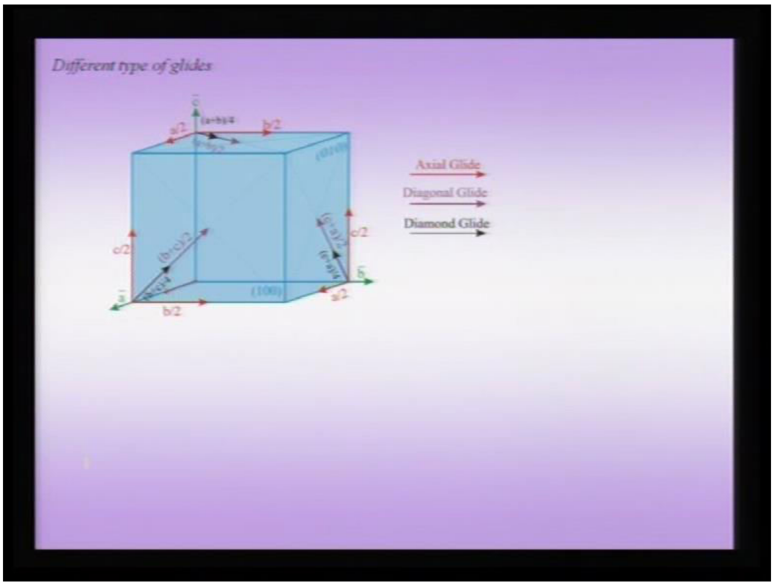

So, this can be seen here, so for instance this is my a glide for instance I can show here, which has a translational component, along the a direction. You could have for instance a diagonal glide, which has a translational component like you can see here a plus b by 2; that means, it is along the face diagonal or you could have, as you have seen before. Here, a diamond glide in this the translational component is one fourth and not half, as in the case of the axial glide or the diagonal glide, to summarize glides we have got axial glide, diagonal glide, and diamond glides, all of which basically take an object to it is enantiomorphic form and involve a translation.

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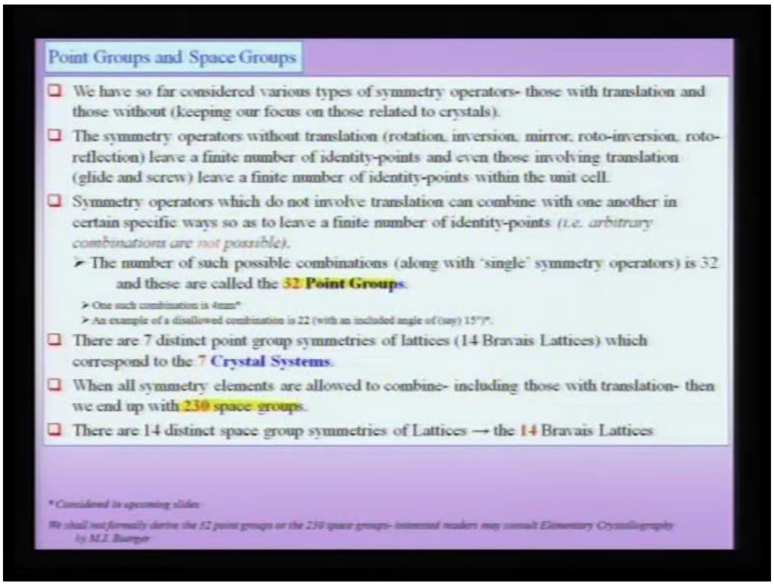

Now, the next important concept in crystallography is the concept of point groups, and a more advanced concept which of course, we will not take-up in this course in detail is a concept of space groups. But, it is worthwhile to be exposed to such terminology, because when someone somebody reads an official text on crystal structure, you will be exposed to these concepts like point groups and space groups.

And especially, this point groups are very, very important from the point of your properties of crystals as we have noted before, so far we have seen various kinds of symmetry operators. And we know that they leave a finite set of points within a unit cell, but are there combinations of symmetry operators, which are possible, we have actually seen some examples. For instance, we have seen a combination like 1 by m or the 3 dot i in which the combination of 3 and inversion, and we have to note that in general of course, all possible combinations are not allowed.

There are only certain distinct combinations allowed, which can leave a finite set of points in space, like the case of the normal operators which also leave a finite set of points in a unit cell. Therefore, there are only certain allowed combinations of symmetry operators, and is, so happens luckily that this number is very not very large. And there are only 32 allowed combinations of symmetry operators, which are not known as the 32 point groups, and if you are talking about those symmetry operators, which involve the translation like the screw or the glide.

Then there are 230 allowed combinations, which are called the 230 space groups, in the point groups you stay around a point you do not move the point from one place to another. But, suppose I am talking about those symmetry operators, which involve translation like the glide or the screw; that means, that I am going to move the point. And if you include those symmetry operators 230 such combinations are allowed, which are known as the 230 space groups.

It is very, very important to have these numbers in mind because the we will later on be exposed to the concept of seven crystal systems, and in fact and also additional concept known as the 14 Bravais Lattices. The 14 Bravais Lattices are created purely by translational symmetry, but it is interesting to note that, if you are talking about these 230 space groups, and those which are compatible with among those which are consistent with lattices, then these 230 space groups will lead to the 14 Bravais Lattices.

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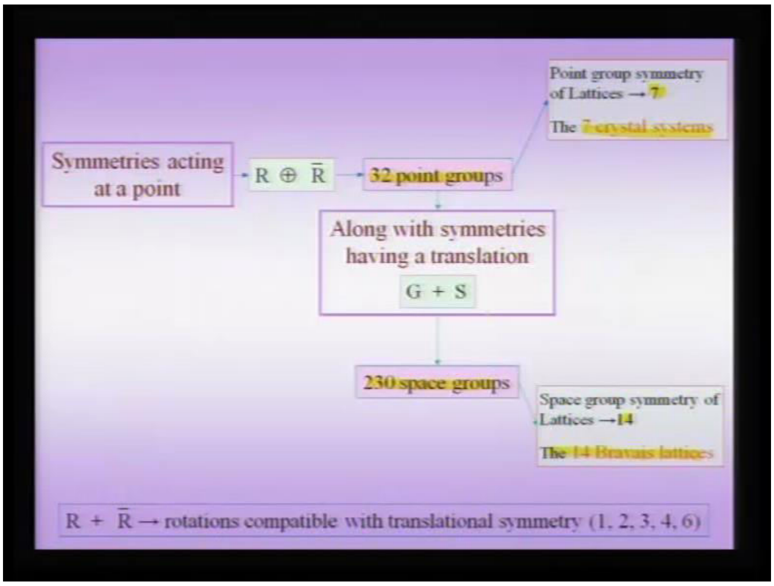

So, let me summarize this rather complicated slide that, if you are talking about symmetries acting at a point, then the allowed combinations will lead to 32 point groups. And we will see some at least couple of examples, if What we mean by allowed combinations. Then among these those symmetries, which survive when I am talking about symmetries of lattices are 7 in number, which are nothing but, which correspond to the 7 crystal systems.

Simply, suppose I am talking about allowed combinations of symmetry operators, which involve translation, then I land up with the 230 space groups. And out of those if I am only considering those symmetries out of these 230 symmetries of the space groups, those which are compatible with lattices, then I will land up with the number 14 which are known as the 14 Bravais Lattices. Of course, one could land up with the 14 Bravais Lattices, as we shall see that by purely considering translations

So, this is a what you might call a real look ahead or a very difficult concept, but here we just want to introduce the important, what you call essentials of these concepts, because some of these would form the basis some of the descriptions you would read. For instance when you are studying about crystal structures, in an interactional tables or you're studying about the report about some crystal structures.

So, for instance suppose I am talking about allowed combinations, one such allowed combination is a 4 mm symmetry. And for instance, suppose I am talking about a disallowed combination, for instance a 2 2 symmetry with 14 degrees included angle would be a disallowed combination.

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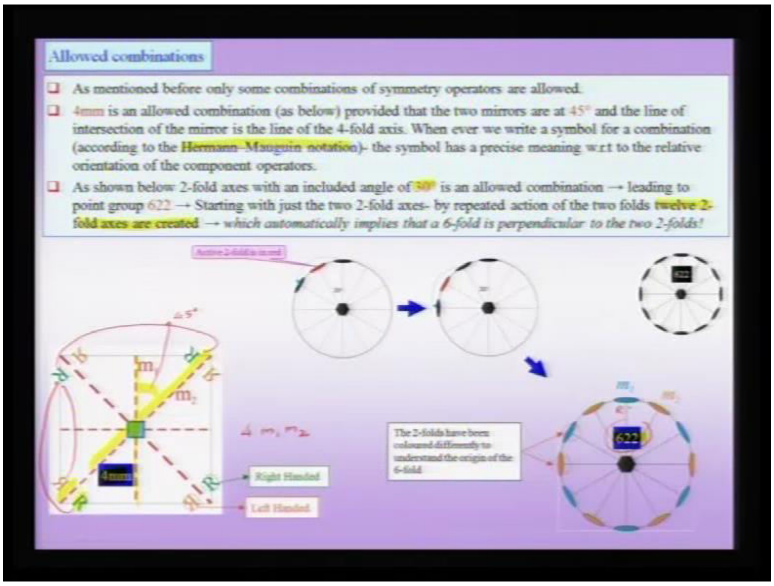

So, let us see how is for instance how can we talk about an allowed combinations 4 mm suppose I am talking about a 4 mm symmetry, here I am talking though the symbol does not tell all the details about this allowed combination. What we exactly mean by this 4 mm symmetry is a fact that, you got a fourfold you got one vertical mirror, and one diagonal mirror, and the orientation between the 2 mirrors is 45 degrees.

So, these are things which are implied, which are not expressly written out, but which are implied in the symbol. So, when I am talking about 4 mm, actually what we are talking about is four fold in combination with m 1 and m 2, if you call this m 1, the diagonal mirror will be m 2. And as you can see the line of intersection of the 2 mirrors m 1 and m 2 is the line of the rotation axis which is the fourfold, now suppose I start with the general point which is a right-handed are drawn here.

Then my fourfold will take me lead me from this green to this green to this green, and finally to the fourth green, and finally it will close space on itself, but this mirror for instance will produce a left-handed R. And this horizontal mirror will produce take this to this right-handed, in other words; however, how many ever times this 4 mm symmetry acts, either individual mirrors or this combination or the fourfold you will notice that I will land up with 8 objects only.

And if I had started with a point I will land up with 8 points, if I am talking about this right-handed objects R, then I will have four right-handed objects then I would have 4 left-handed objects, which are shown in orange color. Therefore, we know from the mere action of this operator 4 mm, that it does not allow combination, because first of all I will land up with an finite number of points starting with or a number of objects starting with one object R a green R.

For instance, I will land up with 4 green R's and 4 red R's or 4 orange R's, therefore I have only 8 objects, if I start with an one object, therefore I can clearly see 4 m m is an allowed combination as far as crystals go. Now, another allowed combination is shown here, for instance which is the 6 2 2 and these combinations are typically written out using what is known as the Hermann Mauguin symbol, which is a short hand notation for these symmetry operations.

And in the second example shown here, as I had pointed out before if I am talking about 2 2 folds any arbitrary angle between the 2 2 folds is not allowed, but a 30 degree included angle. For instance, as shown here is an allowed combination, and in that case suppose I start with 2 2 folds, and an included angle of 30 degrees, then I will land up with, you can see here 12 twofold axis.

And which automatically implies that, there is a 6 fold rotation axis and the total Hermann Mauguin symbol for this combination is 6 2 2. And I can actually perform an experiment like I had done with an green R right here, I can put one of those objects here and I can confirm to myself that actually I will land up with a finite set of objects if I am talking about this allowed combination of 6 2 2 symmetry.

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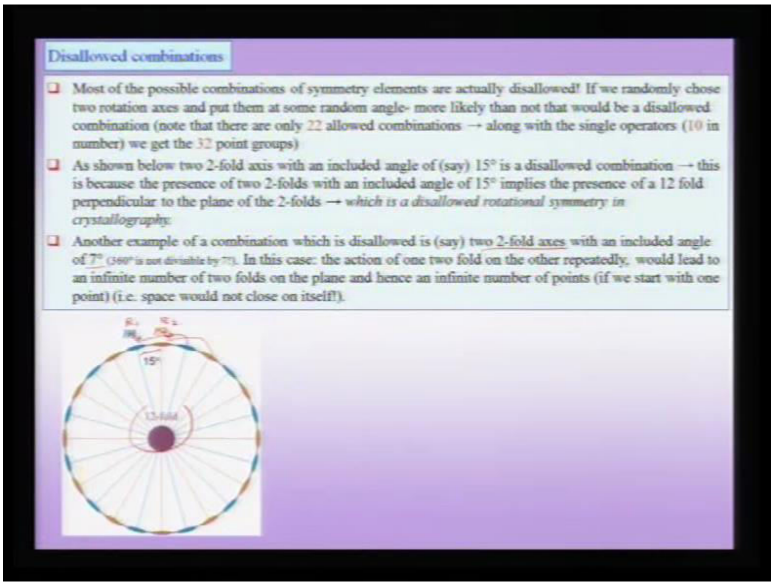

There could be a couple of reasons why symmetry combination is disallowed, one of the reasons is that suppose I talk about to mirrors at 15 degrees apart, then this mirror will keep on this mirror will rotate it to this mirror. And this will rotate it to this mirror and so forth, you land up with a array of rotation axis, for instance this is now. So, suppose I am talking about disallowed combinations, and going back to the previous slide we have talked about allowed combinations.

And one small error here is that these are actually rotation one and rotation 2 which are nothing but, 2 fold axis, and here we are considering disallowed combinations of symmetry operators. In fact, if you randomly already seen the number of allowed combinations is only 32, for symmetry operators which act around a point. So, that that implies that most of the other combinations are disallowed, we cannot have a random combination of 2 symmetry operators, which will leave space closed.

For instance, suppose I talk about a combination like a twofold axis another twofold axis, which are 15 degree apart then this twofold axis will rotate it to another twofold and so forth. And I will have an array of twofold axis as shown here, but this combination of 2 folds would imply a 12 fold axis perpendicular, and if you had we go back to a the place, where we had sent that 12 fold is not a symmetry, which is crystallographically compatible.

Similarly, another reason why a particular combination may not be allowed is that the combination would start producing, an infinite number of symmetry operators, which also mean that if you start with the general point. You may land up with an infinite number of symmetry operators, such example would be 2 twofold axis with an included angle of about 7 degrees. Then you will land up with an infinite number of points starting with one point, and therefore we shall restrict ourselves to only the allowed combinations which are crystallographically allowed.

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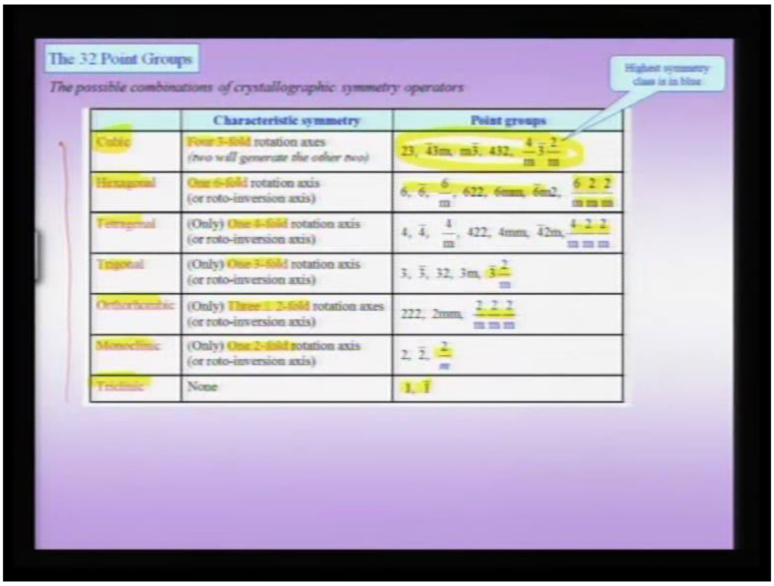

Now, let us briefly talk about the 32 point groups, which are nothing but, the 32 ways in which symmetry operators can combine, and leave of one start leaving with a point, it gives you a finite number of points in region of space. So, these 32 point groups, in fact can if you consider them to have the highest symmetry, which is compatible with lattices then you will land up with 7 which we pointed out.

Where, the symmetries of the 7 crystals systems, which we will take up later during the course, though and important point is that at this we can actually, associate these point groups. Like you have a allowed combinations like 2 3, the 4 bar 3 and the m 3 bar, the 4 3 2 and the 4 by m 3 bar, 2 by m, these point groups come under the cubic class. In other words if I have a cubic crystal, then it has to fit into one of these symmetry classes, and typically if you take for instance we will consider examples like copper crystals or for instance polonium crystal or for that matter iron crystal.

These would have the highest allowed symmetry, which is four by m 3 bar 2 by m symmetry, while it is possible that there are certain lower symmetry cubic crystals, which does not have the full or the higher symmetry allowed for a cubic class. Similarly, we can talk about hexagonal crystals having the higher symmetry which is 6 by m, 2 by m or anyone of the lower symmetries, which is allowed for a hexagonal crystal.

And by noting all these different point groups, and the different crystal classes into which or the crystal systems to which they belong, we can actually sort of come out with a characteristic symmetry or a symmetry which is basically required for a crystal. For instance if you have a cubic crystal it needs to have four threefold axis, a hexagonal crystal needs to have at least one 6 fold axis, and that is all possible there is only one 6 fold axis.

A tetragonal crystal needs to have at least one fourfold axis, a hexagonal crystal has only 1 3 fold axis, and if it if a crystal ends up having 2 3 fold axis then it will end up having 4 3 fold axis and actually then it will start coming into the cubic class. And not in the triangular class, similarly an orthorhombic crystal has 3 perpendicular 2 fold axis a monoclinic crystal has 1 2fold axis, a triclinic crystal at best can have an inversion symmetry or at worst can have only translation symmetry.

In other words if a crystal does not even have a translation symmetry, it cannot be called a set crystal, then it'll be classified as an amorphous material, on the other hand if it at least has translation symmetry we will qualify to be at least a try triclinic crystal.

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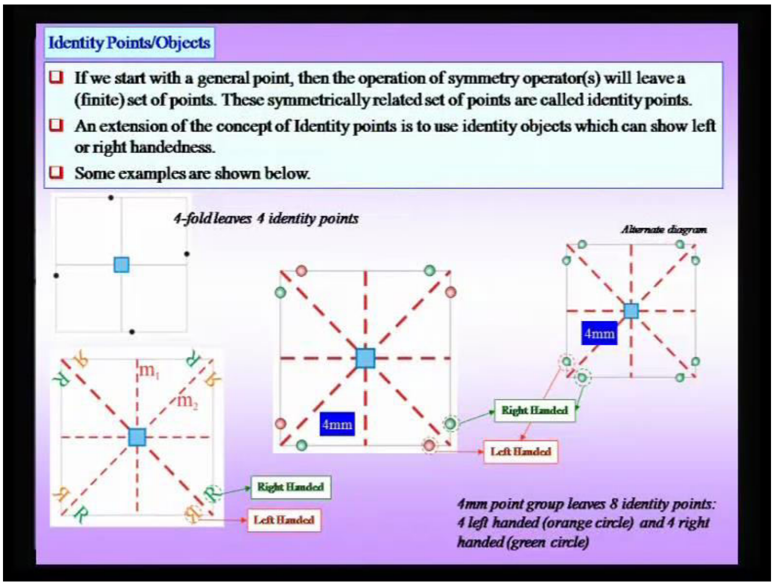

And if any more symmetry is possible in the system, then it can climb up the ladder and go all the way up to the cubic crystal, which is a crystal having very high symmetry, and it can have a symmetry up to 4 by m 3 bar 2 by m.