Condensed Matter Physics
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Lecture - 2
Symmetry in Perfect Solids

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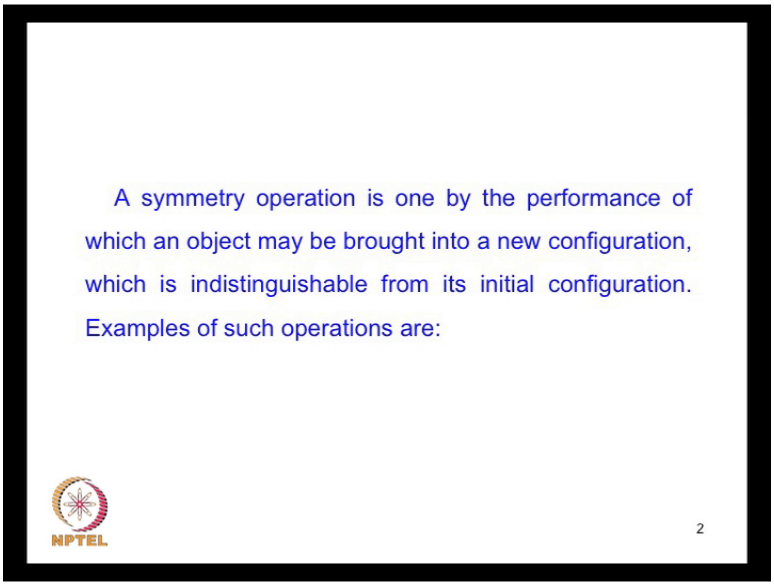

From now on for the next few lectures, we will be dealing with perfectly crystalline solids as prototypes of condensed matter. As we have already seen such perfectly crystalline solids have a good dealer symmetry and the symmetry place a central role in the understanding of the behavior of such solids. We have also seen in lecture one that when they are in phase transitions, there are symmetry changes. So, we need a method for describing quantitatively in a standard sort of way, the symmetry imperfect solid. So, we first talk about what is known as a symmetry operation, what do we mean by a symmetry operation. A symmetry operation is something we will come to various kinds of symmetry operations later, the general definition is if you perform a symmetry operation on an object then the operation will bring it into a new configuration, but this new configuration cannot be recognized from its original configuration. So, if you perform the symmetry operation, and ask someone to observe the object before and after, you would not been a position to say that this operation has to be performed. So, this object goes into a symmetry related new configuration.

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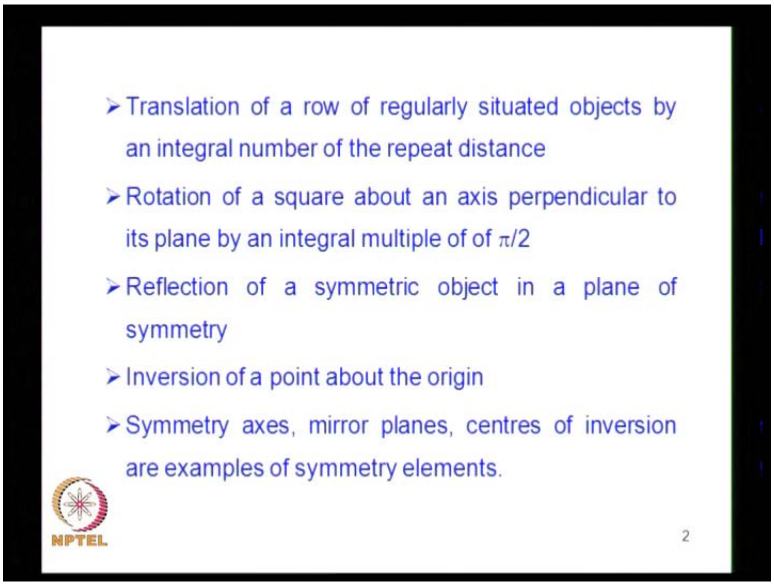

Examples of such operations are translation.

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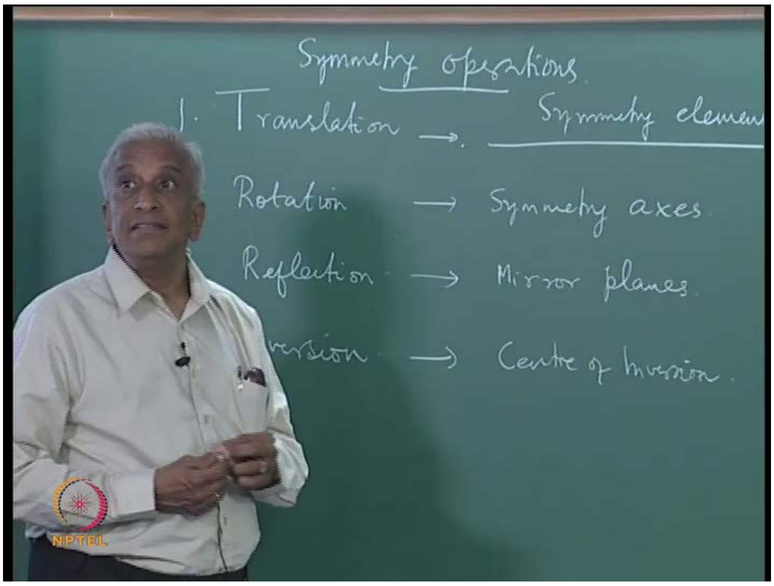

Translation of a row of regularly situated objects by an integral number of the repeat distance. There is also another class of operation namely rotation, for example, rotation of a square, if you take a square and rotate, it about an axis perpendicular to its plane by an integral multiple of pi by 2 something like this. So, if I have a square like this and rotate it by pi by 2, it goes to a new symmetry related configuration, but this square looks the same. So, there is no way of saying that there has been such a rotation by either pi by

2 or pi or 3 pi by 2 and so on. The third classes of symmetry operations are reflections. If you have a symmetric object and if you have a planer symmetry then if you you can reflect the object at this planer symmetry, so that the object gets comes here on the other side and does not look different.

The fourth category of symmetry operations are inversion of an object about a point. So, you have translations by regular repeat distances. Then rotations so these are also known as symmetry axis because rotation is always a form about an axis of rotation. So, then a plane of symmetry which causes a reflection symmetry is known as a mirror plane. So, and then inversion is always about a point which is known as the centre of inversion. So, these are all examples of symmetry elements.

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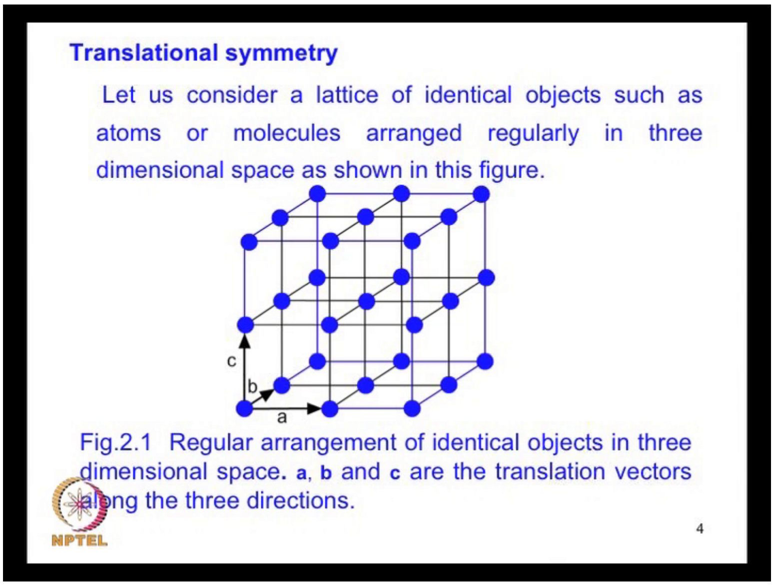

Let us go to translation symmetry, you can see from figure two one where we have a regular arrangement of identical objects in three-dimensional space. And a, b and c are the translation vector along the three mutually orthogonal directions. So, you have each object can be a setter atoms or molecules arranged they are arranged regularly at various points along this three-dimensional array, so that obviously, has translation symmetry.

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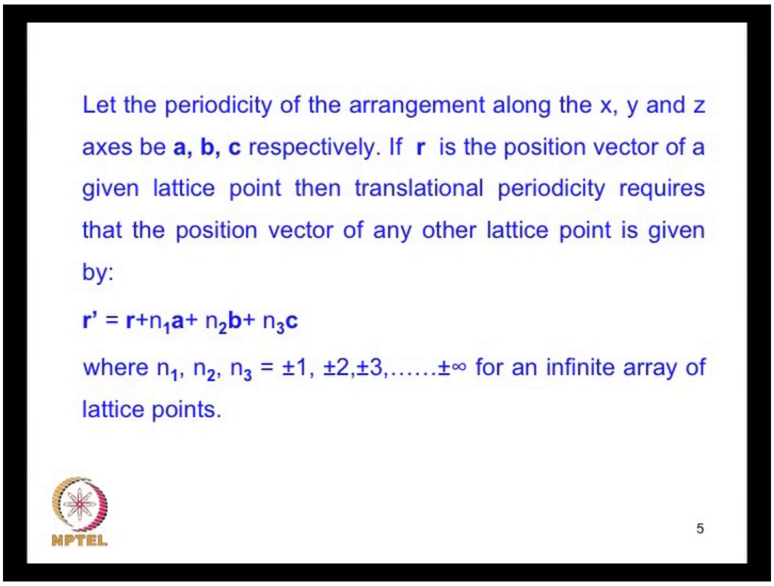

So, if you take this periodic distances, periodicity along the three axis which we will call x, y and z axes, if they are a, b and c respectively.

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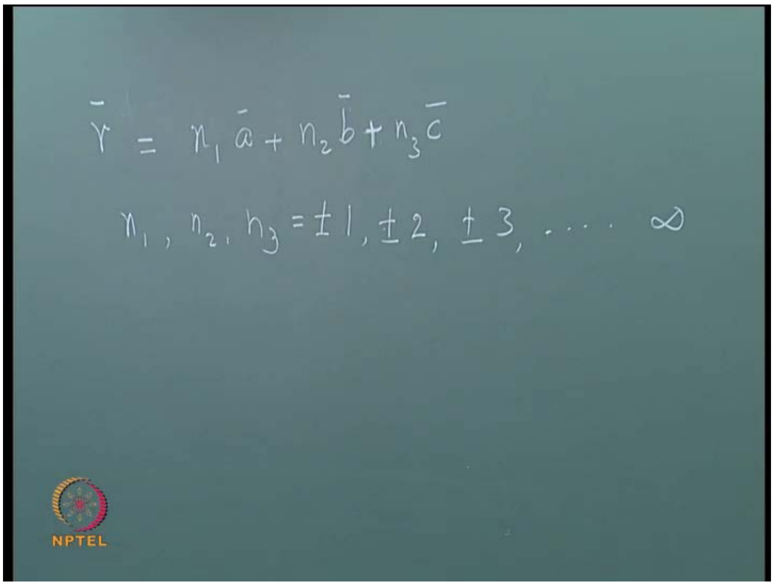

And if r is the position vector of a given lattice point then the translational periodicity requires that any other lattice point in this array is given as the position vector r prime which is n 1 a plus n 2 b plus n 3 c starting from the origin of course. So, n 1, n 2, n 3 are integral numbers integers which can be positive you can go in the positive x direction or in the negative x direction. So, it will be plus or minus 1 plus or minus 2, you can go through two repeat distances, you can go by three repeat distances and so on, you can have an infinite number up to infinity for an infinite array of lattice points, so that is what is being shown in figure two one.

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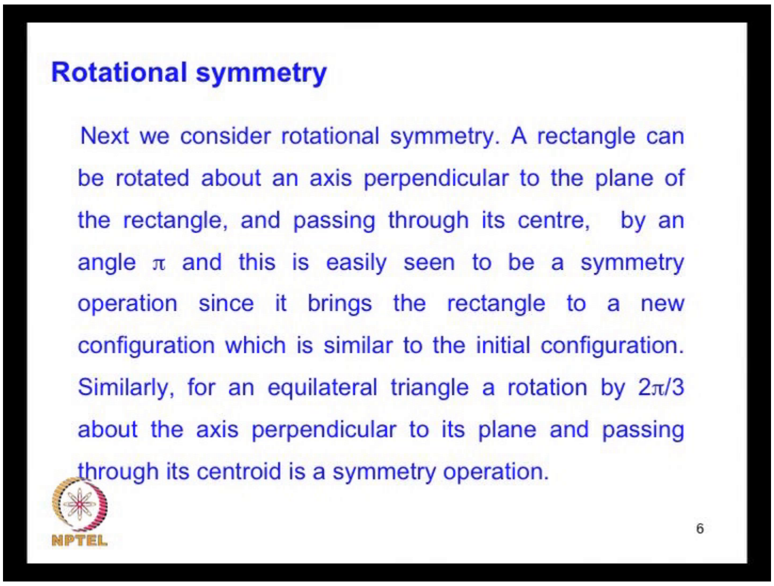

Next we go on to rotational symmetry.

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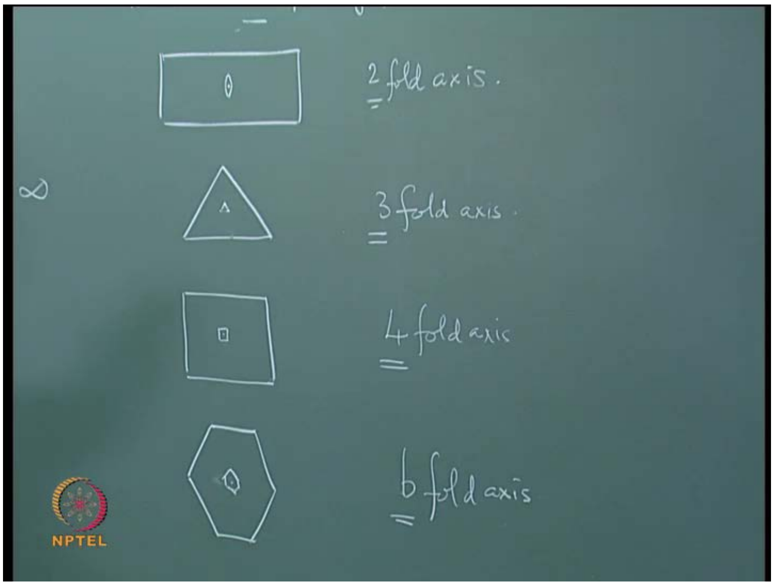

This is translation. Now for example, if you take a rectangular object, and if you rotate this rectangular about an axis perpendicular to its plane, and passing through its geometric centre by an angle of pi then it reaches an identical configuration. So obviously, for a rectangle a twofold rotation axis about this point, we easily seen to be a symmetry operation, since this rotation brings the rectangle to a new configuration which is identical to the initial configuration. So, if I have an equilateral triangle, so it has a twofold rotation symmetry about this point - a rectangle. If you have an equilateral triangle, this has threefold rotation symmetry about this axes. So, this is an axis passing through its centroid of this equilateral triangle. So, if you have a square. So, then we have a fourfold rotation symmetry, fourfold rotation symmetry about the geometric centre of the square.

So, this is twofold axis, this is a threefold axis, this is a fourfold rotation. Why do I say twofold, because if I rotate by pi, it comes to a different configuration, and then you rotate again by pi, it comes back to the original, so you need to such rotation in order to bring it to the original configuration. Here you had to do the symmetry rotation, three times in order to bring a triangle into a self-coincidence. Similarly you need four such rotations to bring this square into self coincidence. And if you have a regular hexagon like this, this has a six fold rotations symmetry about its geometrical centre. So, it is a six fold axis for a regular hexagon. So, you can see that twofold, a threefold, fourfold and six fold axis are the common rotation axis in solids which are perfectly periodic and have a translation symmetry.

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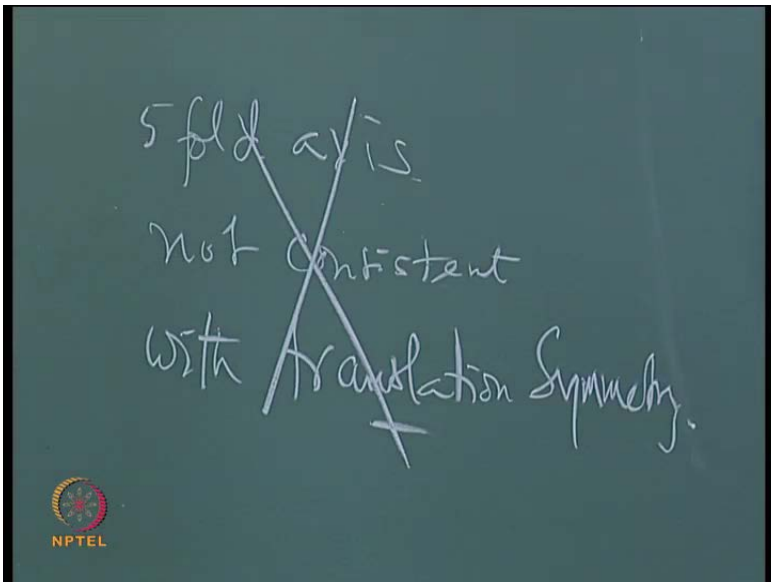

We do not have a fivefold rotation axis, because I do not want to discuss this, but I will simply state that this is not consistent with translation. So, the rotational a fivefold rotation symmetry, if it is present in a perfectly to crystalline solid then it will violate the translation symmetry and for this is not present. So, what we have only twofold, threefold, fourfold, six fold. One fold of course is trivial; it is just nothing, it is just rotation by pi two pi, so it obviously brings into self coincidence.

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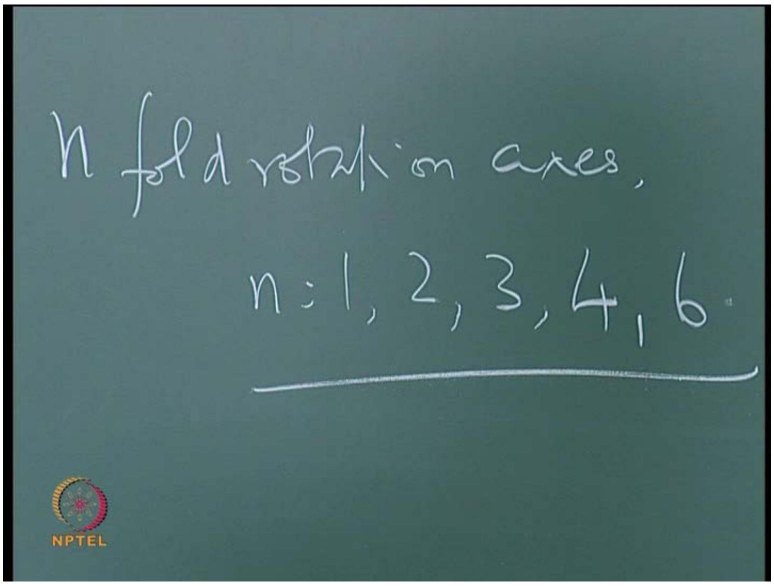

But for just completeness we will also include a one fold rotation. So, 1, 2, 3, 4 and 6. So, here n fold axis where n equal 1, 2, 3, 4, and 6. These are the rotation axis symmetry axis which are consistent with the translation symmetry of a perfectly periodic solid.

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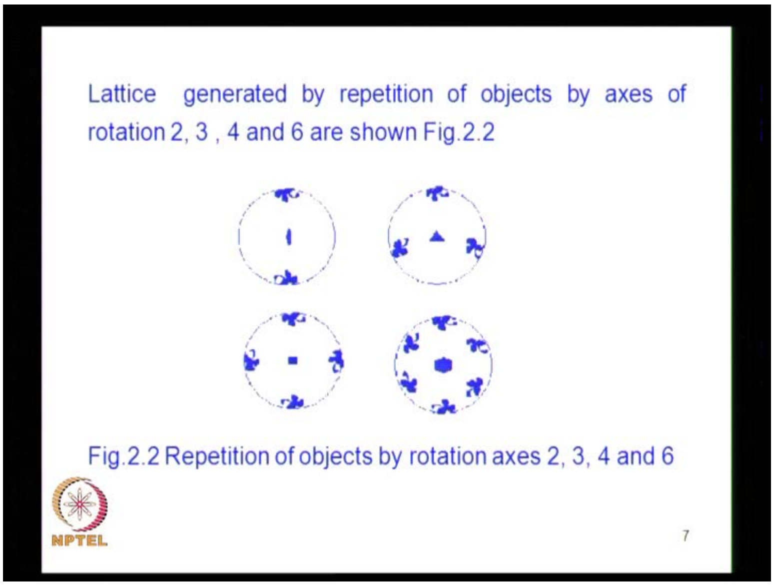

So, figure two two shows what is known as a stereographic projection.

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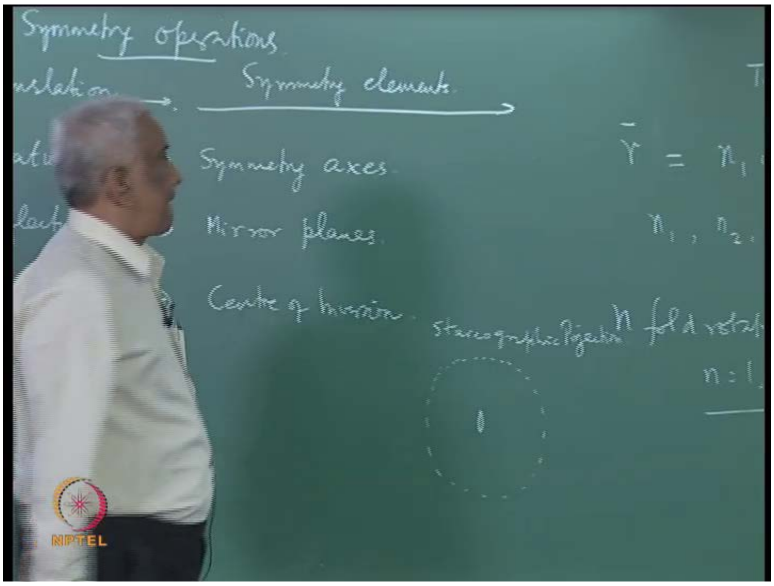

By stereographic projection, what we mean is the project on a sphere like this and the axis rotation axis, twofold axis, for example, is shown like this as in this case. So, we have an object which is repeated by the twofold rotation from here to this. Similarly, a threefold axis is shown like this and the object is repeated like this. Here it is a fourfold rotation and here it is a six-fold rotation. So, these four axis are shown by stereographic projection.

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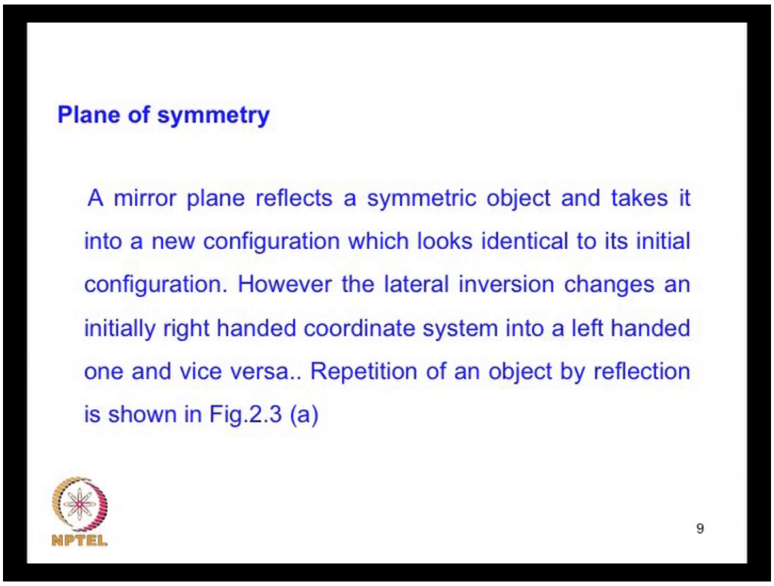

Next we consider a plane of symmetry or a mirror plane.

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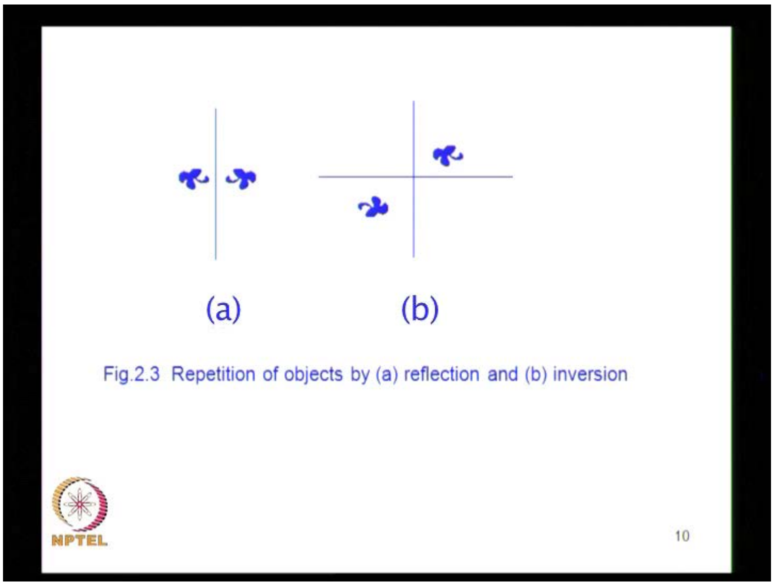

Fig.2.3 Repetition of objects by (a) reflection and (b) inversion

A plane of symmetry or a mirror plane reflects the symmetric object as shown in the figure two three a. So, you can see that there is a mirror plane and that reflects on object about the mirror plane. So, takes the object into a new configuration, which looks identical to the initial configuration. However, the lateral inversion present in the case of a mirror passes a change for the case of a right-handed coordinate system will get inverted at the mirror plane into a left-handed coordinate system.

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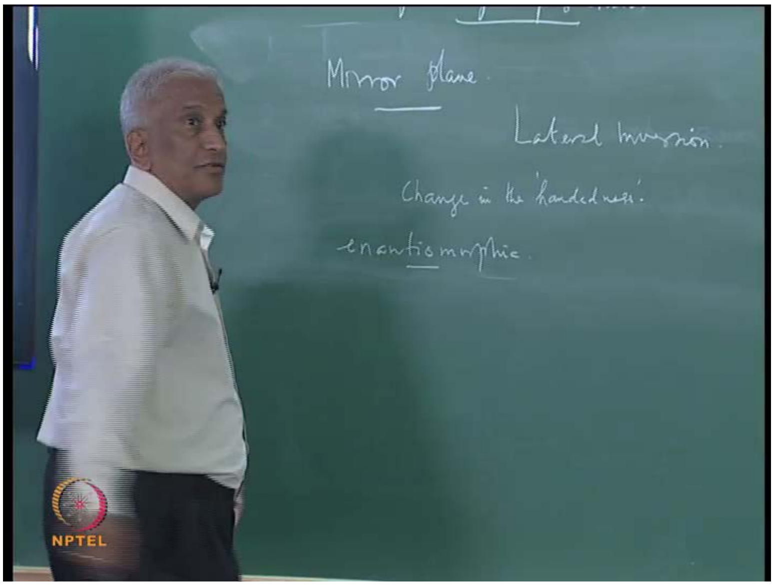

So, because of that the change in the handedness are so such a symmetry operation is known as an enantiomorphic symmetry operation.

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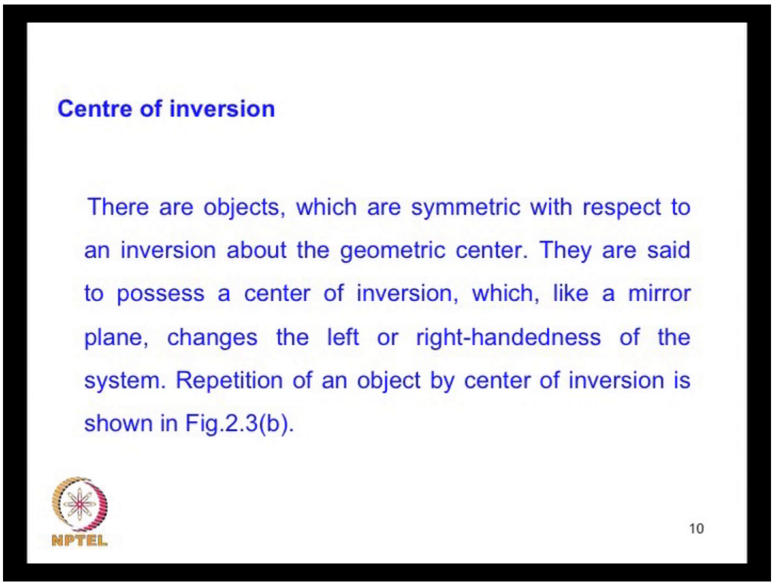

This is also true of a centre of inversion where the object which is symmetry with respect to an inversion about the geometric centre. So, there is a centre of inversion, again an inversion operation also changes the right handed into a left-handed system and vice versa. So, this is shown in the figure to three b where there is a centre of symmetry and this get inverted by at the origin and a there is an accompany change in the handedness.

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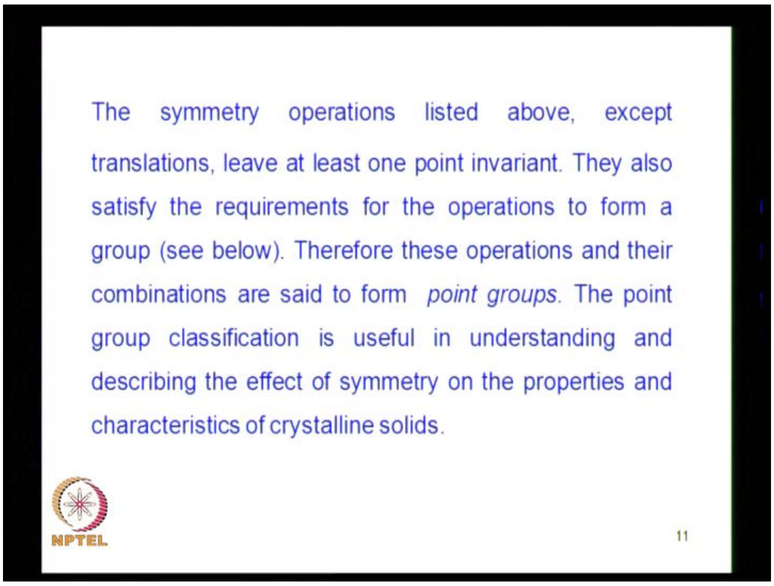

So, in all these cases except translation, in the case of the all these rotational axis, there is an axis of rotation and that mean that any point which lies on the axis of rotation is not change. So, you have to have some other it should a point should be outside in order to for it go to a new configuration. So, it leaves all this symmetry operation a rotation axis whether it is one fold, twofold, threefold, fourfold or six fold lives all the points which lie along this axis of rotation invariant, they do not change.

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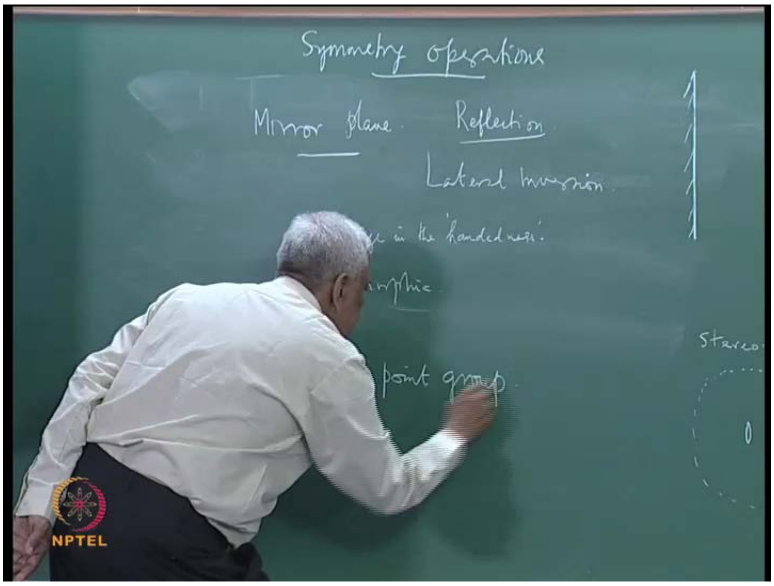

Similarly, in the case of a mirror plane, I will show this like this a mirror plane. Again all the object lying in these mirror plane, do not change the point has to lie outside the plane in order to get reflection and go to a new configuration any point which lies on this mirror plane does not undergo any change by the operation and the mirror symmetry. Therefore, all these points are left invariant by the mirror plane. Similarly, in the case of inversion, the inversion is about the origin and nothing happens to the origin then you perform an inversion operation. So, at least this centered symmetry remains invariant.

So, all these three symmetry operation rotation, reflections and inversion, all these leave at least one point invariant in space. Therefore, these rotation, these rotation, reflection and inversion operations are collectively known as defining this so-called point group of the solid. The solid is set to possess by virtue of the symmetry elements, they belong they are said to form a point group the point group classification is very important for describing and understanding the effecter symmetry on the properties and characteristics of crystalline solid.

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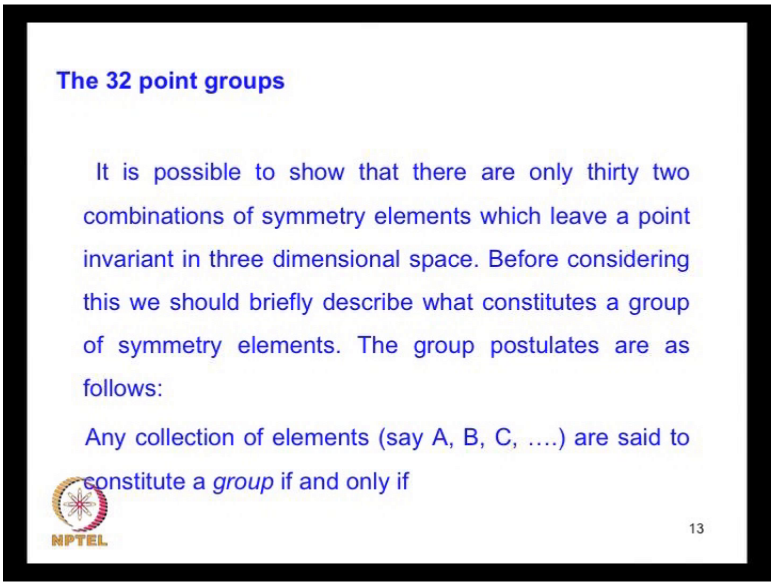

So, we have it can be shown that there are 32 point groups in three dimensional space. We have only 32 combinations of the symmetry element, which leave a point invariant in three-dimensional space. We say that they are they form this so-called point group at this point, we should understand what is meant by the term group here. Now this group is a mathematical group of symmetry elements now what does it mean then it can be say that a set of elements constitute a group, this is important for us to understand.

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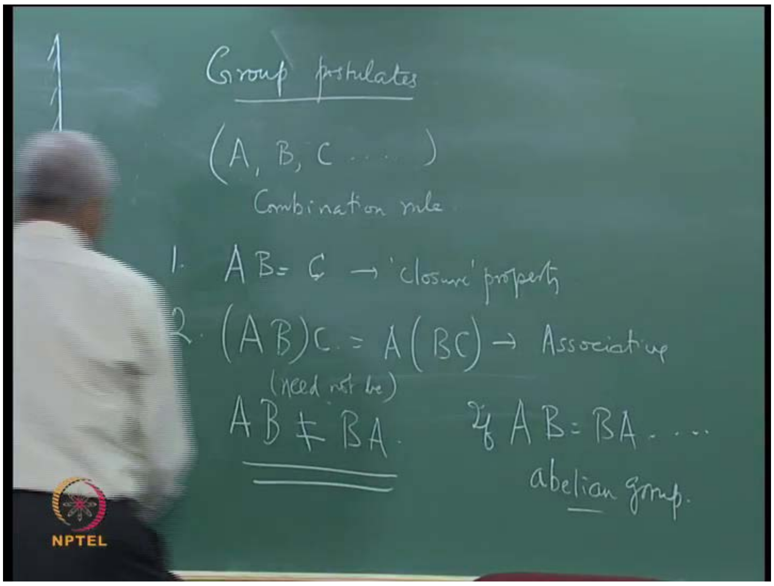

So, let us now go on to describe the so-called the group postulates group postulates what constitutes a group any collection of elements do not form a group. So, if you have a collection of elements let us write them as A B C etcetera. So, this is the collection of elements they can be objects they can be a collection of symmetry element they said to constitute a group.

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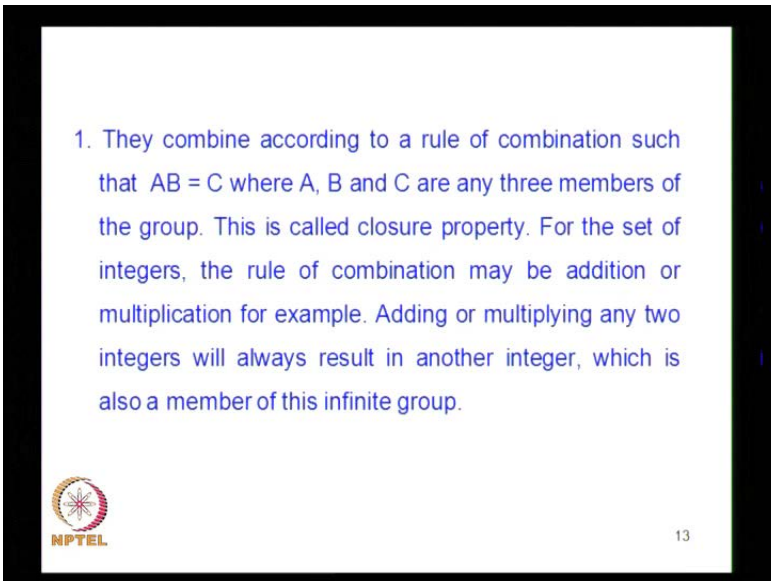

If and only if the following requirements are satisfy what are the various satisfy in the requirements to be satisfy in any such collection in order for them to form a group you must first specify what is the role of combining these elements the role of combination combination role should be specified. For example, in the set of elements known as integers numbers 1, 2, 3 like that plus and minus, positive and negative integer. The role of combination can be, for example, addition, so that you can write one plus one or one plus two one plus three like that.

You can combine the various elements, what do you get, if you say one plus one, if you combine the element with itself you get two which is also an element of the group is you combine one and two you get three which is also an element. So, in general rule is that if you have A B by A B, I mean the combination of A and B elements and this should reserve in an element c which should also be a member of the group for any A and B. So, this is known as the closure property any two elements and b if you specify the role of combination and then combine A and B then they should lead to a third element c in general which should also belong to this collection.

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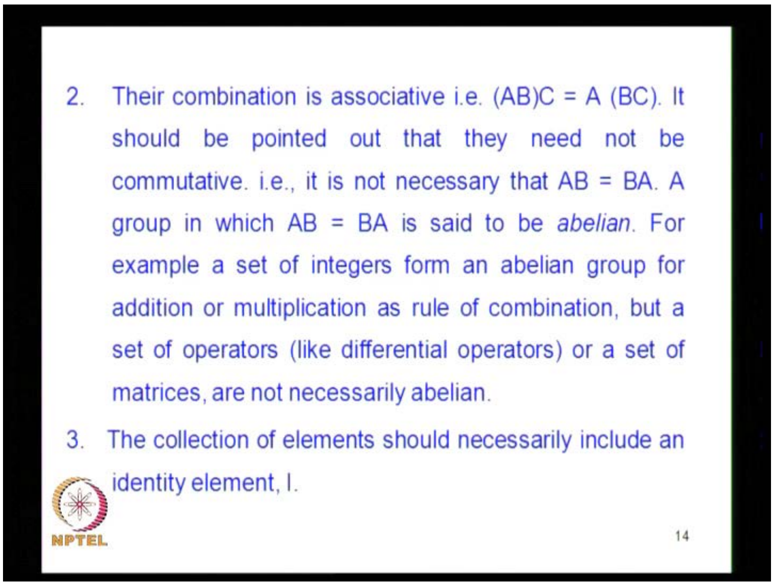

Then only this is one property, which as to be satisfied for the elements A B C etcetera to form a group. The next property which should be satisfied is the the following A B times C should be equal to A times BC, this is associate the combination is associate. So, here for example, you have two and three give you five and then one that is one and two is three and then you combine it with three, you get six and same is the result here two and three is five and then you combine it with one you get six again. So, you get the result. So, this is very necessary for the collection to form a group, but it is not necessary that a b should be equal to b a this is not necessary need not a can b, but if they are then in that specific case if A B equal to B A. Then this group for all the element then it is known as an abelian group then you must always have the third property which is with there should always be in this collection of elements a b c there should always be an identity element.

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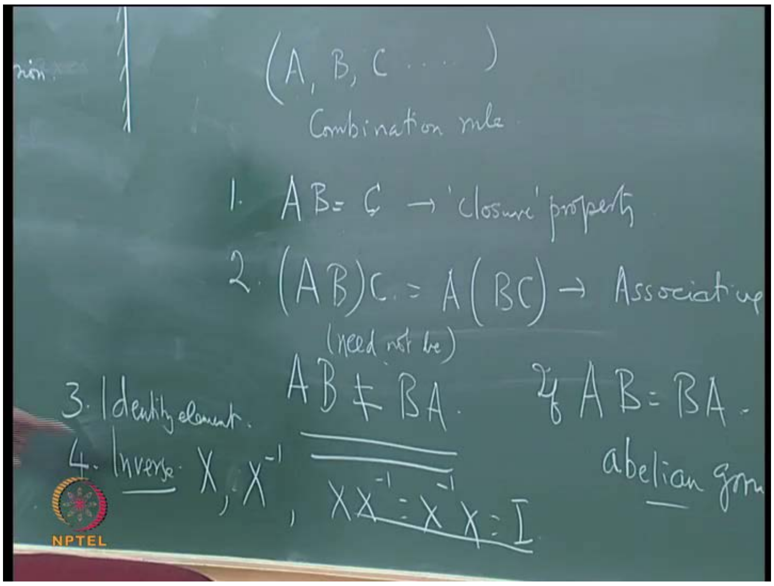

So, the identity should be necessarily an element of this collection.

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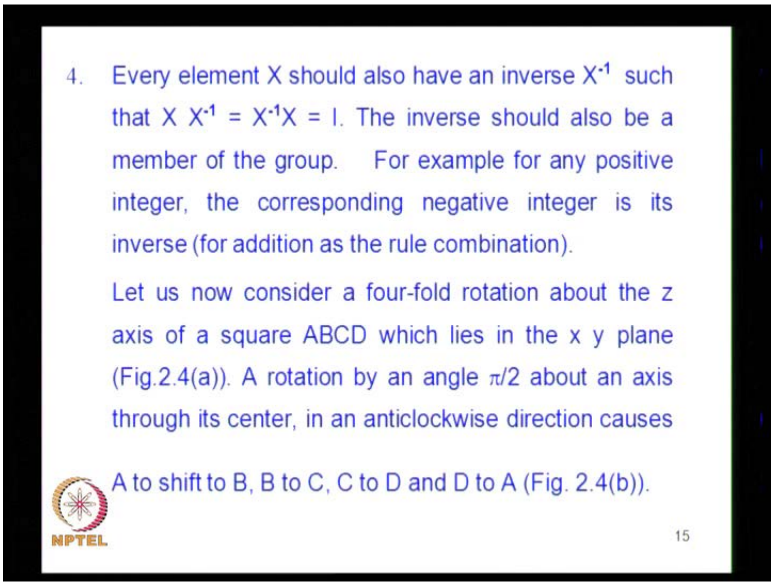

Then in addition, there is a fourth property which is known as the inverse of an element if you have an inverse; that means, suppose we have a general element x in this group of collection of element when you have also X to the power minus 1. So, that the x x inverse equals x inverse x equals i that is the definition of an inverse. So, the inverse of an any element should also be a member of the group, for example, if you have the collection of positive integers then the corresponding negative integer is the inverse of have given positive integers these also true these group postulates are satisfied by for example, here four fold axis. Let us see a fourfold rotation axis and see how the group requirements are satisfy in this case.

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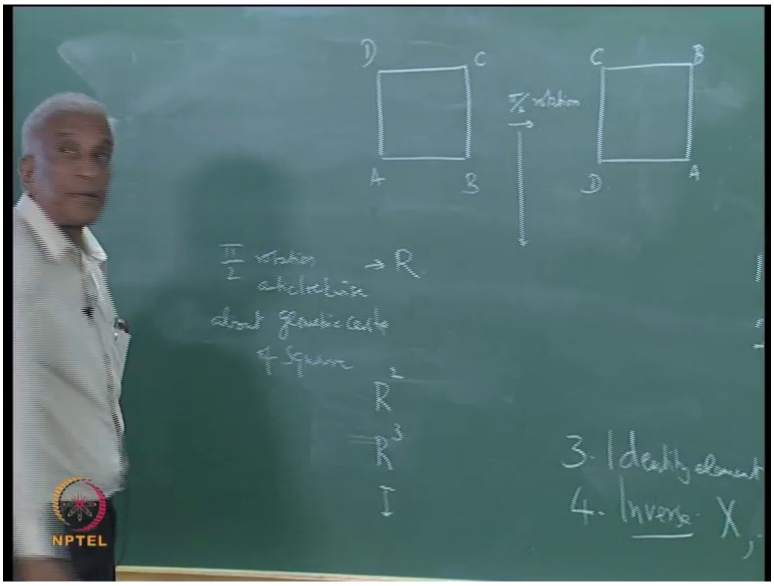

So, taking a fourfold axis i have the collection of elements.

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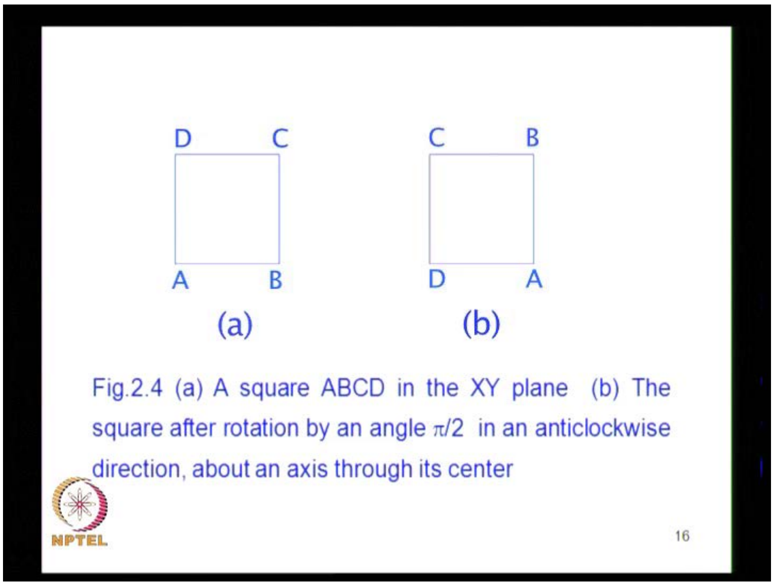

In this if I take a square like this I have ABC and D, a rotation by pi by 2, takes it pi by 2 rotation anticlockwise brings rotates the square and brings it a configuration. Where A goes here, B goes here, C goes here, and D goes if we did not have these later then these two are in destination.

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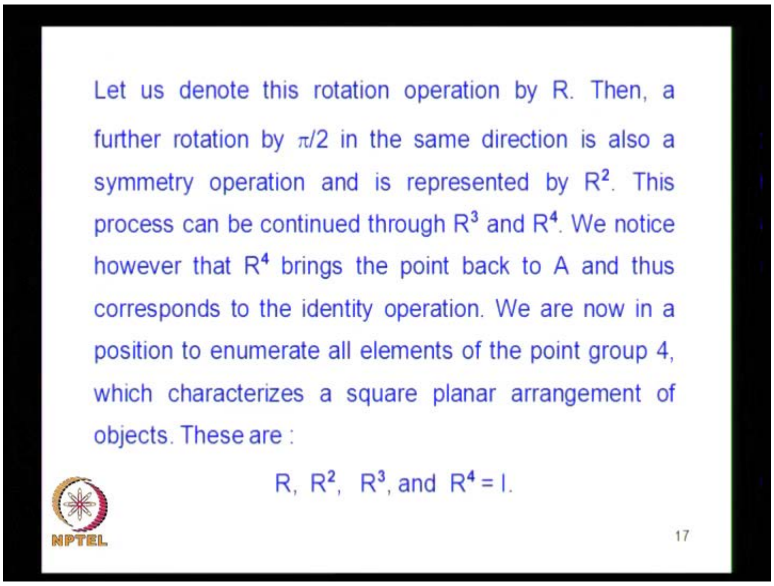

So, what happens let us see what happens to the group postulate. So, the various operation or associate. So, let the operations associated the this rotation a let us say this rotation by pi by two let us call it R is pi by 2 rotation anticlockwise about geometric centre of square suppose we call it R. Then if I rotate it subsequently by another pi by 2 it will again going to a self coincidence. So, that is no shown as r square a second rotation we can go further and make a third rotation by pi by two which we call r cube and then r for four brings it the to the original configuration I, call it I. So, these are the various R, R square, R cube and R to the power 4 equal to I. These are the symmetry elements are the element of this group which corresponds to a square the symmetry operations of a square.

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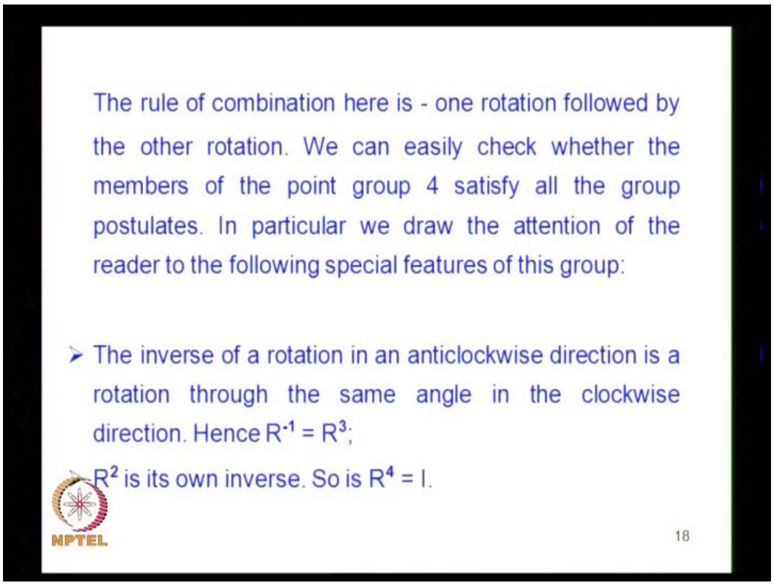

So, we can easily check that all these group postulate or satisfied in the case of these four elements, for example, the rotation by pi by 2 in an anticlockwise direction its inverse is a rotation by the same angle pi by 2 in a clockwise direction.

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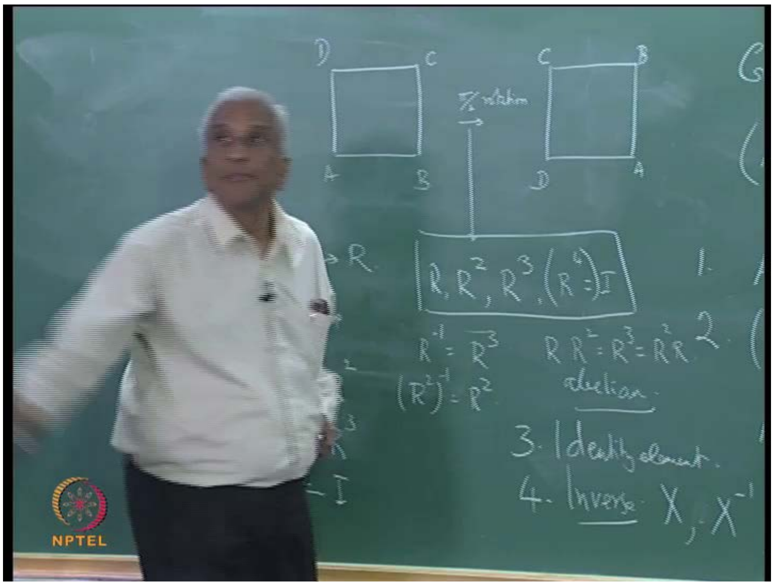

So, R inverse for equals R cube R square inverse equal to R square leg can easily verify these things. So, this is in all these cases we had the situation a b equal to b a R, R square is R cube which is also equal to R square R. So, which is an abelian group.

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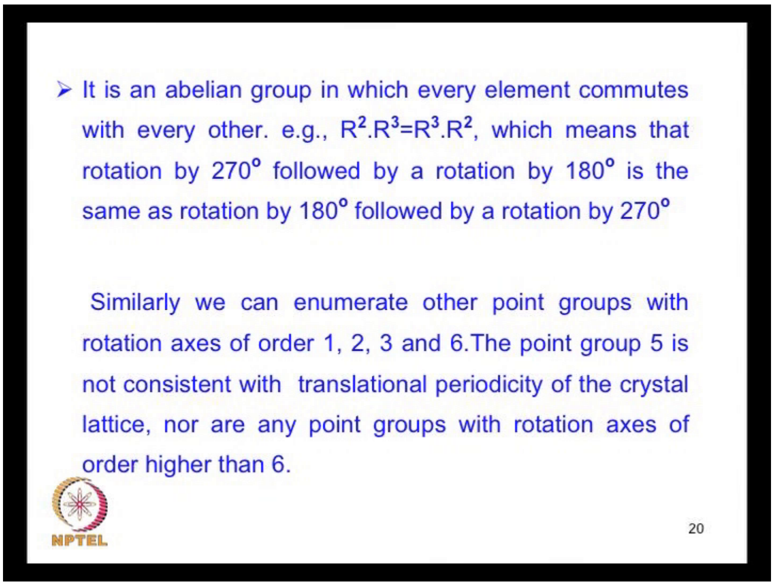

So, we can see that this is the point group corresponding to the four fold rotation axis acting on a square. We call it a cyclic group, because these elements are forming a set of elements which perform a cyclic set of operations to brings is back into a cycle the river original configuration.

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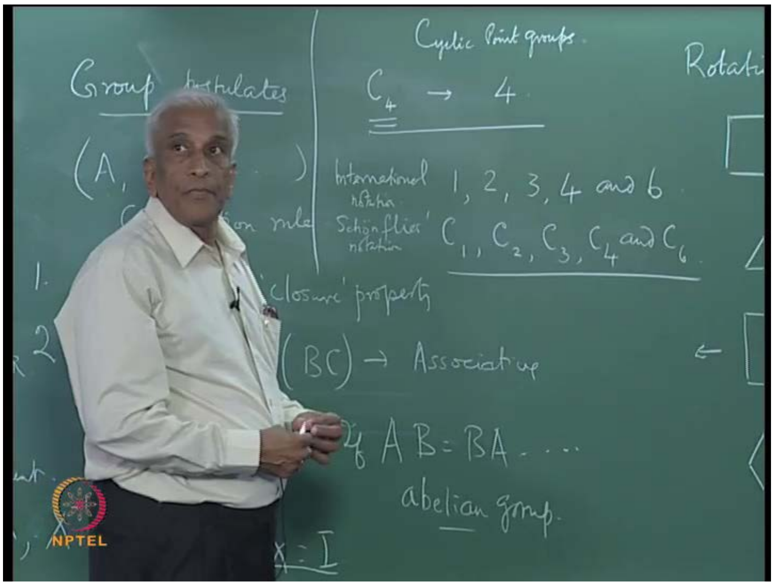

So, this symbol c means cyclic cyclic point groups and to say it is a fourfold rotation we call it c four we also can represented simply as four point group four. So, in this way, we can see that we have the point groups 1, 2, 3, 4 and 6, this can be written also as C 1, C 2, C 3, C 4, and C 6. These are two independent notations one is known as the international notation, this is known as the schon fliers notations the second notations schon fliers notation is usually preferred by spectroscopic whereas, the international notation is preferred by x ray. So, these are the five pure rotation point groups there are no point groups. The symmetry rotational symmetry higher than six and we already saw a fivefold rotation is not allowed because of translation symmetry.

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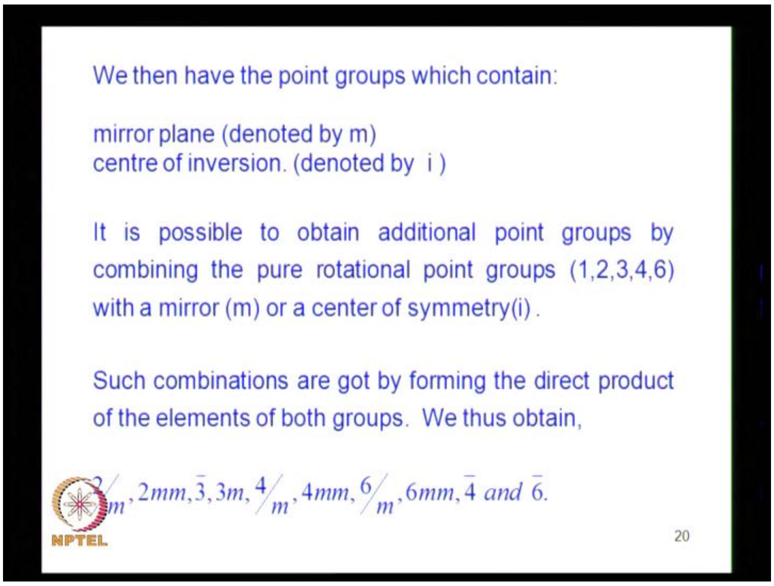

So, these are the five point groups which are the most basic points.

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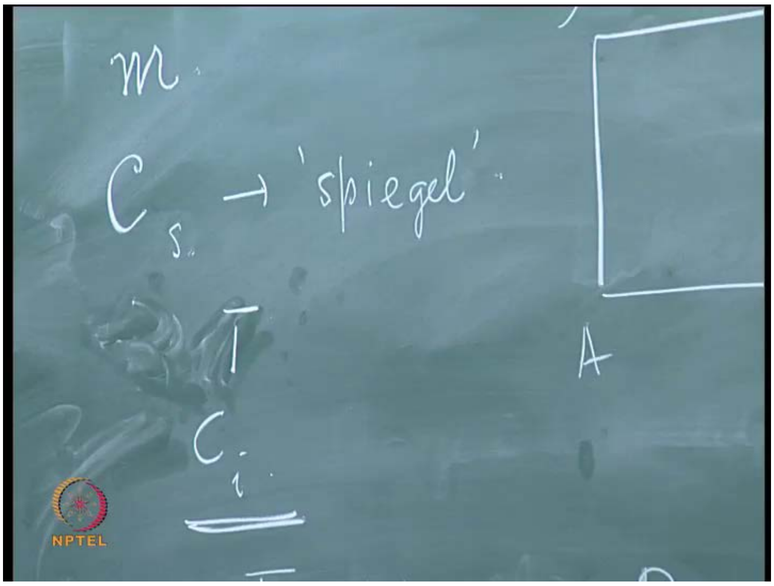

In addition, we have the plane of symmetry a mirror plane, which is shown as m for a mirror or it is also call it is also a cyclic group as you can easily check it is also called c s s being the letters for Spiegel the word Spiegel in German, which means a mirror. So, that is another point group which is cyclic which is also a sixth point groups in addition to these five and then you have an inversion which is shown as simply I or it is also shown as R, it is known as a one bar. So, a one fold axis with an inversion enter gives you this are this also reflects return as C i in shown an notation. So, the pure rotation axis mirror planes and symmetry have a symmetry a centre of symmetry constitute the cyclic point groups.

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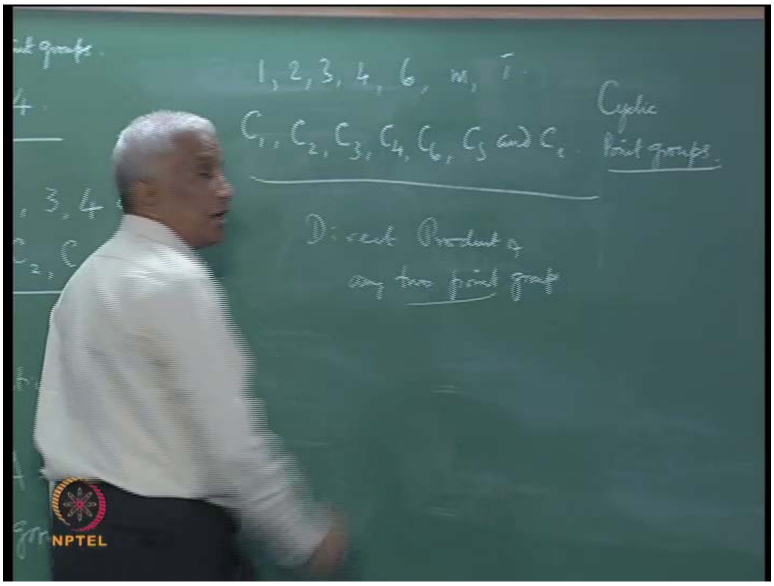

Which are which maybe represented as one, two, three, four, six m on bar or equivalently C 1, C 2, C 3, C 4, C 6, C s and C i, these are all the cyclic point groups. We said that there are thirty-two point groups of which now we have a numerated seven, how do you get an additional point group? Additional point groups are got by combining these various points. So, you can combine any two point groups in way to satisfy group postulate then you can derive new point group, what do we mean by combining point groups. Two groups can be combined the forming the so called the direct product of two groups of any two point groups leads to combinations of the different rotation axis among themselves. Or the rotational axis with a mirror symmetry or the rotational axis with a centre of inversion, all this would give rise to new point groups.

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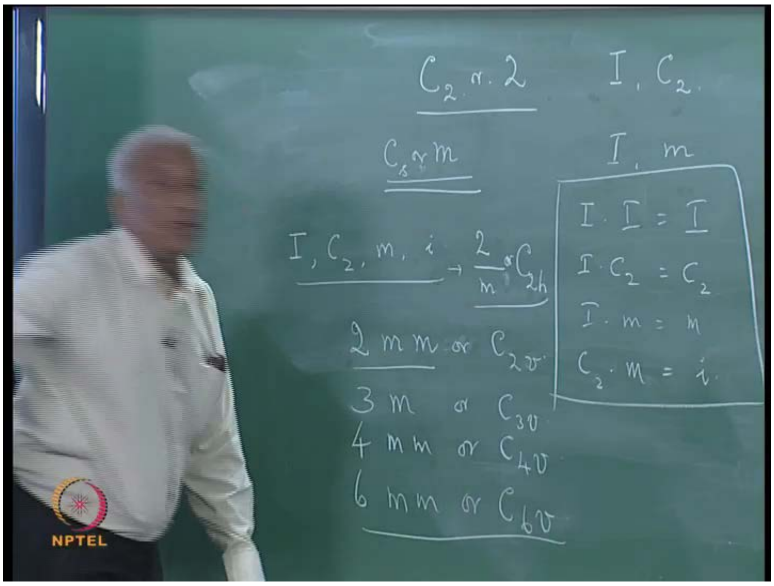

Let us see one example. Let us take a twofold rotation axis which gives rise to the point group known as c two are simply two let us take this how do you form the suppose we take a combine this with a mirror plane or c s suppose the combine these two points. So, what are the elements in this case c two i have the identity and then a c two axis c two square will be i. So, we do not have anything else and here in the case of a mirror we have the identity and a mirror if you repeat the mirror operation it comes back to identity. So, these are the two elements in a twofold point groups two and these are the two elements in the point group m.

So, suppose I form the direct product, direct product means combining the various elements together all the elements. So, I have the products like i into i which obviously, is i identity product of identity with identity and the identity itself. Similarly, identity into C 2 is the C 2 identity with m is m and then you have C 2 and the m. If you combine a twofold rotation axis with a mirror plane then you can easily verify that this leads to n inversion centre. So, these are the four elements derived by the direct direct product of these two. So, we have got a new group which as the elements i C 2 m i, i means the centre of inversion.

So, these four elements give rise to a new point group which is represented as two by m a twofold rotation axis with a mirror plane lying perpendicular to a which this combination leads to an inversion centre a automatically. So, this is a new point group it is also known as c two h the two fold axis is taken to lie along the vertical direction. So, that the mirror plane perpendicular to a is a horizontal mirror plane. So, C 2 h means a C 2 axis which is combined with the horizontal mirror plane. So, that is the schon flies rotation for two by m this is international notation similarly we can also combine a twofold axis with a vertical mirror plane vertical axis with a parallel mirror lying parallel in the same plane. So, that is a vertical mirror plane then you can see that the combination of these you can verify that this will give you rise to at seconds set of mirror plane which are like this.

So, you have two mirror planes. So, two vertical mirror planes which are parallel to the rotational axis. So, you write the m and next to the two fold axis and this is known also as c two v a vertical mirror. Similarly, we can have a threefold axis with a vertical mirror which is known as c three v a fourfold which is known as c four v and a six fold which is known as c six. So, these are the additional combination which we can obtained by combining the rotational and plane of symmetry now you can also combined the various rotation axis this kind of combination will give rise to a twofold axis combined with another two fold axis perpendicular to a will also lead to a third set of third two fold axis.

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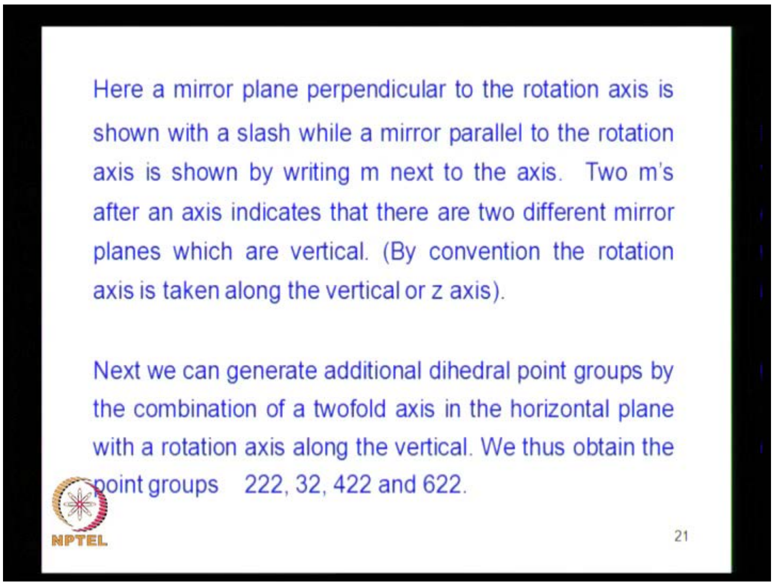

If you have one fold axis like that another like this in that will generate the third two fold axis perpendicular to so this is two to two.

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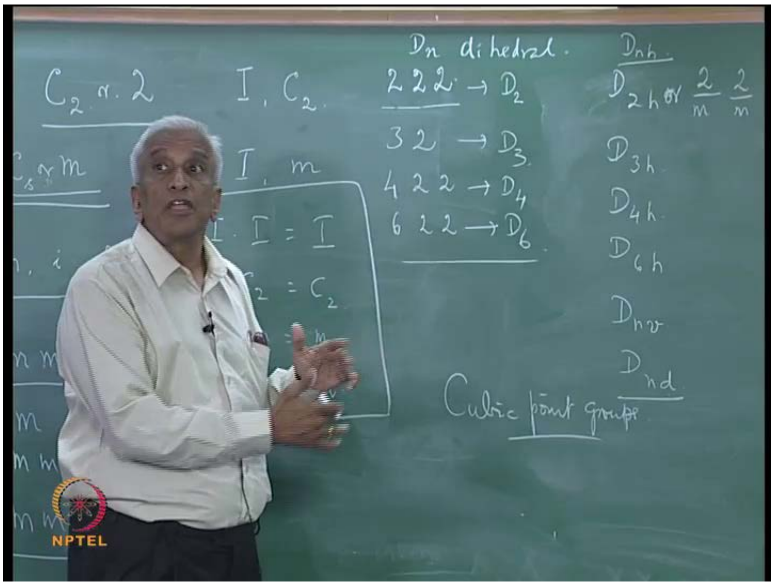

Similarly, you can have three two four to two and six two. So, you have dihedral axis. So, these are all known as the d n the dihedral point groups. So, this is known as D 2, D 3, D 4, D 6.

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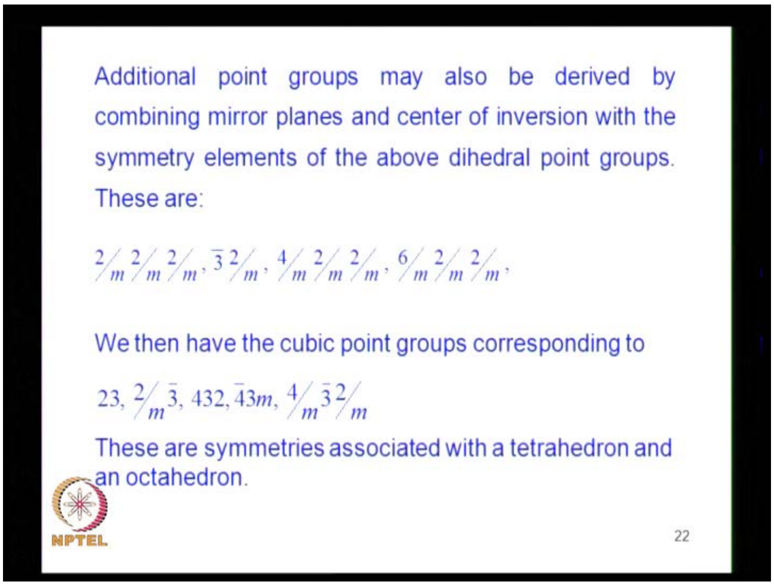

Additional point groups can now be obtained by combining these group dihedral groups with mirrors or inversion centre. So, we get in this way additional point groups which have the following nomenclature, you can add mirror planes lying perpendicular add mirror planes lying perpendicular to the principle rotation axis two fold axis here. So, You will get D 2 h where the mirror is perpendicular to the z axis the vertical axis therefore, it is a horizontal plane. So, this is also this is can also the written as this way. Similarly I can have D 3 h, D 4 h, D 6 h we can also have D n v, these are the D n h. We can also have D n v and we can also show that we can also add mirror diagonal mirror plane diagonal mirror plane, so it is called D n v.

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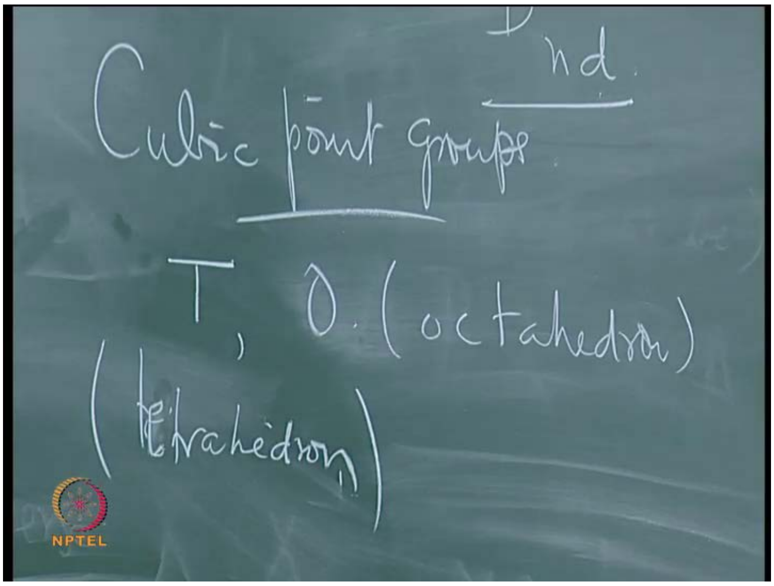

In addition to all these, we have so-called cubic point groups. Cubic point groups are symmetry are associated with the tetrahedron or an octahedron, both of which can be inscribed in a cube. So, it is known as a tetrahedral point group or an octahedron; T for tetrahedron and this is for octahedron. Tetrahedral and octahedral symmetry are implicit in a cube in cubic symmetry.

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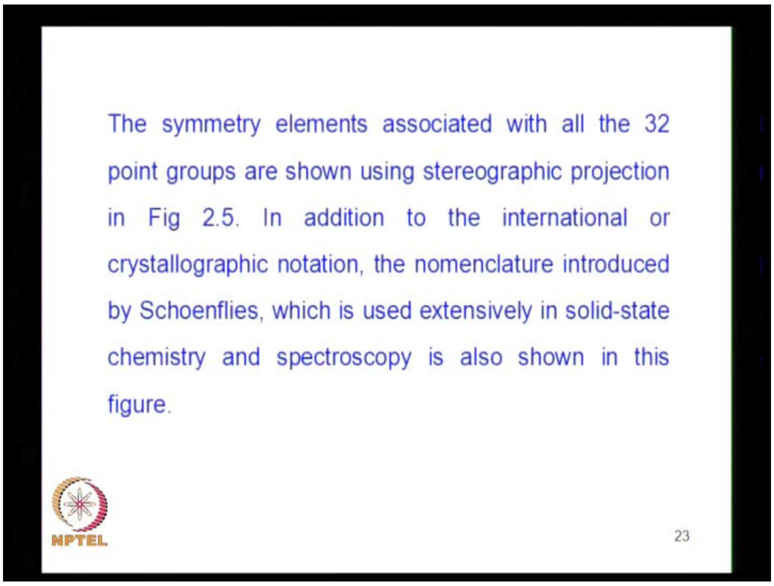

And you can also have additional symmetries like T h, O h by containing the elements of tetrahedral or octahedral symmetries with horizontal mirror plane or we can have other symmetry which we will see in related equation. Now these symmetry elements all together this gives you a thirty-two point groups.

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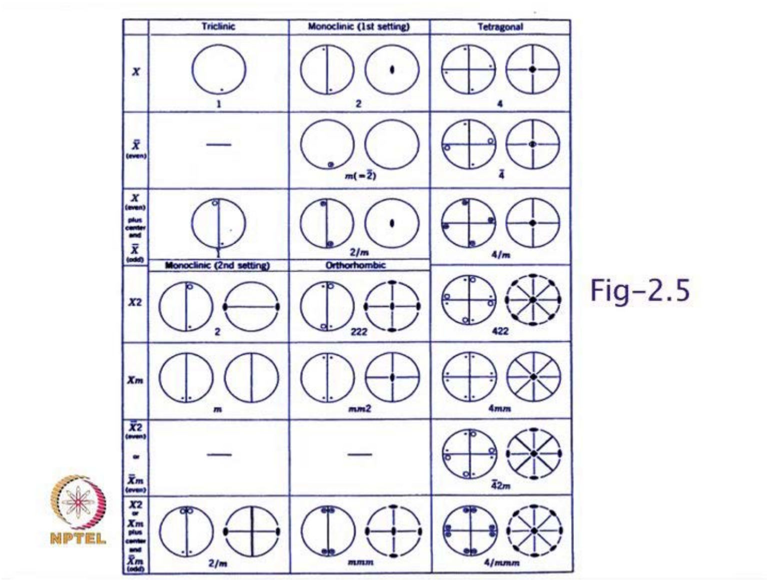

So, all these are shown in stereographic projection.