Crystals, Symmetry and Tensor

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Types of Symmetry Operation

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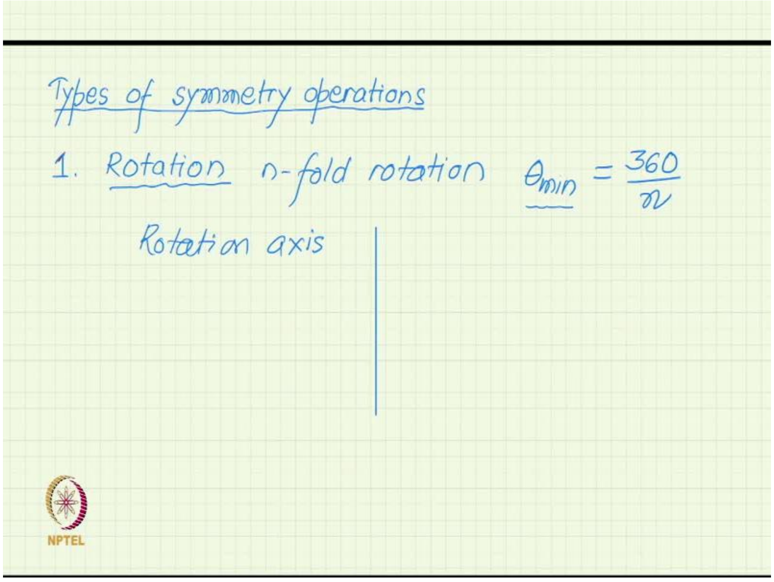

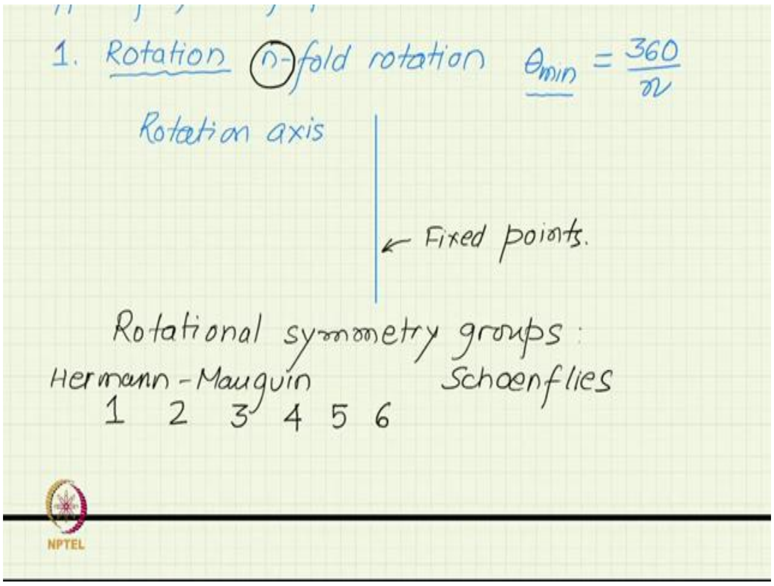

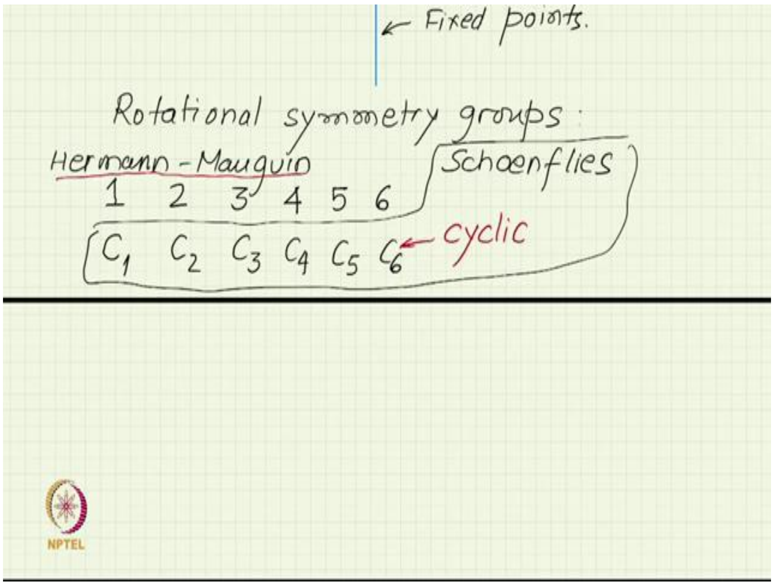

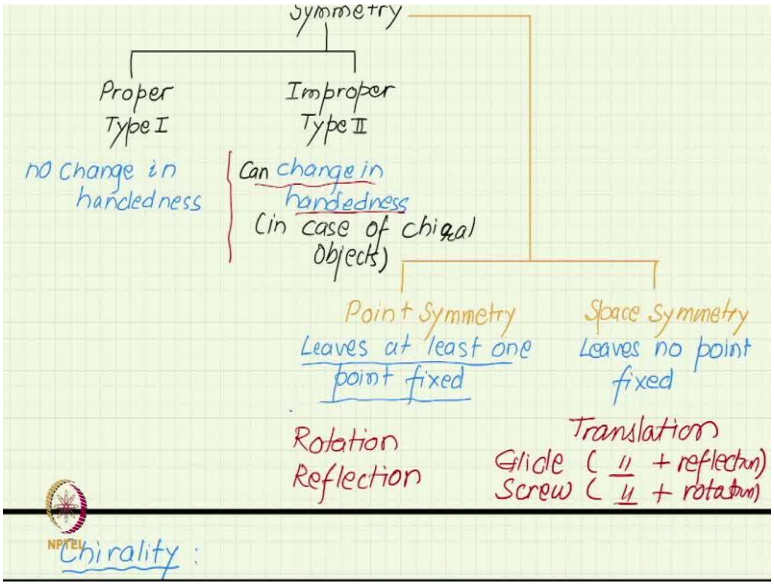

Let us now make a list make, a list of what are the possible symmetry operations can be there. So, we have already seen some of them. So, we have seen for example, rotation and we define the fold of rotation also n-fold rotation, which is defined by theta min is equal to 360 by n. So, when we say four-fold rotation theta min is 360 by 4 that is 90 degrees. So, minimum rotation by which it will come into self-coincidence is 90 degrees.

If that is the case, we call it that four-fold axis. Minimum is required, because see if it comes into coincidence by 90 degrees, 90 degree applied two times is 180 degrees and in 180-degree rotation also it will come into self-coincidence. So, square comes into self-coincidence by 180-degree rotation also. So, if you do not be a specific of theta min, but just theta, so you will say 360 by 2 is equal to 180 degrees. So, square has two-fold symmetry.

It does have two-fold symmetry but as a subgroup of four-fold symmetry. So, for actual description of its symmetry, we will say that it is has a four-fold symmetry rather than saying two-fold symmetry, because two-fold, it has two-fold symmetry but, it is not a complete description of its symmetry, because it has a higher symmetry. So, that is rotation and so that is so you have a rotation axis.

The point symmetry that leaves at least one point fixed so like rotation. So, rotation leaves the axis and change through rotation, the points on the axis are invariant, then reflection, points on the reflection plane are invariant, these points do not change after the flexion. But if you talk of a space symmetry, if you talk of translation, then all points move, for translation there is no fixed point. So, that is a space symmetry.

So, rotation is a point symmetry, reflection is a point symmetry, but translation is space symmetry. Similarly glide, we will come to that, that is translation plus reflection or we have a screw which is translation plus rotation. Since they have translation component these also will not leave any point unchanged in variants. So, all these are space symmetry operation. So, rotation since it is a point operation it leaves points fixed.

And we know that those point fixed are what is the called the rotation axis those are the fixed point. And in terms of we define groups, so when we say rotational symmetry groups, the symmetric group nomenclature there are two of them, one is the Herman Mauguin, I think we had discussed this and the other is Schoenflies. So, the Herman Mauguin notation is 1 2 3 4 5 6 just the number the fold, the n-fold is used as the representation of the group itself.

So n-fold rotation is actually a symmetry group of four-fold rotation is a symmetry group. And that symmetry group itself is represented by the letter 4. So, 4 takes a different meaning in this notation. It is not just the number 4, but it is the name for the symmetry group or four-fold rotation axis. So, and the corresponding Schoenflies symbols are just with C. If you write C with 1 as subscript, so C1, C2, C3, C4, C5 and C6 this becomes the Schoenflies notation.

So, and C stands for cyclic. So, Schoenflies tries to tell us that these are cyclic group cyclic group of order 1 cyclic group of order 2; whereas the Herman Mauguin notation it is you just have to know that it is cyclic and only the order is given.

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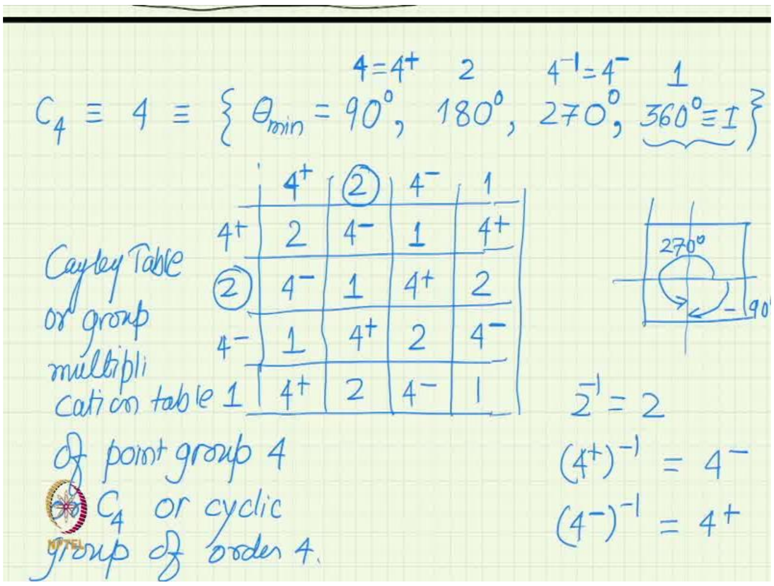

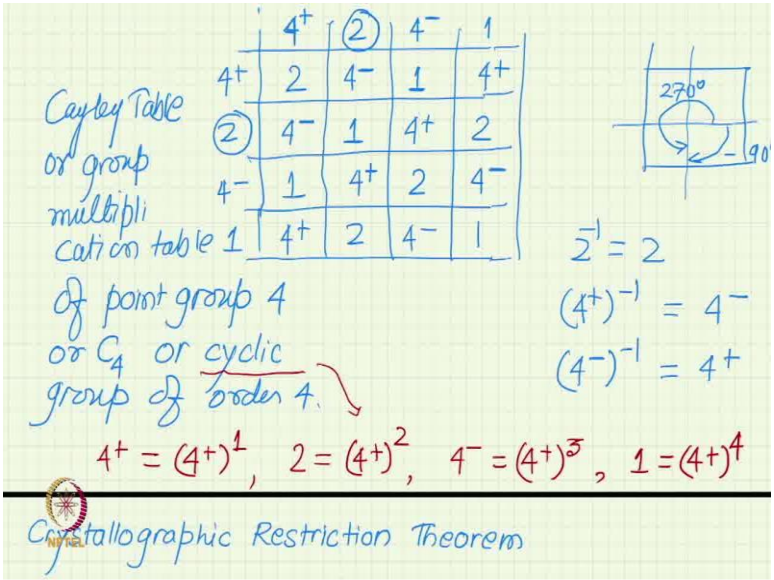

So, let us say C4 the Schoenflies notation. So, either you call it C4 or you call it 4 is actually a symmetry group of rotations and what are those rotations so you have you had theta min is equal to 90 degrees, but then 90 applied by two times 180 degree also should be in the group by the group property that combination of any two operations also has to be an operation. So, that is 180 degree.

Then 90 further applied is 270 degrees. So, that is also should be part of the group. So, instead of rotating by 90 degrees if you rotate by 270 degrees, still the square will come into self-coincidence. And finally, 360 degrees, but 360-degree rotation is equivalent to no rotation, because points come to the same place. So, this is what is the identity the operation of the group, every group should have an identity, you know that.

So, if you make the table the Cayley table or the group multiplication table, so you can write, you can use different symbols. So, for example, for 90 itself, so there is little so for little confusion can be there here, but context makes it clear. If I write for operation 4 as an operation, then it is showing as, it should be interpreted as a 90-degree rotation. So, I have 4 then since 180 degrees a two-fold rotation, I can call it 270-degree rotation.

But 270-degree rotation is equal to minus 90-degree rotation, you get to the same location. So, 270 is nothing but inverse of 4, 270 is inverse of 4 or sometimes you can call it 4 plus so you can call it 4 minus. And 360 degrees is identity we call it 1. So, let us call it 4 plus 2, 4 minus and 1. And here we have 4 plus 2, 4 minus and 1. I have gone a little bit unconventional here, usefully 1 starts with identity.

So, identity usually is the first element in the row, both the row and the column, but does not matter this will also work. And then you just multiply and get your table. So, two times 4 plus and 4 plus, 2 times 4 plus that is 90 plus 90 180. So, that becomes 2. 4 plus and 2 is 90 plus 180, 270, so that is 4 minus. And 4 plus and 4 minus plus 90 and minus 90 is an identity. So, they are the inverses and then 4 plus and 1 is 4 plus.

Similarly, you can complete the table so 2 and 4 plus it will be 4 minus 2, and 2 will be identity. 2 and 4 minus will be 4 plus and 2 and 1 will become 2. So, inverse of 2, 180-degree rotation is itself because 2 combined with 2 gives you the identity, so it is a self-inverse. So, you can say 2 inverse is equal to 2, 4 plus inverse is 4 minus and 4 minus inverse will become 4 plus. So, that group property that every element should have an inverse is being satisfied.

So, we you can complete this, so you will get 1 here, 4 minus and 2 will become 4 plus 4 minus and 4 minus will become 2 become 4 minus an identity, of course, we will leave everything unchanged. So, 4 plus 2, 4 minus and 1. So, that is the so called Cayley table. Why it is called cyclic group is that in this group, I have an element which in terms of which all other elements can be expressed as powers of that element.

So, 4 plus is 4 plus 2 the power 1 applied one times 2 is 4 plus a square 90 degree followed by 90 degrees 180 degree 4 minus is 4 plus cube, 90 plus 90 plus 90 is 270 which is 4 minus and 1 the identity itself is 4 plus is to the power 4. So, 4 plus is a element whose powers give you all other elements of the group. So, this is what is defined as a cyclic. A cyclic group is a group in which all elements can be expressed as powers of a single element.

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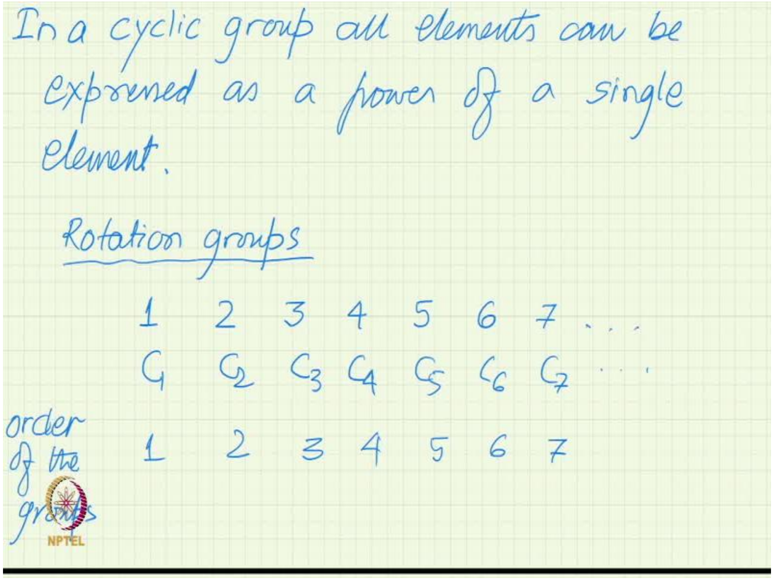

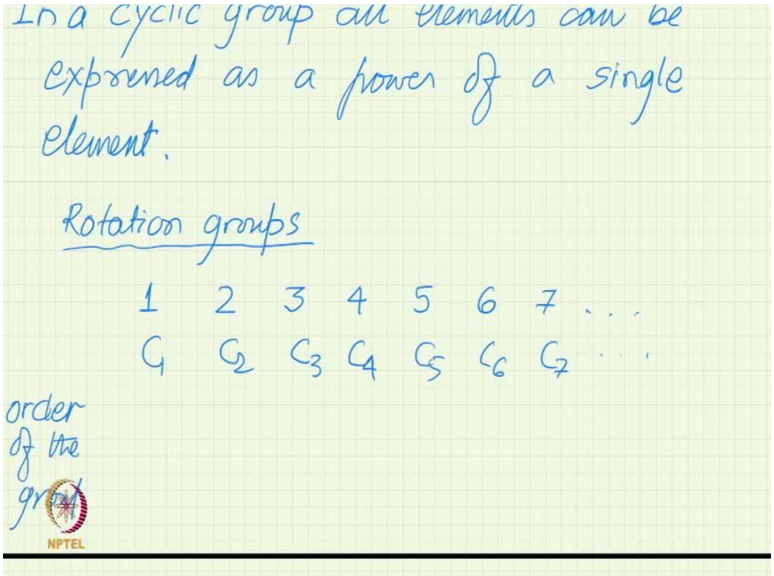

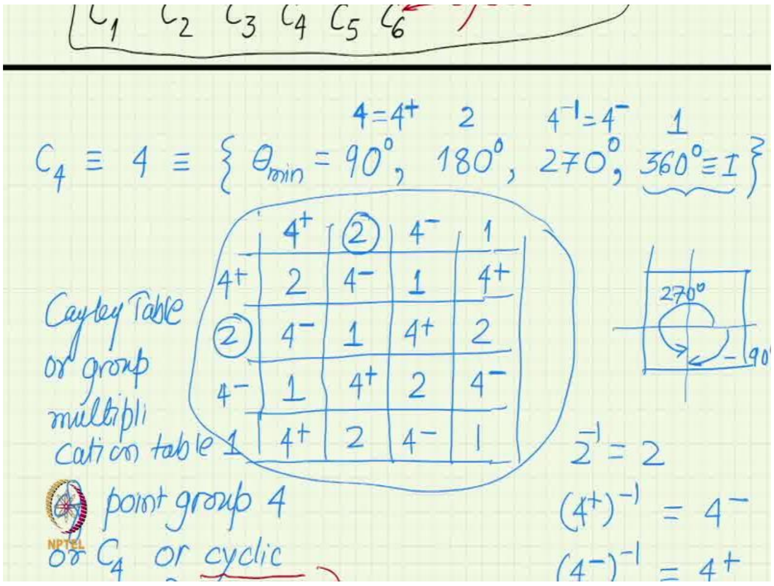

So, in rotation, this will always be true, but you will see we will see other groups where this will not always be true. So, all the rotations so the rotation groups the possible rotation groups are in finite, you can simply keep writing your integers all positive integers correspond to rotation and group. And the order of the group is the number of elements in the group so that is also the same as the integer.

So, how many rotations the group 4 had, the 4 rotations, 4 plus 2, 4 minus and 1 or 90 180 270 and 360 if you saw this. So, that is the order, so ordered is the same number. So, Harman Mauguin notation of these groups are just the order of the group, the subscript in Schoenflies is again the order of the group.

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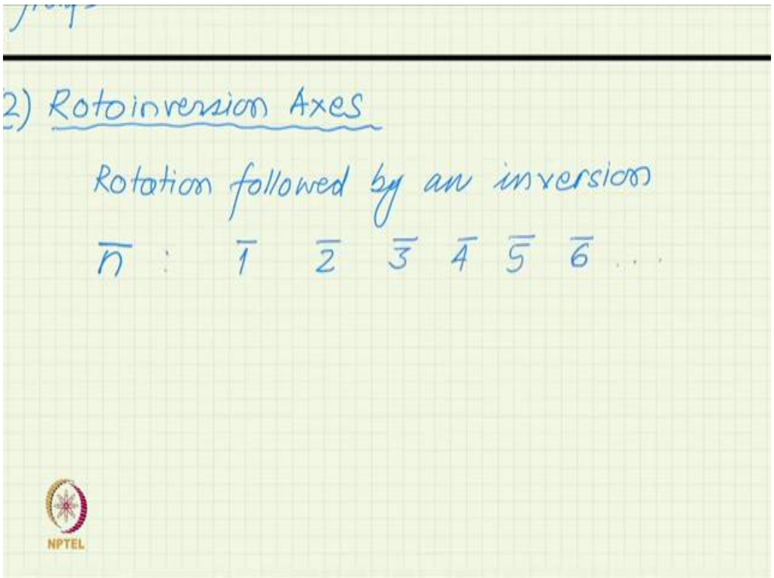

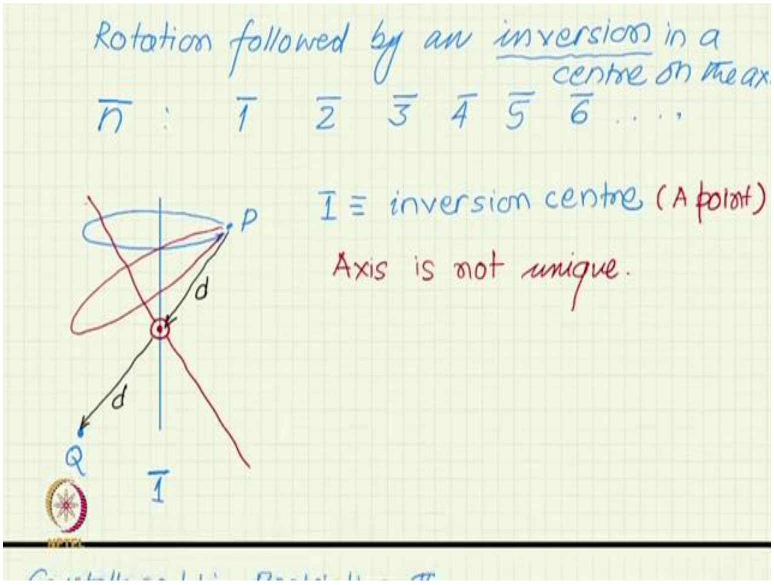

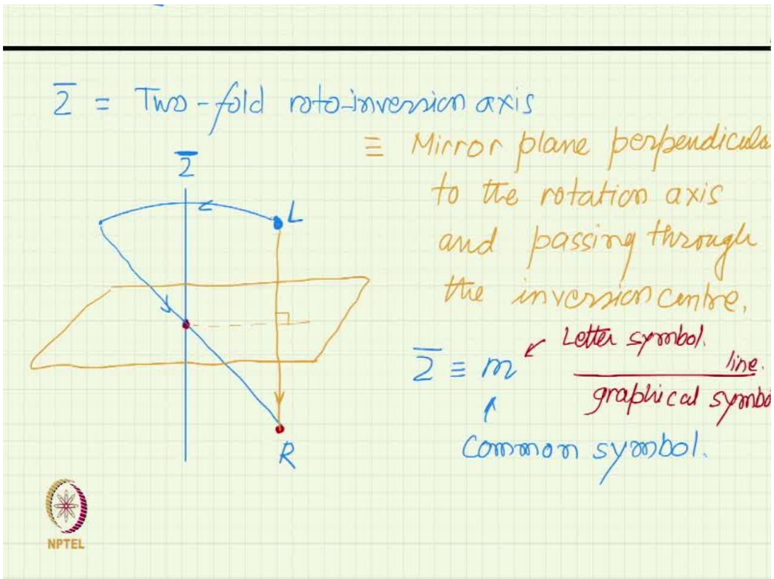

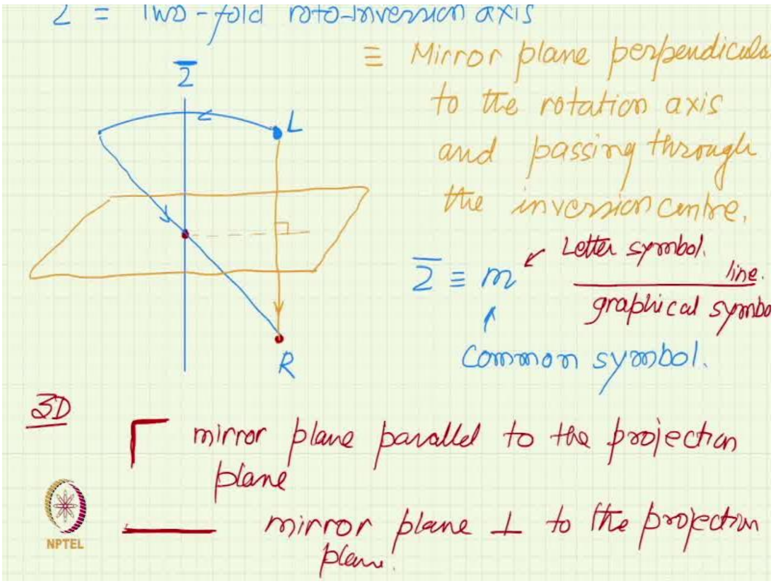

We can have roto-inversion, the second type is roto-inversion axes. So, in the roto-inversion axes rotation followed by an inversion. Then notation here is n bar 1 bar 6 bar. So, n-fold rotation axis always indicates rotation by a minimum angle, n-fold roto-inversion axis will indicate rotation by that same minimum angle, but you do not have to stop there it is followed by an inversion process.

So, let us look at the one fold rotation roto-inversion axis 1 bar, so if I have this as the 1 bar axis and if I have a point, then by how much I have to rotate, 1 bar axis means rotation by a complete 360 degrees, which is equivalent to no rotation. So, I come there itself and followed by an inversion, inversion requires a center, inversion requires a center on the axis. So, I have to identify a point also on the axis then only it will become a roto-inversion axis otherwise it will remain a rotation axis.

So, a roto-inversion axis has an axis with a point. Now, if I rotate this blue point by 360 degrees and then invert it into this red inversion point, inversion means taking the point to the inversion center and going in the opposite direction or continuing, sorry, continuing in the same direction by same distance. So, if this was a distance d, this is further distance d and then this point, the point which is generated is the image point.

So, this is the original point P, this is the image point Q. So, this is called, this operation is called inversion. So, since 360-degree rotation was an identity, so if that did not do anything, so just for the namesake we said that rotate by 360 degrees. If we would not have said rotate by 360 degrees and said just invert into the point, invert in the red point. So, I would have still got from P to Q.

So, the operation is equivalent to 1 bar is just is equivalent to an inverse in center. And rotation axis is superfluous here because that actually plays no role. Because even if you would have taken some other axis, let us say some other axis, and rotated 360 degrees about that axis, again you will come to P. So which axis you are rotating about is really not important. So, it is not really an axis it is just a point.

So, 1 bar axis is really an inversion center. It is just a point. So, we will use the designation 1 bar, but we will always, we will not draw it as an axis because drawing the axis edge superfluous and we will always draw it as a point. Although we may call it a 1 bar axis. Two-fold roto-inversion axis is also interesting. Now, consider a point, since this is a 2 bar axis, so its axis and there is a center, there is a center.

And you now rotate by, since it is a two-fold you rotate by 180 degree and after rotation you invert, so just like a rotation does not change the handedness, but inversion changes handedness, inversion is type 2. So, of course, a point does not have an handedness, but you can think of that there was a left handed object there. So, after inversion it will get converted into a right handed object there. Can you think of any other relation between this L and R?

So, instead of doing all that operation, if you would have done just, take from the, start from this L and reflect in a mirror plane which is perpendicular to the axis and passing through the center you will get the same phenomenon, exactly the same point and same handedness change also. So, a left handed object goes to right handed object by mirror plane. So, two-fold roto-inversion in axis is nothing but a mirror plane passing through the inversion center.

So 2 bar is usually be written as m, we will usually not write it as 2 bar. So, the common symbol is m, if you write it as 2 bar, nobody can say that you are wrong, but since it is equivalent to mirror and mirror is easier to imagine, so this is the common symbol. And common symbol in diagrams, in 2d diagrams is a line, graphical symbol.

Graphical symbol is line, letter symbol is m or written symbol. You can say written symbolism is m, m graphical symbol is a line. In 3d, there is some difficulty that because it is a plane, so it is not a line. So, but in usefully in 3d, we will have the orthographic projections. So, in orthographic projections, either our mirror plane will be parallel to the projection plane in which case you show it like this.

So, in the corner, in the corner of your projection in international table you will see sometimes something drawn like this. Then you know that the projection plane is a mirror plane. And if in the projection you are seeing a line like this, then you know that a mirror plane perpendicular to the projection plane.

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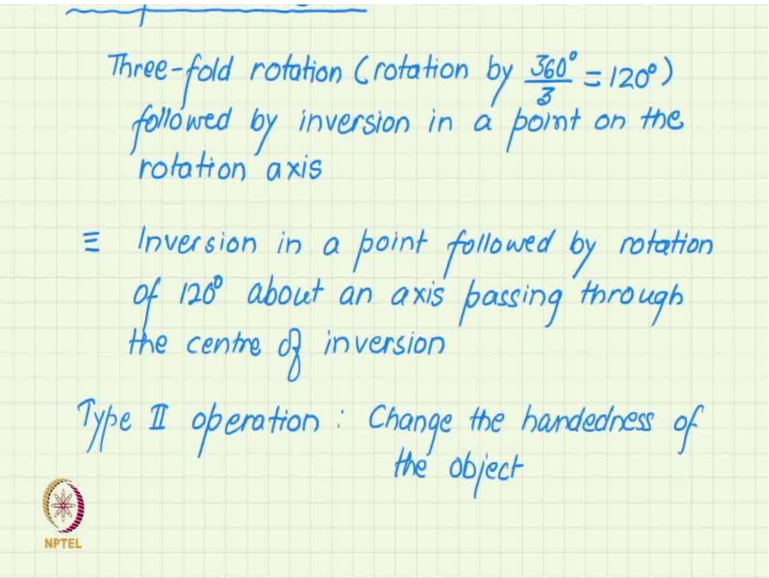

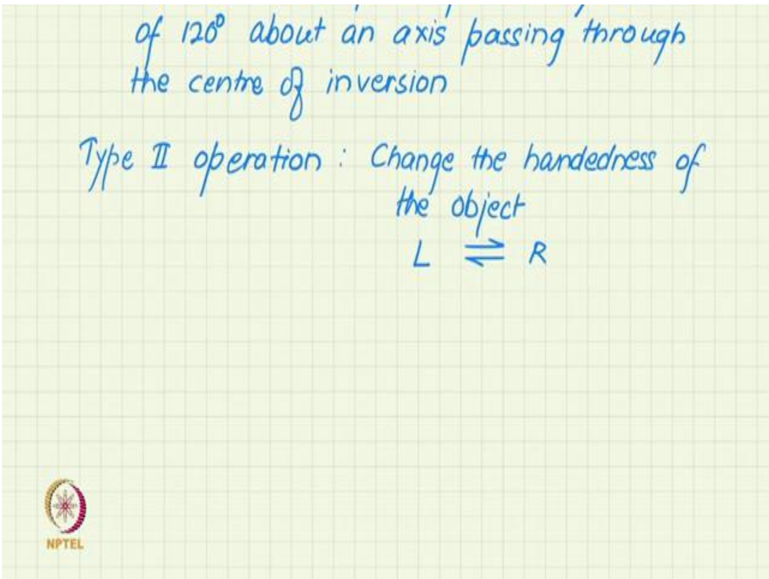

So, let us discuss three fold roto-inversion. As the name suggests this is a three-fold rotation. Three-fold rotation means rotation by 360 degree by 3 equal to 120 degrees. So, a rotation of 120 degree followed by inversion in a point on the rotation axis. The two operations, the three-fold rotation and the inversion are commutative. So, they can be inverted also. So, this process is also equivalent.

If we do inversion first, so we can say inversion in a point followed by a rotation of 120 degrees about an axis passing through the center of inversion. So, the two process is equivalent, whether we do the inverse in first followed by rotation or rotation first followed by inversion. Also you can see that this is a type 2. This is a type 2 operation which means that it will change the handedness of the object and this is because rotation does not change the handedness, but when inversion is done handedness change.

So, a left handed object will become a right handed object and vice versa a right handed object will become a left handed object. So, let us look at this process stereographically.

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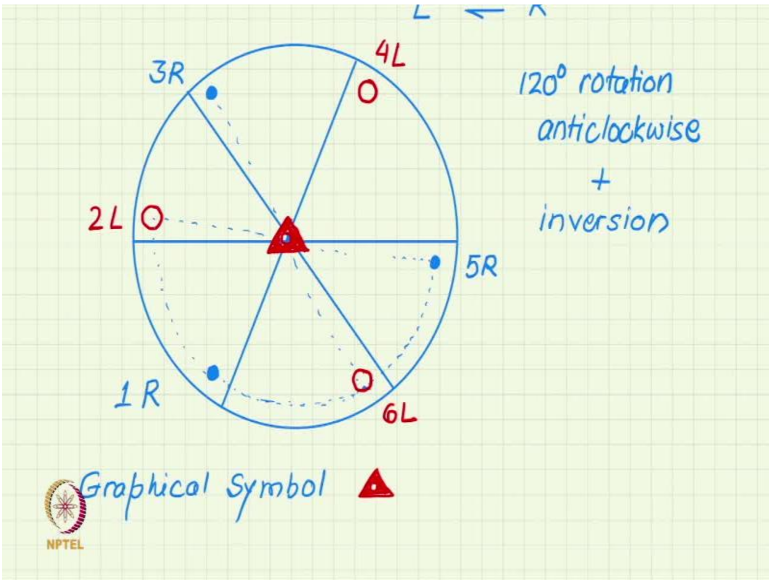

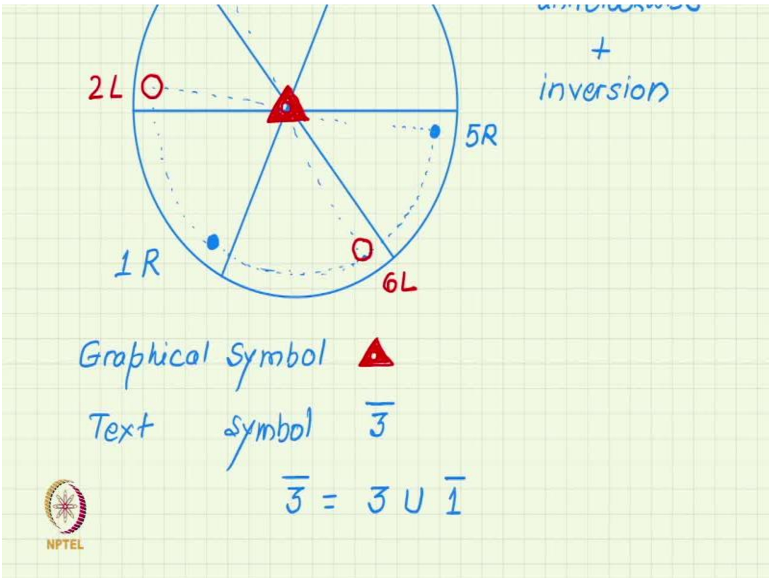

So we draw a primitive circle and let me draw the three reference lines at 60 degrees so as to guide me in my rotation. And start with an object with a say a left handed object let me draw a left handed object in blue and I am using a point or a closed circle to represent an object, a right handed object above the plane, above the equatorial plane.

So, this is the right handed object and this is the first pages and the starting position, so let me call this 1R. Now, the first operation which I have to apply is 120-degree rotation and of course, we have to be concerned about the sense of rotation also, and positive sense is anti-clockwise. So, let me take it 120 degrees anti-clockwise rotation that 60 and that 120.

So, the object reaches there, remains right handed at the moment, but I have not completed the three-fold roto-inversion operation because this has to be followed by inversion. And here we are considering the inversion in the origin and we are assuming the inversion in the rotation axis to be vertical that is in the stereogram, the rotation axis is at the center.

So, this is an intermediate stage in the journey, 120-degree rotation, after this I will invert it in the origin, so it will go there after inversion and since it was above the plane, now it goes below the plane and since it was right handed by inversion it will become left handed. So, to show left handed I use the red color and to show that it is now below the plane, I am using an open circle. So, this is the second position and I now have a left handed object sitting there.

So, this is one operation of a three-fold roto-inversion. If I apply this roto-inversion again. So, you can see, I again come 120 degrees, so I come somewhere there, and then I invert, so I go there, and I started with a left handed object, inversion again changes it, so it becomes a right handed object, so I again use the blue color. And from below the plain inversion will bring it above the plane. So, the next position 3R there. So, now you have got an idea.

So, as I operate again then 4L will come there, 5R will be there, 6L will be there and finally, you will come back to 1R. So, that will complete the operation. About the axis there is a graphical symbol for three-fold roto-inversion. And so let me place that at the center of the stereogram, the graphical symbol is a triangle, a filled triangle, but with a hole left in the center. So, I filled the triangle except the central hole.

So that is the graphical symbol of the three-fold roto-inversion axis, a triangle with a hole. So, the hole actually, why this symbol is being used, the hole in the center of the triangle, triangle shows the three-fold axes. So, you can see everything is related by the three-fold axis also, so the three-fold roto-inversion axis includes three-fold axis as its subset or subgroup.

So, you can see the three blue points above the plane are at 120 degrees, so they satisfy the three-fold symmetry and the three red points below the plane are also satisfying the three-fold symmetry. So, it has three-fold symmetry as its subgroup. And hole in the center shows an inversion center, represents the inversion center. So, you can see that all points are related to each other by a center of inversion also.

So, for example, if I take 1R point and invert it in the origin, I will get 4L. From right handed it will become left handed. So, from blue it becomes red, from above the plane it goes below the plane. So, these two points 1R and 4L are related by a center of inversion. Similarly, 2L and 5R are related by center of inversion and 3R and 6L are related by center of inversion.

So, the 3 bar axis, I can show another symbol, the text symbol for this is, the text symbol is 3 bar. Let me write it, like a graphical symbol we have a text symbol, 3 bar and what I showed you that 3 bar is nothing but a union of or a combination of a three-fold axis and a center of inversion, which I represented by 1 bar.

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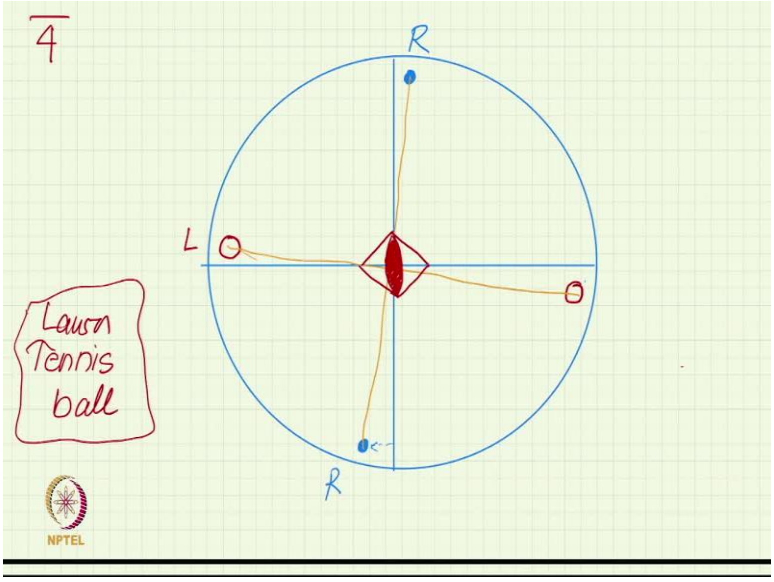

Now, you have got you should have got a hang of it. So, four-fold roto-inversion you should not have any problem, 4 bar is now easy start from a general point there. So, these blue lines are not symmetry lines, these are just reference lines for me to help me rotate. So, since this was left of this line, a 90-degree rotation brings it here, inversion will bring it there.

But take it down and change the handedness, change of handedness read, going down circle, open circle. Then again a 90-degree rotation and inversion from down comes back on top, changes handedness again, so becomes blue. So, both blue are right and both red are left. So, then the next two you will get the red here.

So, you can see that these two lines, these two lines will be 90 degree apart, so just like in the three-fold roto-inversion, you had three points and three points and twisted. In four-fold roto-inversion, you have only two points and a two points 90 degree twisted but vertically downwards. So that is a four-fold roto-inversion. 4 bar and the symbol for 4 bar is you can see that the two blue points satisfies two-fold rotations.

Two red points also satisfied two-fold rotation. So, if you just do not think of four-fold roto-inversion, you will think that it is a two-fold axis. So, two-fold is part of a four-fold roto-inversion. So, the symbol also is made like that, that what you do is draw a square, square was for four-fold. So, you draw a square, but inside a square you draw a lens for two fold.

That since it is a two-fold is complete, but the four fold is not. It is a four-fold roto-inversion, but two fold is subgroup of that, so the symbol becomes this. Square with a lens inside diagonal, a square with a diagonal lens inside and the lens filled. So, that is the symbol for four-fold roto inverse. If you an object which has the symmetry is a tennis ball, lawn tennis ball, lawn tennis ball with its lines marked on it.

If you try to see with the lines marked on it, it will have a… no other object comes to my mind which will have the symmetry, means familiar object, but crystals of course have such axes as part of atomic arrangement. Thank you.