3D Space Groups IV: Screws Axes and Screw Operations
Professor: Rajesh Prasad
Department of Materials and Engineering
Indian Institute of Technology Delhi
Lecture 22 d

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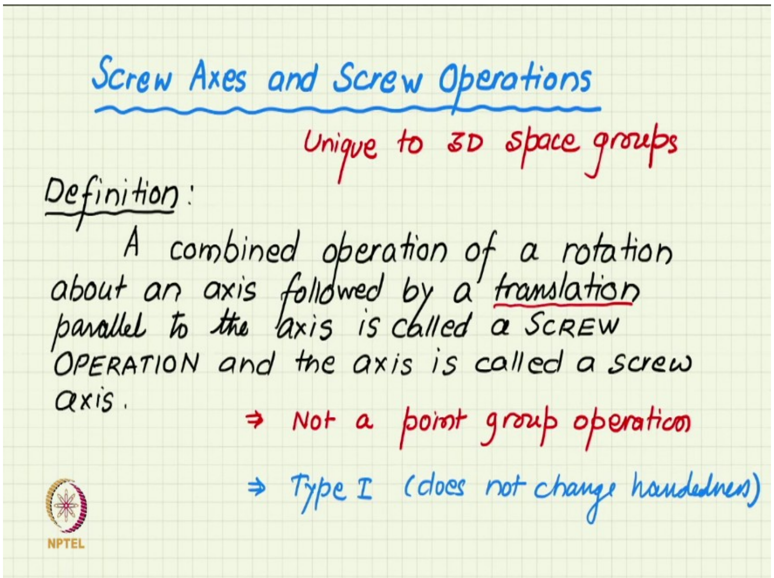

Let us discuss a Screw Axes and a Screw Operations, these are unique operations in 3D, by that I mean that they are in the 3D space groups. So, let me write that unique to 3D space groups, because they are not in they do not exist in 2 dimensions, they exist in 3 dimensions and even in 3 dimensions, they were not part of the point group. And that is because they involve a translation component.

So, here is the definition that are combined operation of a rotation about an axis followed by a translation parallel to the axis is called a screw operation and the axis is called a screw axis. So, because of the translation, it cannot be a point operations operation and since both may translation and rotation are type one, this is also a type one operation it will not change handedness.

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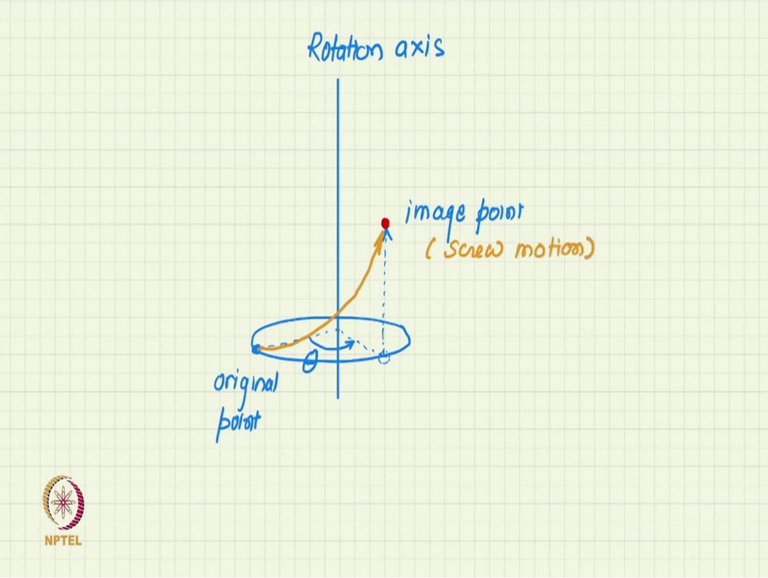

So, let us see this geometrically. So we have a, we have a rotation axis. And let me consider a point in a plane perpendicular to the rotation axis. So, when we talk of his crew motion, I will first rotate this by some angle theta. So, we will get a point here, but that is not the image point. That is an intermediate reference point, because I have to combine it with the translation. So, I further combine it with a translation. So, this will be the final image point. So, this is the original point this is the image point.

So, the imaging process you can see imaging process can be thought of as a screw motion, because its rotation as well as translation, it is a result of screw motion.

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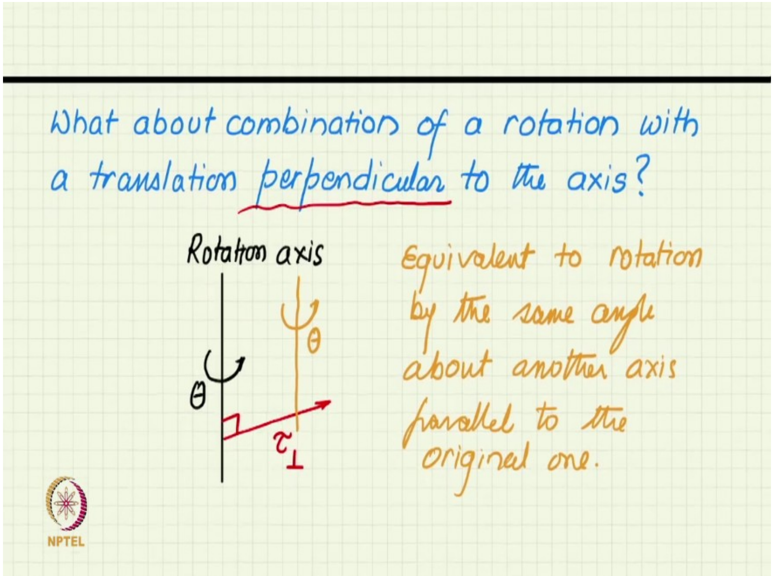

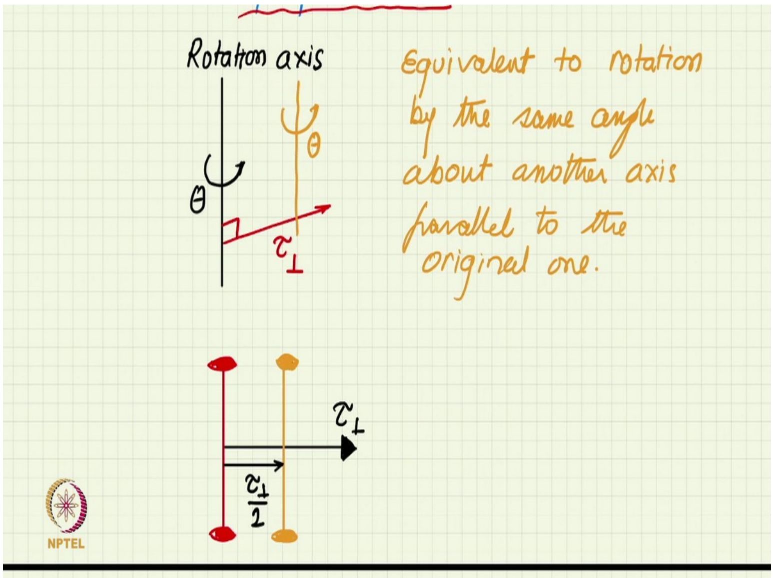

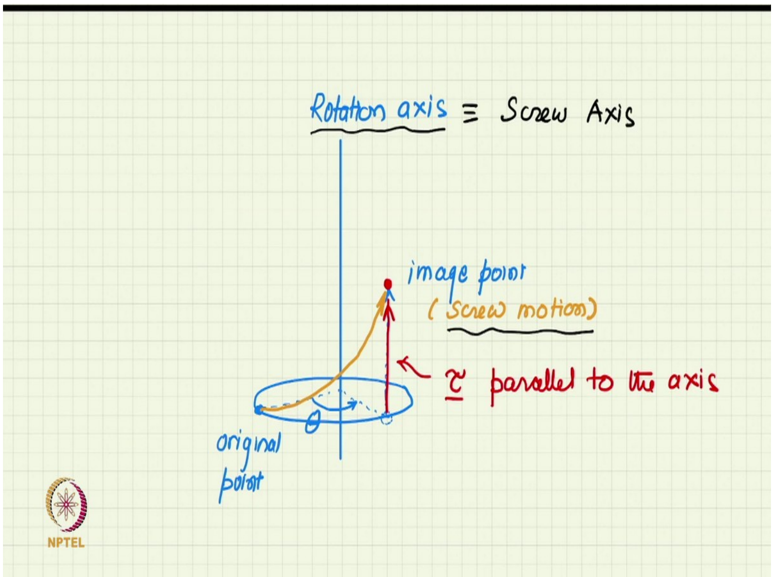

Now, why are we thinking of combination of rotation with translation, this translation component here this translation component was parallel it is the translation tau parallel to the axis. So, why are we insisting on parallel, why not perpendicular? Can we not combine a rotation operation with a translation perpendicular to the axis in fact we can and in a space group this kind of combination is always possible? However, here if we have a rotation axis and we combine it with a translation, which is perpendicular to the axis this will result in this will result in a rotation by the same angle.

So, if there was a rotation by theta about this, this will result in rotation by the same angle theta about another axis parallel to the given axis. So, another axis one can imagine and which will be parallel to the given axis and the same angle theta will be there. So, this is equivalent to rotation by the same angle about another axis parallel to the original one. So, in this sense it is not really a new kind of operation, but just a new rotation about a different axis, we can see this as I will not prove this, but let me just give an example the simplest possible example, which we are already familiar with in our discussion with plain groups.

So, let me consider a 2-fold axis a 2-fold axis. So, if we have a 2-fold axis in a space and I combine it with a translation which is perpendicular to the 2-fold access then, we know in plain groups we have seen this and it will also be true for a space group, that this results in. So, this is a translation let us say this translation is tau perpendicular. So, this will result in another 2 fold which is parallel to the original one but shifted to it by a vector t by 2, t perpendicular by 2.

So, we are familiar with this case and this will always be the case it will not always occur at t perpendicular by 2, but somewhere in space which can be calculated on the basis of the translation vector, there will be another axis about which same rotation is possible. So, that is why this case is not considered a special is not given any special name, it is just combination of 2 operations resulting in another operation, but this particular case is a new case for 3 dimensions and is given name is screw rotation, the screw motion or a screw rotation and the rotation axis is called the screw axis, where the translation is parallel to the axis.

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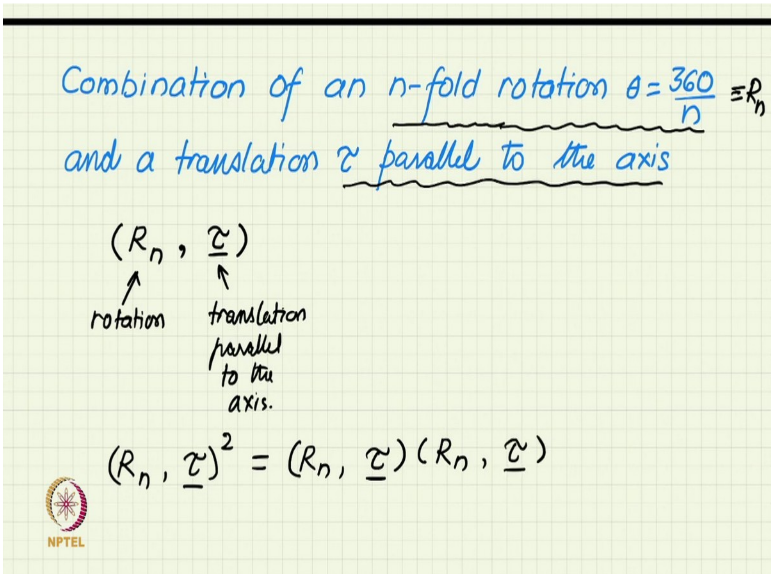

combination of an n fold rotation $\theta = \frac{360}{n} = R_n$

and a translation τ parallel to the axis

$(R_n, \underline{\tau})$ — Intrinsic translation associated with screw operation $\equiv$ pitch

R_n: rotation

$\underline{\tau}$: translation parallel to the axis.

$$(R_n, \underline{\tau})^2 = (R_n, \underline{\tau})(R_n, \underline{\tau})$$
$$= (R_n R_n, R_n \underline{\tau} + \underline{\tau})$$
$$= (R_n^2, \tau + \underline{\tau})$$
$$= (R_n^2, 2\tau)$$

$$(R_n, \underline{\tau})^3 = (R_n, \underline{\tau})(R_n, \underline{\tau})^2$$
$$= (R_n, \underline{\tau})(R_n^2, 2\underline{\tau})$$
$$= (R_n^3, R_n(2\underline{\tau}) + \underline{\tau})$$
$$= (R_n^3, 2\underline{\tau} + \tau)$$
$$= (R_n^3, 3\tau)$$

$R_n \quad \frac{360}{n}$

$$(R_n, \tau)^n = (R_n^n, n\tau)$$
$$= (1, n\tau)$$

$$= (R_n^3, R_n(2\underline{\tau}) + \underline{\tau})$$
$$= (R_n^3, 2\underline{\tau} + \tau)$$
$$= (R_n^3, 3\tau)$$

$R_n \quad \frac{360}{n}$

$$\underbrace{(R_n, \tau)^n}_{\text{Symmetry operation}} = (R_n^n, n\tau)$$
$$= \underbrace{(1, n\tau)}_{\text{Symmetry translation}}$$

$\equiv$ Lattice translation

$n \times$ pitch $=$ A Lattice translation parallel to the axis $(\underline{T})$

$n\underline{\tau} = \underline{T} = p \times \underline{T}^{min}$

integer; $\underline{T}^{min}$ = shortest lattice translation $\parallel$ to the axis

$n\underline{\tau} = p\, \underline{T}^{min}$

$\Rightarrow \boxed{\underline{\tau} = \left(\frac{p}{n}\right) \underline{T}^{min}}$ direction of screw

$\boxed{0 < p < n}$

If $p = 0 \Rightarrow \underline{\tau} = 0 \Rightarrow$ No translation

$\Rightarrow$ Proper rotation axis

If $p = n$

$\underline{\tau} = \underline{T}^{min} \Rightarrow$ Simpliy a combination of symmetry rotation and Lattice trans.

Now, let us try to see what a combination of enfold rotation and translation parallel to the axis will give us. So, let us try to represent it in our sights notation. So, I write it as rn tau rn is this rotation and fold rotation by 360. So, let us call that rn and tau is a translation parallel to the axis. So, rotation this is translation parallel to the axis.

Now, let us see what will happen if I apply this operation 2 times, that is a square of this operation given under bar to show that it is a vector and rn is a matrix. So, this is a matrix column representation and I am applying 2 such operators recall how we apply multiply the sides operator to the 2 matrices will get multiplied that will be the resulting matrix of the product and rn will multiply with tau from here the first matrix rn multiplies the second vector tau, and then we add the first vector, which is also tau in this case.

So, we get this as the product of our sites operator, which we have discussed in detail in previous videos, I am using round brackets here for sites operator, there is a little bit of variations in this case. In some of the previous videos, I have used the square brackets, sometimes angular brackets are also preferred. In this case, I am just using normal parenthesis now for representing sites operator this comma also is sometimes replaced by a vertical bar. But I think writing comma and writing parenthesis is simpler in this case, so, let us go ahead with that.

And so, continuing with this product this becomes rn square note that tau notice what is tau. So, tau is a translation parallel to the axis what will... so, what will this product be rn tau. Rn is a rotation and tau is a translation parallel to the axis, if you apply rotation to a translation parallel to the axis, it does not change, a translation parallel to the rotation axis is an invariant translation for that rotation. So, rn tau will actually result in simply tau and you will get tau plus tau. So, we will get rn square 2 tau. You can continue this let us do one more multiplication.

So, let us find out rn tau cube which is rn tau multiplied by rn tau square we have already solved the case for square, so we can write it as rn square 2 tau. Now, if I use our multiplication rule, so, we get rn cube rn of 2 tau plus tau and using the linearity of rn over 2 tau, this is simply 2 tau because 2 if tau is a translation parallel to the rotation axis 2 tau is also a translation parallel to the axis and will remain invariant under the rotation rn. So, I get to 2 tau plus tau which gives us rn cube 3 tau.

So, you have got the pattern now, when I squared it, I get rn squared 2 tau, when I cubed it I got rn cube 3 tau. So, now you can write the general expression rn tau to the power n, what will happen if I take an n fold rotation, combine it with translation and this combination I applied n times. So, this is what I want to find out soon. This will become rn to the power n, n tau. But notice that rn was a n fold axis. So, it was a rotation by 360 by n. So, if you apply it n times, so, the total rotation will be 360 by n into n. So that will be by 360. So, rn raised to the power n is nothing but an identity operation, it is no rotation at all or a rotation by 360 degree which I represented by 1, which is our identity in international notation.

So, I write it as 1 and n tau is the translation associated with it. So, that means there is no rotation if I multiply a screw rotation, and n fold screw rotation n times I will get a pure translation parallel to the axis which is n times tau. Tau was the intrinsic translation associated with so, sometimes it is called let me note that, n times intrinsic translation associated with screw operations and sometimes it is also called pitch just like we use it in engineering for pitch of a screw. So, this tau is either pitch or the intrinsic translation.

So, n times multiplying or applying the screw motion n times results in a pure translation, which is n times the pitch n into tau. Now, let us assume that rn tau was a symmetry operation, if rn tau was symmetry operation, then this also is n times applying a symmetry operation is also a symmetry operation. So, if the screw operation was a symmetry operation, then this left hand side is a symmetry operation. So, which means this is also a symmetry operation, but this is a translation.

So, this has to be a symmetry translation, we do not use phrase like symmetry translation, we simply call it lattice translation. So, this means that n times operation of a screw operation n times applied gives you a lattice translation. So, let us write this n into pitch is equal to a lattice translation and not an arbitrary lattice translation because remember pitch is a translation parallel to the axis. So, this lattice translation is also parallel to the axis. Now, we do not know which lattice translation it is.

So, if we have a screw axis what we are saying and we had a tau which was the pitch or the intrinsic translation associated with this screw. Then we are saying that n times tau it is some lattice translation. Let us say let us call it T, parallel to the axis T, since it is a lattice translation, it has to be a multiple of the minimum lattice translation in this direction. So, I write this as p times t min, where t min is the shortest lattice translation parallel to the axis so, p in that case will be another integer.

So, this gives us an interesting result that n times the pitch of the screw is p times the minimum lattice translation parallel to the screw which means, if I want to write the pitch of the screw I can write it as p by n into T minimum. This is an interesting result so, any screw operation will be characterized by a lattice translation which gives the direction of a crew and also by this fraction also by this fraction p by n which finally gives that what fraction is of the minimum translation is the pith, of course, you can see here that the meaningful values of p has to be between n and 0 because if p is 0 then tau is 0. Which means you have no translation associated with the rotation so, that is a pure rotation axis.

So, n is equal to 0 will not give us a screw axis, but a pure rotation axis and if p is equal to n then tau will be equal to T min so, it is simply a translation. So, lattice translation so, then you are combining a rotation with a lattice translation that is a combination of 2 symmetry operations, which because of the group property of the symmetry operation is always possible. So, this is not a special case simply a combination of lattice translation. So, the special cases which gave us the screw motion or a screw axes are these cases. So, this is what will define the types of his crew which we can have in crystal.

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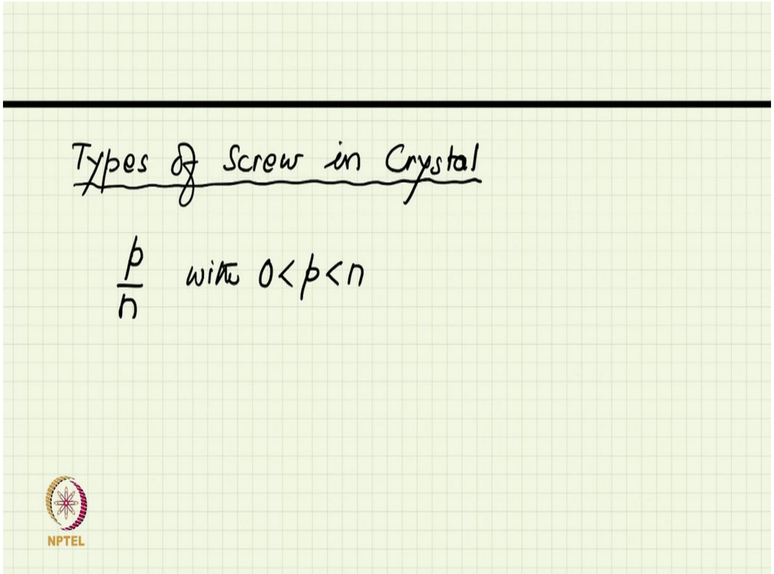

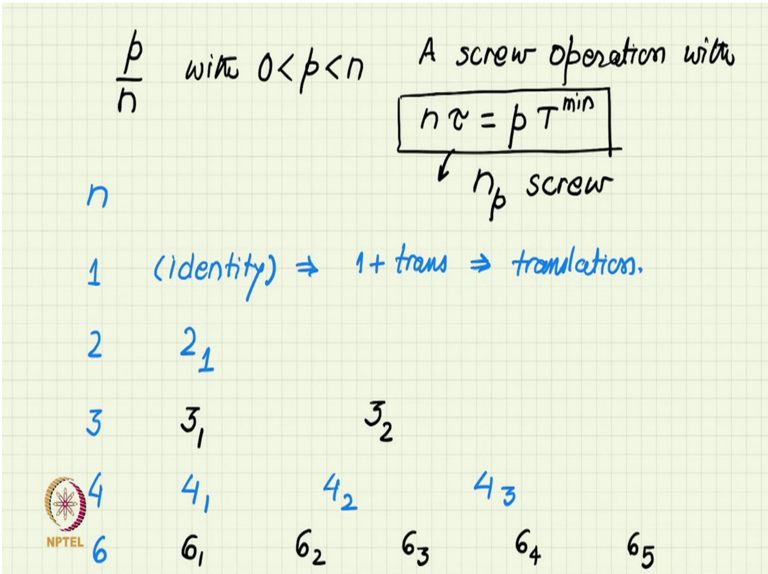

So, it is defined by we have seen 2 integers, p and n would be less than n and greater than 0. The possible values of n we have seen are 1, 2, 3, 4 and 6. So, n is of course, one folder rotation is an identity and if I combine it with translation, I will get a pure translation. So, that is not a screw. So, 1 plus will just give me translation. So, not a screw with the 2, the only value of p possible is 1. So, I will use the notation 2 1 to represent this is crew. So, as crew for which let me define that. So, a crew operation when n tau is equal to p T tau min that is what we established, what is character.

So, this is designated as np screw. So, for 2 fold the only value possible for p between 0 and less than 2 is 1. So, I get one possible to screw operation 2 1, for 3 you can see that we will have now, the values of p can be 1 or 2. So, I have 2 kinds of access 3 1 and 3 2, 2 operations. In case of 4 we have 3 values 4 1, 4 2, and 4 3 and for 6 we have 5 different screw axes 6 1, 6 2, 6 3, 6 4 and 6 5. So, if you count these are the 11 screw rotations which are possible in a crystal.

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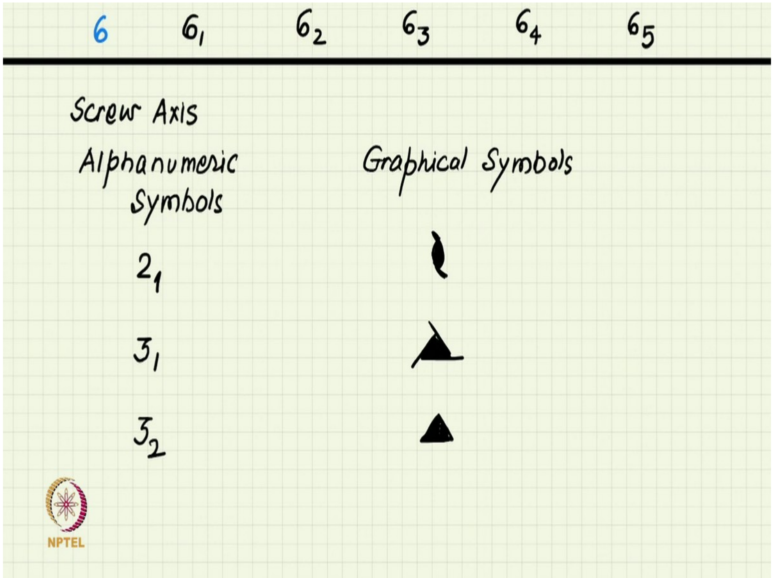

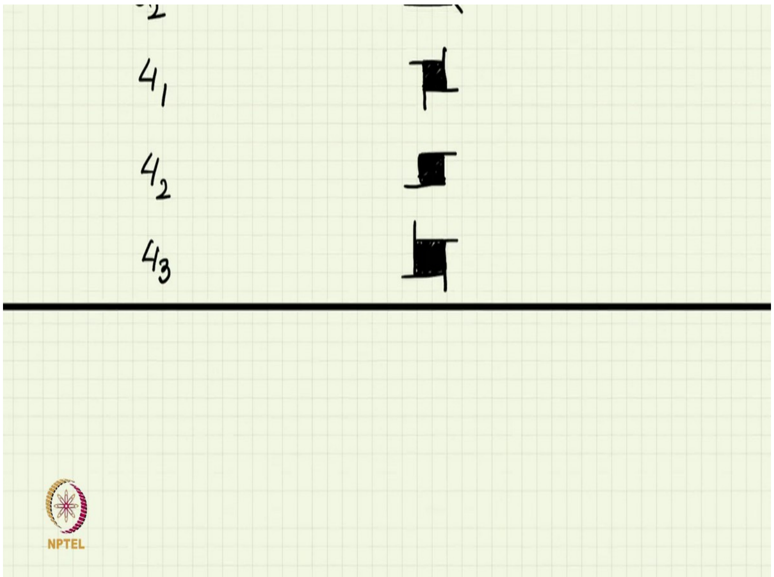

4_3

6_1

6_2

6_3

6_4

6_5

2_1

3_1

3_2

Enantomeric pairs

4_1

Achira' 4_2

4_3

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6_1

4_2

4_3

6_1

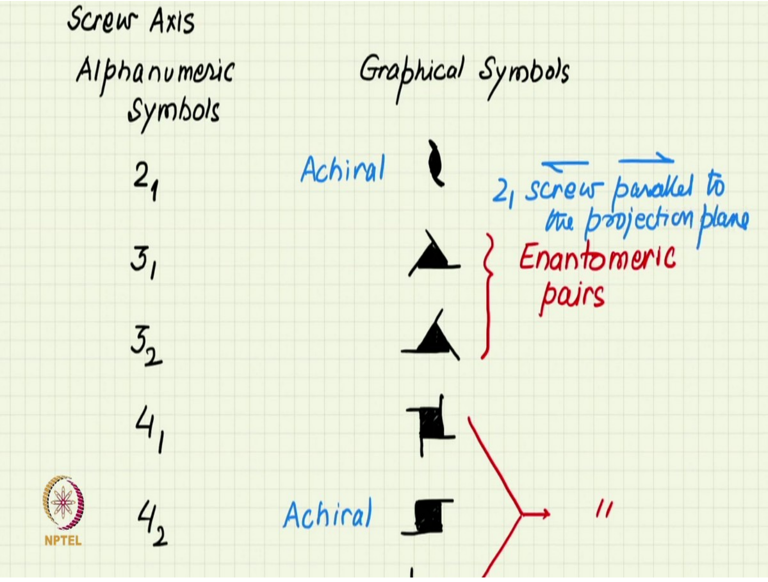
6_2

Achirc 6_3

6_4

6_5

Mirror image pairs



So, let me give you let me give you a table of graphical symbols which are used to denote this in international tables, So, screw axis we can call the symbols which I have just given you alphanumeric symbols and now, I also want to give you the graphical symbols. These are used in even in the international tables, the space groups are represented and their symmetry elements are shown. So, those graphical symbols will be used. So, 2 1 is screw it just remember the 2 folded axis, 2-fold axis at the symbol, I just have to extend this 2 sides to make it a screw symbol and 3 1. For the 3 fold we use triangle 3 1, we extend the sides of the triangle to represent a screw. 3 2, we are going to extend the sides of the triangle, but in the opposite way. That is 3 2.

4 1 4-fold is a squared and I extend the sides to the present 4 1. 4 2, only 2 opposite sides are extended will represent 4 2. 4 3, Again all sides all sides are extended, but in the opposite sense to 4 1. And finally, for 6-fold we have the 5 screw axes 6 1, 6 2, 6 3, 6 4 and 6 5. 6 4 is represented by hexagon, and you extend the sides represent 6 1 screw. 6 2 screw you extend the alternate sides. So, only 3 sides in 6 3, only 2 sides the 2 opposite sides. 6 4 again 3 sides, but in an opposite sense to 6 2. And 6 5 all the sides, but opposite sense to 6 1.

So, these are the graphical symbols which are used in the international tables, just a comment here that 3 1 and 3 2 are actually mirror images of each other. So, they are enantomeric pairs that is they are opposite handedness. So, if you reflect 3 1 in a mirror, you will get 3 2. So, they have opposite handedness, same thing is true for 4 1 and 4 3. So, they are also in enantomeric pairs. In the case of 6 1 and 6 5 are enantomeric pairs and so are 6 2 and 6 4, in fact that is why the notation of using the opposite extension which I was showing you, that the arms are extended in opposite sense is to show that they are mirror image of each other, these are also mirror image pairs.

4 2 is left and 4 2 is achiral does not have handedness. So, if you reflect 4 2 in a mirror, you will get the same 4 2 and this happens here in 6 3 achiral and 2 1 is also achiral does not have handedness. 2-fold screw sometimes lie in the projection plane in International Table and for that there is a special symbol. So if they screw axis is line, all these symbols which I have shown you are for screw axis lying perpendicular to the plane. But if they screw axis lies parallel to the plane, then the symbol shown is by a pair of half arrows. I think for the moment, we will end our discussion of screw axis here and we will discuss more later. Thank you.