3D Space Groups XIV
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Interpretation of International Table Page
Part 7: Generators Selected

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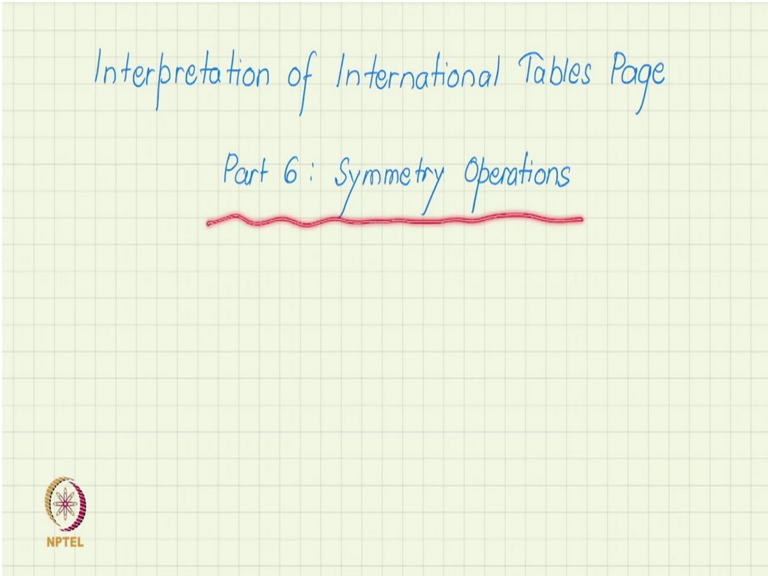

Hello, we will continue our discussion on the Interpretation of International Tables Page and in this part, we will look at the symmetry operations. So, one of the important information which is there in the international tables is the so called symmetry operations after all, if you think what is the space group? So, a space group is a group of symmetry operations of a crystal. So, the symmetry of operations in the sense is one of the most important information.

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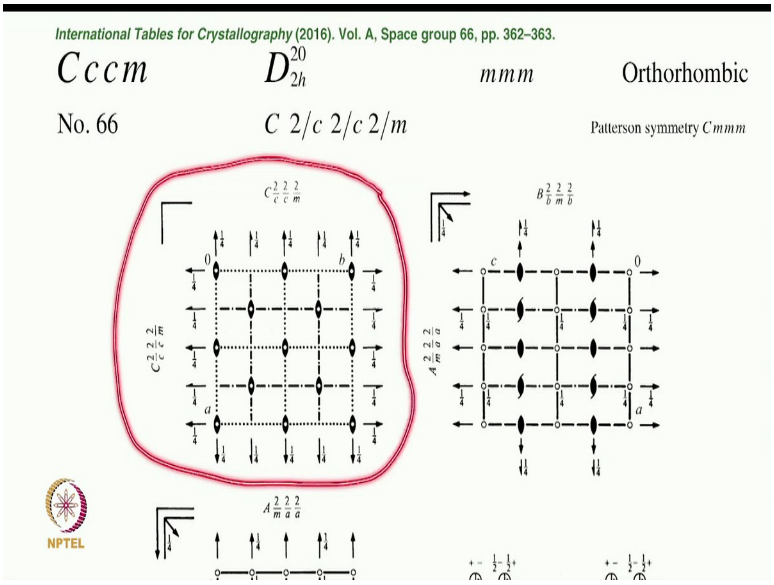

The way the symmetry operations are discussed. Actually, there are 2 ways and one of them diagrammatically where the symmetry elements are shown there is a slight difference between symmetry elements geometrical symmetry element and symmetry operations, we will look at that.

So, these diagrams show the symmetry elements, geometric symmetry elements, we are in the space group 66 and the space group Hermann Mauguin symbol for the space group in capital C followed by 2 small c's and m.

So, the capital C, is C centered lattice and the small C's are showing that there are glide operations, C glide operations perpendicular to a and b axes and there is a mirror plane perpendicular to the third axis that is the C axis. So, that is the space group we are in, we have discussed the symmetry element diagram a little bit detail in a previous video.

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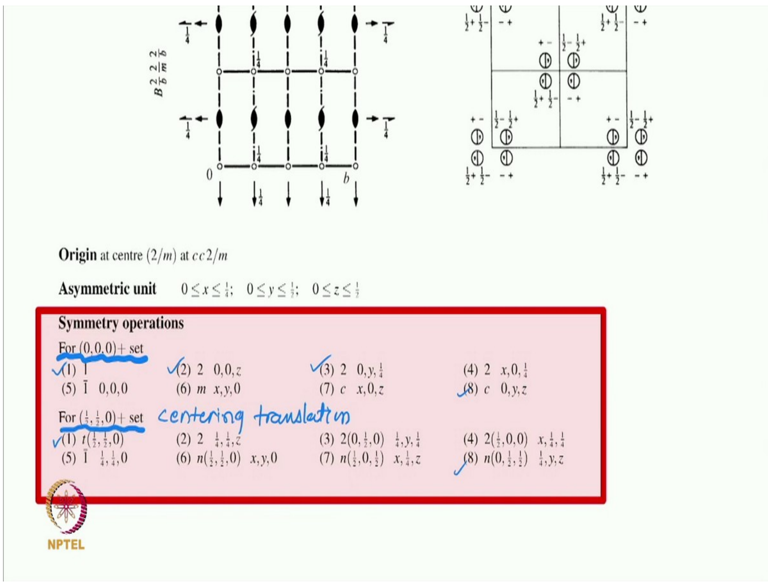

And now, we will look at this block, this particular block which is called the symmetry operations this block. And this block has a you can see there are 2 parts, 2 sub blocks to this, one is for set 000, and another is for set half half 0, that is because this is a C centered lattice, the second block half half 0, as you can see is the centering translation for this particular lattice.

So, 000 is the origin you can say and half half 0, is the centering translation you can see that there are 8 operations listed in both the sub blocks and they are numbered 123. They are serially numbered up to 8, in the first block and then again 123 to 8 in the second block. And each of these with the details associated with the serial numbers are details about the symmetry operation present in the space group. So, we will like to look at how to read the information about symmetry information given in this symbol.

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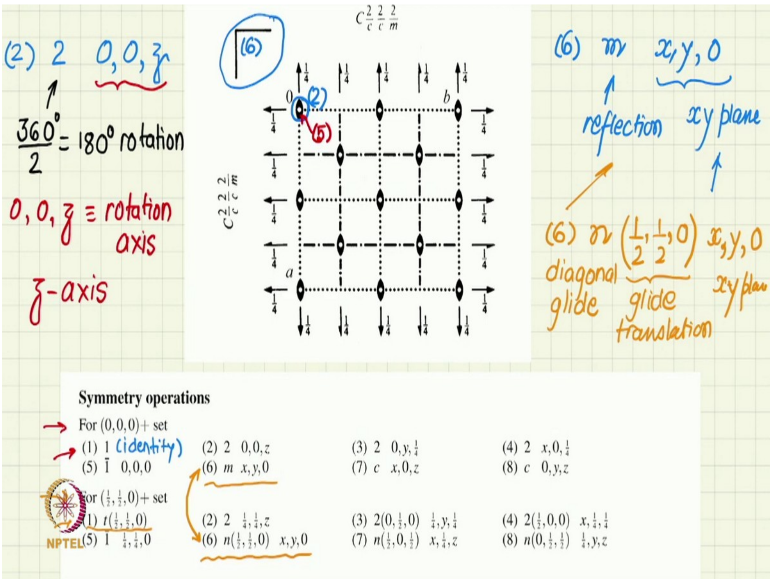

So, let us look at it we will look at it one by one carefully. So, to do that, let me try to put the symmetry element diagram and the symmetry operations list close to each other, which I have done here and let us look at one by one.

So, in the first block in the first set, the 000 set the first symmetry operation given is just one and as you know one represents identity and that has to be there in any symmetry group. There is a requirement of the group property every group has to have identity as one of its symmetry operation. So, our space group also has this identity. Of course, identity cannot be represented by any geometric symmetry element. So, it is not there in the diagram. We just have to assume its presence and we have to know that it exists. So, one is the identity.

Let us now come to the second operation, the second list, which is written as 2 and then o comma o comma Z. So, what is this showing? So, the first the first letter 2, the first number 2 is, so, let me write it here we are talking about the operation 2 with the information 2, and then 0 comma 0 comma z. So, this 2 the first 2 is telling us that it is a rotation, a 2 fold rotation that is a rotation by 360 degree by 2.That is 180 degrees. So, it is 180 degree rotation.

The next 3 numbers and letters the triplet OOz, tells us about the rotation axis 00z is the rotation axis. Now, you can see that the 2 of the coordinates are 0 means x is 0 and y is 0, and z is left as a variable. So, all points for which x is 0 and y is 0, but z can take any value is the rotation axis, which means this itself is the z axis.

So, that means the symmetry operation 2, which we are discussing now is a 2 fold rotation 180 degree rotation about the z-axis, axis passing through the origin and parallel to the z direction.

So, similar information is there, there are other 2 fold axes represented as operation 3 here and then there is an operation 4 there. So, all these are 2 fold symmetry operations. Then, operation 5, you can see is a one bar, one bar is an inversion and for inversion center, the coordinate of the inversion point is given, in this case it is given as OOO, which means it is origin. So, you have an inverse in about an origin.

So, let us relate these to symmetry element diagram. So, the operation 2 which we discussed was a 2 fold parallel to the z axis. So, that was the operation 2. And then this operation 5, which is the inversion center in the origin is just the dot inside the lens. That is the operation 5.

Let us look at Operation 6. The symmetry operation 6 is shown as m and then x comma y comma O, m represents a mirror reflection. So, this is a symmetry operation which is a mirror reflection let me write it here. 6, m, this represents reflection, it is a reflection operation. And if it is a reflection operation, we need to give the plane of Reflection, the mirror plane and that is being given by this triplet x y O, so, z coordinate is fixed 0 and x y is left variable. So, that means it is a xy plane passing through the origin.

So, there is a mirror reflection in the xy plane passing through the origin, the xy plane, the mirror plane is what is being shown here by the symbol here. So, that is the representative of Operation 6. So you can see, it is, I am saying it is representative of Operation 6, it is not actually the operation, what is shown in the diagram is not the operation, but the symmetry element or the geometric symmetry element associated with the operation. And what is being shown in the table here, below it are the representations of the operation that work.

So, m represents here in number 6, m represents the reflection operation, and x comma y comma o represents the xy plane, which has the geometric symmetry element, and it is only the symmetry element, which is finally shown in the diagram.

An interesting thing to note here, when we come to the second block the half half 0 set. So, the first operation now is t, half half O, t represents the translation and as you know, this is a C centered lattice. So, there is a half half O translation available in this lattice or in this space group. So, that is the first operation is the translation in the second block.

So, this second block, second block is given as half half O plus set, which means, for every position, you have to add this half half O to get to the new position described by the set. So, identity does not do anything. So, identity represents the position somewhere in this space group and then that is the number one of the first block the OOO block, but the number one of the second block is the translation half half O.

So, these numbers are given the same numbers in the 2 blocks, because they are correlated. So, the number 2 in the second block is representing a symmetry operation in which, which corresponds to the symmetry operation of the 2 of first block let me write it this way. These for example, these 2 twos in fact, a more interesting case which I will like to handle and discuss with you is the 2 operations which are listed at 6 in the first block and 6 in the second block.

So, what does it mean is that these 2 operations listed at 6 are related to each other. If you add a translation to the operations 6 if you add the half half 0 translation, the C centering translation to the operation 6 of the first block you will get operation 6 of the second block let us see how does that happen.

So, the first block the number 6 we have already seen here is a mirror x y 0, but the same number 6 in the second block is being shown as n glide, n glide and for glide operation, glide always is associated not only with the mirror plane, but also with the glide vector. So, the representation of glide operation is given by the symbol for the glide here it is n, which is symbol for diagonal glide and is diagonal glide and this is the glide translation and finally, you have the glide plane.

So, if the mirror is there, there is no glide translation. So, you only give m and the mirror plane, but when you represent the glide operation, you have to give the symbol for the glide which is n here, then the glide translation which is half half 0, and then the glide plane which is x y 0, so, this is also the xy plane.

So, note this interesting thing the xy plane is present in this operation 6 in the second block and there it is being shown as an n glide operation, a diagonal glide operation, this xy plane is present in the operation 6 in the first block also, but there it is shown as a mirror reflexion and if you see in the xy0 plane the symbol which is shown here is only for the mirror, not for the n glide. So, how is miss… this can be a little confusing, but the clarity will come once when distinguishes between the geometric symmetry element and the symmetry operation, what is shown in the diagram this particular line at 90 degrees, which is showing a mirror plane parallel to the xy plane.

So, this this is a mirror plane which is a geometric symmetry element and the same mirror plane is present in these 2 symmetric operations which means, there are more than one symmetry operations which can be associated with the same geometric symmetry element.

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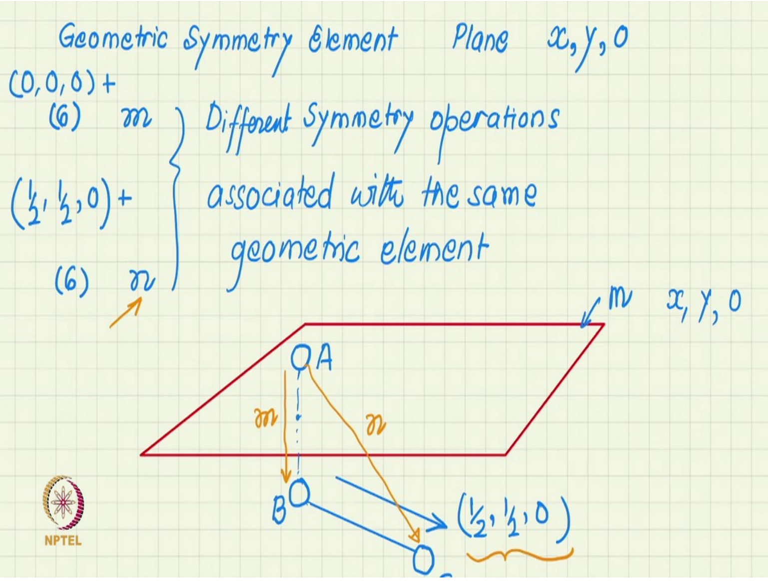

Let me try to write this for the greater emphasis. So, one has to distinguish between Geometric symmetry element which for both the operation is a plane and in this case it is an xy plane represented as x y 0, but this geometric element is associated with more than one symmetry operations and in this case symmetry operations 6 for the 00 plus block you get an operation 6 in which case it was a mirror reflection.

So, it was a mirror reflection and when we looked at half half 0, block that is the same operation with centering translation it became an n glide operation. So, these are symmetry operation both of these are symmetry operations, let me call it different symmetry operations associated when the same geometric element in fact, if you have a mirror plane in a space group, if you have a mirror plane then there are also infinitely many translations parallel to the mirror plane.

In this case in this particular example, is a half half 0, translation which is parallel to the mirror plane the mirror plane itself is the xy plane. So, if there is an object which is operated upon by the mirror so it reflects in the mirror and comes here and then it translates by the translation vector because translation vector also is part of the space group. So, that will act the mirror is there, you get that object. Let me call this and we call this 1 let me call this A, we call this A, Let me call this B, which results from mirror and now, I translate it and I get it get the object C due to that translation.

So, if you now relate, now relate A directly to B. It is a combination of reflection followed by a translation parallel to the mirror plane. And since the translation vector is half half 0, this is called diagonal glide or n glide operation and this particular operation, so, this was the n glide operation, and this operation directly reflecting here was the reflection operation.

So, both are given this number 6, because the 2 are related, one was without the half half 0, translation. So, that is in the O plus group, the another is with half half 0, translation. So, that is in the half half 0, plus group.

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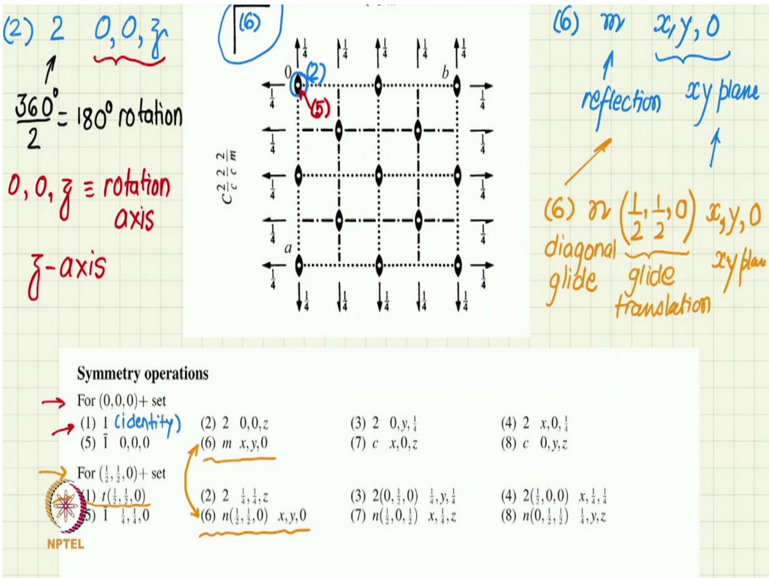

So, I think we have discussed in quite a bit detail, the symmetry operation, other symmetry operations, which I have not explained, you can try to work out and correlate with the symmetry element diagram, which is also present. Thank you very much.