Fundamentals of Computational Materials Modelling
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Translational symmetry operators

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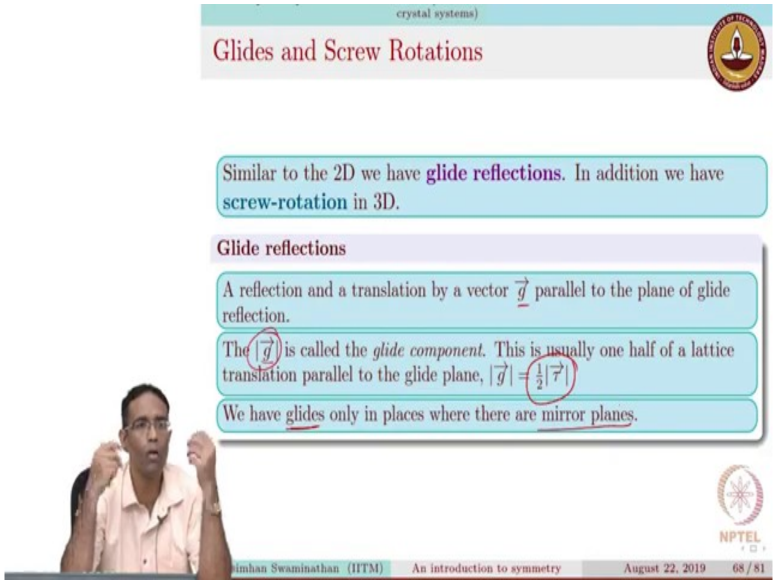

So in so far as far as 3 dimension of space lattice is concern we have only looked at the rotations and the mirror planes. We have not looked at some translational symmetry operators which are also present. For example, in case of 2D you did have this glide plane, you are able to reflect it about a line and then move it by half the translation vector. That was the new symmetry operation that was possible in 2D.

In 3D also the same thing is possible, it is called as glide plane or glide refection and in addition to that we have something called as screw rotation. You rotate it by a certain amount. The amount is basically either 1 fold, 2 fold, not 1 fold, 2 fold, 3 fold, 4 and 6 fold and then you move it by a certain amount. You move it in the same direction parallel to the rotation axis by a certain amount. These are called as screw rotations.

Now glide reflections involves a translation by a vector g which is parallel to the plane of the glide reflection always. And the glide reflection is called the component, the absolute value by which you are moving it is called as the glide component and is usually one half of the lattice vector in a direction that is parallel to the mirror. We will some examples you will understand it better. So the most important thing is that you can have glide planes only in the regions where you can have mirrors.

Because you are always going to reflect the only thing that differentiates between pure glide and a mirror is that, in mirror you just reflect it whereas in a glide you are reflecting it and moving it either, if this is the plane of the mirror you can reflect an object like that and then move it like that or you can move it like that. Either way is possible.

So each of these movements have a specific name associated with them so that we are able to identify what direction the movement has actually taken place.

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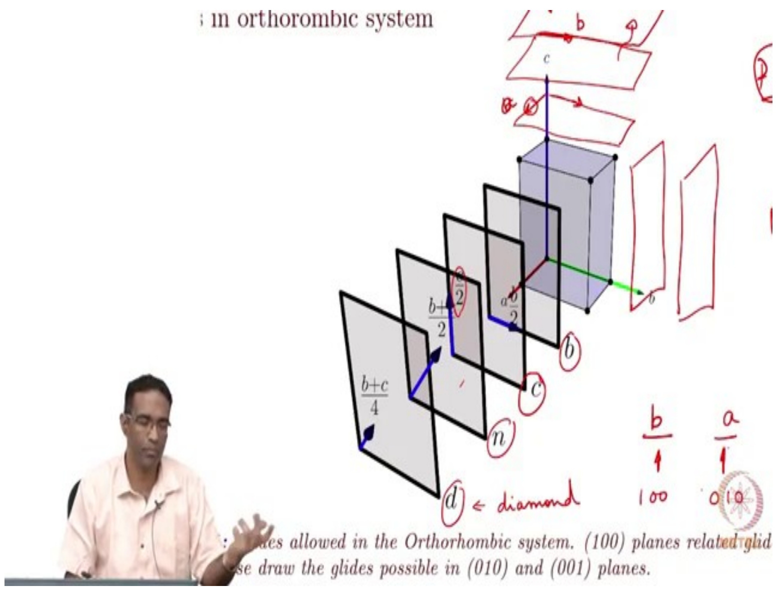

So a good example to take a look at would be this, the glide planes that are possible in orthorhombic system. So in orthorhombic system we basically have mirrors which are having either the A axis or the B axis or the C axis as a normal. Those are the mirrors. So you obviously have the same set of mirrors here as well and here as well.

It is enough for us to understand the kind of glide operations that are possible on 1 face or one kind of mirror and to so that we can introduce the associated nomenclature with the glide reflections. So the first one what happens so this is a mirror this black line that is thick line that is there as a mirror and it has the 100 as the normal and suppose we perform a reflection about this mirror and move it in the B direction by half the lattice vector then that is called as a b-glide, that is called as a b-glide.

Similarly if you have the same mirror except that now the glide is happening along the c direction here by half the lattice translation along the c direction. And that is called as a c-glide. So you have c and b. Now it is also possible for us to have a glide that is along the diagonal of this mirror so you can reflect it about, you can reflect an object about this mirror and then glide it by b plus c by 2. That is called as an N glide and then finally you have what is referred to as a diamond glide where instead of going b plus c by 2 you go b plus c by 4. So the same set of b, c, n and d are also possible for these mirrors except that the glide now cannot happen in the c direction. On this plane you can either have a a-glide or you can have a b-glide. Or you can have a but so this will be called as this this if only this is present it will be called the corresponding b, if this is present it will be called sorry it will be called a and only if this is present it will be called b and if you have a combination like this it will be b plus a by 2 and it will be called as the N glide and so on, b plus a by 4 will be called as the corresponding d-glide.

But remember even though b-c-n-d, b-c-n-d, b-c-n-d would essentially or something else would essentially be the same for all the 3 orthogonal mirror planes possible. The Herman Mauguin symbol will clearly tell us what the plane is because each of the slot will correspond to specific planes. For example, if you had a, b and c so this one cannot have a a-glide so let us say a b-glide, a a-glide and c-glide. So you clearly know that this b-glide corresponds to this mirror.

Because this slot corresponds to the mirror which has the 1 0 0 as the normal. This slot corresponds to the mirror which has 0 1 0 as the normal, and this one corresponds to 0 0 1 as the normal. So by looking at the slot in which the glide is happening it is possible for you to say in what direction or in what plane mirror plane this particular glide is actually taken place. As far as orthorhombic is concern.

So you know this may not be clear to you right now but when we look at the space group symbols for those crystals which have a glide plane it will be you will understand what exactly that means. So you will have this basically is a space group, so if I say p, b, a, c this is actually a space group. Instead of saying p, m, m, m , I am saying p, b, a, c so instead of saying instead of having the mirror I am actually having a glide plane in positions of the mirror.

This is actually a space group. Now what would be the point group of p, a, b, c? mmm because you just have to remove all associated translational symmetry operators and you will get the corresponding point group. The same thing applies to every other space group that you can have.

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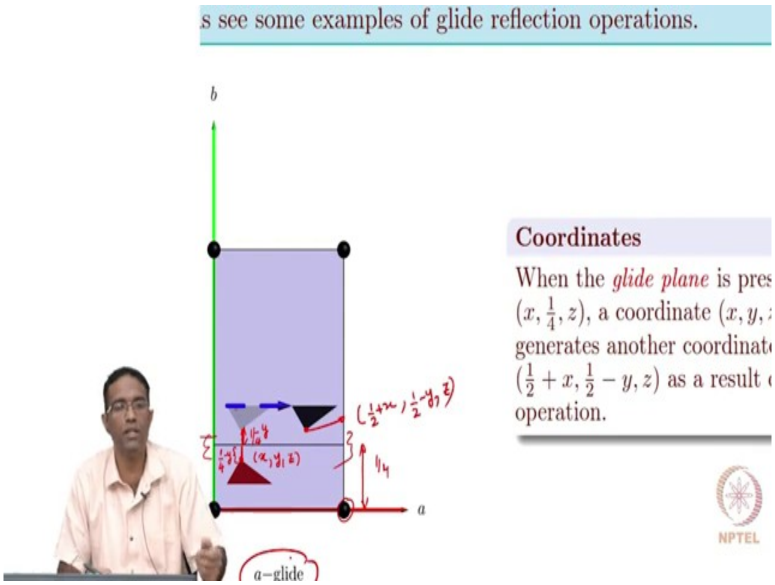

So let us see some examples of glide reflections just for clarity purposes. So this is a glide pane is present at x, ys quarter or bs quarter so this line that you are seeing here is basically the mirror. And this scalene triangle is what is being reflected and moved by half the translation vector. So this is obviously an example of an a-glide because you are reflecting this object about this mirror and this shaded, lightly shaded triangle is what is found after you reflect it. And then you are going to move it by half the translation vector, half the distance between 0 and this point here, this point here and you get the new position of this point.

So it is possible for us to find out if this is having a coordinate of x, y, z and this is actually having a fractional coordinate of quarter because the mirror is actually present at x quarter z. It is actually long mirror which is coming out of the plane of the board. So what would be the corresponding coordinate here is what we would need. Remember the Wyckoff positions, we talked about the Wyckoff positions, the Wyckoff positions were all generated by applying the various symmetry operators to some point.

Like we applied for example, the 4 fold rotation to an arbitrary point x y z and we generated all the other points within the unit cell. So even when we talk about the week off positions for a general position for a space group which has this glide thing, then you would have to apply this refection and also the movement and also the glide component.

So you would have to calculate what is the new position after applying this symmetry operation, which is reflection plus a translation. So how do kind of get these coordinates? Just to give you an example. So if we have x y z then what would be this? This component here? Quarter minus, quarter minus y, this would also be quarter minus y,right?   correct? So the actually y coordinate here would be into 2 plus y that will be half minus y.

And the corresponding x coordinate here, so this has what would be the x coordinate here? This x coordinate will be half plus x because there is just being moved half the lattice translation vector. The corresponding y component would be half minus y and the z component would exactly be what it is, z, so this is an example of a a-glide right here, so this sort of operations which are actually applied in order to generate appropriate week off positions for the space groups which have these symmetry, the glide operations.

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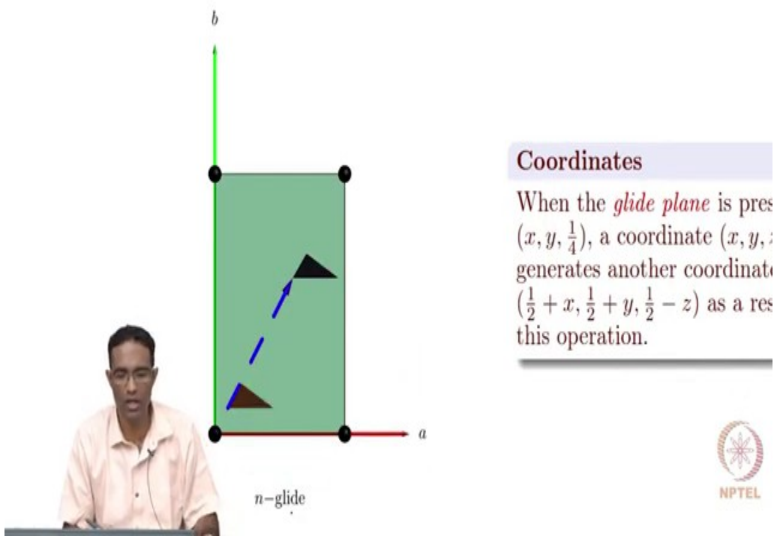

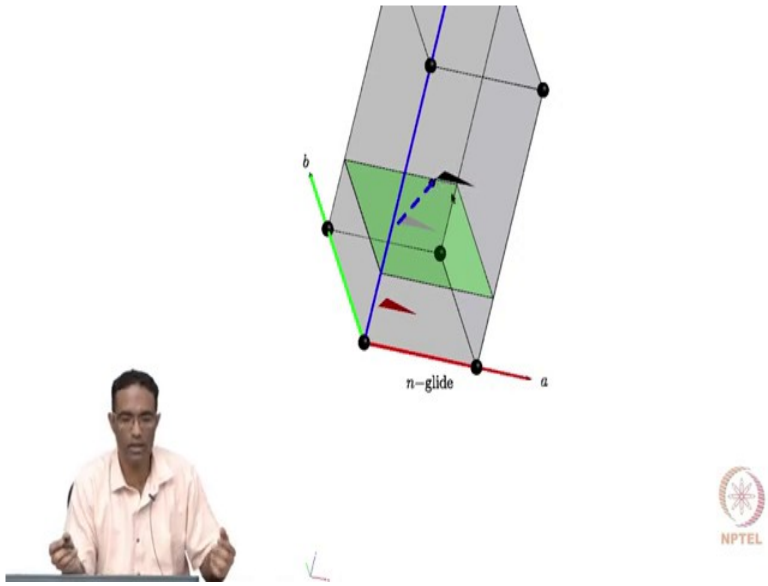

Now let us look at an n-glide, so this is an n-glide. The n- glide where is the n-glide present? The n-glide is present at x, y at z is equal to quarter so it is present somewhere. So this is a mirror plane, this greenish thing is a mirror plane. So we are taking this triangle, the triangle that is there in the bottom. We are reflecting it about this plane, and performing a glide which is half a plus b, half of a plus b, and it takes this particular triangle to this particular spot.

So again it is possible for you to generate the corresponding coordinates of these, of the triangle after this entire symmetry operation is being applied that is going to be half plus x half plus y and half minus z, will be the coordinates all these triangles right here. When you look at it from the top it just appears is moving there but actually it has been reflected about that plane and then moved. Like what you saw in the 3 dimensional image that I just showed you. Is that clear?

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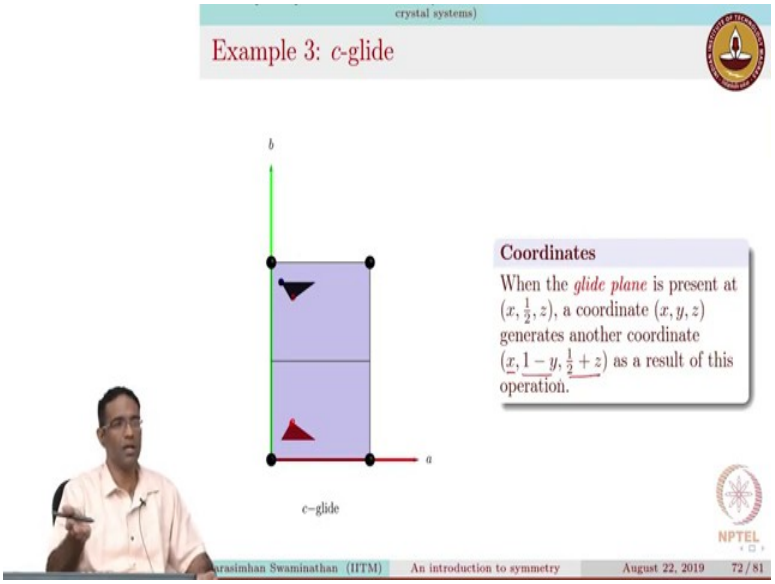

You can look at another example where you have a c-glide, so this is an example of a c-glide, so you have a glide plane that is present at x half z. A coordinate x, y, z is present right here, is being reflected. But after reflection instead of moving it in the a direction I am now moving it in the (c) in the direction perpendicular to the plane of the paper.

And that will generate these as a new coordinates. Any arbitrary points x y z will actually become x 1 minus y and half plus z by the application of this glide. So if I am giving you a glide I am giving you an arbitrary point I am expecting you to be able to look at it carefully and find out the corresponding coordinates after the symmetry has been applied. The symmetry does not involve only the mirror plane or the glide, it involves a combination of both, it involves a combination of both.

So this is glide. So what happens when you are talking about space groups is all the mirror planes you are enhancing the possibility of all the mirror planes also being glide planes, which increases the number of possibilities of symmetry that you can actually have for various crystals. Another thing what happens which is only unique to space lattice are the screw rotations.

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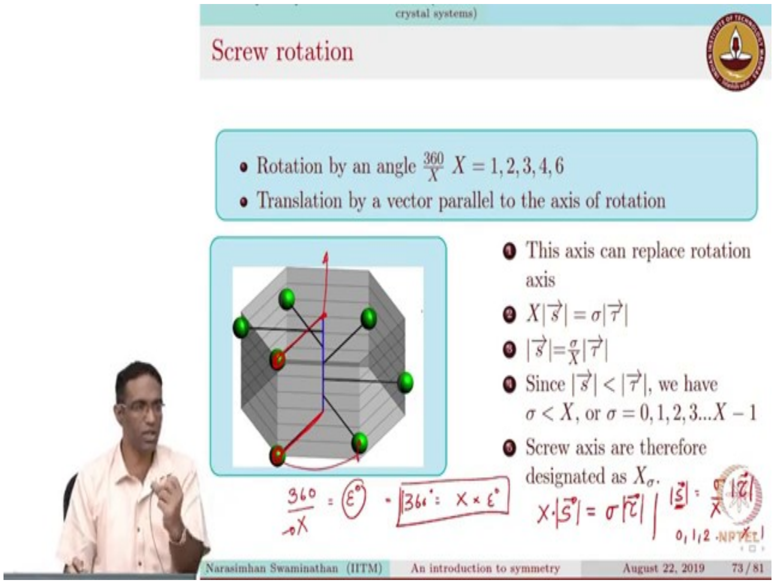

Screw rotations, so screw rotations are actually going to involve rotation and movement in a direction parallel to the direction of rotation. So this is the axis of rotation I am just taking an arbitrary example. So I am going to take this atom here, I am going to rotate it by 60 degrees but instead of keeping it there, I am going to move it up by some amount.

Now this some amount cannot be some arbitrary amount, because our symmetry operations has got to be compatible with lattice translations. So if you imagine this entire thing that I have drawn to be a unit cell then if there is one structure like this at the base of this unit cell you are going to have to have another one right on top. Otherwise they do not repeat themselves in the direction of axis of rotation.

So there is specific rule that you have to be careful about when you are actually applying the screw rotations and there are very simple formulas that you can actually come up with. So if you talk about the screw rotation, so let us say you are rotating it by 360 by x would essentially where x is basically the order of rotation basically 1, 2, 3 and 6 or 4 and 6 this would be the corresponding degree or the angle by which you are going to rotate that particular atom.

Now if you perform this rotation or this can also be written as if 360 degree is equal to x multiplied by epsilon. If you perform the 60 degree rotation 6 times you essentially get back the same position equal to 1, 360 degree rotations. Now the question is by how much can you actually move it after the rotation, by how much can you actually move it after the rotation? So let s vector be the vector by which you can actually move it following the rotation x times s must be equal to the translation vector, x times s must be equal to the translation vector.

So we will put the absolute values here, so but you need not actually be the entire translation vector, it so happens that it can be an integral multiple of the translation vector. We will see some examples and this will be a little bit more clear. Consequently what happens? s vector is equal to sigma divided by x times the lattice vector, since s is the amount by which you are moving it, it is obviously less than tau.

It is less than tau, so by how much can it be, how will you find out you know what are all the various values that it can have? So sigma can have values between 0, 1, 2 to x minus 1, correct? So it can have if this is a for example if you are performing a 2-fold rotations we will see an example so that we will make things much clear. So I have some figure here.

Student: when you are refferring tau, this is lattice or general tau ?

Professor: This is a, the question is what is tau? Tau is basically a Lattice vector, the distance between two Lattice points.

Student: So in that case you should not be having the sigma that side, Sigma should be this side so that the integral multiples of the distance which we obtained from rotation should be equal to lattice Vector.

Professor: So yeah, so the thing is it need not be equal to one full lattice vector it can be integral multiple of any lattice vector. You are rotating it you are moving it, you are rotating it and you are moving it, you are rotating it and moving it. So let us take for example the 6 fold, so let us rotate by 60 degrees and move one sixth of the unit cell let us rotate by 60 degrees which is precisely the example that is shown right here.

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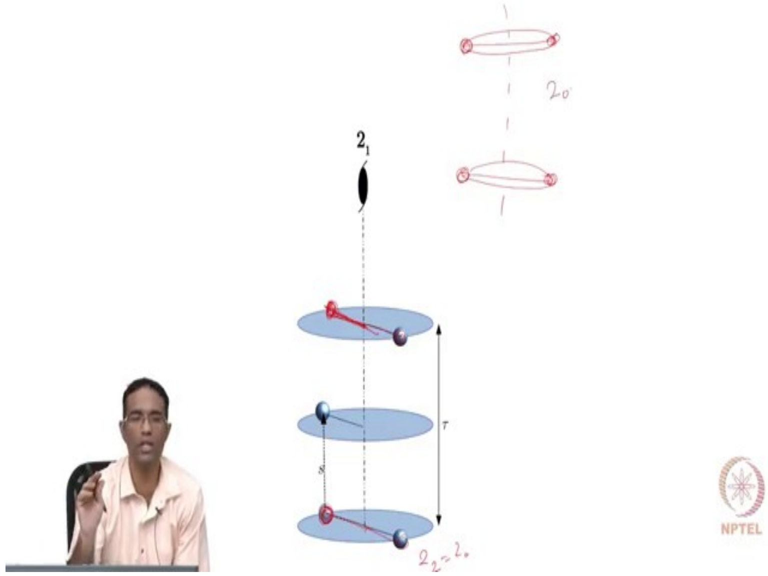

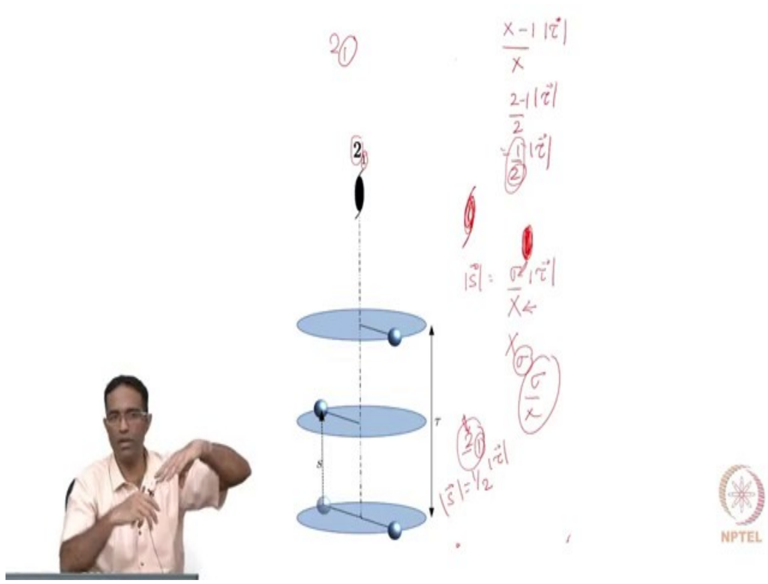

So sixty degree is rotated I have a better picture so if you just allow me to open that, if you perform a 2 fold rotation, this is the unit cell whatever is marked tau that entire thing is a unit. We perform a 2 fold rotation and move it up here and move one full unit cell what does it mean? I told you that this is a unit cell, this entire thing is a unit cell which means if there is an element like this here there should be also be an element like this here, correct.

Now performing a 2 fold rotation and moving it up by the entire tau made this new element, correct? Now if this entire thing has to have translation symmetry it only means that this should also be present. So this is nothing but 2 2, what is 2 2? Is nothing but just pure 2 fold rotation is equal to 2, 0. This entire thing now is just 2 0 or just possessing a 2 fold symmetry, it does not possess any screw rotation.

But now look at what happens when you do two fold rotations and it up by half the amount, I perform a 2 fold rotation moved it by half the unit cell, again perform a 2 fold rotation or moved it by half the rotation. So now this can keep continuing and this pattern does have the 2-1 screw rotation axis, so how will you identify from this work, from this you can identify two things, one is you can identify what is the order of rotation that has been applied and you can also identify by how much of the unit cell the this entire thing has been be moved.

All you have to this take this and divide it by this, so 1 by 2 of tau has been moved. So the s or the vector s through which this has been moved after the performance of rotation is tau by 2 or modulus of tau by 2, is this clear? This is for the 2 fold rotation is fairly simple, so in 2 fold rotation the only thing that is possible is screw rotation that is possible is 2 1, because 2 2 is nothing but the 2 fold rotation.

So extend by which you can move it, will be what? Will be the maximum value it can have is x minus 1 by x times the lattice translation vector. So x is 2, so 2 minus 1 by 2 times the lattice translation vector which is 1 by 2 time the lattice translation vector, correct. Now let us see some slightly more involved examples and of course every screw, this was the symbol for just the 2 fold rotation axis present and this one. This ellipse with this tail right here is basically the symbol for 2 1. So if you want to know, so in our mathematical derivation of the expression for s we had sigma which is an integer by x which is order of rotation times tau. So the screw rotation is represented instead of in the Herman Mouguin symbol. If you want to represent the rotation axis you just say 2 or 3 or 4 or 6. If you want to represent the screw rotation axis you represent it by x suffix sigma, x suffix sigma.

So in this case x was 2, 2 orders of rotation and a sigma is 1. Consequently the amount which you want to move is nothing but sigma by x, yes.

Student: Why is it not tau by 4?

Professor: In this case you have, tau by 4? No there cannot be tau by 4, why you have tau by 4 in this?

Student: You will be able to move 2 or more 3 rotations in same direction.

Professor: no, this, no-no-no, if you put 4 here that means you are saying 4 fold rotation, this is actually the order of the rotation you will see 4 fold rotation later.

Student: No sir, if you have lattice as such, like in this case, if you have 1 point 4 here and 1 point here and start rotating by 2 by 4 then shifting by 1 by 4 of the lattice vector

Professor: I have rotated it 2 by 4 and then?

Student: And then I am shifting it by 1 by 4^{th} of the lattice vector

Professor: 1 by 4^{th} of the lattice vector, tau by 4.

Student: So in that case after doing it 4 times the 4^{th} time I will be reaching the same.

Professor: No, then the unit cell is actually tau, it is shrunk yeah, the unit cell shrinks, if you look at that one particular unit cell you only have two times that is happening.

Student: Even on rotation should be 2 by tau.

Professor: Yeah, it cannot be more than that, yes.

Student: Whenever we are writing a symbol for a particular symmetry element like I said what it essentially means is that the entire unit cell is subjected to that symmetry operations and when that happens the unit cells coincides with itself. So do one actually means that all the atoms of the unit cells are rotated by 180 degree and all of them are moved by translation vector and after that the unit cell will constantly.

Professor: Absolutely, it will do that, but do not ask what happens to the free surface, if you are rotating it and move, the crystal actually, the free surface actually moves up we are not looking at the free surface. We are just assuming that they are just infinitely large.

So performing this operation is still able to coincide with an infinite array of atoms, that is what it exactly means. It means that the entire thing which has a symmetry when rotated and moved will just coincide with itself and you will not be equal to find out the difference. Now let us look at slightly more involved examples for another 5-6 minutes.

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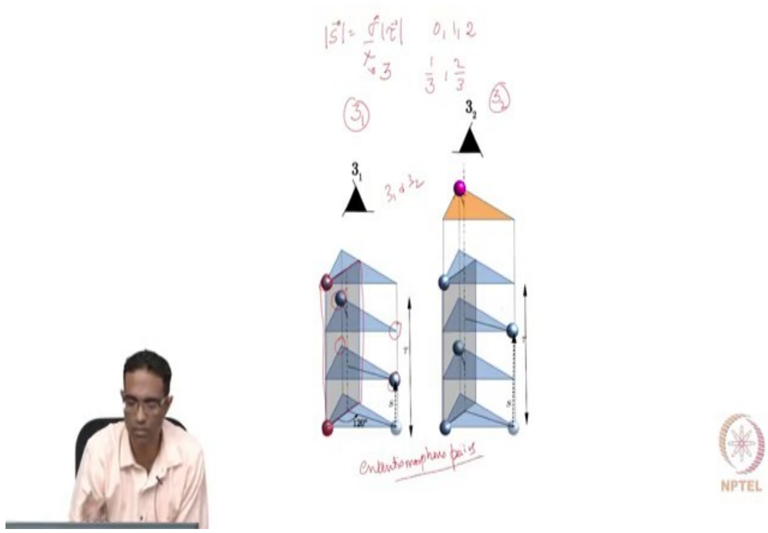

So this is the example of 3 1, so when you have the 3 fold rotation what is, so s would be equal to sigma by x times tau, so what are all the various possibilities? Sigma is nothing but an integer x is 3, so sigma can be 0, 1 and 2. So you can either have a movement of 0 does not make just the absolute rotation. You can have 1 over 3 and 2 over 3, so which means you can have a 3 suffix 1 screw rotation axis and 3 suffix 2 screw rotation axis as you have written here.

It is interesting to see what happens when you perform a 3 1 and a 3 2 just to be clear on these things. So I have marked the entire unit cell as tau. This is the base atom right here, moving it by 120 degrees and moving it by one third of the unit cell tau by 3, moving it up 1 third of the unit cell. This is just the shaded atom which is just indicating an intermediate step there is no atom there.

Then again I am performing a 3 fold rotation and moving it up, 3 fold rotation and moving it up. So this entire thing is basically 1 unit cell which is commensurate with the lattice translation in the along the axis of rotation. You can keep repeating this unit cell and it will have this feature of 3 suffix 1. Now what happens when we do 3 suffix 2, when we have 3 suffix 2, we rotate it by 120 degrees but move it by 2 thirds of the unit cell. So consequently this atom comes here first and then it goes here.

Next this one rotates by 120 degrees and goes to the unit cell that is present on top of it. And it appears now if you are not paying attention you can get a little bit confused. So now you have to carefully see that this is what you defined as your unit cell. So if there is a structure here like this, there has got to be 1 like this. The application of 3 2 took this atom to this part. Now this one is only 1 layer above the base of the previous unit cell, correct?

Which means there must be an atom even here, if lattice translation is to be respected in that direction correct. Now you rotate this by 120 degree and move by 2 thirds you will end up in this part. So now this and this in what way they are different?

Student: Seems one is clockwise other one is anti-clockwise

Professor: Yes, one is seems to be a counter clockwise rotation and going up the other one is a clockwise rotation and going up. So these, if you put a mirror right here right here and see how these atoms are been reflected you will see that since this is the atom and the mirror is passing through it, it would not get reflected at all. However this layer this atom will get reflected over here correct, and this atom will get reflected over here which is exactly 3 2.

Can you all see that? So 3 1 and 3 2 are mirror images of each other and such pairs are called as enantiomorphous pairs. Is that clear?