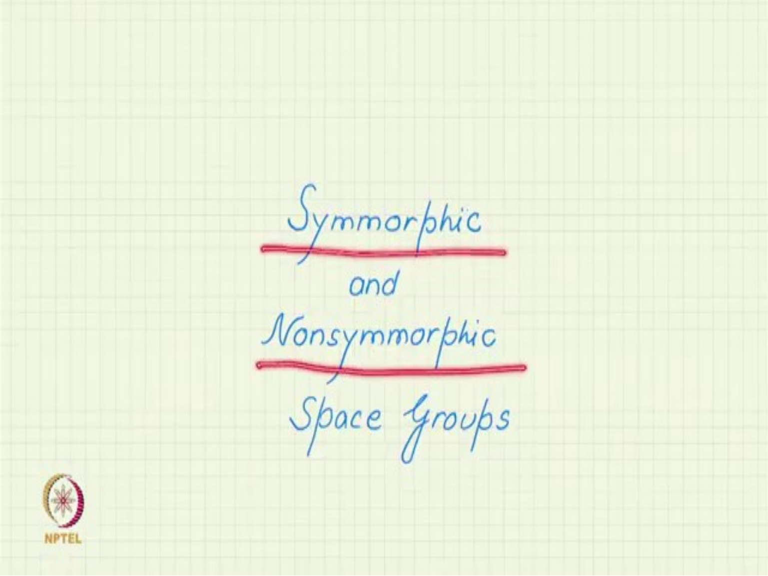
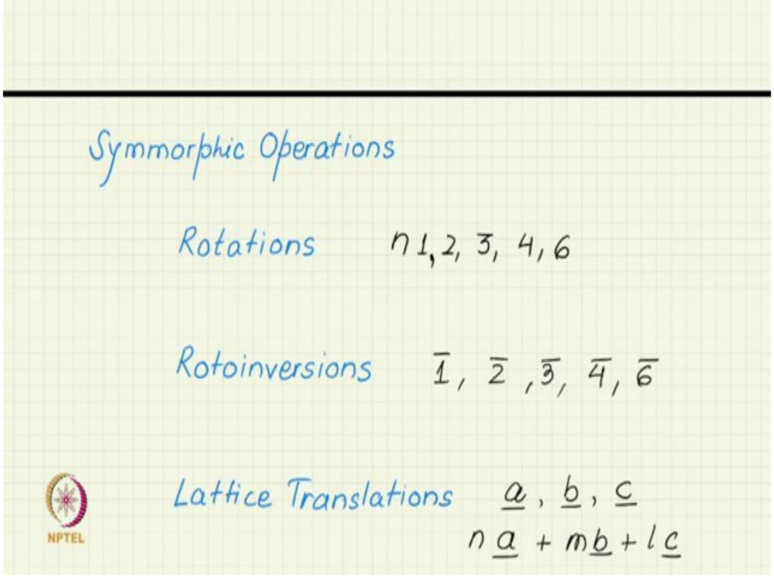
Crystal, Symmetry and Tensors
Professor Rajesh Prasad
Department of Materials Science and Engineering
Indian Institute of Technology, Delhi
3D Space Groups Vl:
Symmorphic and Nonsymmorphic Space Groups

(Refer Slide Time: 0:13)





Symmorphic Operations

Rotations n 1, 2, 3, 4, 6

Rotoinversions $\bar{1}, \bar{2}, \bar{3}, \bar{4}, \bar{6}$

Lattice Translations $\underline{a}, \underline{b}, \underline{c}$

$n\underline{a} + m\underline{b} + l\underline{c}$

$n, m, l \in \mathbb{Z}$

Do not involve non lattice translations.

lattice translations. $n, m, l \in \mathbb{Z}$

Nonsymmorphic Operations

Screw $2_1, 3_1, 3_2, 4_1, 4_2, 4_3$

$6_1, 6_2, 6_3, 6_4, 6_5$

Glides a, b, c, d, e, n

involve non lattice translations.

$\frac{1}{2}\underline{a}$.

Symmorphic Space Groups

Space groups that can be GENERATED using only symmorphic operations.

Can contain nonsymmorphic operations but they are not required as generators.

An important classification of space groups is in 2 types called symmorphic and non symmorphic. So, we will look at this classification in this video. So, we define symmorphic operations. So, a symmorphic operations are rotations, rotoinversions, or lattice translations. So, as you know rotations can be n fold rotation where n is equal to 2, 3, 4, and 6 of course you can count 1 fold also, but that is an identity. Similarly, rotoinversions, you have n bar access of type 1 bar, 2 bar, 3 bar, 4 bar, 6 bar and then you have lattice translations.

So, lattice translations you can write as the basis vector defining your unit cell and linear combinations of these so, you can write n a plus m b plus l c where n m l are integers. Of course, if you have centered cell, then some of the fractions are also allowed but we are taking only the lattice translations either with fraction in the case of centered cell or only integers in case of primitive cell.

So, here I have given you what will be true for a primitive cell none of these translations involve non-lattice translations. So, the symmorphic definition requires that they do not involve any non-lattice translations. So, those operations we call symmorphic operations rotations, roto inversions and lattice translation please keep this in mind that it has to be a lattice translation for some symmorphic operation.

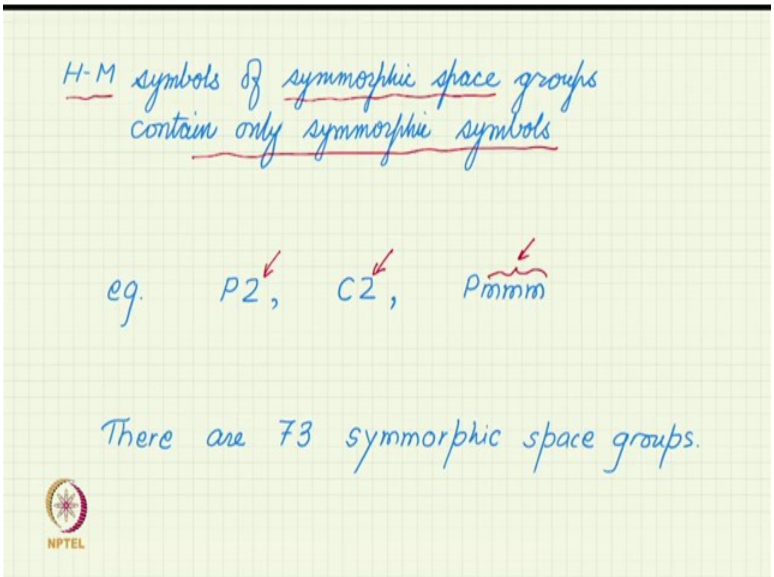
Non symmorphic operations, we have discussed this in some of the previous videos are 2 types is screw and glide, screw as you know there are 11 different kinds of screw let me begin with 2. So, 2 1 then 3 1, 3 2 and 4 1, 4 2 and 4 3 and finally 6 1, 6 2, 6 3, 6 4 and 6 5 these are the 11 screw axis and operations associated with them. And then there are glides which have the symbol a b c these are axial glide then you have d the diamond glide e the double glide and n diagonal glide.

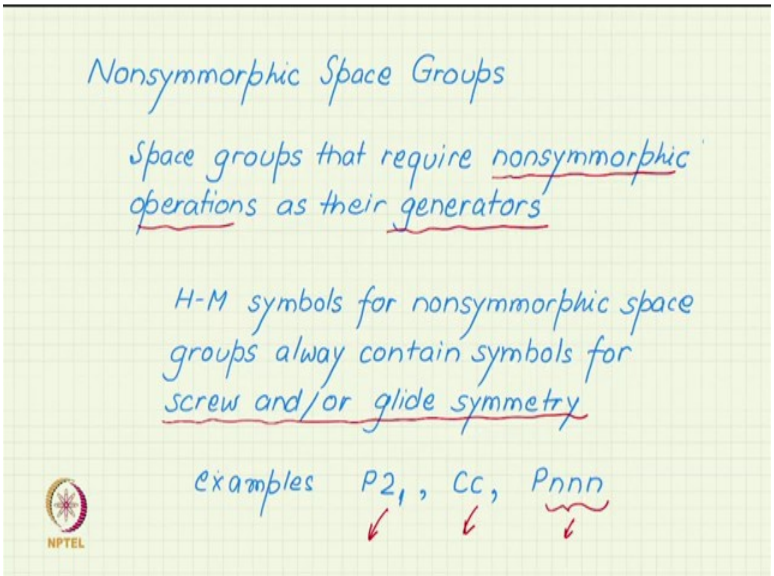
So, we have discussed these operations these operations always involve some non-lattice translation. For example, glide involves half the lattice translation. So, half lattice translation is not a lattice translation so they involve translations. So, for example, a glide will involve a translation by a translation by half a. So all operations which involve non lattice translations and there are up these 2 categories of screw and glides are called non symmorphic operations. This is what is used in defining the symmorphic and non symmorphic space groups. So, when we define symmorphic a space group we define them as the space groups that can be generated using only symmorphic operations.

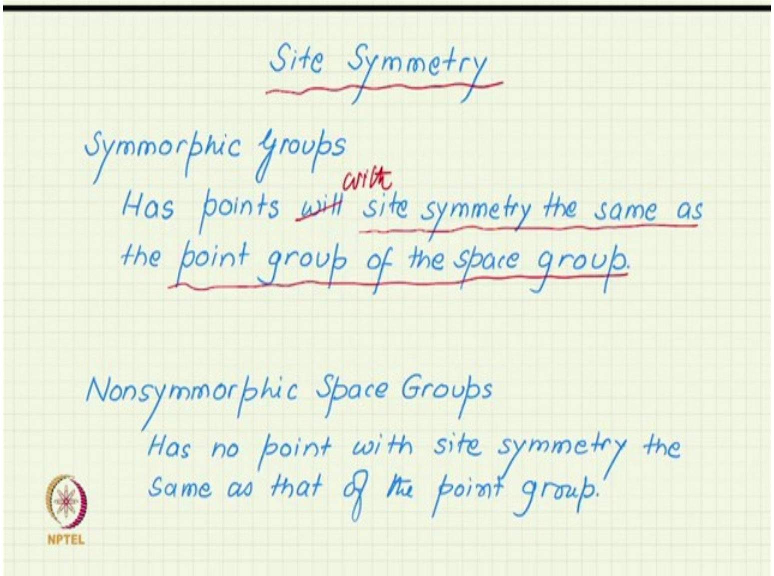
So, that is very important. I have already written generated in capitals and in a different color. I am further highlighting it by putting it in a box that is this word is important is space groups that can be generated using only symmorphic operation that is they will involve they can be generated only using rotations, rotoinversions or lattice translations they will not involve as their generator screw or glide.

I emphasize the generator is important sometimes there is a misconception that the symmorphic space groups do not contain screw or glide that is not true. They may contain a screw or glide but screw glide are not required to screw and glide operations are not required as generators they can be generated purely by symmorphic operations. We will see this will become clearer when we look at some examples.

(Refer Slide Time: 6:07)







Now, let us look at Hermann Mauguin's symbols. So, in the Hermann Mauguin symbols one of the characteristics of Hermann Mauguin's symbols is that they give you all the generators all the essential generators of any space group. So, the Hermann Mauguin symbol itself is a collection of generators and since the symmorphic space groups, the symmorphic space groups do not require non symmorphic generators they do not require a screw and gliders their generators in the symbols of symmorphic space group there will be no screw or glide operations.

So, they will contain only symmorphic symbols. So, some examples some of the simple examples are for example, P 2 so you can see 2 is a 2-fold accesses a symmorphic operation, C 2 again symmorphic operation m m m, the mirror are symmorphic operation. So, and these are the generators of these groups. So, once these symbols are known in Hermann Mauguin's symbols we can generate the entire group just using this information.

There are 73 symmorphic space groups we will devote another video to the listing of the 73 symmorphic space groups. Let us now define the non symmorphic space group. So, by contrast symmorphic space group was defined as those which can be generated only using symmorphic operators or a symmorphic operations non symmorphic is space group in contrast is defined by those which will require non symmorphic operations as their generators.

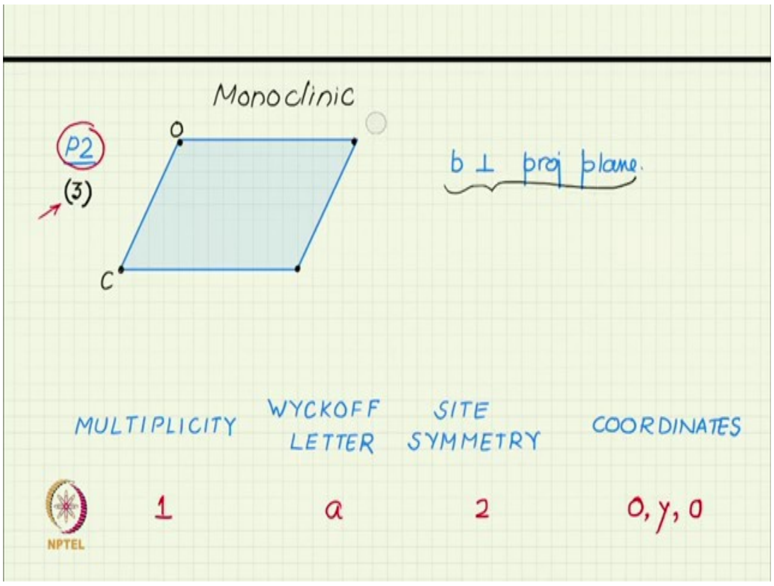
So, they cannot be generated only by symmorphic operations. So, they are not only contains non symmorphic operations they also require those non symmorphic operation they screw or glide as they are generated. So, obviously since the Hermann Mauguin's symbol as we saw contains the generators of the space group the symbol will contain symbols for screw and glide symmetry. So, it is very easy to identify from the symbol itself whether the space group is symmorphic or non symmorphic if you see a screw axis in this space group symbol in the H M symbol then it is non symmorphic.

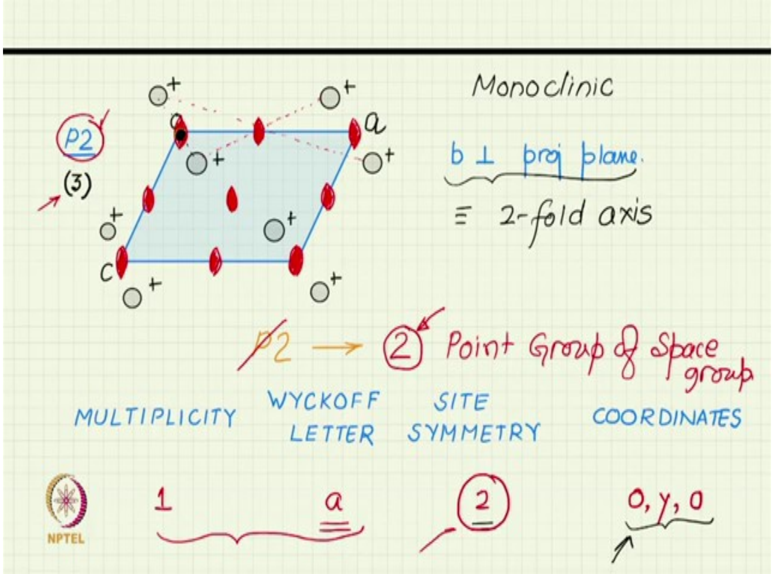
So, here there is a 2 1 screw. So, non symmorphic as c glide non symmorphic n n n non symmorphic. So, these are non symmorphic operators, which are required as generators. Another interesting distinction between the 2 groups 2 types of groups symmorphic and non symmorphic is in terms of the site symmetry. Now, by site symmetry as you know we mean symmetry point group symmetry of a particular site not the point group symmetry of the entire crystal not the point group symmetry of the space group.

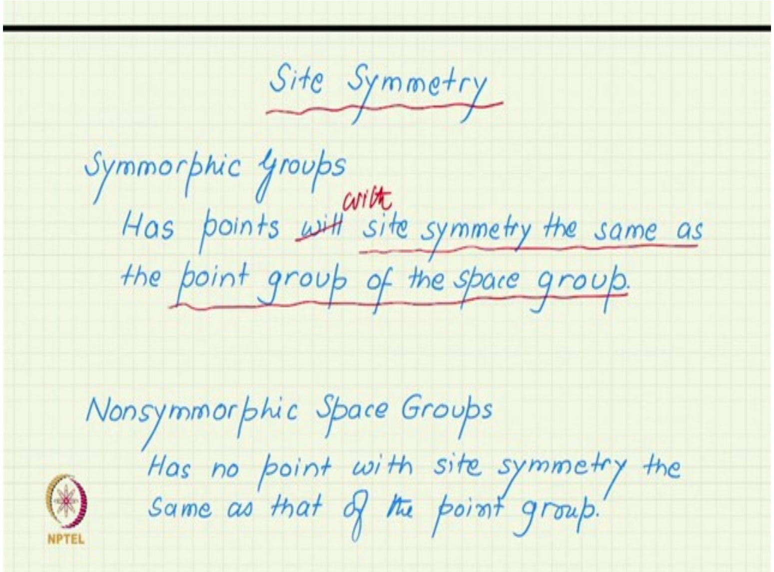
But point group symmetry at a site at a given site means what symmetry operations are actually leaving that particular site invariant that particular site fixed. So, if you look at from this point of view then symmorphic space groups has points, points with site symmetry the same as the point group of the same space group. So, every space group has a point group and every point in the space group every point in the space has it is own site symmetry group.

These 2 need not be equal but in the case of the symmorphic group you can find some sites all sites will not have this property but you will have some site which will have the same point group as the space group and non symmorphic space group this property is not true. So, there are no points with site symmetry the same as that of the point group of the space group.

(Refer Slide Time: 11:11)







So, again, this will become clearer when we take the examples. So, we now look at some of the simpler examples very simple space group. So, for example, I am taking a space group number 3 as you can see it is one of the very early space groups in the table of 230 space groups and this one is a monoclinic space group monoclinic crystal system for that requires only a 2-fold as you know and you can see from Hermann Mauguin symbol that this has a generator just a 2-fold.

So, P stands for capital P stands for primitive lattice. So, that means the lattice is primitive drawn the unit cell in the projection this is a b perpendicular the projection plane. So, let me fix this labelling this direction is a so this direction coming down slanting down is c the direction parallel to the horizontal direction on the page is the direction of a vector an O is the origin.

So, this is the projection of the unit cell the b axis is taken to be perpendicular to the plane of the projection and b axis is taken to be the 2-fold axis this is called the b setting and this is what is taken as the standard setting for monoclinic, although of course, you can make your 2-fold parallel to the c axis or you can make your 2-fold parallel to the a axis, but those are not common not so common and it is preferred to keep the 2-fold axis parallel to the b axis. So, if we now using the this 2-fold information if we start putting the 2-fold at a lattice point then obviously I will get 2-fold all the lattice points because all lattice points are equivalent.

Now, let me try to put a motif in a general position the 2-fold will rotate it 180 degree so will create a motif somewhere there I write a small plus there to designate that it may not it may not be exactly on the ac plane, but may have some high of plus y let us say so this is above the ac plane these notations you are of course familiar.

Now, since all lattice points equivalent you will have identical points identical pair of points at each lattice point. So, that completes the general position for these 2-folds at the corner. But you see that because of these positions now there are 2-folds already in between. So, for example this 2-fold is relating these 2 objects in this way and of course it will relate all other objects I want to draw all the lines, but these 2 also you can see are related by that 2-folds.

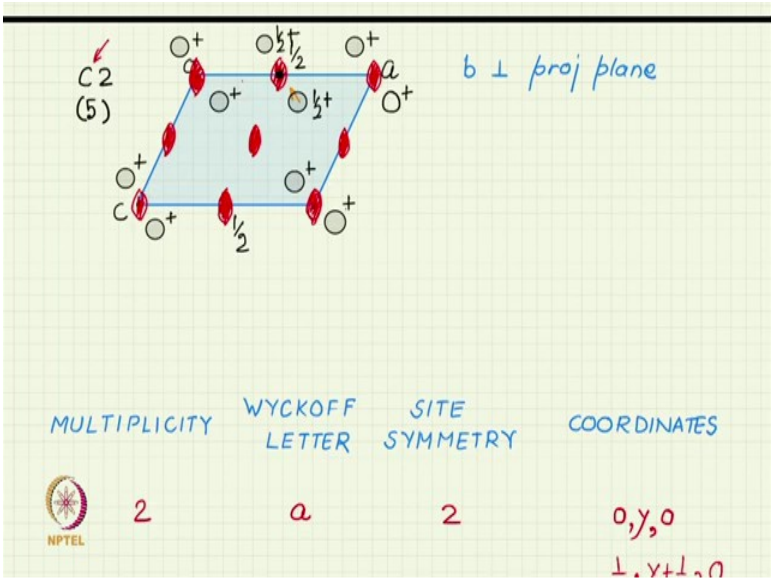
So, there is a 2-fold which comes in between this property we are familiar when we were looking at the plane groups also that whenever you have 2-fold axis passing through a lattice point, then in every translation direction, there will be another 2-fold axis at half the translation. So, similarly, you generate a 2-fold at c by 2 there are 2-fold here and 2-fold here and note the diagonal of this parallelogram is also a translation lattice translation that is the a plus c translation and they are also the same principle we have and you will get 2-fold in the center.

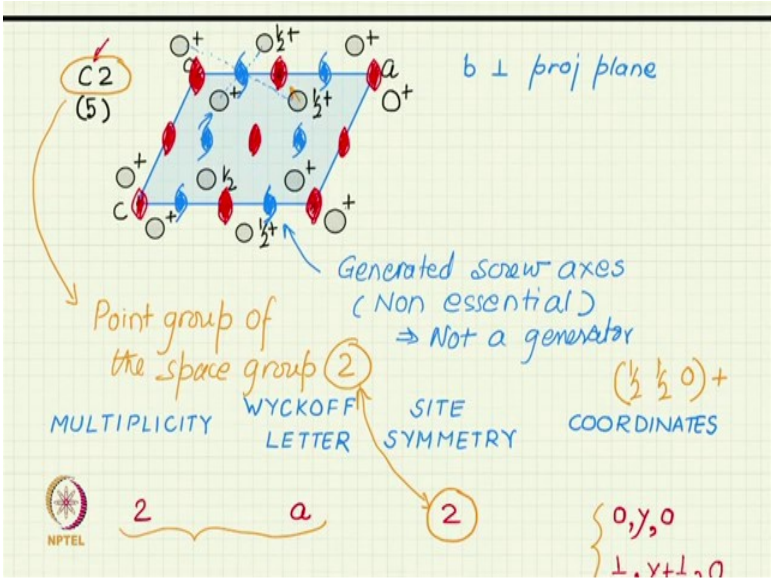
So, these 2-folds all get generated by our starting 2-fold if you look at the point with highest symmetry, remember Wyckoff letter a always gives you a point of highest symmetry. So, according to the international tables, the point of highest symmetry in this is a point with site symmetry 2 that is it is on a 2-fold axis and coordinate 0 y 0 if you look at that so 0 along a, y along b, so it is actually this special point by the circles which I showed you initially those were the general points but now we are talking of a special point and I am showing this let us say in some other color maybe black was better.

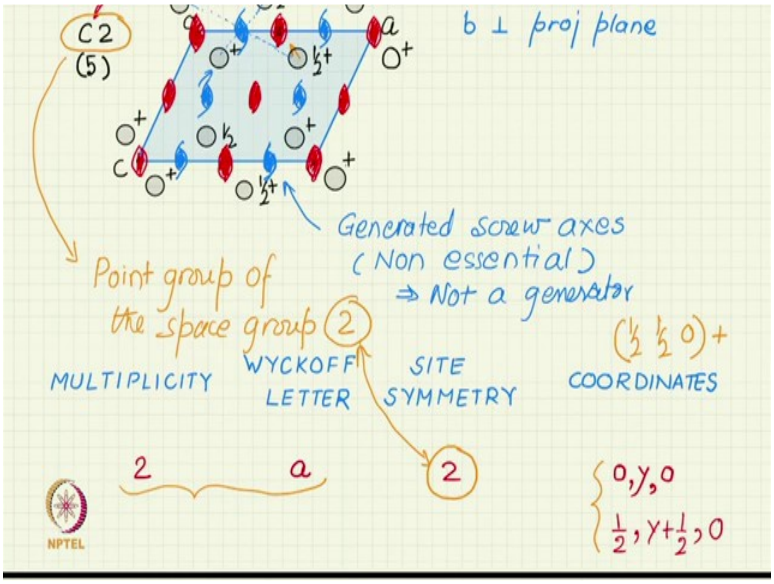
So, this black dot is representing this a special point 0 y 0. Now, if I try to create equivalent positions for this you can see that unlike this open circle which got rotated by 180 degree and gave you another equivalent point this will rotate on itself because it is on the rotation axis. So, it will not create any new equivalent position. So, that is why it will remain where it is and it site symmetry is 2 Hermann Mauguin's symbols gives you the point group of the space group and the method of data meaning that is to simply forget the letter symbol the centering symbol and convert any screw or glide to the normal rotation and mirror plane here that is not required we do not have a screw and glide.

So, the point group of this space group is 2 and you can see that the site symmetry of this location of Wycoff location 1 a generally Wycoff locations are named after by combining the multiplicity and the Wycoff letter. So, I will call this site one a. So, site one a had site symmetry 2 the space group also had the point group symmetry 2. So, this is what I meant when I said that has points with the site symmetry the same as the point group of the space group.

(Refer Slide Time: 19:15)







Now, c 2 is another interesting example by the letter c we mean c centering, c centering means the a b phase so I have lattice points at the corners but I have an additional lattice point on the a b phase which on the projection is there and it is on the center of the a b phase. So, come there and since it is on the center in the projection it is coming there but these will have a height half in the y direction.

So, you have 2 additional lattice points on these 2 faces that have half the y height. So, that is what will give you the c centering. But then I again start with my start generating the space group symmetry y put the 2-folds, 2-folds at the lattice point now the lattice point is on the centering face also. So, we get 2-fold there as well. And we have seen that it half positions also you will get so you get these 2-folds.

Now, again if I start putting my motif positions so in a general position I get these get like I had got the previous example but now the center of this this edge here this is all this was also a lattice point because of the c centering. So, I will have to place identical motif there also, but that is at half height. So, I will get a pair of points half height in the b direction but they are at I will write half plus indicate they are at half i you can get rid of some of these.

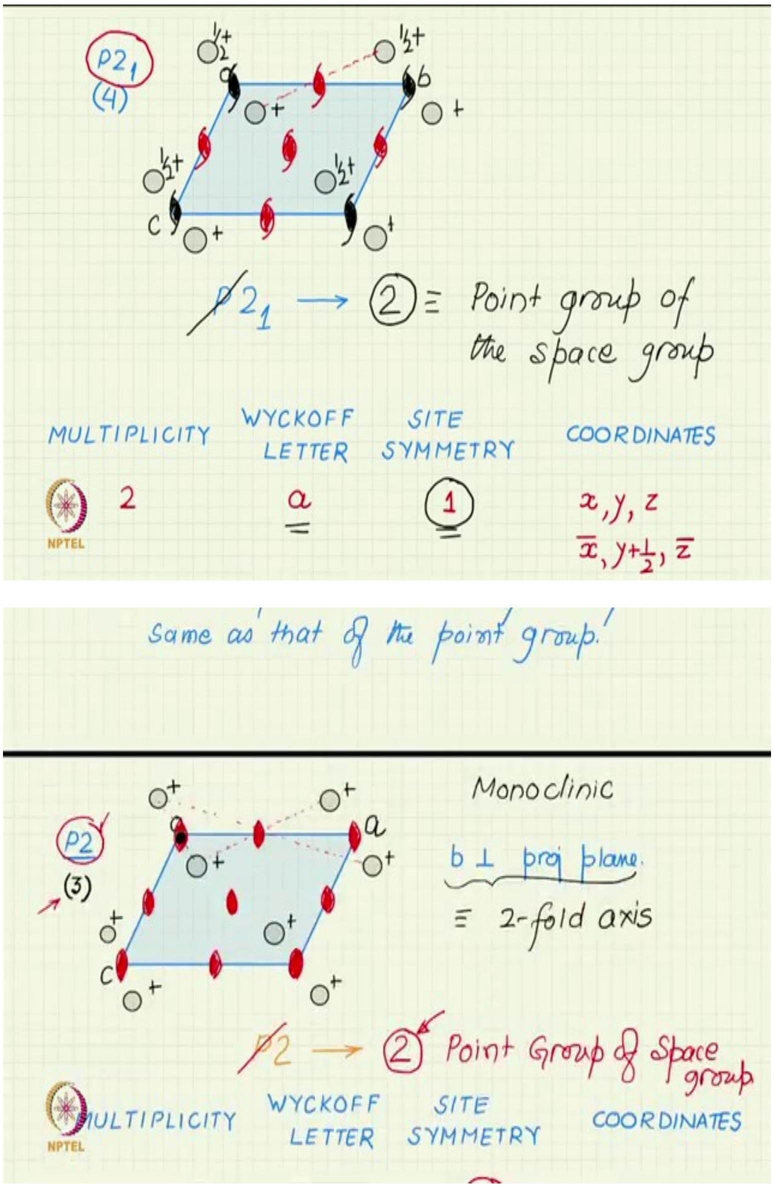
Similarly, for this face centering now an interesting thing happens that you can see now that because of these half positions, you find that you have actually introduced we have to many reds so, let me use blue for this purpose you have actually introduced a screw axis at these locations. So, if you take any point let us take this point and you rotate by 180 degree. So, it will get there but then you translate by half. So, you can see this was just plus it was plus y whereas this is half plus. So, this is half plus y. So, you have a y translation of half relating these 2 so there is a screw axis there.

Similarly, if you look at these 2 points now being connected so you rotate by 180 degree and translate by half. So, several screw axes get generated between these red 2-folds I do not have to create any new position the positions which were created by the 2 pure 2-fold also automatically gets related by the screw axis. So, this screw axis get generated by the action of the 2-fold and the translations.

So, this is a generated the screw axis, screw axis but they are not essential because you can see all the equivalent positions I could generate only by the pure 2-fold. So, that is why this is not a generator so in this space group symbol we are only using c 2 the pure 2-fold which shows the generator. Again, if you look at the location now the Wycoff location to a. So, it has a multiplicity 2, multiplicity is 2 because of the c centering now because 0 y 0 also gets replicated at half y plus half 0 because you have half, half 0 as you are centering translations.

So, any position will also have another equivalent position if you add half, half 0 so 0 y 0 and half y plus half 0 gives you take 2 coordinates to justify the multiplicity 2 but what is important that if you see the site symmetric 2 and again c 2 will give you the point symmetry 2 and these 2 are equal indicating another property of the symmorphic space group that this is a c 2 is also a symmorphic space group but I gave you this example to show that this is just a symmorphic space group but it is still contains non symmorphic operations it contains a screw axes.

(Refer Slide Time: 26:33)



But our final example, we take the P 2 1. So, here the 2-fold is the 2-fold a screw itself is the generating operator. So, y put it on the lattice points let it pass through the lattice points. It is again a P lattice. So, there is no centering translation here. So, I get these screws. So, compared to the with respect to the screws if I now put the equivalent positions. So, if this is plus y this will be half plus y because of the screw translation of half or lattice point will have identical set.

But now again you will see that just like between 2 2-fold axes, we found that another 2-fold was get generated between 2 screw axes also you are seeing that another screw axes is getting generated because these 2 points for example you can see a related by this is screw I can add all these additional screws but here there is no pure 2-fold only a screw access. So, for the generation of a space group that is crew symmetry is required. So, the Hermon Morgan's symbol has this screw operation as it is generator.

But if you find its point group so by the method of finding point group we cancel the letter but we also convert the screw axes to simply 2 so the point group of this space group is also 2 but the highest site symmetry in this case is just the identity. Site symmetry is 1 that is there is no point in the space group which remains fixed by any symmetry operation other than the identity. That is because in the 2-fold case in the pure 2-fold case points on the axis were invariant but in the case of a screw axes even points on the axis are not invariant because the rotation part will leave them invariant. But when you translate by half the point will move up or down along the axis.

So, there is no point which has a 2-fold rotational symmetry as it site symmetry. So, the point group of the highest point group or point with highest point site symmetry is simply 1 whereas point group of the space group is 2 and these 2 are not equal indicating that this is a non symmorphic space group. Thank you very much for your attention.