3D Space Groups XIV Interpretation of International Table Page

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Lecture-26a

Part 8: Positions

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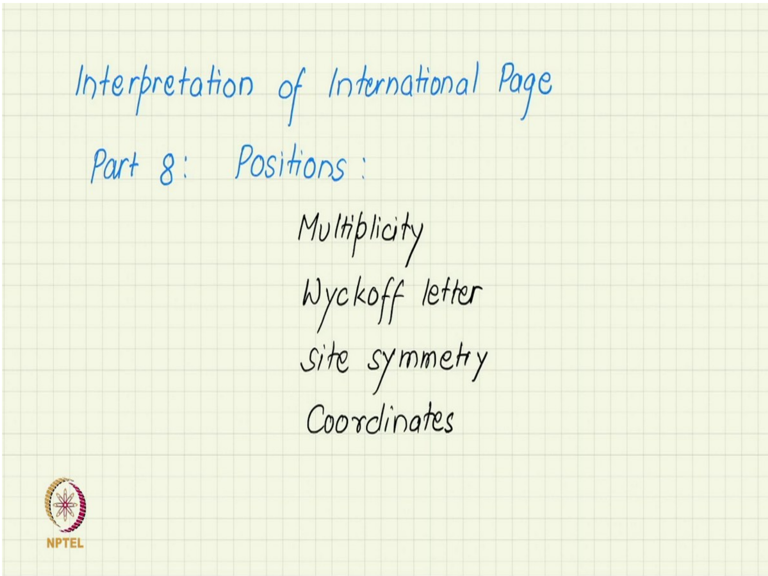

Let us continue the interpretation of International Table page, we are looking at one particular example as you know, the space group number 66 and using that example, we are explaining various concepts which are there on the international tables page.

So, in this part, we will look at a very very important section important block of international table, which is labeled as Positions. And this had several other important concepts, which are sub headings of within positions, which is called Multiplicity, Wyckoff letter, Site symmetry and Coordinates. So, we will look at these concepts in this video.

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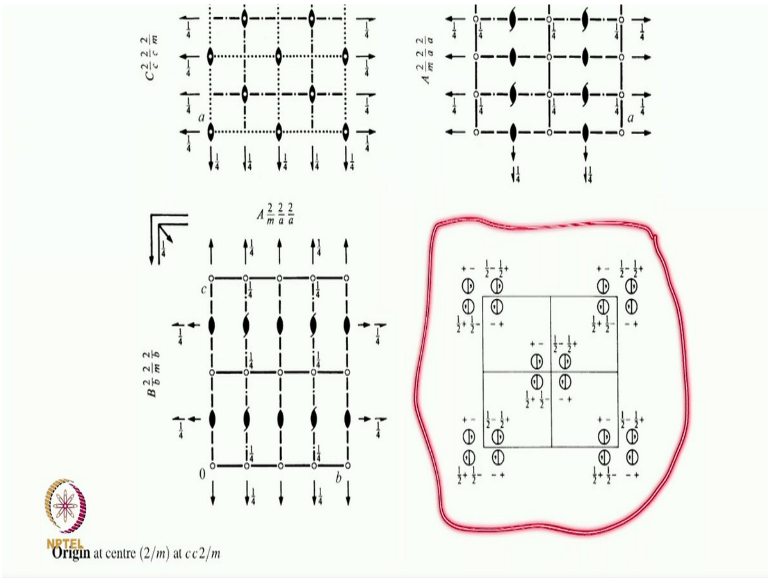

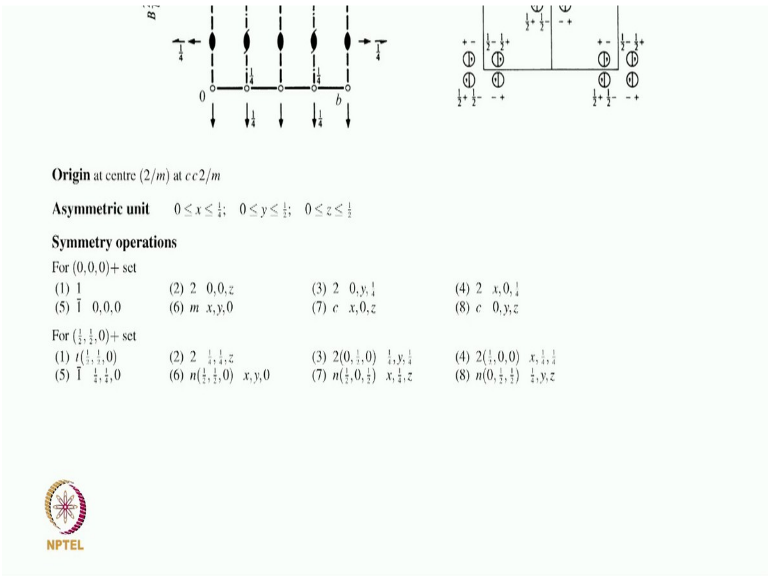

CONTINUED No. 66 $Cccm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
16	m	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x},\bar{y},z$ (6) $x,y,\bar{z}$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$ (7) $x,\bar{y},z+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}+\frac{1}{2}$ (8) $\bar{x},y,z+\frac{1}{2}$	hkl: $h+k=2n$ $0kl$: $k,l=2n$ $h0l$: $h,l=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
8	l	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
8	k	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl: $k+l=2n$

CONTINUED No. 66 $Cccm$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

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							Special: as above, plus
8	l	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
8	k	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl: $k+l=2n$

8	j	$..2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
8	i	$..2$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl: $l=2n$

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
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8	l	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
8	k	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl: $k+l=2n$
8	j	$..2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
8	i	$..2$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl: $l=2n$

8	h	$.2.$	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl: $l=2n$
8	g	$2..$	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl: $l=2n$
4	f	$..2/m$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	e	$..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	d	$..2/m$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
4	c	$..2/m$	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$

So, back to our tables page, this page group number 66, we have looked at much of the details on this page just to remind you, so, the headline giving the name of n number of the space group, the point group, encryptosystem and so, on.

Then symmetry element diagram, infact, there are 3 symmetry element diagrams which is 3 different projections, the ab, bc and ca projection in case of orthorhombic and the general projection diagram, this general projection diagram will be relevant for today also. So, we will look at that and then we discussed origin asymmetric unit, symmetry operations, all these are on one of the page, if we go to the next page the first item is generators selected which we discussed and then comes today's topic, which is the position.

So, look at the heading here. So, position and it has subheadings multiplicity, Wyckoff letter and Site symmetry and then it also has coordinates and then, there are list of these positions starting from and given by so called Wycoff letter starting from a at the bottom and then goes to b, c as you can see, going all the way up to m this m is not mirror, this m is simply the Wycoff letter giving the type of position, type of Wycoff position which these coordinates represent.

So, for each position, so, each of the line, each of the line here is one set of Wycoff position or example, this line is one set of Wycoff position and within that line, you have the first number. So, for example, in this case, the first number 8 is the multiplicity, second l is the Wycoff letter, and then dot dot m is the site symmetry followed by these coordinates. So, these 4 positions belong to this Wycoff site, the Wycoff site itself will be designated by multiplicity and the Wycoff letter.

So, we will call this we will name this row as 8 l, we will say Wycoff site 8 l. So, multiplicity and the letter is used as the designation of the positions themselves. So, this is just a brief introduction of the structure, let us look at the exact meaning of these terms one by one.

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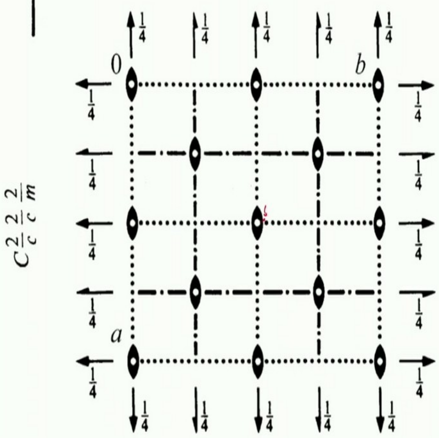
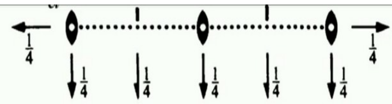
$C\frac{2}{c}\frac{2}{c}\frac{2}{m}$



							Special: as above, plus
8	l	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditions
8	k	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl: $k+l=2n$
8	j	$..2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
8	i	$..2$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl: $l=2n$
8	h	$.2.$	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl: $l=2n$
8	g	$2..$	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl: $l=2n$
4	f	$..2/m$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	e	$..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	d	$..2/m$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
4	c	$..2/m$	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$
4	b	222	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
4	a	222	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$

$C\frac{2}{c}\frac{2}{c}\frac{2}{m}$



Positions
- General Position
- Special "

So, to do that, I have pasted the cut and paste of the crystal symmetry element diagram on the same page to be able to quickly refer, but let us now define what these terms mean. So, the most important term here are the positions. So, positions can be either general position or a special position.

So, if you look at here, we started with the bottom row 4 a and then we went all the way up to the topmost row, which was 16 m. And now, the topmost row in every space group, the topmost row is what is called the general position, this row will be considered general position and all other rows other than the top row are special positions these are a special position. So, we will see what is general and what is special about them that comes from the general and especially comes from the concept of site symmetry.

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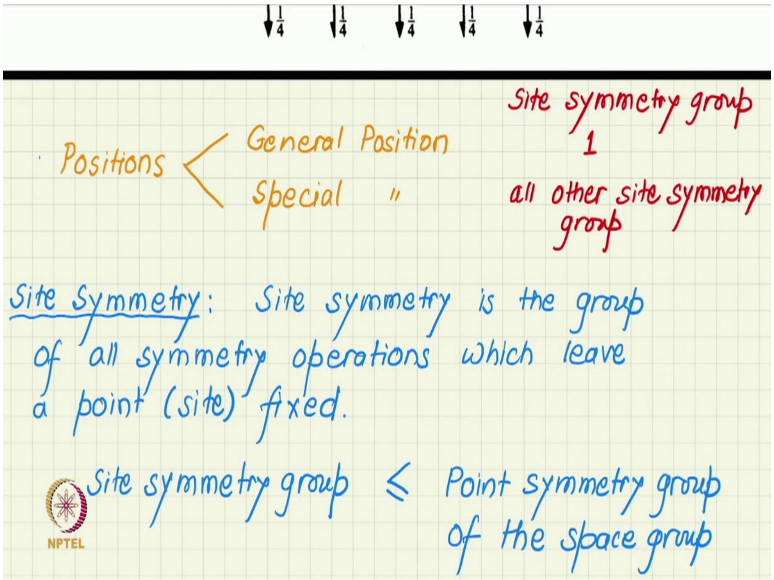

Let us define that, site symmetry is the group of all symmetry operations which leave a point the point is what we meant by site here. So, site symmetry is the group of all symmetry operations which leave a point fixed that is what is called Site symmetry.

So, all operations which leave a point of space fixed is the site symmetry group of that point and this will also be a point group and it will be a subgroup of the point group of the space group. So, site symmetry group is a subgroup of points symmetry group or point group of the space group, if so, when we are dividing general position and specially position we can add here now, this classification is based on the site symmetry group.

So, general position means the site symmetry group is just 1. So, only identity is the site symmetry group for general positions, which means, there are no operation in space group which will leave the point fixed only identity will leave it fixed, any other symmetry operation of the space group will move these points to some other point.

So, that is the general position special position all other sites symmetry. So, your site symmetry group includes any non trivial operation a 2 fold rotation mirror plane or a 4 fold rotation or whatever other than identity, then those positions are considered as a special position.

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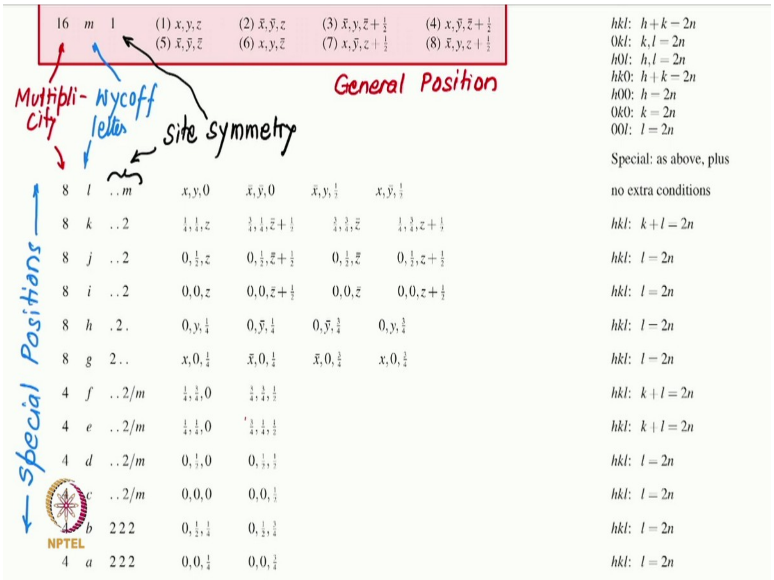

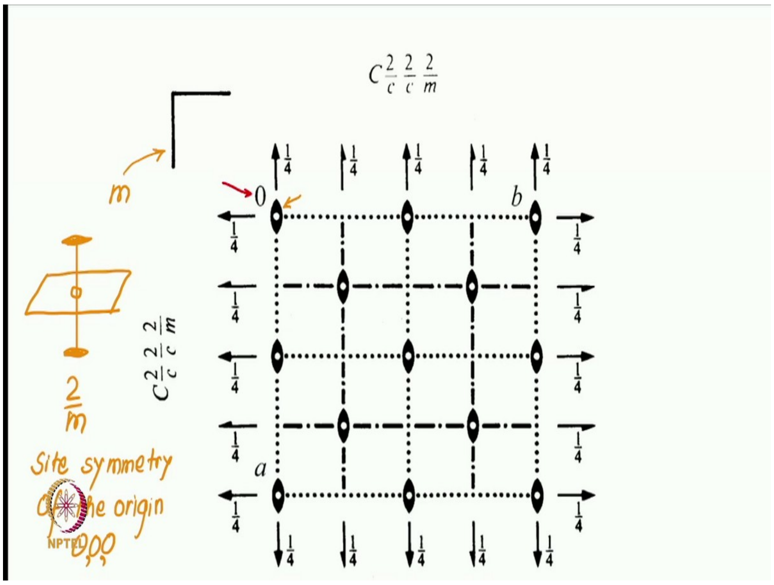

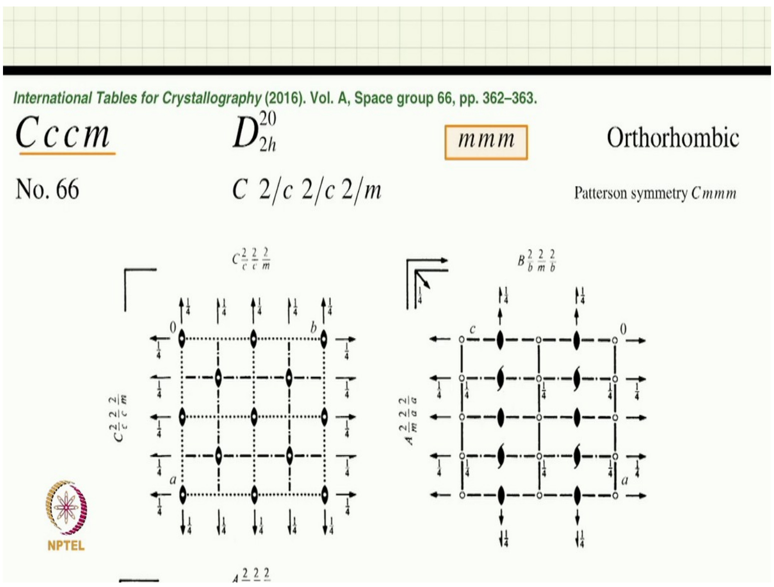

So, let us look at our diagram again. So, you can see that this last column, this last column here, this is what is giving the site symmetry group the sequence is explained here first multiplicity, so this is the multiplicity. This is the Wycoff letter and this part is the site symmetry of course, I have missed out the general position, the same thing is true for these also we can see that the general position the site symmetry is just 1.

Whereas, for a special positions always some non trivial operation is there in the site symmetry m or 2 or 2 by m or 222. So, they are special from the point of view that they have some symmetry operations, which leave these points fixed.

So, let us examine a particular site. So, the whole idea of this division into different Wycoff positions is to classify them by symmetry and by their symmetry equivalence. So, we will see that so, first of all let us look at the site symmetry. So, please note that when we were discussing the symmetry element of this space group, we realized that the center the origin of the space group is taken at the center.

So, this is the origin and origin is taken at the center, which is shown by a white dot inside the lens. Also, through that origin, the black lens, so is that a 2 fold axis is passing. And then this particular symbol of 2 orthogonal lines is showing that a mirror plane is also passing through the xy-plane. And since origin is located on the xy-plane, this mirror m also passes through the origin through the origin, a 2 fold axis passes that black lens, the center is located at the origin and a mirror plane passes through the origin, this symmetry you are now familiar, this is what is called a 2 by m symmetry.

So, if we draw it in perspective, so you have a 2 fold axis, that is what is shown by a lens in the projection, then you have a mirror plane that is what is shown by the orthogonal 2 orthogonal lines. And you have a center of inversion, which is shown by the white hole inside the lens. So, this point group is called 2 by m.

It is actually a monoclinic point group. But here, it is appearing as a site symmetry of the origin. So, site symmetry, this is the site symmetry origin that is points with coordinate 000. The point with coordinate 000 has the site symmetry.

If you look at the point group symmetry of the space group that is m m m. Remember, to convert or to derive the point group from the space group symbol, all we have to do is to remove the first letter, which is the centering symbol. So, in this case the capital C and then convert any glide plane or screw axes to normal mirror plane and normal rotation axes. In this case, there are no screw axes, but there are 2 glide planes CC, so the both of them get converted to m m. And that is why you get the point group, which is mmm.

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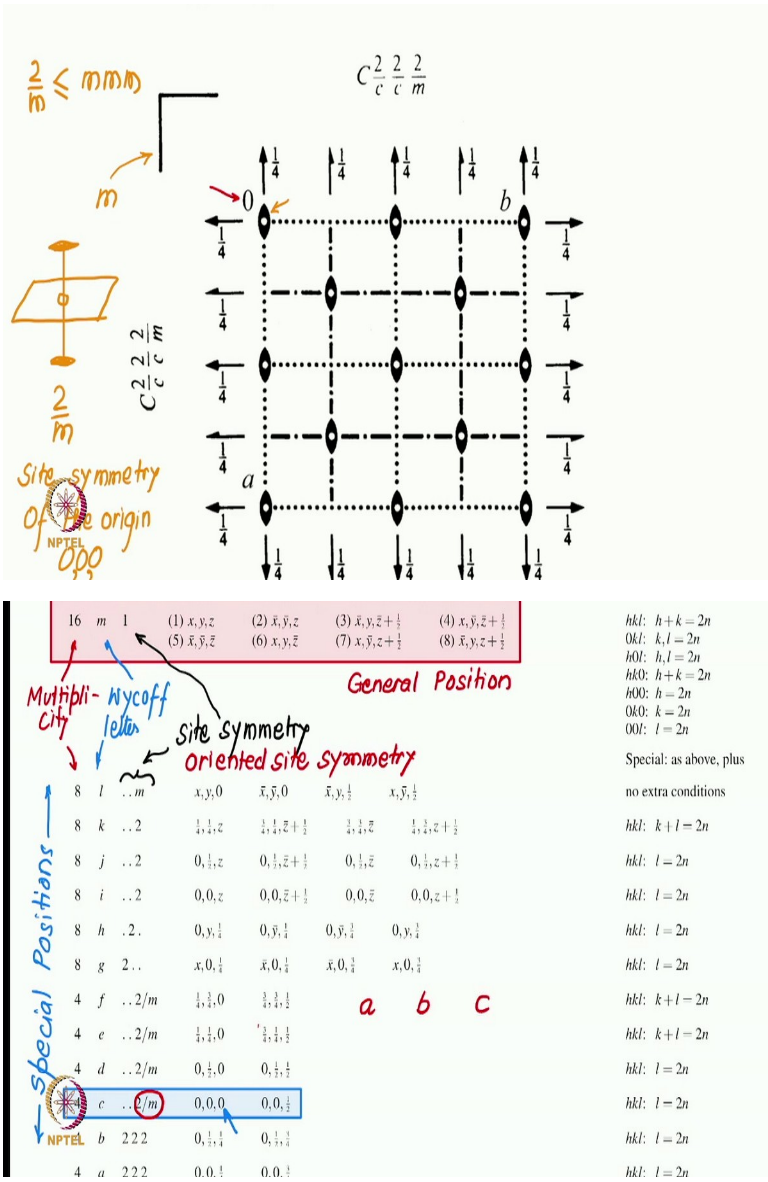

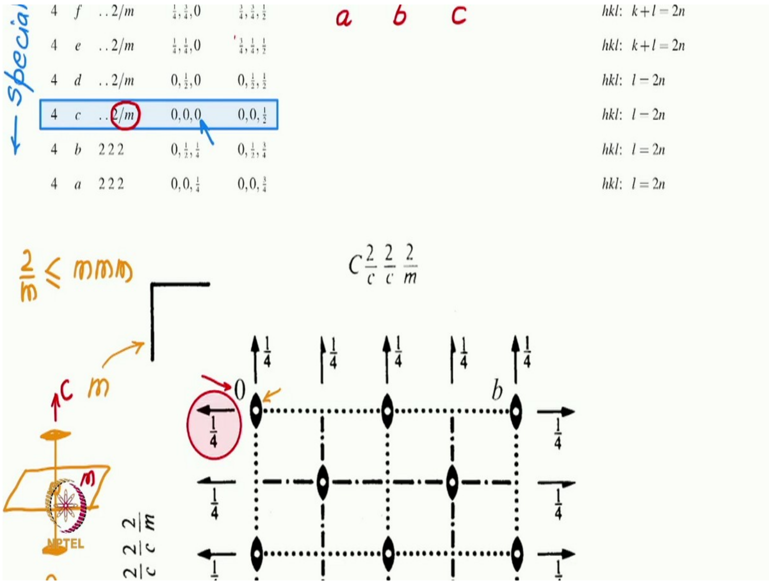

Now, coming back to the Site symmetry of the origin you will see the other site symmetry of the origin is 2 by m. And this 2 by m is a subgroup of mmm, so the site symmetry will always be a subgroup of the point group symmetry of the space group.

Let us look at in the list, in the list the coordinate 000, is coming here. Let us highlight that. So, we are looking at this the origin is coming there. And you can see that the site symmetry is listed as 2 by m only thing is that there are 2 dots which are preceding this 2 by m. And that is because this site symmetry is actually what is called an oriented site symmetry.

The symbol is slightly different from normal point look, if I was describing the normal point group, I would have just said 2 by m. But in this case, I am calling it dot dot 2 by m. So, this is because this is an orthorhombic system. And in orthorhombic system, you know that the symmetries are listed along a b and c axes. And in this case, you will see that the 2 fold axis is along the C axis the mirror plane is perpendicular to the C axis and center of inverse and of course does not have any orientation.

So, both the axis 2 is and m are in the sense along the C axis. But what about the x and y axis? So, along that you do not have any symmetry, in this case, because you have, you can see that along the x axis, there is a 2 fold axis shown here, but its height is 1 by 4. So, it is not really passing through the origin, it is parallel to the x-axis, but it is not it is missing the origin, it is not going at 0 high.

Similarly, the same thing is true for the one along y-axis. So, it is passing at height 1 by 4. So, it misses the origin. So, origin just have this 2 by m and along x and y, there are no symmetry. So, finally, we have this dot dot 2 by m as the site symmetry for this particular point.

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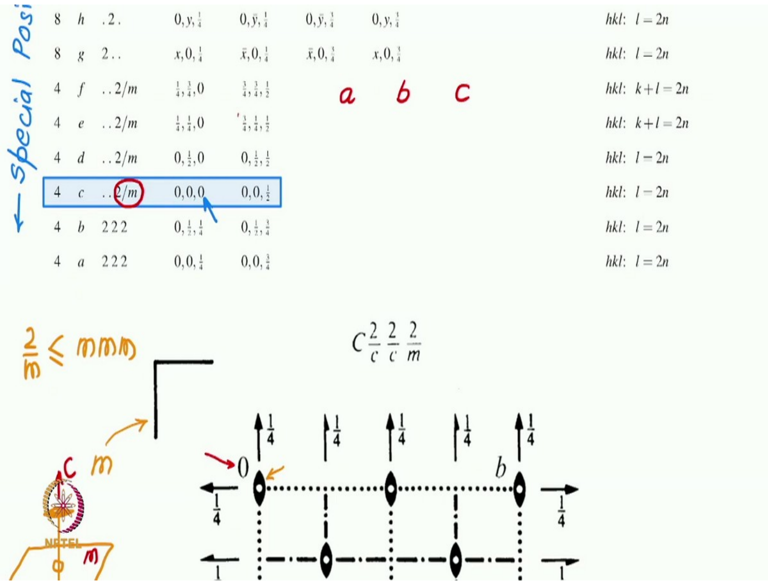

Now, let us come. So, similarly, you can interpret site symmetry of any other points, which are given here. So, let us take one more example. This 2 2 2 is looking interesting just now, I told that we did not consider 2 as part of the site symmetry for origin because it was missing the origin, but these 2, 2 folds you can see here these 2, 2 folds both of them are at height quarter.

So, obviously, at quarter height, they will be intersecting and the z axis is anyway the 2 fold. So, they at quarter high at this location, you will have at quarter height at this location, you will have 3, 2 folds intersecting one along x axis, one along y axis and one along z axis. So, the point group at height one fourth, 1 by 4 will be 222. That is exactly what is being indicated here. You can see that at 0011 quarter, that is the point where 3, 2 fold along x along y and along z are going.

So, you get the site symmetry there 222 there are no dots here, because along all 3 axes, you have some symmetry or 2 fold symmetry, but that is for the coordinate 004.

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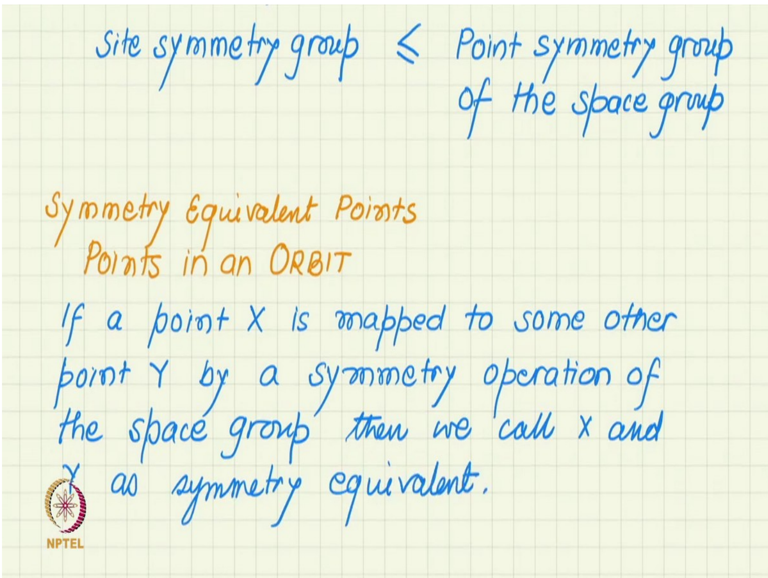

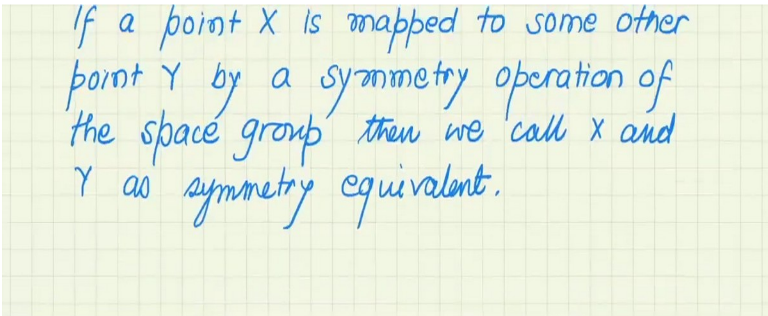

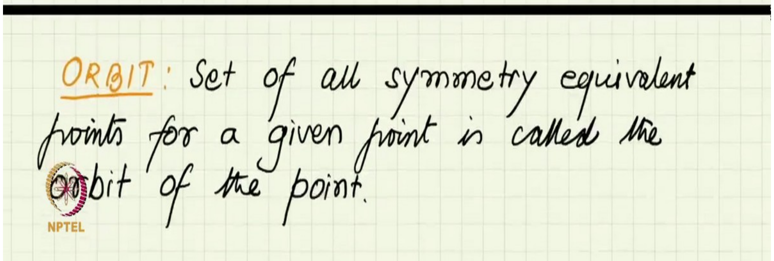

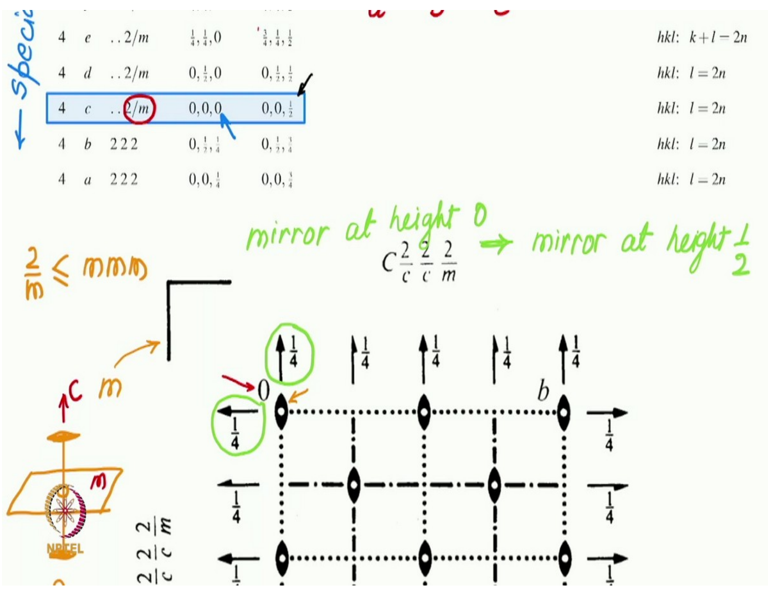

Now, the next one set is so, we have understood the site symmetry and next concept is of symmetry equivalent points. Sometimes these are also called points in an orbit. So, this concept is related to the symmetry of the space group, if one point is mapped to some other point by a symmetry operation.

So, let us define this also. If if a point X is mapped to some other point Y by a symmetry operation of the group this group here is a space group symmetry operation of the space group then we call X and Y as symmetry equivalent and set of all symmetry equivalent point.

This orbit concept not very common, commonly used with this is nothing but a set of all points for a given point. So, if we take a point and find all points which are symmetry equivalent to it, they are called to form an orbit. So, this set will be called an orbit it will be unique orbit for a given point is called the orbit, or a point is set to belong to that orbit or all points form the orbit.

So, so, in this so, let us look at this idea now. So, when I was talking about the origin, o, I said that, o has a site symmetry 2 by m, but If you can see that another point is also listed along with that, 000 along in the same row that is 00 half.

So, that is a point along the z-axis with coordinate half is in the same Wycoff row, in the same Wycoff position as the origin, why is it so? So, please recall that this means that there is some symmetry operation of the space group which will take me, take the origin to 00 half.

What is that symmetry operation, which takes the origin to 00 half, that symmetry operation is we will have to recall some of your symmetry principles which you have learned the mirror is shown here at 0, 0 height mirror at height 0 because no no height is specified.

So, this is a mirror at height 0, but then a mirror at height 0, also implies no but sorry I was getting diverted the mirror, I was just going to say let me complete this, but this will not be relevant to the discussion we are having at the moment mirror at height 0, also implies mirror at height half because the translation distance between mirror is half the lattice translation in that direction.

So, that is fine, but I got diverted that is not the symmetry operation which can map 000 to 00 half, the symmetry operation which is mapping the origin to 00 half is actually this one, the 2 fold at quarter, you can see that if you rotate the origin about this axis, which is at quarter height, then origin will move by 180 degree rotation about this axis to height half.

So, in fact, this is not the only operation there is another 2 fold in the other direction, both these operations will map 000 to 00 half. So, that is why they are symmetry equivalent. They are symmetry equivalent by this 2 fold rotation and they belong to the same orbit.

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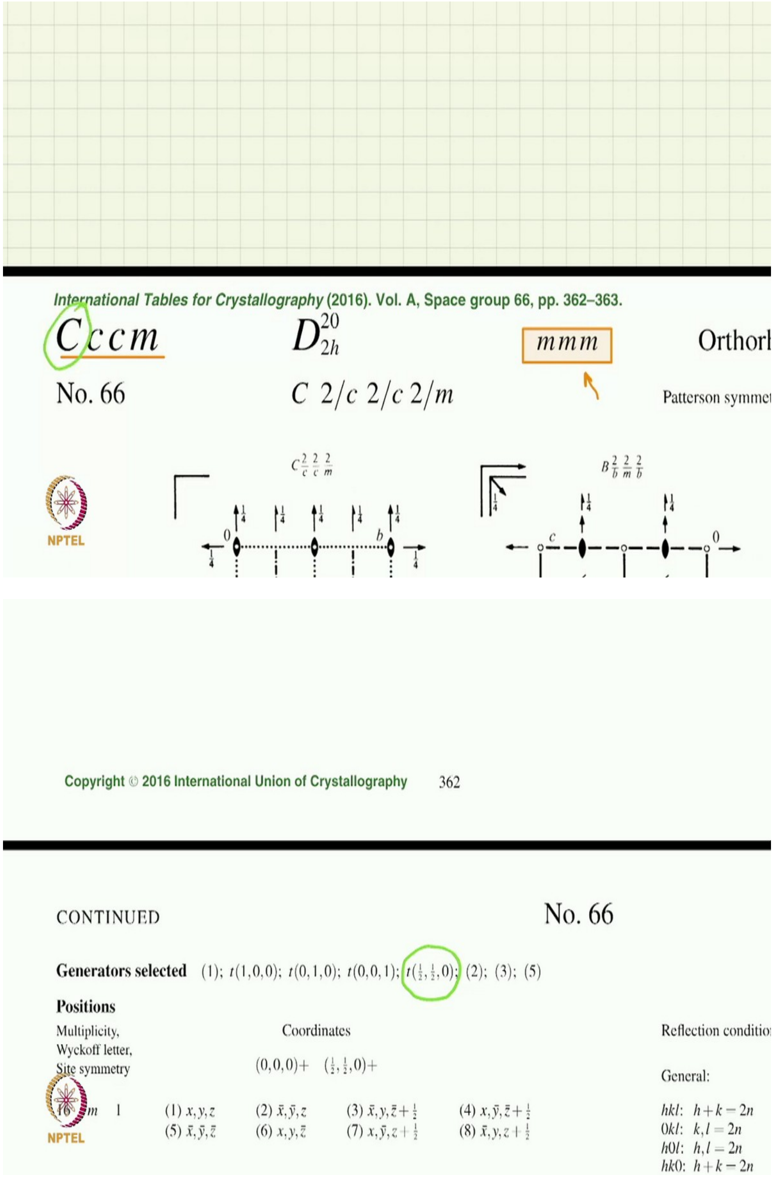

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(\frac{1}{2},\frac{1}{2},0)$; (2); (3); (5)

Positions

Multiplicity, Wyckoff letter, Site symmetry

Coordinates

$(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$

Reflection conditi

Mult.	Wyckoff	Site sym.	Coordinates				Reflection conditions
							General:
16	m	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}+\frac{1}{2}$	hkl: $h+k=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x},y,z+\frac{1}{2}$	$0kl$: $k,l=2n$
							$h0l$: $h,l=2n$
							$hk0$: $h+k=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above,
8	l	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditior
8	k	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl: $k+l=2n$
8	j	$..2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
8	i	$..2$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl: $l=2n$
8	h	$.2.$	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl: $l=2n$
8	g	$2..$	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl: $l=2n$

General Position

Multipli-city

Wycoff letter

site symmetry

oriented site symmetry

Positions

NPTEL

Mult.	Wyckoff	Site sym.	Coordinates				Reflection conditions
16	m	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}+\frac{1}{2}$	(4) $x,\bar{y},\bar{z}+\frac{1}{2}$	hkl: $h+k=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x},y,z+\frac{1}{2}$	$0kl$: $k,l=2n$
							$h0l$: $h,l=2n$
							$hk0$: $h+k=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above,
8	l	$..m$	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra conditior
8	k	$..2$	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl: $k+l=2n$
8	j	$..2$	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
8	i	$..2$	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl: $l=2n$
8	h	$.2.$	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl: $l=2n$
8	g	$2..$	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl: $l=2n$

General Position

Multipli-city

Wycoff letter

site symmetry

oriented site symmetry

Mult.	Wyckoff	Site sym.	Coordinates				Reflection conditions
4	f	$..2/m$	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	e	$..2/m$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	d	$..2/m$	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
4	c	$..2/m$	$0,0,0$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $l=2n$
4	b	222	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$

a b c

Special Positions

NPTEL

Y as symmetry equivalent.

ORBIT: Set of all symmetry equivalent points for a given point is called the orbit of the point.

NPTEL

Now, are these the only point 2 points no, because this is a C centered lattice, C centered lattice. Remember this C centering. And C centering gives you if you remember the generators. So, one of the generating translation is half half 0, that is exactly what is meant by centering.

So, if you apply half half 0, half half 0 is supposed to be added to any of the coordinates listed here. So, this is simply for to reduce the effort of printing or reduce the effort of writing that those coordinates are not written or they are written in a shorthand notation here.

Notice that once and for all on the top block itself, it is given that all coordinates we have to add 00 Plus and half half 0, 000 adds nothing. So, the coordinates given corresponds to 000. But coordinates not given has to be implied has to be understood that I have to create new points by adding half half 0. So, if I add half half 0 to these coordinates, then I will get to more coordinates half half 0 by adding it to 000 and half half half by adding the centering translation to 0 0 half.

So, these positions are also symmetry equivalent to the origin. So, in the end, you get these 4 points within the unit cell. Now, orbit, the concept of orbits which I told you is a set of all symmetry equivalent points.

So, what is the size of the orbit? How many members are there in the set? Well, this set is infinite, because we are talking about the space group the symmetry, which we are talking about the space group and in the space group, you know, that there are infinite operations, the translations themselves are infinite and the rotations are distributed about infinitely many axes.

So, there are infinitely many operations. So, each point will be mapped to infinitely many different points. So, the orbit is actually infinite, but what is listed here is only those points of orbit which belong to a given unit cell.

So, that is why within the unit cell in in the orbit of origin 000, only these 4 points are there 000, 00 half, half half 0 and half half half and out of these also as I told you, half half 0 and half half half are not explicitly listed, but is left to be interpreted from the sign here, half half 0 plus.

So, I have listed it explicitly and these 4 points are now belonging to the same orbit, they are all symmetry equivalent, they all have site symmetry 2 by m. And so, they belong by definition to the same Wycoff position.

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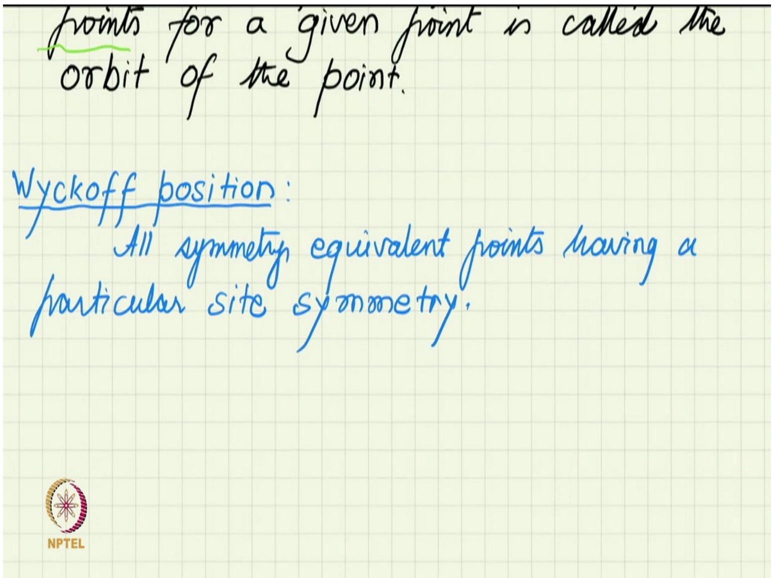
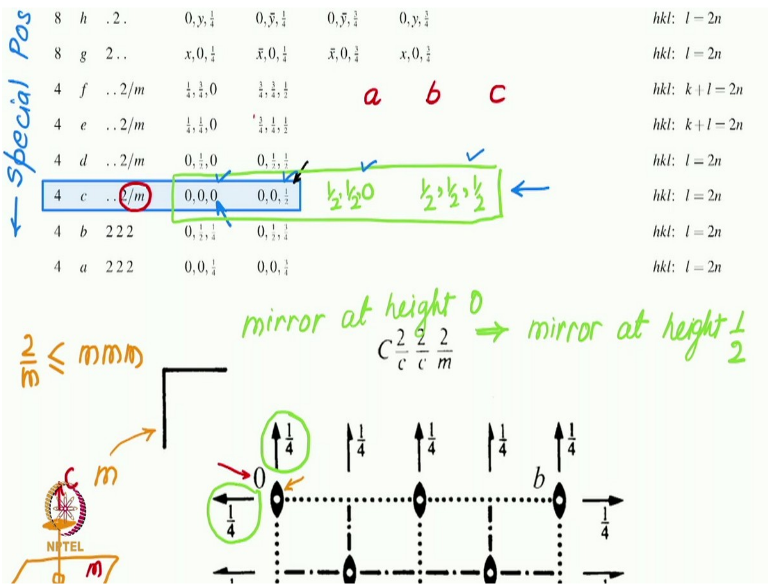
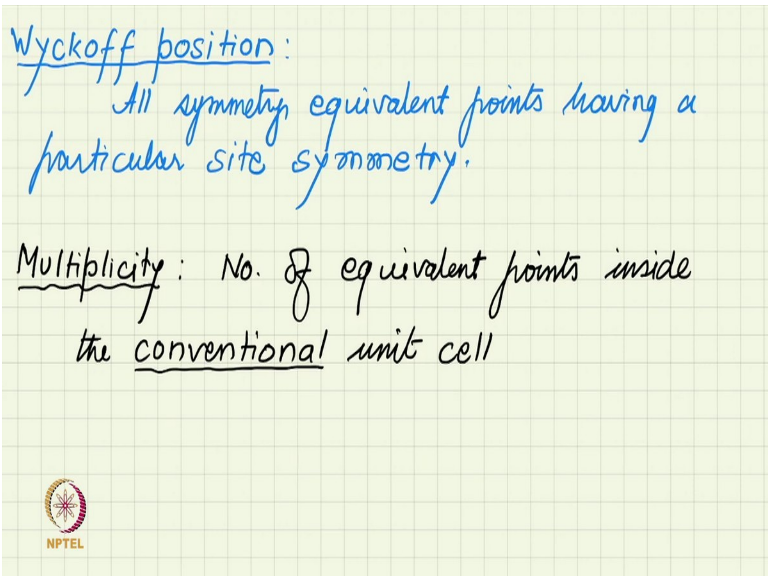




8	h	.2.	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl: $l=2n$
8	g	2..	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl: $l=2n$
4	f	..2/m	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	e	..2/m	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	d	..2/m	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
4	c	..2/m	$0,0,0$	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $l=2n$
4	b	222	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
4	a	222	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$



← Special Positions —

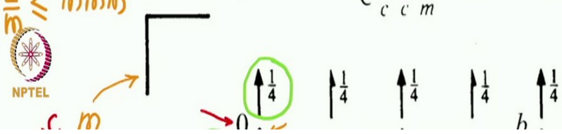
8	k	..2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl: $k+l=2n$
8	j	..2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
8	i	..2	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl: $l=2n$
8	h	.2.	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl: $l=2n$
8	g	2..	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl: $l=2n$
4	f	..2/m	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	e	..2/m	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	d	..2/m	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
4	c	..2/m	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$
4	b	222	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
4	a	222	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$

a b c

→ 4c Wyckoff position.

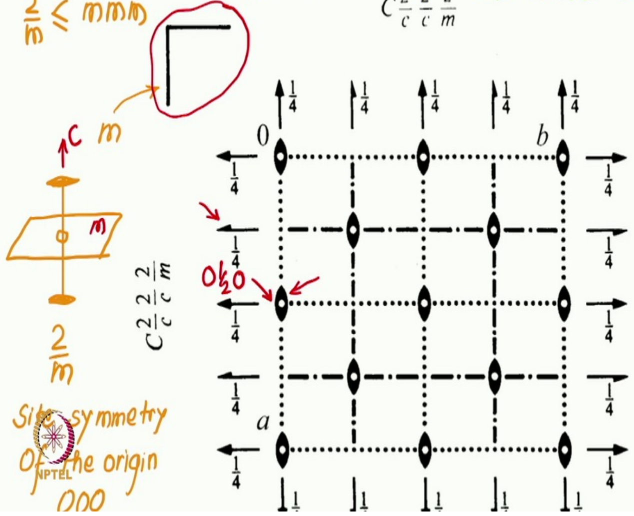
mirror at height 0 $C\frac{2}{c}\frac{2}{c}\frac{2}{m}$ ⇒ mirror at height $\frac{1}{2}$

$\frac{2}{m} \leq mmm$



mirror at height 0 $C\frac{2}{c}\frac{2}{c}\frac{2}{m}$ ⇒ mirror at height $\frac{1}{2}$

$\frac{2}{m} \leq mmm$



16	m	1	(1) x,y,z	(2) [illegible]	(3) [illegible]	(4) [illegible]
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x,y,\bar{z}$	(7) $x,\bar{y},z+\frac{1}{2}$	(8) $\bar{x},y,z+\frac{1}{2}$

Reflection conditions:
hkl: $h+k=2n$
$0kl$: $k,l=2n$
$h0l$: $h,l=2n$
$hk0$: $h+k=2n$
$h00$: $h=2n$
$0k0$: $k=2n$
$00l$: $l=2n$

General Position

Multipli-city

Wycoff letter

site symmetry

oriented site symmetry

Special: as above, no extra condition

← Special Positions —

8	l	..m	$x,y,0$	$\bar{x},\bar{y},0$	$\bar{x},y,\frac{1}{2}$	$x,\bar{y},\frac{1}{2}$	no extra condition
8	k	..2	$\frac{1}{4},\frac{1}{4},z$	$\frac{3}{4},\frac{1}{4},\bar{z}+\frac{1}{2}$	$\frac{3}{4},\frac{3}{4},\bar{z}$	$\frac{1}{4},\frac{3}{4},z+\frac{1}{2}$	hkl: $k+l=2n$
8	j	..2	$0,\frac{1}{2},z$	$0,\frac{1}{2},\bar{z}+\frac{1}{2}$	$0,\frac{1}{2},\bar{z}$	$0,\frac{1}{2},z+\frac{1}{2}$	hkl: $l=2n$
8	i	..2	$0,0,z$	$0,0,\bar{z}+\frac{1}{2}$	$0,0,\bar{z}$	$0,0,z+\frac{1}{2}$	hkl: $l=2n$
8	h	.2.	$0,y,\frac{1}{4}$	$0,\bar{y},\frac{1}{4}$	$0,\bar{y},\frac{3}{4}$	$0,y,\frac{3}{4}$	hkl: $l=2n$
8	g	2..	$x,0,\frac{1}{4}$	$\bar{x},0,\frac{1}{4}$	$\bar{x},0,\frac{3}{4}$	$x,0,\frac{3}{4}$	hkl: $l=2n$
4	f	..2/m	$\frac{1}{4},\frac{3}{4},0$	$\frac{3}{4},\frac{3}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	e	..2/m	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},\frac{1}{2}$			hkl: $k+l=2n$
4	d	..2/m	$0,\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$			hkl: $l=2n$
4	c	..2/m	$0,0,0$	$0,0,\frac{1}{2}$			hkl: $l=2n$
4	b	222	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$			hkl: $l=2n$
4	a	222	$0,0,\frac{1}{4}$	$0,0,\frac{3}{4}$			hkl: $l=2n$

a b c

→ 4c Wyckoff position.

So, we come to the definition of Wycoff position role symmetry equivalent points having a particular site symmetry. So, 2 conditions are required for belonging to the same Wycoff position, they should have the same site symmetry and they should also be symmetry equivalent.

So, these 4 positions, which we are considering here listed within the unit cell are symmetry equivalent, all of them have the site symmetry 2 by m, or dot dot 2 by m if you so, please. So, all of them belong to the same Wycoff position and this Wycoff position is then given a letter which is more or less arbitrary chosen by Wycoff letter c.

So, we will call this particular row on which we are focusing the Wycoff petition containing the origin as Wycoff Site C. Infact, we will call it Wycoff site 4 C, because as I told you in naming of the particular Wycoff position multiplicity is also included, but then what is this multiplicity.

So, we have seen the multiplicity is nothing we have not defined yet, but we are seeing that 4 equivalent positions are there within this unit cell for the origin. So, origin belongs to an orbit out of which 4 points belong to the unit cell. So, the number of equivalent points belonging to the unit cell is what is called the multiplicity and that is why the multiplicity is given here as 4.

So, let us write that as definition. So, multiplicity number of equivalent points inside the conventional unit cell, conventional unit cell, meaning the unit cell shown in the space group, the very definition of conventional unit cell is the unit cell used by International Table to depict or to show that particular space group.

So, you just have to count how many equivalent positions are there in any Wycoff position and that will be the multiplicity of that position. So, let me let me clean this up for the moment. And let me remove these annotations.

So, so, this particular one is the Wycoff projection we were considering, see there are only 2 coordinates, but the multiplicity is 4 because it is a C centered lattice and we do not have to forget this particular instruction. That half half 0, has to be added to all positions. So, the number gets duplicated. So, only 2 pages is shown, but multiplicity is 4 and this site will be called 4C site.

Now, notice that 4D, the row just above it, let us focus on this 4D that also has point group 2 by m, dot dot 2 by m. So, that means, these points also have exactly the same site symmetry, but still they belong to different Wycoff position, why is it so, not the definition of Wycoff position we required 2 things that points should be having the same site symmetry, but they should also be all symmetry equivalent.

In this case, what happens that although these 2 points the points in position 4C and points in position 4D although they have the same site symmetry, but they are not equivalent to each other that is, there is no symmetry have a space group which will take origin to origin which belongs to 4C to a point 0 half 0 which belongs to 4D, let us see whether that is true.

Let me clean up some of the notations here also and so, there is an origin and we are saying that it cannot be taken to let us say this particular point 0 half 0. So, 0 half 0 so, that is a point midway on the x-axis here, 0 half 0.

Why is there no symmetry in which can take 000 to 0 half 0, you can see here that there is means I can apply all the symmetry elements are already shown here. And if you apply any symmetry operation, so, for example, if you apply the only suitable ones look like for example, this true axis at quarter.

So, this is true axis at quarter will bring 002 at the same level as this point, but due to the translation associated, it will shift it away. And also since it is not in the plane, it is at quarter height. So, it will take 000 to half height first of all and then after half heght it will give a translation also in the y-axis.

So, you cannot bring it to 0 half 0 by this 2 fold similarly, you can explore other symmetry operations present in the space group, you will not find any symmetry operation in the space group, which can map 000 to 0 half 0. So, they belong to different Wycoff positions.

But if you look at the symmetry at 0 half 0, so what is the symmetry at 0 half 0 you can see that the 2 fold axis is passing there also parallel to the C axis, 0 half 0 is in the, at height 0. And at height 0 there is a center of innovation shown and at height 0, there is a mirror plane shown here by these 2 orthogonal lines.

So, the symmetry here also is exactly 2 by m or dot dot 2 by m. So, these 2 positions 000 and 0 half 0, they have the same site symmetry 2 by m, but still do not belong to the same Wycoff position, because there is no symmetry operation which can take points from one position to another position. So, that is also important.

So, this way, you can analyze and see other Wycoff positions yourself, I have just taken a simpler example here. And similarly, the multiplicity and Wycoff letter will keep changing as we go up in the table. The beauty of this Wycoff classification is that it has classified all possible different kinds of sites, symmetries, which you can have.

So, in this space group, these are the only possible sites symmetries, you can have either 2 2 2, we are going from bottom to top, I am seeing 2 2 2, or 2 by m, or just a 2 fold axis. And you can see that 8 G is a 2 fold axis along the a-axis. Whereas 8 H is dot 2 dot. So, it is a 2 fold axis along the y-axis, 8 i is dot dot 2. So, it is a 2 fold axis along z-axis.

So, with this, I think we have discussed in quite a bit detail, this Wycoff nomenclature and other concepts associated with this position, general position and specially position. So, I think we will stop here. Thank you very much.