Electron Diffraction and Imaging

Prof. Sundararaman M
Department of Metallurgical and Materials Engineering
Indian Institute of Technology, Madras

Lecture - 06
Symmetry in 3-D Crystals

Welcome you all this class on a diffraction and imaging, in the last class we considered symmetry elements associated with the 2 dimensional lattice both the point group symmetry and the 2 dimensional space group symmetry we will discuss. On the same length today we will discuss the 3 dimensional point groups and space group symmetry. I have told you earlier itself that what is the need for having information about the point group symmetry, because the properties of the material essentially exhibit point of symmetry including when crystals form their external crystal form one can look at it and identify the symmetry elements which are associated with it. What are the symmetry elements which we considered for point to pin 2 dimensional crystal symmetry elements which we consider.

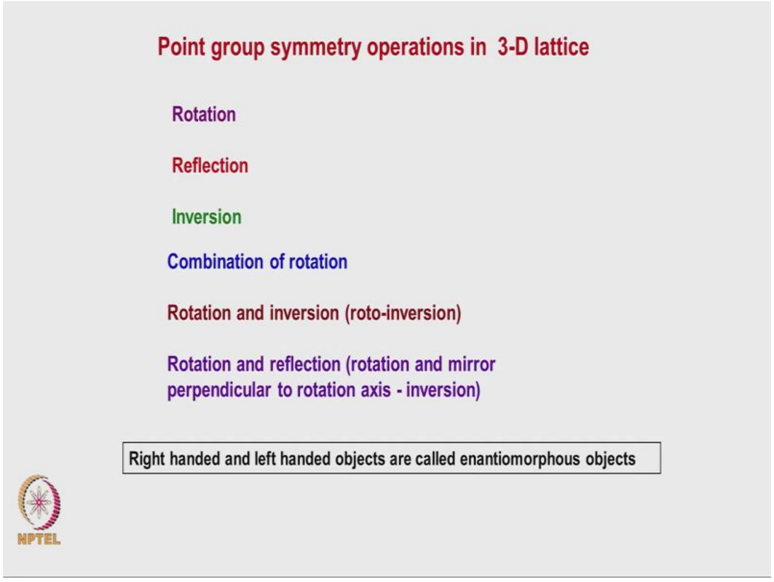
Student: Rotation (Refer Time: 01:23).

Rotation then.

Student: Rotation mirror (Refer Time: 01:26).

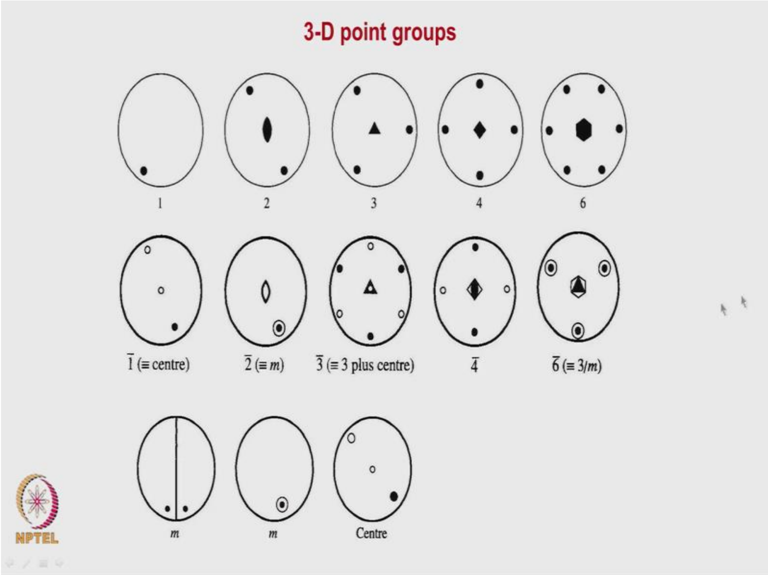
Rotation mirror these are all the 2 symmetry elements which we consider. In the case of 3 dimensional lattice we have to consider in addition to rotation and mirror, we will be considering inversion also, but I had already mentioned about what an inversion is.

(Refer Slide Time: 01:49)



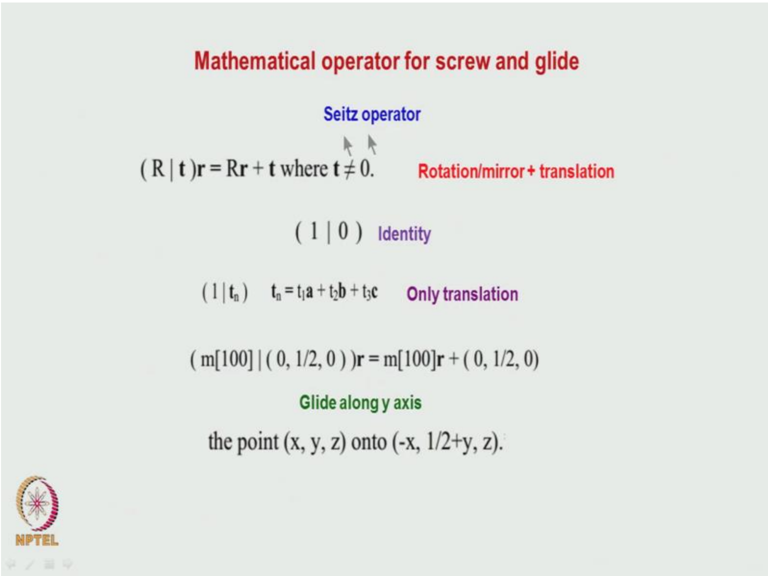
So, rotation, reflection are a mirror, inversion and we can generate symmetry elements taking combination of these, then we can have what is called as a roto-inversion that is that in the last class and Saturday I explained to you how this roto, what roto-inversion means and how it is done. So, if you take the combination of all these we will be getting different type of symmetry elements which we will be generating. This will constitute some distinct number of symmetry elements that in general turns out to be (Refer Time: 02:31) to find to. Looking at the type of symmetry elements one can talk about what is the sort of property which the crystal will exhibit how to construct the stereo gram, and now for different point to symmetry elements that we have done as an exercise in the last class.

(Refer Slide Time: 02:55)



So, that is what essentially I had shown it here, this is a an 1 fold symmetry, then a 2 fold symmetry that a point which we take that is rotated once 180 degree and then again rotated this is a symbol which corresponds to 2 fold symmetry; like this we can have 3 fold, 4 fold, 6 fold. So, far we have considered the various symmetry operations like rotation, mirror, inversion, screw and glide all these operations can be represented.

(Refer Slide Time: 03:42)



In mathematical terms to find out the coordinates of the different motives after these various operations by what is called the Seitz operator. what us the Seitz operator is represented in this (Refer Time: 03:47) that is R stroke t that is operating on small r, the small r represents nothing but the position of that motif r the lattice point and R represents essentially the type of symmetry operation, t represents the translation with is associated with the symmetry operation, this itself can be written as R into r where that this plus t where t is not equal to 0.

These r essentially what we mean by rotation r symmetry r in where rotation are mirror or translation, suppose we consider a identity operation that is a 360 degree rotation around a point then this r will become 1, that is 1 stroke and there is no translation associated with it then it becomes 0 then this called as a identity operation which brings the point after the symmetry evaporation back to it is original position. Suppose it is only here translation which is involved, but that is only a translational symmetry is operating no other symmetry, no other rotation or mirror or inversion symmetry. In such a case we can put it up this way that this one represents the identity, and t n represents the translation then t n could be t 1 t a plus t 2 into b plus t 2 3 t 3 into c, where a b c represents the lattice translation vectors.

Suppose it is mirror and the mirror is and on 1 0 0 plane, then this is the way this could be represented. Similarly if it is a glide which is along that axis he is going to be there then what it essentially represent is that here we will be putting the rotation symmetry plus what is going to be the pitch corresponding the glide that will come us the t, that is the we can represent this.

So, in short using this operator and the matrix transformation matrix associated with the different symmetry elements like a rotation, inversion and mirror we can find out the coordinates of the other points after the symmetry operation. What we have considered there are just pure rotation and rotation and inversion, how it is represented in a stereogram the point group symmetry.

I mentioned also earlier that rotation itself we can consider a combination of it if we take a 3 dimensional crystal, we find that in one particular direction there is a symmetry element which is associated with it 2 fold rotation is there and if we look into other directions which are non coplanar with it, these thing will see there may be some symmetry elements which are associated with it. What are the types of symmetry elements which are possible in other directions also, that is what essentially is given in this table.

(Refer Slide Time: 07:15)

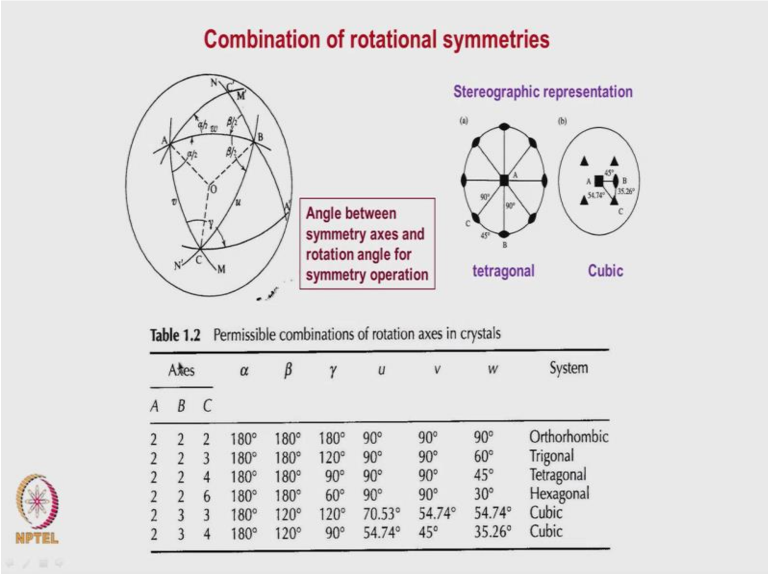


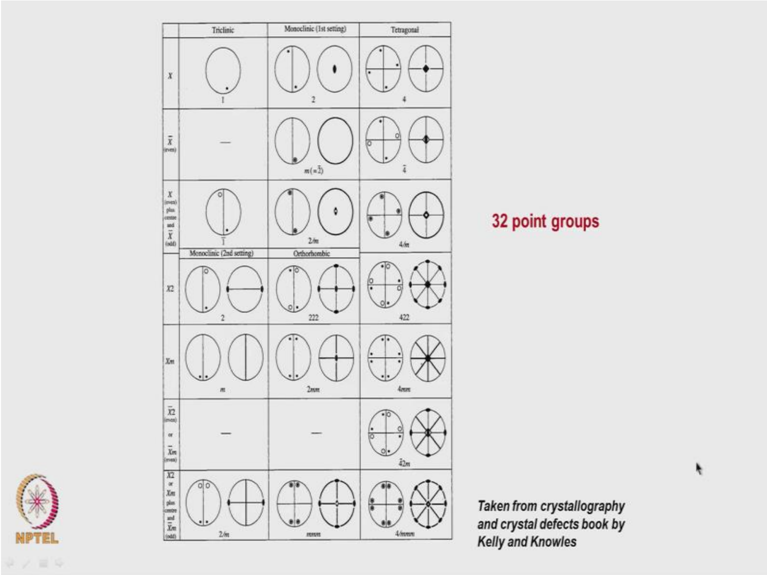
Table 1.2 Permissible combinations of rotation axes in crystals

Axes A	Axes B	Axes C	α	β	γ	u	v	w	System
2	2	2	180°	180°	180°	90°	90°	90°	Orthorhombic
2	2	3	180°	180°	120°	90°	90°	60°	Trigonal
2	2	4	180°	180°	90°	90°	90°	45°	Tetragonal
2	2	6	180°	180°	60°	90°	90°	30°	Hexagonal
2	3	3	180°	120°	120°	70.53°	54.74°	54.74°	Cubic
2	3	4	180°	120°	90°	54.74°	45°	35.26°	Cubic

Here what is being shown is what are the symmetry axis which are being considered, a crystal which we are considered we find that there is a 2 fold rotation is there, then another 2 fold rotation is there along b, and another along c and all these axis are 90 degree with respect to each other. So, 2 fold a 180 degree and the only lattice which can have this sort of symmetry element is essentially an orthorhombic crystal right.

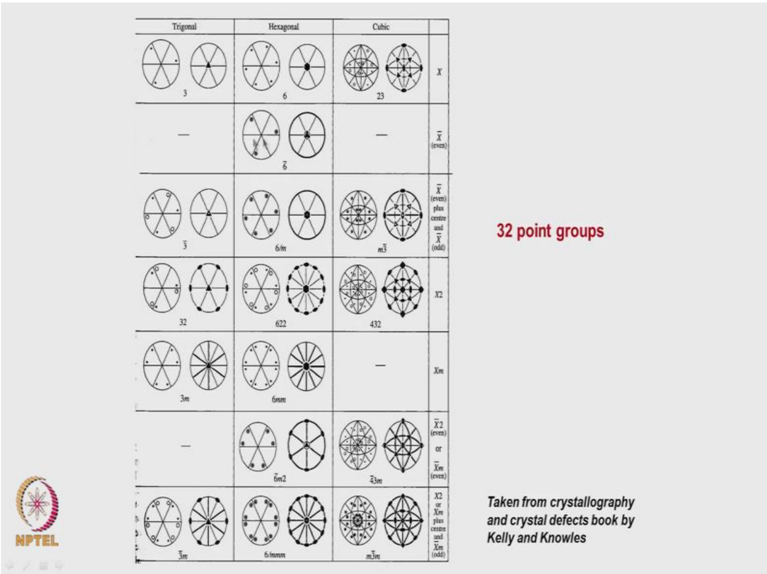
Suppose a lattice has got a 2 fold, the 2 fold and the 3 fold, then that is essentially a trigonal lattice. Similarly if a lattice has got a 2 fold and 2 fold and the 6 fold, that lattice will essentially be a hexagonal right. Suppose the lattice has got a 2 fold, 2 fold and the 4 fold, what it will be? It is a tetragonal if a lattice has got 2 fold, 3 fold and the 4 fold then that lattice will be a cubic type of a lattice right. So, this is the sort of combinations which we can have. Similarly we can have a comic here we have considered only pure rotation the combination could be of pure rotation and the roto-inversion also similarly we can have combinations that also can be considered that will give rise some symmetry elements.

(Refer Slide Time: 09:00)



If we consider all these symmetry elements together the distinct number of symmetry elements which we can have is essentially 32 point groups which we can have. All the point group stereography projection of the 32 point groups are given, in this as well as the next transparency.

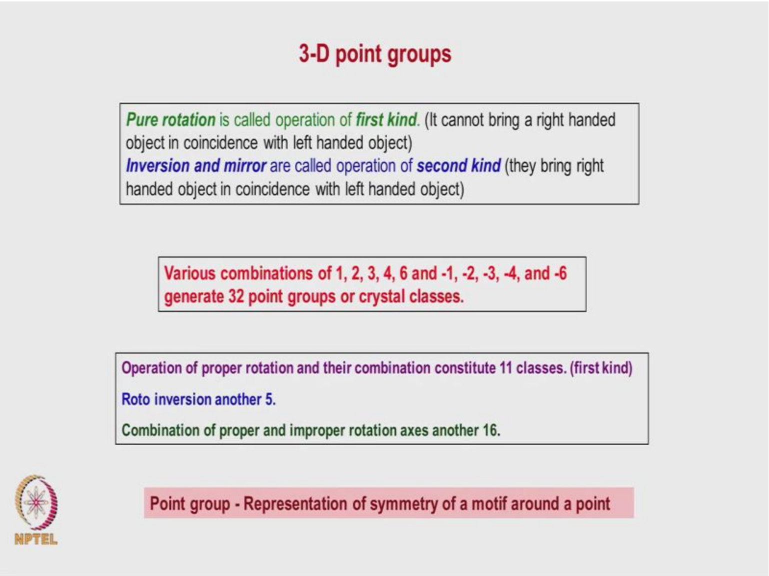
(Refer Slide Time: 09:29)



Are you able to see it, here it is for a cubic. So, essentially what one can make out these that these are all the various symmetry what do we mean by 32 point groups? That is suppose we take a crystal growth itself, that different type of the crystals which can form they can exhibit external shapes corresponding to this sort of point group symmetry correct or if you look at the property of a material, if you are looking at a dielectric property of a material or a magnetic property or elastic constants of the material what are the types of symmetry which the property can exhibit if we measure the property on a signal crystal.

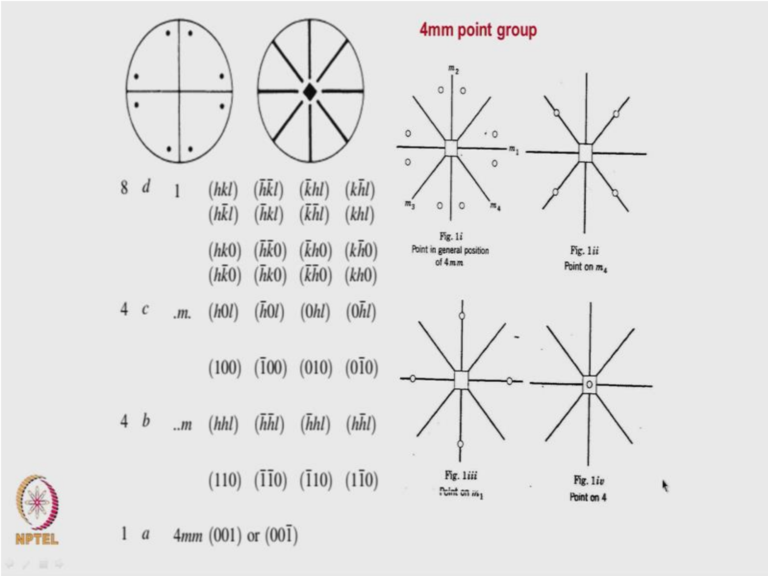
And then if we try to group it into different directions when they are formed, find out what all the directions in which they are there, and we will invariably find that all these axes intersect through a point in some cases, in some cases it will be only a plane some cases it will be only an axis which will be there which is invariant then we say that these are all essentially a point group symmetry. Because at least 1 point is left invariant in that symmetry operation is this clear, but what you can do it is that this slides I will anyway send it to you go through it, I had given a some assignment also to you people to generate, when you do that then you will be able to understand how these stereographic projection of point group symmetries are generated, it will be quite simple.

(Refer Slide Time: 11:20)



So, essentially how many symmetry elements that is rotation if you consider there are 5 mirror 6 right, then roto-inversion these are all the symmetry elements, then I combination of roto-inversion and rotation axis, all of them put together if we see the total number as I mentioned is 32. What I will just describe briefly is so far we looked at only just the stereographic projection of it.

(Refer Slide Time: 11:40)



Now, what we will try to look at it is what does it mean? Generally in a stereographic projection what we are trying to take is a general point pole, and how the pole is repeated if the crystal has got particular point group symmetry, I mentioned that the crystal can have special points also. So, here what we are trying to do it is that whenever we try to look at a as an example the point group symmetry of we wanted to we are trying to identify the point group symmetry of a crystal looking at it is external form.

For example suppose you look at this cube, what are the external forms this has which you can see.

Student: (Refer Time: 12:52).

Only phases which are 1 0 0 type of a phase correct? That is the only way in which it is existing; suppose you assume that these are all the axis then what these phase will correspond to - 1 1 0 type of a phase also it can have crystal can have correct, and what are symmetry elements which are going to be associated with this one, this cube if you look at it? The 4 fold axis along all the 3 coordinates which are chosen, then 2 fold axis is going to be there around 1 1 0 direction, then mirror is going to be there on these axis correct.

So, that is what essentially is being shown in this particular, that is what is being shown is that if a point has got a 4 mm symmetry, the phase it can have is only 0 0 1 type of a phase, that is around this axis if you take it what are the phases which come only 1 0 0 type of a phase which it comes correct.

So, in this one 1 1 0 phase when they come they can have a mirror symmetry associated with it around this as well as this (Refer Time: 14:24) symmetry is associated with it correct 1 1 0, and this phases also is related by a mirror. If I take a mirror axis the mirror plane like this or a mirror plane like this both the sides we have 1 0 0 and maybe here 1 1 0 1 0. So, this type of plane also is there with which it can form. So, 2 types of mirror planes can be there we it can have an external shape which exhibit mirror plane, one is with 1 1 0 phase of the external form or with 1 0 0 type that is what essentially is shown here.

Other than that it can take any other form like suppose I take a 1 1 1, as the phase then how many it can have 1 1 1 phase.

Student: (Refer Time: 15:28).

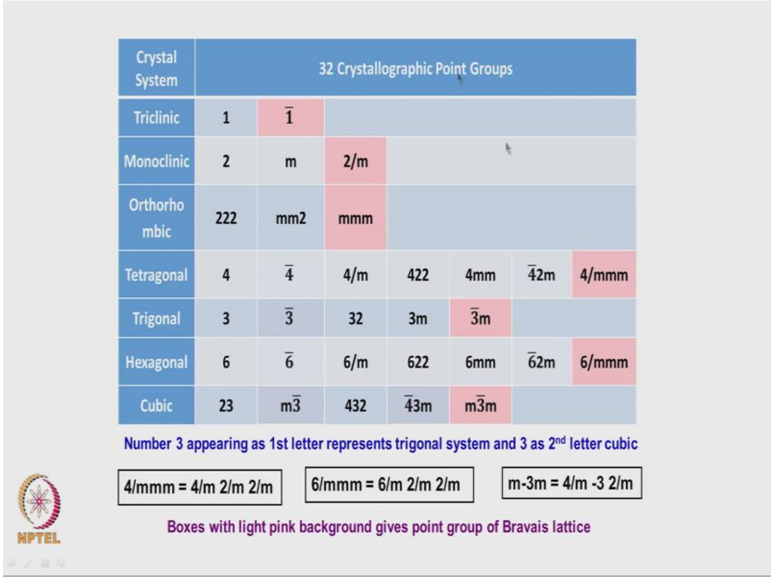
So, 8

Student: 8.

8 phases will be there correct. So, this general one which corresponds to those type of symmetries, h k l which is or it can be 1 2 3 also a phase which it can form. So, these are all the phases with which also the crystal can form.

So, essentially what is being shown here is that like this table a b c essentially like the Wyckoff positions, which I mentioned this is at different points at this particular point because there is a different symmetry elements passes through a particular point right that is the centre of; that is what we chose us the centre of the origin of the coordinate system, with respect to that 4 mm symmetry is essentially exhibited by axis which is passes through it because of 4 fold rotation is there, and mirror is also there correct this axis and the phase which is normal to heat is to this pole is essentially 0 0 1, then we have these 4 phases are there 1 0 0 type of 1 0 0 and 0 1 0 which have essentially mirror planes which are associated with it, then with respect to 1 1 0 a mirror plane is associated with it, then if the crystal has got 1 2 3 type of a (Refer Time: 16:58) then also then it will have 8 for this point group symmetry 4 mm.

(Refer Slide Time: 17:09)



Crystal System	32 Crystallographic Point Groups						
Triclinic	1	$\bar{1}$					
Monoclinic	2	m	2/m				
Orthorhombic	222	mm2	mmm				
Tetragonal	4	$\bar{4}$	4/m	422	4mm	$\bar{4}$2m	4/mmm
Trigonal	3	$\bar{3}$	32	3m	$\bar{3}$m		
Hexagonal	6	$\bar{6}$	6/m	622	6mm	$\bar{6}$2m	6/mmm
Cubic	23	m$\bar{3}$	432	$\bar{4}$3m	m$\bar{3}$m		

Number 3 appearing as 1st letter represents trigonal system and 3 as 2nd letter cubic

4/mmm = 4/m 2/m 2/m

6/mmm = 6/m 2/m 2/m

m-3m = 4/m -3 2/m

Boxes with light pink background gives point group of Bravais lattice

In this table what has been done is that all the point groups symmetry element the 32 crystallographic point groups are represented in a tabular form. You are triclinic because the earlier class I mentioned that this crystal classes other crystal systems, they are determined on the basis of minimum symmetry the crystal of a particular class exhibits correct.

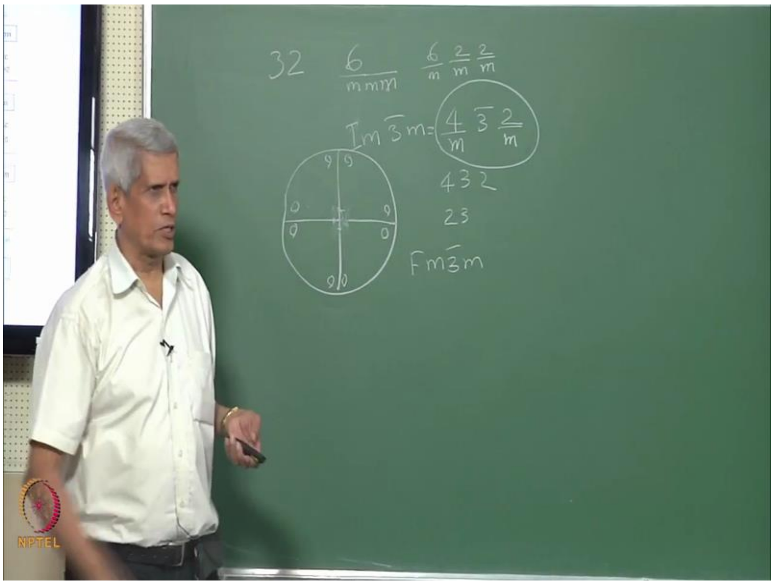
On that basis if you look at it triclinic has got 1 fold total symmetry are 1 bar inversion; then if you look at monoclinic, the minimum symmetry element which is there is only one 2 fold rotation correct, and the orthorhombic is three 2 fold rotation, tetragonal should have minimum one 4 fold axis correct if that is there is tetragonal. Trigonal exhibits minimum one 3 fold axis, hexagonal exhibits one 6 fold axis correct and cubic represents 2 fold and a 3 fold axis four 3 fold axis which are intersecting; these are the minimum symmetry which a cubic crystal should have.

This said what is being exhibited is what is being shown is the maximum symmetry element in this class a crystal we can have. That is essentially if you construct the lattice, because as I mentioned earlier that is when you put a motif around the lattice point depending upon the type of motif and how they are placed, the symmetry of the crystal can be equal to that of the lattice or it can be smaller than that. So, in each of this class which we consider the lattice exhibits the maximum symmetry elements right.

The different classes are defined with respect to minimum symmetry elements which are required, maximum symmetry element which are triclinic can have is 1 bar, monoclinic can have is 2 by m, orthorhombic can have a symmetry which is m m m this will come to later I will show some examples of the crystal structures; then tetragonal is 4 by m m m, trigonal it is 3 bar m, and 6 by m m m is what the symmetry for hexagonal, cubic is m 3 bar m it is written. In between there are different types of groups of symmetry elements which are possible, but what you should notice is that everywhere here 2 fold and that mirror always that 2 is going to be the minimum symmetry element always has to be exhibited by all the crystals, plus some additional symmetry elements are there, but the lattice exhibits the maximum symmetry elements.

So, this total together turns out to be 32; if you look at this table the like the some of the like 6 by m m m which is written many of the symbols are shorten symbols.

(Refer Slide Time: 21:05)

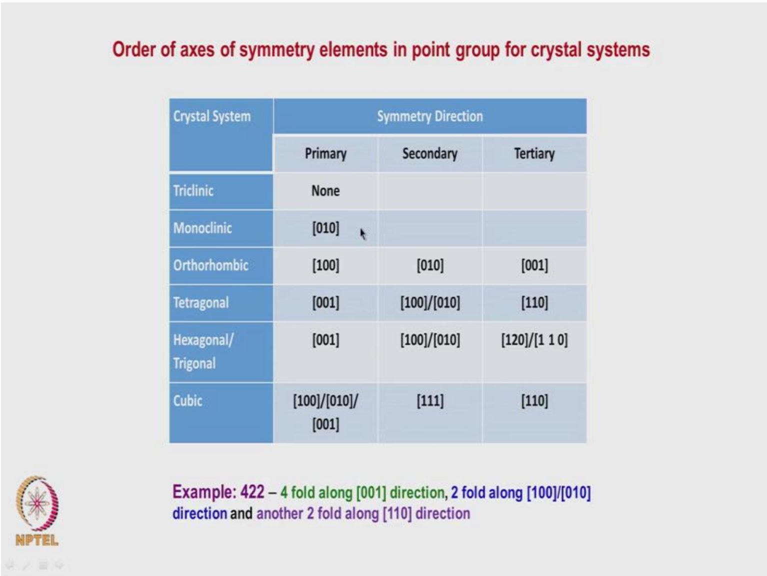


Then actually that symmetry elements are 6 by m, 2 by m 2 by m is the decal symmetry which (Refer Time: 21:27) because in the crystallographic table quite often the to bring no you cannot say the to bring clarity, but to bring some uniformity some shorthand notations are followed; like it is written m 3 bar m for cubic 1 this actually means 4 by m 3 bar 2 by m is the symmetry elements which are associated with it.

Now, I will explain what these symbols each one of this because we are using always 3 symbols to represent it correct is it clear? The convention which is followed essentially is that the rotation axis is a maximum rotation that is taken along the generally along the z axis or in the stereographic projection the centre of the stereogram represents that point through which that symmetry axis passes through either a 4 fold or 2 fold like this is the point through which the 2 fold axis is there or it could be that here we have a. So, this is a 4 fold axis right.

This is how the various axis are represented for a monoclinic we have only that here if you notice it is mentioned as 0 1 0 that is the convention which is being followed that is the 2 fold axis, the 2 fold rotation axis is along 0 1 0 direction.

(Refer Slide Time: 23:24)



Crystal System	Symmetry Direction		
	Primary	Secondary	Tertiary
Triclinic	None		
Monoclinic	[010]		
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	[100]/[010]	[110]
Hexagonal/ Trigonal	[001]	[100]/[010]	[120]/[1 1 0]
Cubic	[100]/[010]/ [001]	[111]	[110]

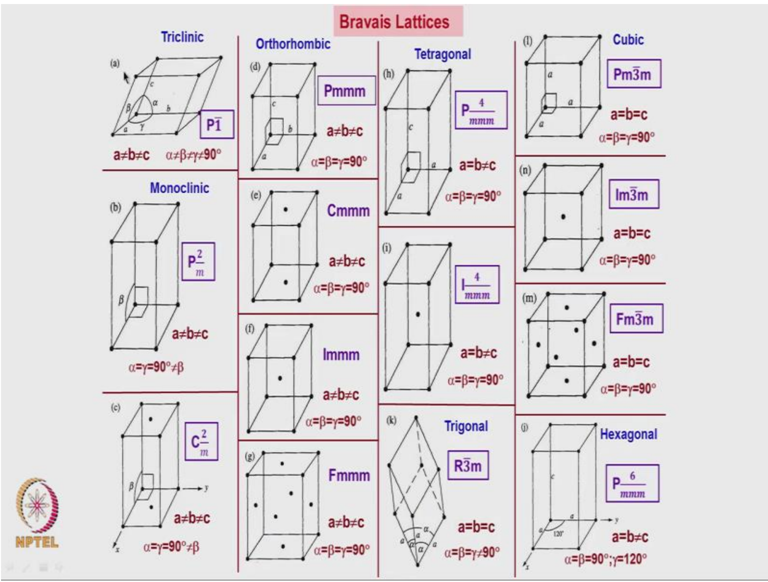
And if we take orthorhombic it is essentially the primary all the 3 symbols 2 2 2 they represent symmetry elements along all the 3 axis.

Then tetragonal if you see the first letter which is 4, the 4 2 2 if you take it or 4 2 m if you take it the 4 represents the symmetry element along 0 0 1 direction and the next one represents symmetry along element along 1 0 0 or 0 1 0, and the third letter represents symmetry elements along 1 1 0 direction. These the convention with which all these symmetry elements are represented in that table hexagonal similarly the 6 fold axis will be along 0 0 1, that is c axis and along 1 0 0 or 0 1 0 it represents the next number which represents and the third one represents either 1 2 0 or 1 1 0 type; whereas, in the case of cubic system the first letter represents the symmetry element along any one of these 0 0 1 direction.

The next letter represents the symmetry element along 1 1 1 direction, the third letter represents symmetry element along 1 1 0 direction this is a convention which is being followed to represent the point group symmetry or similarly the same convention is followed first space group symmetry also when we wanted to represent for all the crystal systems. And if you notice trigonal has got here 3 fold rotation axis correct and cube also has got a 3 fold rotation axis how they are differentiated is, if I write as 3 2 if the first letter is 3 that represents a trigonal, if the second letter is 3 like 4 3 2 or 2 3 then this represents a cubic system, this is the convention which is followed to differentiate between cubic system and the trigonal system is it clear.

On this basis on this basis of the symmetry element we have got the seven crystal system, and then the space group lattice how we decide is on the basis of whether it is a primitive lattice or whether it is body centred, phase centre or one phase centred on that basis we have the various classification. So, we can have 14 Bravais Lattices are possible right.

(Refer Slide Time: 27:36)



In this transparency I had just mentioned the space group symbol which is used to represent these fourteen Bravais Lattices, like here it is a triclinic here if you see these are all cubic one we can have a cubic crystal with a primitive lattice, the symmetry which it exhibits if this symmetry that is equal. So, if I put a symbol P in front of it this represents a simple cubic lattice, if I represent I in front of it becomes a body centre and if you put F then it becomes a phase centre. But the point group symmetry which this crystal exhibits are the this lattice cubic lattice exhibits whether it is primitive or simple cubic is essentially the same is it clear all these symmetry elements will be there. This symmetry elements are only a few symmetry elements which are used to represent the symmetry correct, but the number of symmetry elements which if you consider which this crystal will have is quite a lot, that we have not looked at it that is 4 itself three 4 fold axis are going to be there correct.

Similarly, 3 fold how many are going to be there 8 right; no, 4 similarly 1 1 0 that is 2 fold rotation if you take it they are going to be 6 like that along different directions which are quite distinct. So, there are many symmetry elements are there this we will talk about what are the number of symmetry elements which it can have. In fact, that is also is represented by the number of poles which you see in a stereographic projection. Generally for suppose this is what the stereographic projection shows there are 8 poles which we are seeing right, the total number of symmetry elements which it can have this crystal is going to be 8.

There are many ways in which it can be derived, but you can take it because just looking at the number of poles which are there you get the information about all the symmetry operations which are possible, the total number of symmetry elements operations which are possible is it clear.

Then we considered the various types of that 2 fold rotation there is rotation, inversion, mirror, roto-inversion and combination of rotation, and combination of rotation and roto-inversion we considered it. This number we can take different combinations if you take various combinations the number of systems which we can consider point group symmetry are quite now, quite a lot, because that combination which one can try it, but many of them will turn out to be identical to one another which I think in the last class when you have worked out you could make out how it happens, because of that only we find that only 32 distinct point group symmetry elements are present.

So, far we considered only the point group symmetry, but in a crystal in addition to point group symmetry, because the lattice point gets repeated if you put a motif you also can get repeat itself depending upon where the motif is being kept, in some cases it can exhibit another 2 types of symmetry elements they are one is glide, and another is a screw axis.

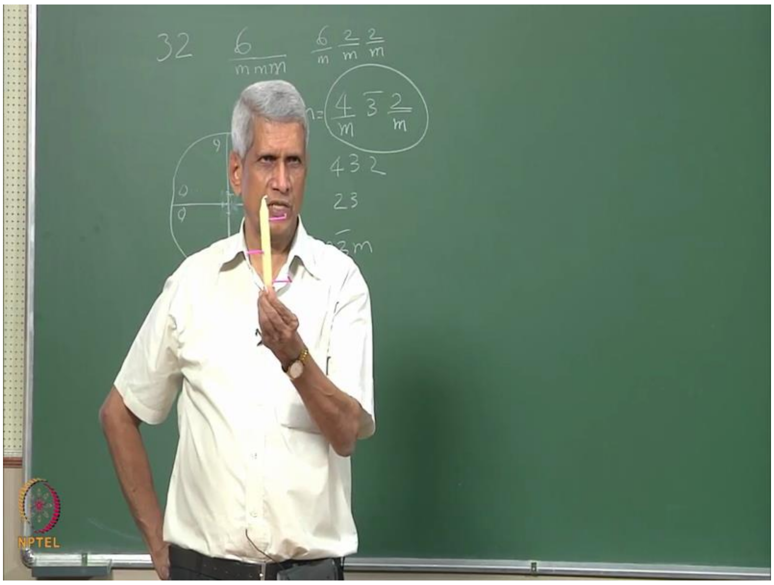
So, for a crystal if we consider apart from this point group symmetry elements these symmetry elements also come into the plane. So, if you take a combination of all these symmetry elements the total number of distinct groups of symmetry elements which we can have turns out to be 230, distinct point group symmetry. So, all the crystal systems which are periodic in nature which represents the translational periodicity, we will observe that they will fall into one of these 230 space groups.

Space group really tell about if you place motif around the point that is what are the types of crystals which we can have; and if we do not consider the motif if you look at only the lattice points then we have only 14 Bravais Lattices are there, to which if you add all the symmetry elements and put motifs around it satisfying the symmetry elements, then the distinct crystal with distinct space group symmetry which we can have the total number turns out to be 230.

About glide we have already considered when we talked about the 2 dimensional point groups. What we have to consider is another type of an axis which is called as a screw axis; that is in a crystal like this, if it place your motif at some particular point to satisfy the symmetry the motif should be kept at some points to satisfy this symmetry, there is an another way in which is a because the rotational symmetry (Refer Time: 34:27) satisfied.

Other way in which it can happen is that along this direction one motif is kept there, another motif is possibly rotated and it comes here, then after some rotation it comes back to from this motif to this motif which is there and this one with respect to lattice there in identical position. But to satisfy that symmetry it is not on a particular plane which is there it is along an axis the motif itself has been shifted. This sort of symmetry elements are exhibited by many crystals, this we call it as a screw axis. This is like a normal threaded screw when we rotate it one round by a pitch it comes back to identical position right exactly like this, but there are some conditions which this screw axis will have to satisfy so that the periodicity of the consistent with the translational periodicity of the lattice.

(Refer Slide Time: 35:41)

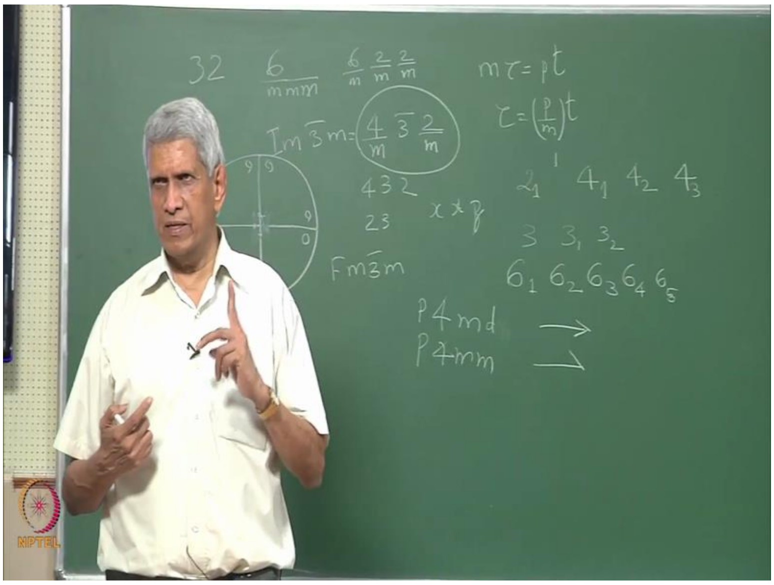


Suppose a crystal has got a 2 fold rotation, the possibility which it can have is that at one lattice point you look at it these are all the 2 atom positions which are there so that the 2 fold rotation will be there another lattice point also there should be at this point you have an another type of a motif which is being kept, the same type of motif which repeats itself. So, that around this axis if you rotate it 2 fold rotation is always being main maintained correct.

You see here, this one is there this repeats itself and the next lattice point it is there in an identical position, in between we have a point this has been rotated by 180 degree, but shifted by half the lattice parameter and again this particular direction you notice that this has got a screw axis associated with that in the lattice, these sort of symmetries are exhibited many by many molecular crystals.

This is essentially a there is a convention which is being followed to represent it, that will come to at this point issue we should make a subtle distinction because this is essentially if you see here it is rotated by 180 degree then it will come like this here. What is the type of symmetry this one exhibits glide, the difference essentially is that it is shift translated by half and then this is a reflection, these 2 you can make out the subtle difference between the these 2 symmetry elements correct.

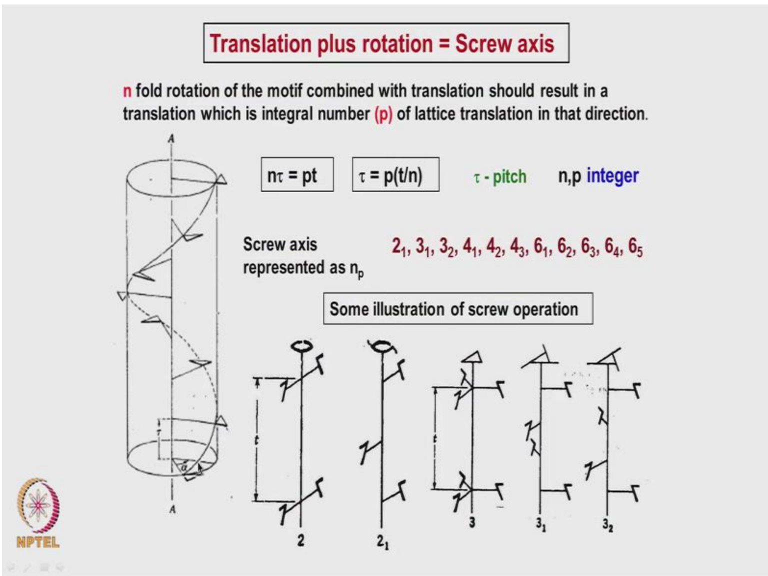
(Refer Slide Time: 37:49)



So, what is the condition essentially is being followed is that from one lattice point to another lattice point if you move through some pitch which you take it to be z that is if m times tau the pitch equals t is the lattice translation vector in that direction either it would be one lattice translation vector or some number n that is what essentially is given as p.

So, what does this m represents m represents the rotational symmetry which it has, then this will be p by m into t if p turns out to be 1 that is like in this specific case which is being shown.

(Refer Slide Time: 38:37)



Here it has a 6 fold symmetry it is rotated by 60 degree; and then translated by 1 6 then after a complete 360 degree rotation at the next lattice point it comes back to identical position correct; that is what essentially is happening. But there are cases where it may not come back to identical position after one rotation maybe after 2 rotation it can then, what will happen is that suppose that happens from here to here what will happen to a pitch which has to be doubled correct, then only such a sort of a translation can occur that is what this expression also tells.

After 2 translation vectors if it has to happen then the P will be 2, and then divided by m which is the number of rotations which that is the rotational symmetry of that in that direction then we can find out what is going to be the value of tau is this clear.

Let us consider this with an example of 4 fold symmetry, in this if you look at it along this axis it has got a 4 fold rotational symmetry right, here also is a 4 fold is there by a parameter t this direction it is repeating itself you assume that is going on like this staged 1 1 top of the other. So, it exhibits a 4 fold symmetry right and the periodicity is t.

You look at this here from here, there is a motif which is being kept here it has been rotated by 90 degree, and shifted by one-fourth of the lattice parameters in that, that is translation vector in that direction it reaches here, again rotated by one-fourth it reaches at the half, again rotated by one-fourth it comes here the fourth one it has come back to an identical position correct.

Student: (Refer Time: 41:00).

No, from here 1 2 3 4 1 is here. So, this has come back. So, this essentially is a 4 fold rotation plus if you look at the pitch is turning out to be t by 4 correct? And the direction if you see it here is in a what way we have taken it with respect to this, it is in a rotation is an anti clockwise right you see this one, the same way you start with here buts in a clockwise rotation it comes. So, both are possible, but both of them are distinct they are not the same correct is it not.

Because here after this position one here it comes here in the opposite direction it comes, see the 2 different types, but one is a clockwise rotation and another is an anticlockwise rotation. You look at this one what do you see, here the motif itself has got a 2 fold symmetries associated with it this motif is rotated by the pitches if this is the pitch it is by not one forth, but half and pitch is half angle is 90 degree. Now it comes like this when I rotate it again another rotation if I look at it now it comes back to this position it looks like similar, but it is not because you understand that suppose I can put a marker on this one this marker would have come here and this marker comes here. So, that is not again if it does one more double the rotation it comes back to a original position correct.

In this particular case the translation period translation is 2 times that is what essentially this expression this p means. So, if you look at it if you compare with respect to these 2, now you can see that they are not the same, this is a 2 what the symbol which is used to 1 that I will come to it and here the symbol which is used as 4 2 because the rotation which is given is 90 degree here the rotation is 180 degree.

So, what we can make out here is that if this p turns out to be 1 in this case, 1 and it is a 2 fold rotation. So, this is represented as 2 1; similarly when we consider the 4 fold we have a 4 1, another is 4 2 that is corresponding to this one then the other one is written as 4 3; why it is written as 4 3?

Student: (Refer Time: 45:02).

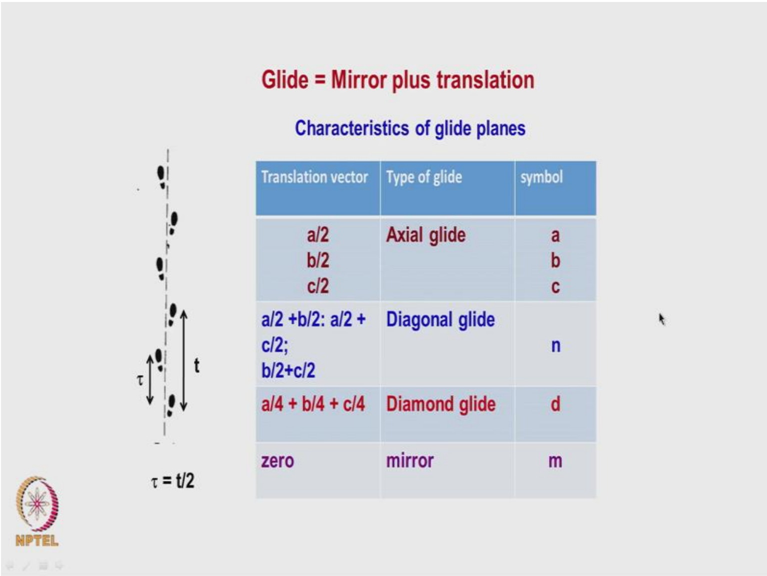
Because if you look with respect to the (Refer Time: 45:06) the clockwise and anticlockwise if we consider, but it is equivalent to the other way down if you do it in the opposite direction it will be one third of it which you have to rotate it to bring it to an identical position.

See here what happens is that, from here in the opposite direction if you rotate how much you have to rotate it to bring it to this position, one-fourth if you rotate it you will be bringing it to a position which is identical with it with respect to this if I rotate it in this direction one-fourth, this is equivalent to 1 minus in this opposite direction 1 minus one-fourth that is how it is being considered.

So, essentially this is equivalent to if we take a pitch of 3 by 4 and then take it along then we will notice that this will turn out to be the same identical (Refer Time: 46:12), but why we are writing it in this way is that we are following one convention of taking the sense of rotation, because here the way we considered is in one case the sense of rotation is a clockwise and another is anticlockwise. If we change take the sense of rotation in that same way, we will notice it that it is going to be that pitch is going to be not one-fourth it is going to be three-fourth.

Now, if we consider similarly 3 we can have 3 1, 3 2, 4 we have considered 6 also we will have 6 1, 6 2, 6 6 will turn out to be essentially the 6 1 itself that repeats itself. So, these are all the number of screw axis which we can have in the lattices; is this clear? This is in addition to that is it some crystals can exhibit with screw axis which is there in some crystals it can be just a simple 2 fold or 3 fold or 4 fold or 6 fold rotation also.

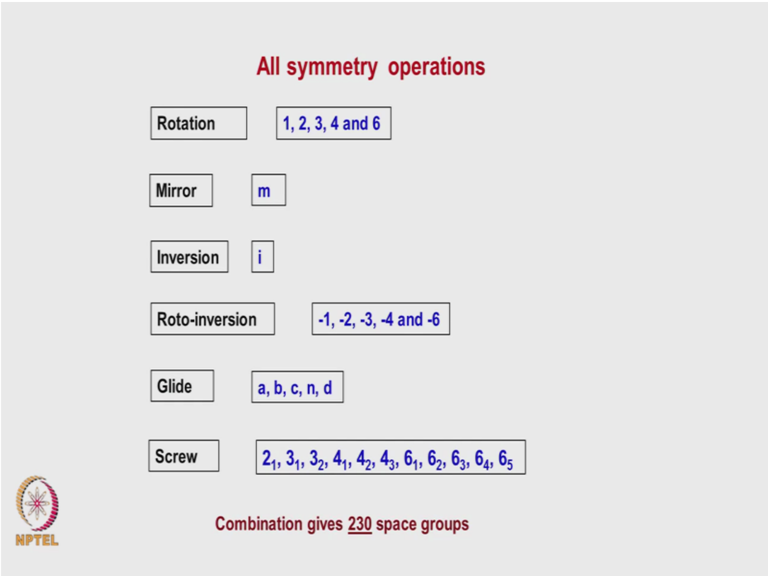
(Refer Slide Time: 47:52)



So, now we know I think 1, 2, 3, 4, 11, 11 types of screw axis are possible then mirror if we consider not mirror glide, glide also essentially a mirror and a translation together right it is a combination of both of them with respect to a crystal it can so happen not only along 0 0 1 axis we have the glide, other axis there is no glide or it can be there along b axis or along c axis or it can be along the phase diagonal, or it can be along the body diagonal all these directions we can have glide axis that is possible in the crystal

If that is the case then what is going to be the translation vector that is what is given in this table, and then this is called as axial glide diagonal glide diamond glide (Refer Time: 48:49) and the symbols which are used to represent them in international union of crystallography is a b and c, because along a axis it will be a, b axis is b, c axis it will be c which will be used and whenever the diagonal glide is there n is used, diamond glide d is the symbol which will be used like we assume that the crystal has 4 mm, in this direction where mirror is there this is along 1 1 0 direction. If there is a instead of a mirror there is a glide is there in this direction then the symbol will turn out to be 4 m d and if it is primitive we will be writing p 4 m d this is the way this space group is represented is this clear? When the glide is not there then the space group will be p 4 mm this is the way it will be.

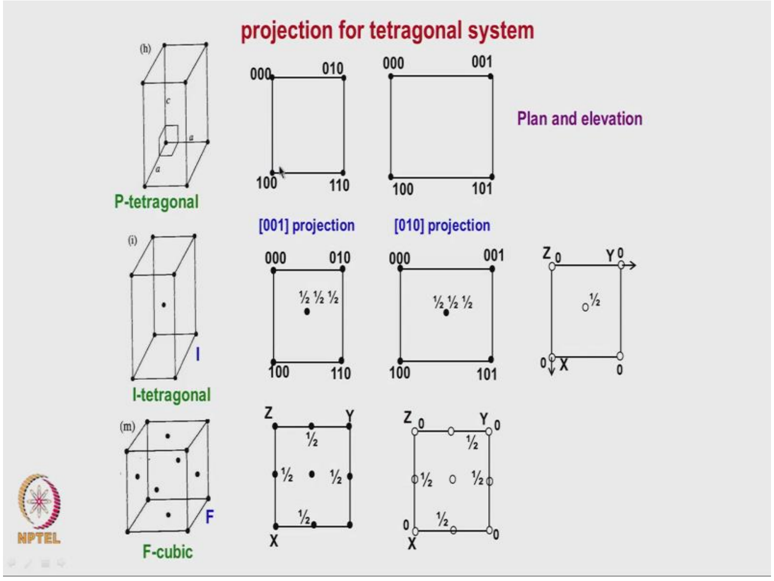
(Refer Slide Time: 49:56)



So, what are the symmetry operations which we have for a space lattice or a we have 1 2 3 4 mirror inversion, roto-inversion, glide, screw we can have a combination of all of this put together that gives totally 230 space groups exhibit is it clear? And in the international union of crystallography if you look at it this space groups if you it has to be represented because we are talking now with respect to a lattice correct; and representing 3 dimensional lattice in 2 dimension if you have to represent generally we draw a cube and we do it, but the cube does not but looking at the cube we cannot tell that whether it is cube or whether it is a tetragonal lattice or an orthorhombic lattice unless and until we mentioned what are the lattice parameters correct; otherwise it could be anything any one of this it could be.

So, the other way in which we can represent it is generally like what in mechanical engineers and civil engineers do is the plan and elevation correct.

(Refer Slide Time: 51:33)



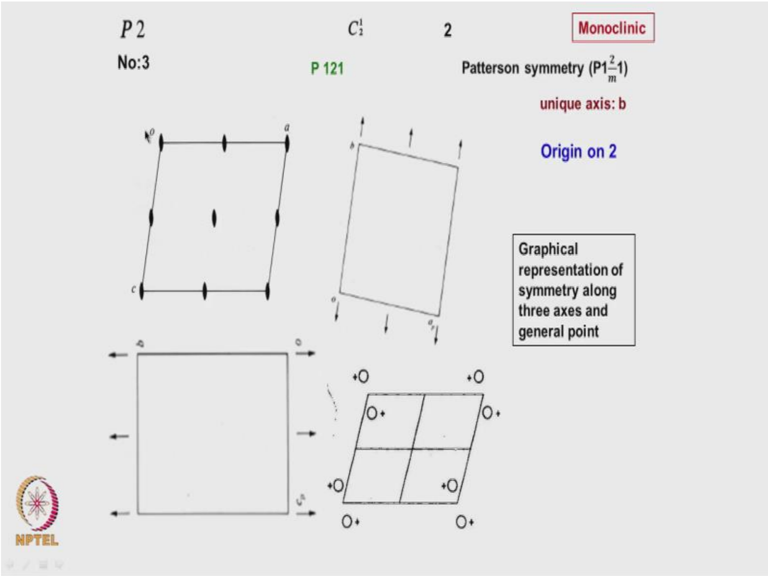
So, you look at the crystal then try to represent it in 2 directions you look at it. So, this is a projection which is given now of the crystal looking along 0 0 1 direction this is how it looks correct for a tetragonal lattice and this is how the projection which it will be in 0 1 0 direction correct. Once these 2 projections are given the crystal is completely specified the lattice is come where the unit cell of the lattice is completely specified correct complete information is available.

Then similarly if it is a body centred then there will be one more atom position is going to be there how do we represent it? The way in which it can be done is that you show this position at the centre because that projection it will be seen this as the projected onto this plane correct, and then just mention half and half means that it is sitting at a position halfway up that is how it is represented.

Similarly, if it is a phase centred 1 cubic, then these positions we mentioned at that half position and others we know that they are in that same plane. So, these are all the way in which we can represent it. In fact, when you see many of the journal papers they are also when they wanted to show the projection of unit cell quite often this method is following. We will just take a few example of. So, this is the way in which a unit cell can be represented.

Then after representing the unit cell in this way we can put motif around different positions and also show the symmetry elements which are associated with the unit cell, that is how it is represented diagrammatically in the international union of crystallography. What I have taken is the one which has got the monoclinic crystal structure which has got only a 2 fold symmetry one 2 fold symmetry axis.

(Refer Slide Time: 53:52)



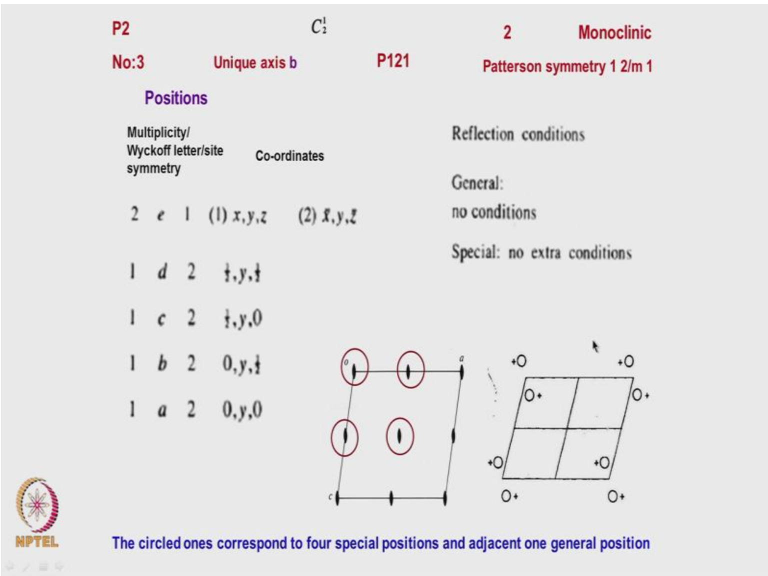
So, the as you remember for monoclinic I mentioned that 2 fold symmetry is taken along the b axis correct. So, here in this projection the b axis is normal to that screen this is a and this is c, then these are all the other 2 directions are also being shown projection when these directions are being shown it is complete in itself correct? Then in addition to it if you see here a symbol which is being shown is an arrow with, if this arrow is shown this exhibits that it is a rotation axis is along this direction is what it means.

These are all the symbols which I think in the book afterwards you will be able to see what each of the symbols mean and in the perpendicular direction what we show this symbol if we show it means a it is a 2 fold rotation is here, the 2 fold rotation around this point here as well as here. If we take it these are all the additional symmetry points which are generated in the lattice and around this lattice if we put a motif around here in this what one should consider is that what is the symmetry axis which is there only a 2 fold rotation correct; only 1 axes symmetry is there then why do we fix the origin of the unit cell arbitrarily you can choose it anywhere on the axis.

Suppose we have a that is what is the case for many symmetry elements where if the symmetry elements do not intersect, then we have to fix the origin arbitrarily like 4 mm or 2 mm all of them the mirror also is on the plane of the symmetry axis correct the symmetry axis, there is a rotational symmetry axis and the mirror plane they are parallel to each other. So, origin you can choose arbitrarily if the symmetry elements intersect the point of intersection is always taken as the origin that is the convention which is always followed. So, because of that here what is being done is that that is why the motif is being placed at some position with respect to a coordinate system which has been chosen origin of the coordinate system plus ok.

Then around this axis which is perpendicular to this plane of the paper plane of the screen, if it since it is a 2 fold rotation is there. So, another one will come at 180 degree rotation correct a motif as to be there. So, this is how the general position is represented, this diagram represents the symmetry elements which are associated with the unit cell this diagram represents the position of a motif when it is placed at a general point.

(Refer Slide Time: 57:21)



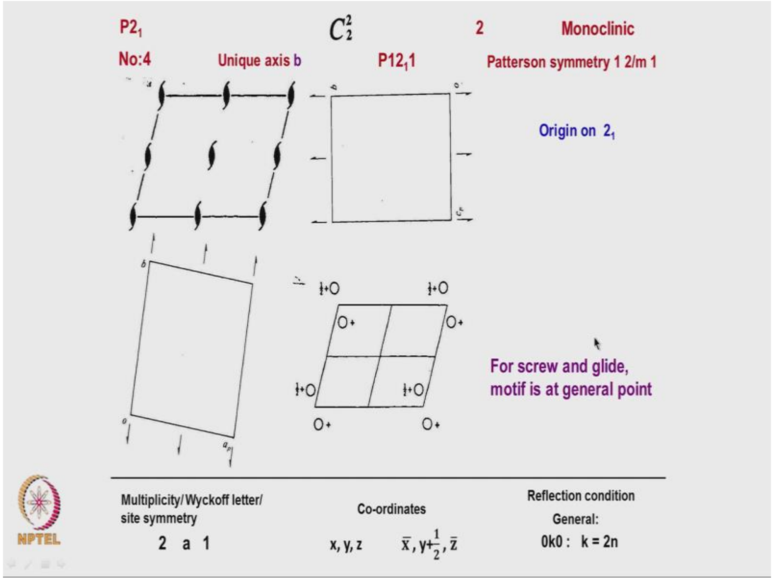
What is essentially important is that to construct a crystal, is this type of information which is the tabular form which is being given about the coordinates of the various positions of special points as well as general points. At this point if you consider what is the symmetry which it has? 2 fold rotation correct is it not. So, if we keep any atom at this point if you put at this point only here, here, here by translation they will be generated the unit cell will be completed in itself, but it can and since the origin is never fixed the atom can may not be kept at the origin, it can be kept on this y axis anywhere also it can be kept that is essentially what it means that 0 y 0, that is 0 with respect to here 0 with respect to here on the y axis it is kept at some position arbitrarily at y. Or the other position where it can be kept is that 0 on the x axis that is a a here, then half in this direction and y on top that is this is also another symmetry element if I keep an atom at this position, and then I another atom at this position will come by translational symmetry, by translational symmetry another will come here another will come here again you notice that the monoclinic structure is being constructed.

Similarly, an atom could be kept at this position that is what this shows, or the third it would be kept at this centre this is what this is the coordinates of the atom position which is being shown where we have to keep the atom, and then there is only one position where we have to keep it because the others are all generated by translational because here the p represents essentially a primitive lattice, primitive lattice means that the number of atoms per unit cell is one. So, that is why essentially we have to choose only one position. Then if we keep it at a general point since it is a 2 fold symmetry there should be minimum 2 atoms per unit cell should be there, that is what you can see that when atoms have been put a general point this position and this position it is going to be there. So, within the unit cell you have to are there that is what this number 2 represents the multiplicity.

There are some reasons the way in which one can reason out and find out how these are derived, that part I am not going to it that those who are interested can read the book and introduction to crystal geometric by just there it is all explained very nicely, and then I had also mentioned that when you know the rotation symmetry axis how to find out when one position is given the coordinates of the other position we can find out correct.

So, this is the one which is very important this table. So, the possibilities is that either an atom could be kept at this position atom are a molecule or at this position or at this position or at this position then by translational symmetry they will be generated at other points, but what is essentially important is that the same atom cannot be kept at this position as well as this position and as well as this position that is not possible that I will come to later to explain it. So, these are all the possible positions either here or here or here or here it is or not and this is essentially.

(Refer Slide Time: 61:49)



Now, in the stable if you see it here in the crystallography international union of crystallography table, each page are corresponding to a particular space group the number is given right here this number is 4 which is given for this one, and then it is written monoclinic and this one shows what is the point group symmetry corresponding to it. The difference between point group symmetry and space group symmetry is that in the space group symmetry if you remove the rotation axis the screw or the glide, what will be left behind if you remove glide then it becomes a simple mirror, if you remove screw it becomes a simple rotation that is how the space groups are mentioned.

So, here if you look at it this is just a shows the point group symmetry this is the shooflies symbol and this is the space group symbol which is followed now that 2 1 corresponds to 2 fold rotation, because these are sharp symbol this is the correct symbol this symbol what is then primitive along x axis there is one fold rotation, along y axis there is a 2 fold screw axis is there then on the z axis that is an one fold rotation correct.

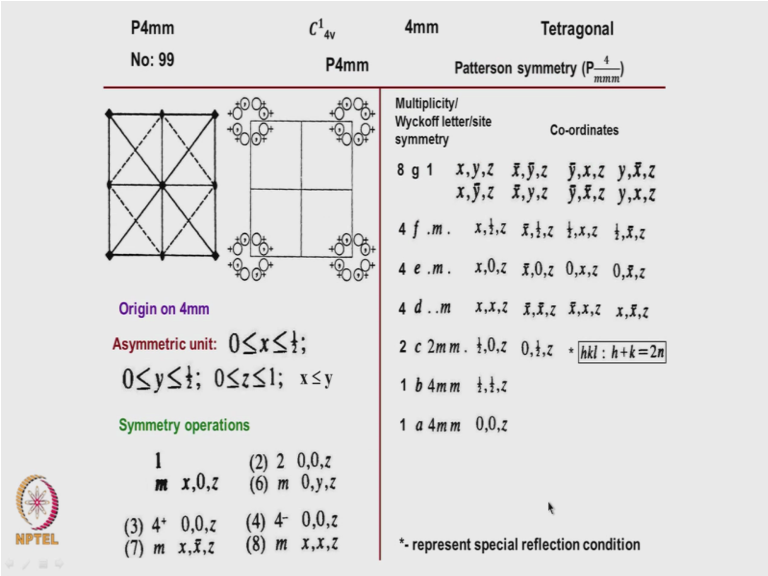
Now, you look at this in this one the symbol which is used for representing screw is this symbol, this is for a 2 fold screw axis 2 fold screw axis is this clear. Then as I mentioned earlier and another thing also is that the projection which is they are taken along the other perpendicular directions of the unit cell. Here the arrow which depicts is 1 side only the arrow is there, if an arrow is put like that this represents just your rotation if we put an arrow like this it represents the screw axis there are various symbols are used to represent that in a separate table all these symbols are given what are symbols which are used.

Here what is going to happen is that if we keep one motif at a particular point, another motif comes at half position that is from wherever it is being kept half the distance if we (Refer Time: 64:49) translate it and do the 180 degree rotation that motif will come that is why wherever this is 0 plus this is the O plus the O half plus it is given.

In this particular case the choice if you look at though here also we have a 2 fold all these are possible, the coordinates if you consider it that positions which are possibly x y z and another is it is x bar y plus half z. There are some ways in which these are represented this I have already mentioned to you with respect to glide how exactly it is done, and this is the method in which it is represented these various types of operations which called as a Seitz operator you do not have to know about it, but I wanted you to be aware that this is the methodology which is being followed. In this symbol this represents nothing, but the rotation operation, this represents the translation operation no mirror operation and this is r is the translation. So, this is what essentially here you can see that 1 0 means that it is an identity operation, here 1 t by n means that it is an one fold rotation is one fold then is only just a translation which is taking place.

Suppose we have a mirror is there, then it is the mirror whatever is the axis which you have to put it the coordinates of this r is the position vector of the motif then plus the translation which is being given. So, that is what it happens that x y z if there is a point is there, that becomes if the glide is along y axis it is shifted by y plus half correct along the y axis then its position and when it reaches that position the when you take the mirror with respect to when the mirror is along the y axis, the glide is along the y axis it will be that x will become minus x that is of this these symbols I had explained already how it come.

(Refer Slide Time: 67:15)



Another case which will consider is a primitive lattice which has got 4 mm symmetry point group symmetric, this is the way it is represented it is a tetragonal point group symmetry is 4 mm, this is the Schoenflies symbol. So, what are symmetry elements which are there associated with at the corner points of the lattice you have 4 fold, at the middle we have a 4 fold correct then at the edges and middle if you look at it we have a 2 fold symmetry is there, then 2 types of mirrors which are seen correct.

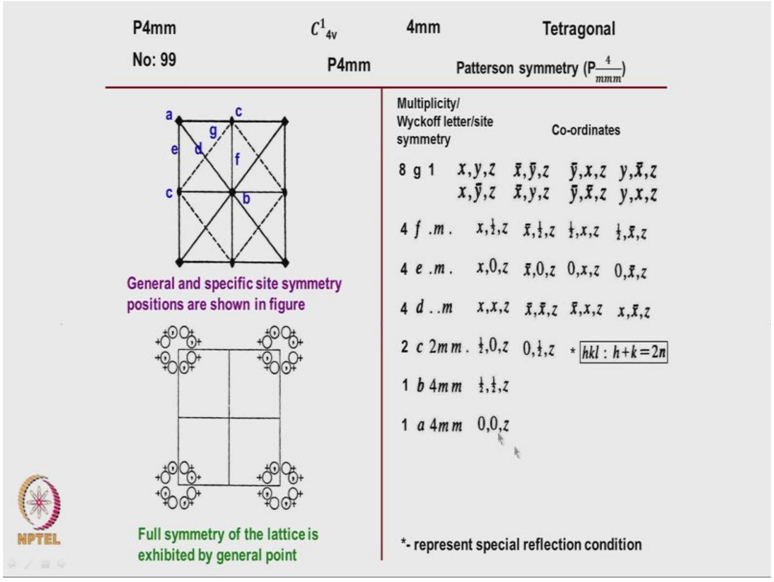
So, all of these and you should understand that here also since it is a 4 mm symmetry the origin is we can arbitrarily fix it, because 4 fold rotation axis the mirror parallel to each other. So, they never intersect that is the reason why when we give the position where the motif are an atom can be kept here it is given 0 0 z is given, because this is the z is the axis around which the 4 fold rotation axis is there.

So, suppose we fixed the origin corresponding to the atom position then this will turn out to be 0 0 correct. So, this corresponds to an atom being kept at this particular position the origin, then it will be 0 0 z or 0 0 0 it can be both possible. Then by translational symmetry other 4 positions atoms will come the unit cell gets completed correct then at the centre of this unit cell also this also another special point where symmetry elements are meeting. So, this also has got a 4 mm symmetry associated with it if you look at it that is mirrors pass through the 4 fold rotation is also there, that is the site symmetry and this position in the Wyckoff position this is given as a, this is called as b and the number of positional atoms which have to be kept or the motif which has to be kept at this point is only one.

Then by symmetry operation the others will be by translational symmetry operation the other lattice points will be generated. If we keep one here which corresponds to 2 mm symmetry, then 2 positions are possible here as well as here then by translational symmetry these 2 will also be generated. So, like that for all the possible special positions what are the places at which the motif should be kept that information is being given here and if you put at a general point like what is being shown in this diagram in the international union of crystallography table, and here that if x y z is a will be a general point right because whenever anything is related by symmetry if you write a coordinate if I write x x z means that x as well as y they have the same distance right, whenever this sort of notation comes; that means, that this point is a point which is related by some symmetry operation that is a special point that is what you can see here, here when that m is there you see that the x x z it is written right.

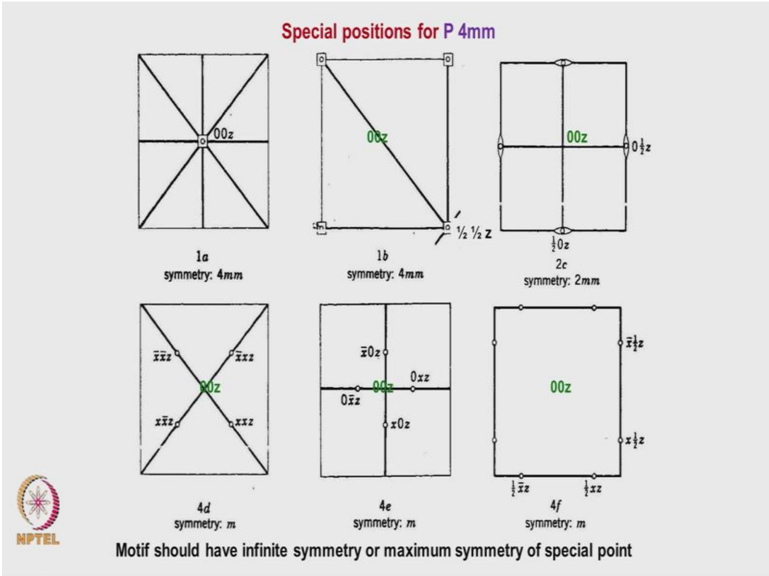
Like here you see that x 0 z similar thing you will notice it, and here when it comes it is x y z which is being used all the 3 are distinctly different; that means, that that represents a general point.

(Refer Slide Time: 72:23)



And here what I have shown is what this a b c means corresponding to this one, these are all the y compositions which are given that site symmetry I have already explained what it means.

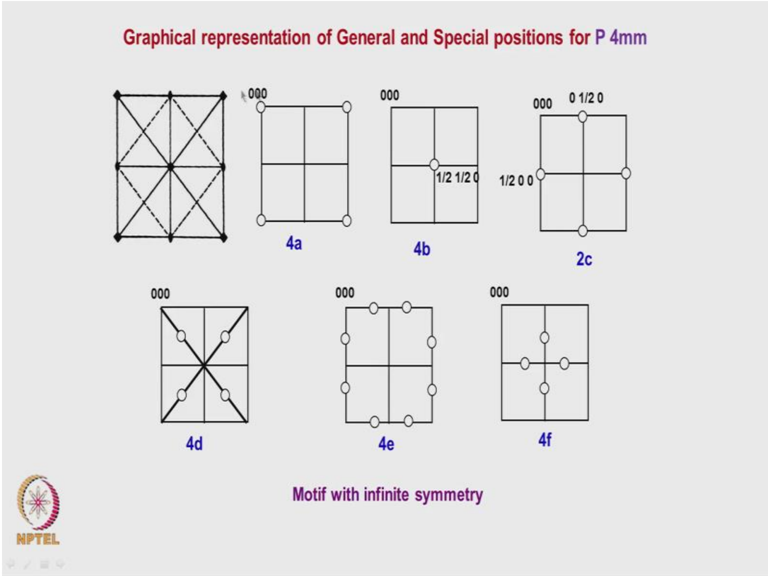
(Refer Slide Time: 72:39)



The same information presented it in a different way that is we can have a position where at the centre we can put an atom position or one we can put it at this particular position or it can be kept at these positions, or at these positions we can put that motifs or we can put at these positions or these positions if we put it motif all of them exhibit 4 mm symmetry is exhibited, but what is essentially important is that suppose I put a one type of an atom here, the same type of an atom at this point then what is going to happen is that this essentially is a p 4 mm correct and if I put 1 here and an identical atom here then 1 has come at the middle then the symmetry changes to I 4 mm. So, that is not the same.

So, same atom cannot be placed at 2 types of Wyckoff positions, but these are all that as I mentioned earlier whatever we are talking about it is a geometrical crystallography. In geometrical crystallography we are looking at what are the possible positions in which motifs can be kept which satisfies the symmetry element that is what we are looking at it.

(Refer Slide Time: 74:17)



Because now, you can see here also the same thing which I am shown like if I put an atom here by translational symmetry, this will be generated this point all these points are generated this is what is generated as a the Wyckoff table mentioned as a 4 a.

This is 1 way in which it can be filled if the same atom I wanted to keep it in a this position then this is the way it will appear in the unit cell or if it is a 2 c which is the 2 mm symmetry is there, these are all the positions with respect to unit cell which is chosen, these are all the positions at which the atom should be placed; with respect to unit cell which is chosen if it is for one type of a mirror atoms will be kept at this position, for an another type of a mirror the atom should be kept at this position, for an another type atoms will be kept at this position with respect to unit cell.

So, any one of this type of any one of this type we can use, or each one of them when we keep an atom at this particular position, each of them independently satisfy the 4 mm symmetry you understand that, whether I keep an atom here and generate a crystal or whether I keep an atom here and generate a crystal with respect to a unit cell or whether I keep an atom at this position and generate the crystal or in these or this one all of them satisfy 4 mm symmetry, is it clear? What I will do it is I will stop here now, we will continue in the next class.