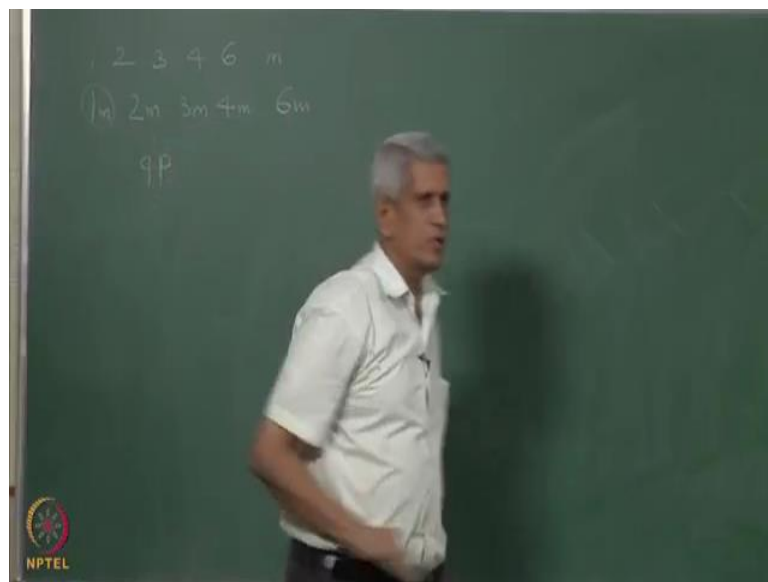


Electron Diffraction and Imaging
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Lecture - 05
Symmetry in 2-D Crystals

Welcome you all to this course on a Diffraction and Imaging. In the last we discussed about the one dimensional lattice, what are the types of symmetry which are associated with one dimensional lattice: both point group as well as the space group we considered right. There are five point groups and the total seven space groups are possible for an one dimensional lattice. Today we will looked at a two dimensional lattices.

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What are types of rotation which was possible in one dimensional lattice? Only 2-fold rotation right and we also considered that we can have 1-fold, 2-fold, 3-fold, 4 and 6-fold rotations are the rotations which are possible for two dimensional lattice, but this is true for three dimensional lattice also. These are all the types of rotations which are consistent with translational periodicity.

In addition to it we have mirror correct. And these are all the independent operations which are possible. If you have a material which exhibits a 4-fold rotation, what are other rot symmetry elements which are possible?

Student: 2-fold.

Twofold and 1-fold is possible correct, is it not? Whereas for 1-fold there is only 1-fold rotation is possible. That means, that it is not only the 4-fold rotation these are also possible right. You consider 6-fold then what are rotations which are possible

Student: (Refer Time: 02:15) two, 3-fold.

Six-fold, 3-fold, 2-fold, and 1-fold, all these operations are possible correct. That means that the group of operations which are possible for a 6-fold is that contains all these symmetry elements. So, like that we can consider various symmetry elements. We can consider combination of these symmetry elements. If we consider the combination of these symmetry elements in 2-fold what are which we can have. 1-fold and mirror, 2-fold and mirror, 4-fold and mirror, 6-fold and mirror, these are all combinations which we can choose, is it not? That six independent rotation symmetry are there then a mirror is there we can have a combination also in two dimensional lattice. If we take that these are all the possibilities which are going to be there; this 1-fold and mirror will turn out to be what

Student: Mirror.

Only a mirror, then this is another one. So, essentially if we add now how many symmetry elements are there?

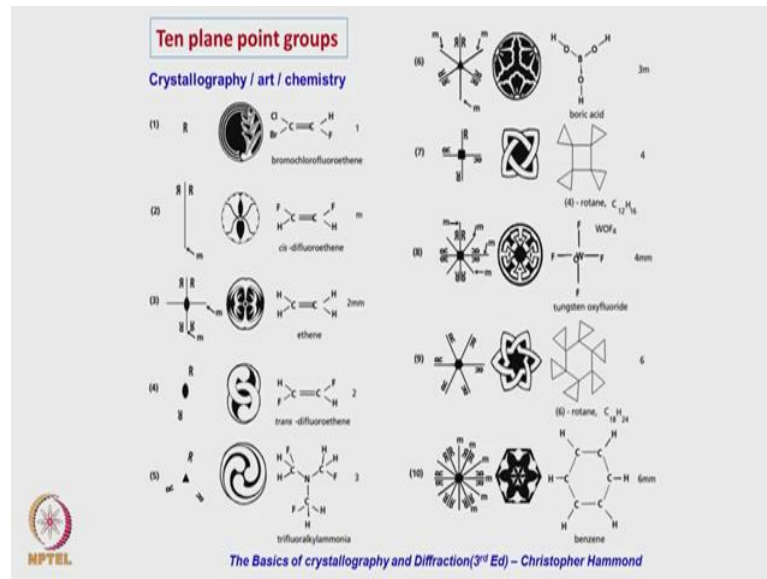
Student: 10.

10. So, essentially we can have 10 two dimensional point group symmetries; crystallographic point group symmetries are possible. This one can easily work out, that is what I wanted to tell; it is not very difficult. And in a two dimensional lattice if we consider it this 1-fold is essentially; if you take an asymmetric motif because the easiest way in which we can do it is take a motif which does not have any periodicity associated with it. Like if we consider r, I will take P if you take this is an asymmetric motif which it could be a molecule, but which does not have any symmetry associated with it. Then only symmetry which it can have is only a 1-fold rotation correct. There can be a case where the molecule itself as got one there is another one if we considered it then what is the symmetry which this has.

Student: (Refer Time: 04:56).

So, this has got only a mirror symmetry which is associated with it correct. So, like this knowing the symmetry operation one can construct the various types of motifs which are possible. That is what we discussed in the last class also.

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So, essentially this sort of motifs itself also could be used to keep it on a points. So, these are all motif around the point correct, that is around some axis we are seeing that these are all the rotational symmetry which are possible, then if rotation and a mirror is also there. Here the mirror is parallel to the axis of rotation in all these cases.

So, then we can have these are all possibilities which exists. So, essentially 10 planar point group symmetries are possible.


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10.1.2. Crystallographic point groups

10.1.2.1. *Description of point groups*

In crystallography, point groups usually are described

- (i) by means of their Hermann–Mauguin or Schoenflies symbols;
- (ii) by means of their stereographic projections;
- (iii) by means of the matrix representations of their symmetry operations, frequently listed in the form of Miller indices (hkl) of the equivalent general crystal faces;
- (iv) by means of drawings of actual crystals, natural or synthetic.

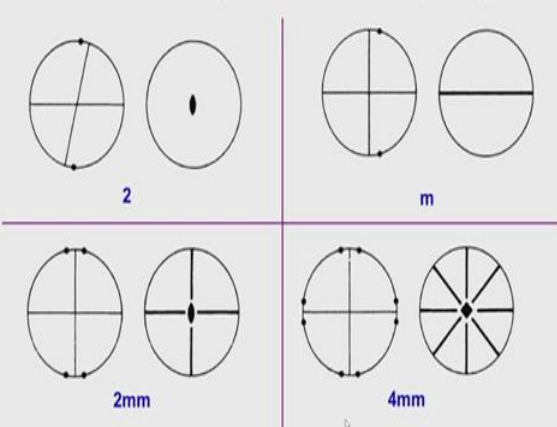


International union of crystallography tables

Then I have also mentioned that this can be described in different forms and different ways represented. The way in which it can be represented is one is using the symbols; Hermann-Mauguin symbol are the Schoenflies symbol. Another is with a stereographic projection we can represent it. Then there is a matrix representation in which what is the type of matrix which you use to transform from one coordinates of one point to a coordinate of another point. Or physically we can draw the picture itself and do this representation. All the representations have been used in crystallography.


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Examples of 2-D Point group representation using stereogram



2 **m**

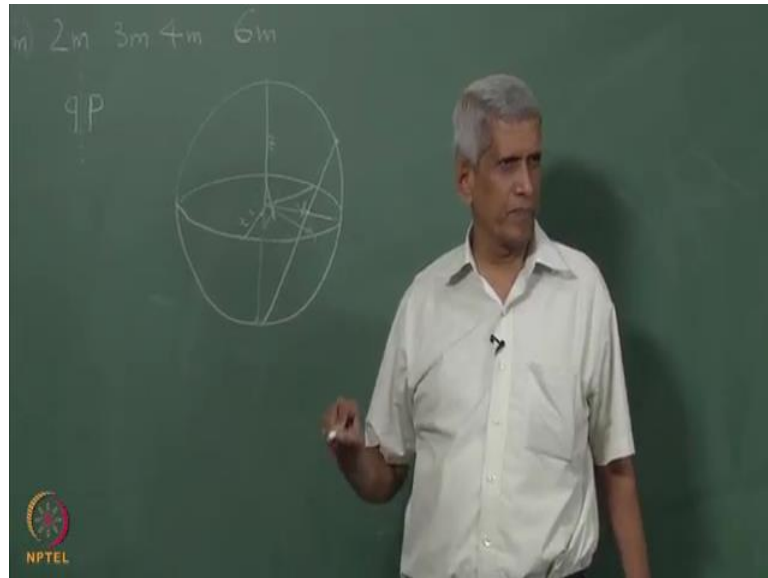
2mm **4mm**



Stereographic representation, general positions as well as symmetry elements are given.

Here what I am trying to do is to show for two dimensional lattice how it is represented in a stereographic projection. You remember the stereographic projection.

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Essentially, assume that this is a sphere, the coordinates x y z and when we are viewing from here, the pole of any point here under surface it will be cutting if we viewed from here; cutting along a particular point on the equatorial plane.

In a two dimensional lattice what happens the z information is not there, so we are keeping essentially; we assume that we are keeping a lattice right at the equatorial plane. How do we construct the pole there, the pole is nothing but a plane normal. Here what will be the plane? That is if this is all the row of atoms which are there in one dimensional to which we will be drawing a normal. So, we can draw the normal they will all be meeting on which plane; on the equatorial plane.

The projection when we see it in three dimensions; projection when we see it in two dimension it is essentially the poles are lying on the circumference of the equatorial plane. Because of that for a two dimensional stereographic projection for any point which we want to represent is essentially represented at the circumference of the circle, whereas in a three dimension for a pole which is going to be here it is representation will be within that inside. So, this is the difference which one should notice it.


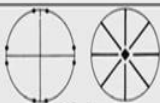
Here if you see it a projection which is being shown; this is the axis which is being shown and the two dimensional projection. If you take a pole of one point this will be rotated by 180 degree for 2-fold rotation it will come here; this is one way to represent. Another way in which it is represented is and the same stereographic projection the symbol used for 2-fold rotation is nothing but an ellipse; that way also we can represent it.

Here I am considering a case for a mirror; there mirror is perpendicular to placed on y axis there is along the y axis it is lying (Refer Time: 10:03) So, then what is going to happen if we have any point on the circumference this point will be represented here. Suppose this is for a three dimensional crystal possibly what may happen is that instead of this point may come inside and it is reflection will be come inside. That we will come to later, but this subtle difference one should know that for two dimensional lattices all the poles which we show are going to be on the circumference.

Similarly, we can do it for a; and not only that with a thick line in the stereographic projection the mirror will be represented. This we also one can represent it. For 2 mm if we consider we take a ort rotate it 180 degree it comes here, another rotation it comes back. And if we take a mirror along keep a mirror and the y z plane then what is going to happen is that this will get reflected here, this point will get reflected here. So now we have four poles are going to be there this represents 2 mm symmetry on a stereogram. That is what essentially is being shown here by. And once a mirror has been kept and these sorts of poles have been generated we can immediately see that it is equivalent to putting a mirror on the x z plane as well. So, that is why here you see that the symbol which are used is 2-fold is with the ellipse and two mirrors are being shown. This we can see it: this is for 4 mm.

(Refer Slide Time: 11:47)

Examples of 2-D point group

SQUARE SYSTEM			
4			
4	a	1	Square Square (d)
			 $(hk) (\bar{h}\bar{k}) (\bar{h}k) (hk)$
<hr/>			
4mm			
8	c	1	Ditragon Truncated square (g)
4	b	.m	Square Square (f)
4	a	.m	Square Square (d)
			 $(hk) (\bar{h}\bar{k}) (\bar{h}k) (hk)$ $(\bar{h}k) (hk) (hk) (\bar{h}\bar{k})$ $(11) (\bar{1}\bar{1}) (\bar{1}1) (1\bar{1})$ $(10) (\bar{1}0) (01) (0\bar{1})$

International union of crystallography tables

In addition to it, there is some other information which is also being provided; that I will come to later after a do it. Essentially what is being done is that if you have crystal with this symmetry, because all these point group symmetry has been found out by looking at material looking at the external forms. What all the types of shapes which can give raise to the same type of a; shapes can be external shape if you look at it can be different, but still the same symmetry can be exhibited. For example tetrahedron, what is the symmetry it belongs to cubic correct? You take a cube if a crystal goes in to shape; that also will have cubic symmetry. But if you look at the shape they have a different shape correct. Tetrahedron is not the same as a cube, but both can exhibits the same symmetry.

So, these what is being shown is what are the types of surfaces which it can have, what is the symmetry associated with it; that information is also given in this tables.

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Classification of 2-D point groups

Symmetry type	No.	Specific type
Pure rotation	5	1, 2, 3, 4 and 6
Reflection /mirror	1	m
Rotation plus reflection	4	2mm, 3m, 4mm, 6mm

Generation of 2-D planar groups / crystals

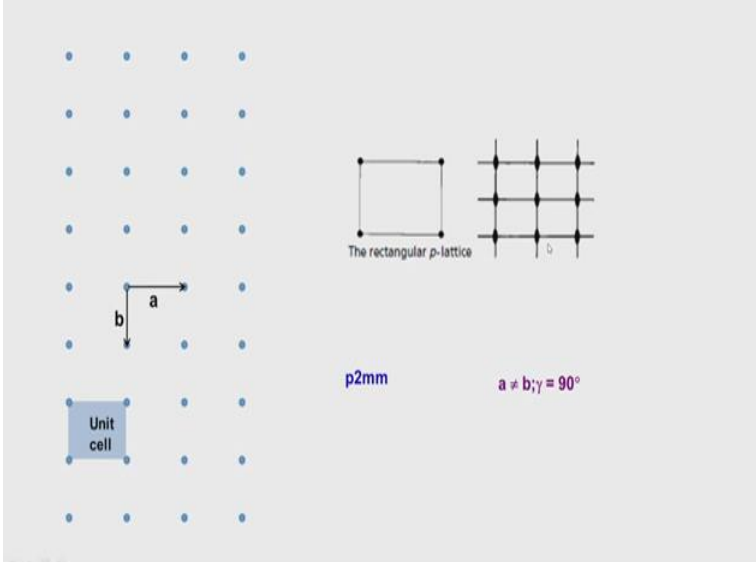
Ten 2-d point groups are consistent with translational symmetry.
Keeping motifs with these symmetry elements around each lattice point in a lattice one should be able to generate 2-D crystals.
Some examples of distinct crystals that can be generated are shown in next few slides

First let us look at the symmetries associated with 2-D lattices



So, essentially what we have is that in a two dimensional lattice if we consider the point group symmetries which we can have are only done. Now, let us look at some symmetry associated with two dimensional lattice, because we have looked at only the point group symmetry. That is around the point which we have considered, which is consistent with the periodicity of the lattice.

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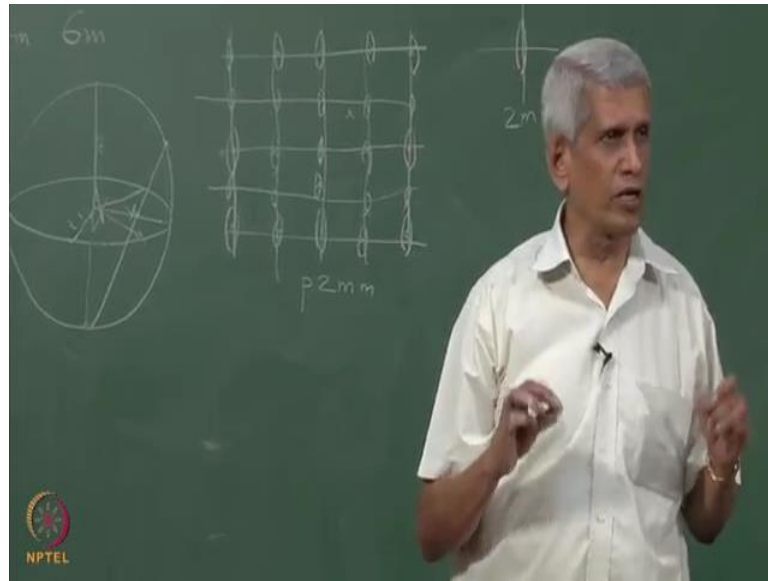


The rectangular p-lattice

$p2mm$ $a \neq b; \gamma = 90^\circ$

So, here what I have done is we are taking a rectangular lattice.

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In this rectangular lattice by inspection looking at it what are symmetries which it can have.

Student: 2-fold.

Two-fold, where it can there because once we fix a lattice there where we can have the symmetries also fixed. So, one we can have 2-fold here.

Student: (Refer Time: 14:26).

That is any of the lattice point we can have right, because we are only just showing part of the lattice; lattice is an infinite one. So, we can have 2-fold symmetry around all the lattice points. Is there any other place where we can have any other symmetry? That is if I take a point here or here or here or here, all these points also I can have a 2-fold symmetry, is it not.

Student: Yes.

If I take an axis here at this particular point rotate the lattice by 180 degree all these points will come back to original position, identical position. Again rotate it to once more it will come back to original position. That means that this point also has got a 2-fold symmetry.

So, now 2-fold symmetry is there like this here, points are there. In addition to it if I take this point, around this point also if I given 180 degree rotation around this point then also it will be coming back to an identical position. So, here also we have two dimensional that is 2-fold symmetry is there. So, these are all the points which we have 2-fold symmetry. What is it which is the rather than this? If I see with respect to plane like this, we have mirror symmetry. We have plane like this if you take mirror symmetry. So, that is also going to be there.

So, we have a 2-fold and mirror symmetry, and this is generally represented as a $p2mm$ that is how it is. And we say that for a crystal having the sort of symmetry a equals b not equal to c that angle between them is 90 degree correct. This is exactly what we are showing only a 1 unit cell. What are the symmetry element which are associated with it this?

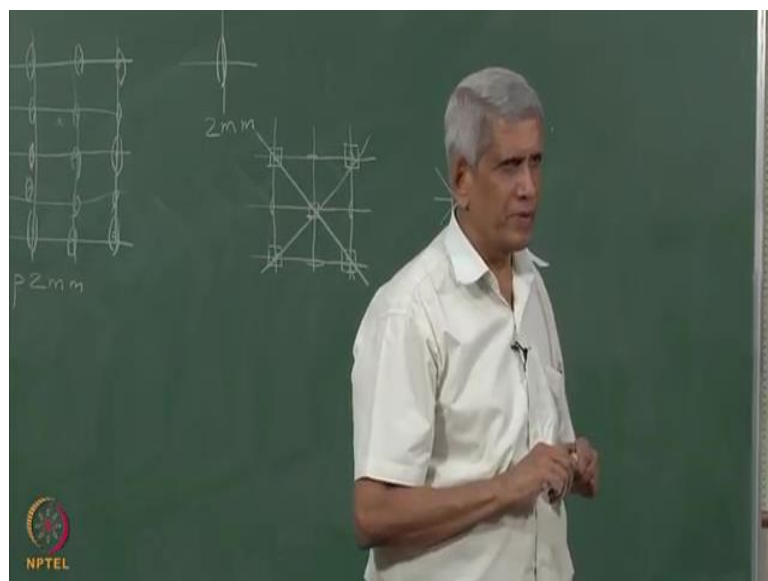
Student: (Refer Time: 17:23) mirror chose (Refer Time: 17:25).

Mirror?

Student: Chose and (Refer Time: 17:30)

That is here. These are all the symmetry elements which you have. Mirror and these symmetry elements are there, is it not?

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And if you look at any lattice point, what are symmetries which are associated with it now here. This has one 2-fold; these are all the symmetry elements which are associated with it mirror. Is it exactly what the point group symmetry also right, what we have looked at it point groups symmetry around the point is this corresponds to 2 mm.

So, here if we looked at all these points all of them mixing with the same type of a symmetry; 2 mm. And any point which is there here the centre, here if you consider it what will be the symmetry which it will exhibit. Only on 1-fold rotation symmetry, because around this point except for 360 degree rotation around this axis any other rotation it will not come back to identical position.

From consideration of this lattice you can immediately understand that apart from the lattice point which are having an identical symmetry there are other points in the material which also exhibit some symmetry elements associated with it. These types of points are called as Special Points in the crystals; the unit cell of the crystal.

Now, let us consider a square lattice. In a square lattice what are types of symmetry which we can have here.

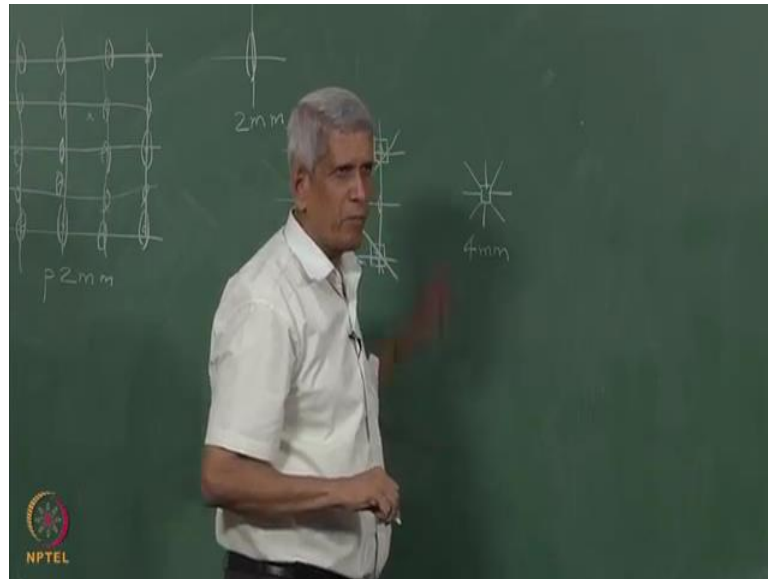
Student: 4-fold.

Fourfold symmetry is possible; that means, that 4-fold symmetry is the symbol is just putting square to represent it, I am just showing one unit cell is it 4-fold. By looking at this is that any others symmetry elements which are possible at any other place.

Student: (Refer Time: 20:18) 2-fold (Refer Time: 20:20).

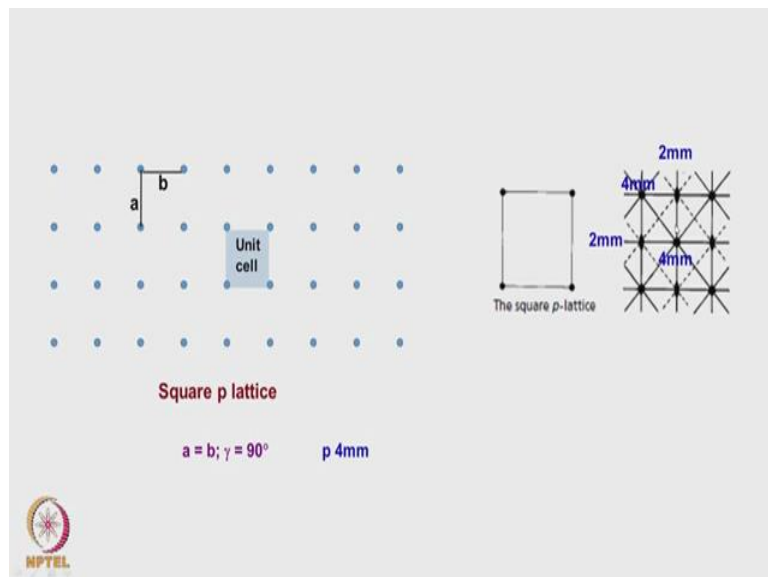
Here 2-fold will come here, 2-fold will come, and here also again at the centre you will have a 4-fold. Then in addition to it you will have a mirror symmetry which will come passing through this correct, is it not. Then along the diagonals correct. So, if you now look at any of this point you have a 4-fold. These are all the symmetry elements which are there correct.

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This is essentially for 4 mm symmetry, point group symmetry it is going to be 4 mm; for a 4 mm symmetry if you look at it this is the symbol which we use right point groups there are point groups these are all the two mirror planes which are cutting each other. So, that is exactly what we have.

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In addition to that if we consider an axis like this here what happen suppose we assume that on these points an atom is being placed at n r motif with an infinite symmetry being placed. Then what is it which is going to happen. That is if I put the plane like this, a

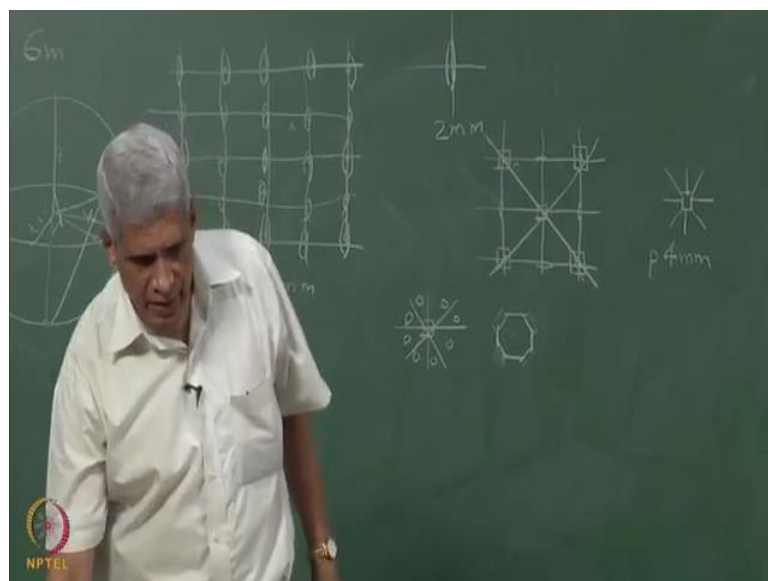
mirror plane like this what it will happen is that this will be reflected and it should come here, but there is nothing is going to be there. But if from here to here what is the distance? This is a by root 2 with respect to the, if a is there side of the unit cell. Then from here to here you shift it, and then around this if you take a reflection this point will be generated.

And again from here to here you shift it by half the lattice translation vector in this direction and again take a reflection around it you get it. This is what you we have discussed earlier that this is a nothing but a glide. So, in addition to mirror a glide also is inherently there in this one it is not separately added, but this structure has got glide also present in it.

So, if you look at all the points that are this is the unit cell which we are considering it here what are the symmetry elements which are associated with it around any of this lattice points we have a 4 mm symmetry. Here on this point we have 4 mm symmetry, then around this point 2 mm symmetry similarly we have a here 2 mm symmetry is there, then there is a mirror, there is a glide, 1-fold symmetry, all these symmetries. Except for that 1-fold there are some symmetry elements of the other is present.

Now what I wanted to remember here is that we talk with respect to 10 point groups, what are the types of symmetries which can be associated with it?

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Here also if we look at it that same type of a symmetry element being associated with it. If I take that motif like 4 mm symmetry if I take it r it will be; I will just put it with the circle that means that, that will be just to represent that one of the points that is at anywhere if I put it for a 4 mm symmetry around this there should be a eight equivalent point should be there then only the 4 mm symmetry will be satisfied. This you assume a it represents as an asymmetric motif, is it clear.

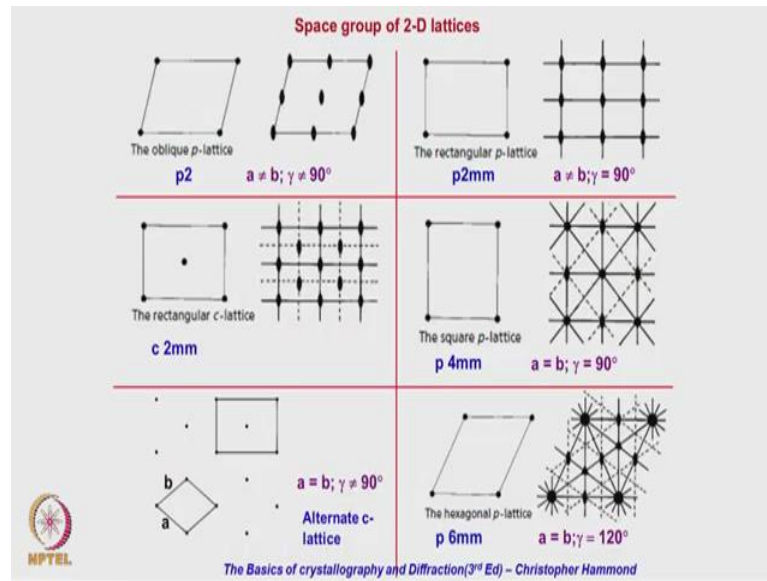
If I take this and put it here then what will happen? With respect to the lattice the motif which I have chosen all its symmetry elements match perfectly correct. Then only this putting one motif at that point is good enough to satisfy the full symmetry of the lattice, is it clear. See this could as well be, this is a eight sided one. Suppose this is the motif symmetry. If you take it and keep it here at this point all the symmetry elements match. If the symmetry elements match with this one motif keeping it there at the lattice point, the lattice could be generated, is this clear. Suppose I keep the motif in such a way that instead of keeping it here suppose I keep this motif somewhere here, then what will happen?

Student: (Refer Time: 27:07).

Because I am putting at the point where is 1-fold then at eight positions around that it has to be kept. Even though it has the full symmetry it has to be kept to satisfy the complete symmetry you understand that. That is a point which I want to emphasize. So, the point where we keep it what are symmetry element which are associated with it; we have to locate it. And whether the symmetry elements match or not, are also has to be seen, is this clear.

So, essentially in this structure if you look at it we have many positions are there where we could place, because this is a lattice. In these lattice atom could be kept at the lattice points or at this middle of this each of this lattice translation vector sites or at the centre of the unit cell or at any point here. So, there are many possibilities are; or on this mirror planes we could keep it. Any way we can keep it and create a lattice; two dimensional. The same is two for three dimensional lattice also.

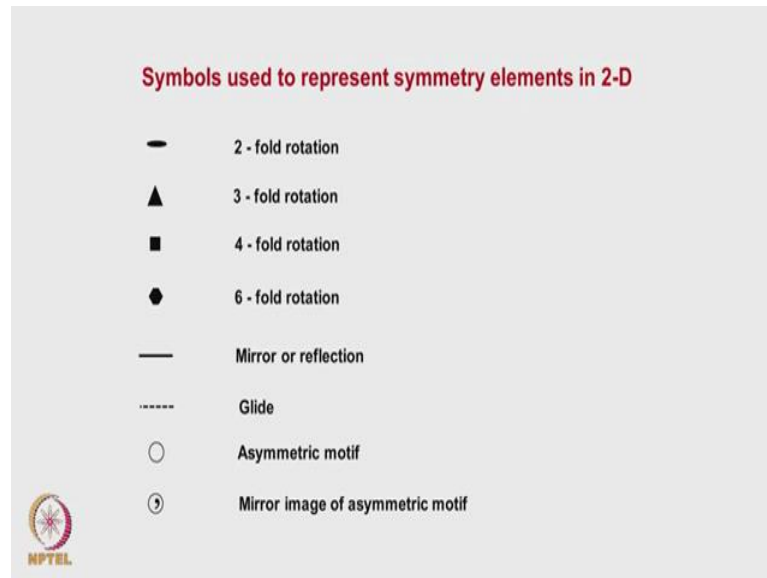
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Before going in to it those detail further what I have done it is that just shown that this is the way we can find out the symmetry of the lattices. So, for the 5 two dimensional lattices the symmetries which are associated with it together representation because this is c centred so it is 2 mm, others are all. And this is the maximum symmetry a crystal can exhibit, because around each lattice point suppose we put an atom and we generally assume atom to be spherical.

If an atom is spherical one single atom if you put it, then since it has got infinite symmetry associated with it all the symmetry around each of the lattice point are the sides each satisfied by that. Because of that the maximum the symmetry which the crystal will exhibit is this particular one. But depending upon the shape you can exhibit symmetries which are less than this also.

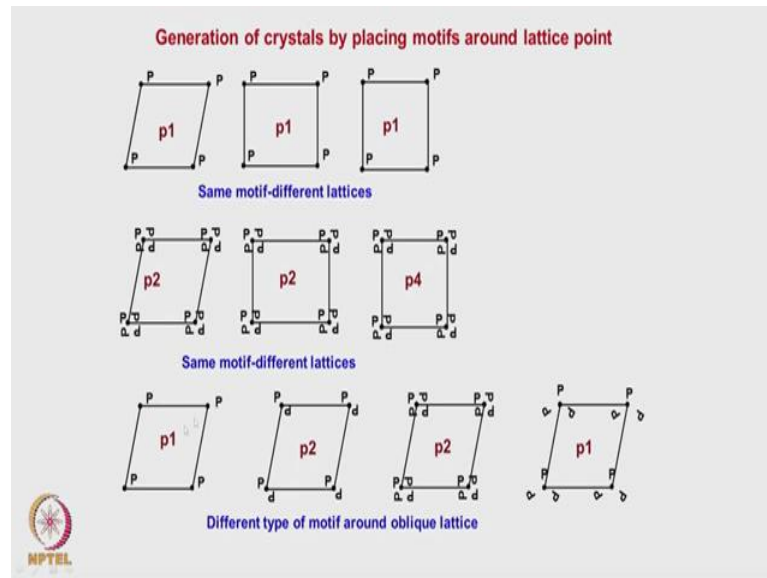
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In fact, these are all the types of symbols which we use for 3-fold, 4-fold then 6-fold. And in this, another one also which we should consider it is that if you look at the factors of 4; the 4 is a 4 into 1 right; 2 into 2 it will come 4 can come. And here similarly if you look at 6; 6, 3, 2, 1, so these are all the groups which you can see. So, if a crystal is having a 6-fold symmetry are; what all the symmetry lower than that which it can have. They are also given by this root; that is a 6-fold crystal can exhibit a 3-fold symmetry. What can happen is that when a phase transformation takes place? From one structure to another structure when it under goes a transformation, phase transformation or transition you called physics you called it as a phase transition.

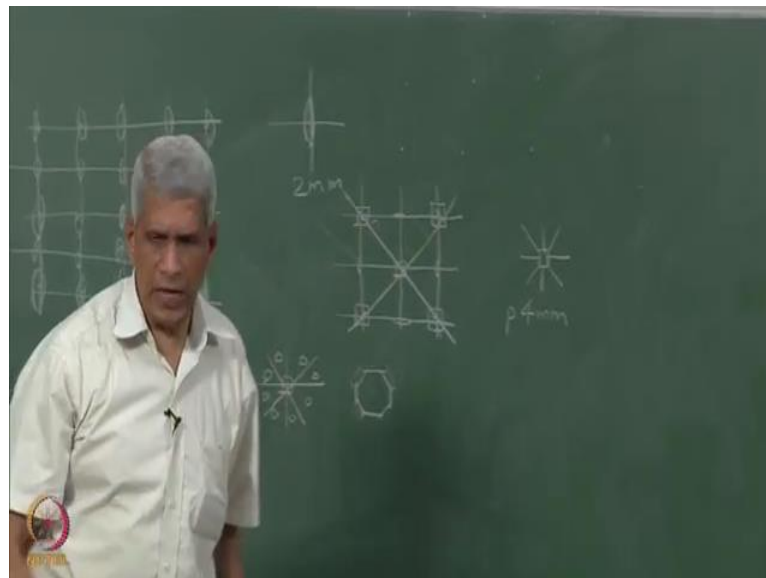
Then there is a relationship between what sorts of structures which it can form when it goes from one structure to another structure. What is very important is that from this between 4-fold and 6-fold that is between cubic or cubic and hexagonal if you look at it there is nothing common between them these are two different classes of structures. That is in a cubic structure in a cube by whichever way you arrange atoms around the lattice point you cannot create a hexagonal lattice. In a hexagonal lattice whichever way you try to put the motifs around them you cannot create a lattice with a cubic symmetry; you understand that. Is this clear? This you might have noticed in many of this phase transformations (Refer Time: 31:59) you might not been aware of it that why it happens, but this is because of this reason it is; related to the symmetry.

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Here what I have considered is a let us take a different type of motifs, where no different type of a two dimensional lattice put a motif around it. This is a parallelogram to the oblique lattice. And what is the symmetry which is associated with it has? 2-fold symmetry which is associated with this lattice; what is the symmetry of the lattice 2-fold.

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That is around this point if I around this axis if I do an 180 degree rotation I will be able to bring it back, this has got a 2-fold rotation. But around each lattice point around it I am putting an asymmetric motif. When an asymmetric motif has been placed then at the

identical position we have to place that motif. So, when we do that? Now we should look at this crystal what is the symmetry which it has only in a 1-fold symmetry. The 2-fold symmetry is last. And here you see that it is essentially a rectangular lattice where when we keep a motif asymmetric motif; only 1-fold symmetry is present right p 1. So, this is what essentially it happens with all the irrespective of though the lattice has got a higher symmetry. The symmetry of the motif also decides.

So, not only the symmetry of the motif, if symmetry has got an infinite if the motif has got an infinite symmetry associated with it then it can exhibit the complete symmetry of the lattice. If the motif has got a symmetry which is higher than that of the lattice and depending upon how the different axis of symmetry match that decides what is going to be the symmetry that which is common to them between both of them that group that decides the symmetry of the crystal. Is it clear? Like here what I have done it is. Similarly I have taken a for loops motif which has got a 4-fold symmetry right. So, if you look at this motif it has got a 4-fold symmetry associated with it around this axis if we take its rotational symmetry.

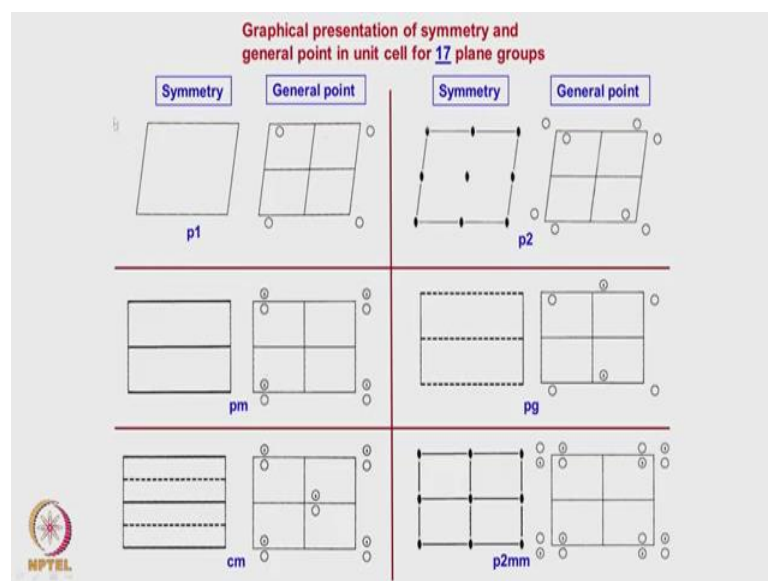
This lattice is essentially an oblique lattice which has got only a 2-fold symmetry when I keep this around it, since the axis of rotation the 4-fold as well as the 2-fold because when I say it as a 4-fold it has got a 2-fold rotation associated with it. So, which is common to them both is the 2-fold. So, these exhibits now were 2-fold rotation. And like here it is essentially a rectangular one where when I put a 4-fold again around each of this lattice point its essentially a 2-fold rotation is what the lattice has got and motif has got a 4-fold rotation and the 2-fold rotation, since the axis coincide it will exhibit only a 2-fold.

Whereas, here if you see it is a square lattice around which I am putting a motif which has got the 4-fold rotation. Now this exhibits the 4-fold symmetry, is this clear? But you should understand that this exhibits only a 4-fold symmetry. What is the symmetry of this lattice square lattice generally 4 mm. But that mirror do you see that? No mirror is not there that is because the mirror planes of the lattice there, but this has got no mirror symmetry associated with it; you understand that. I am just taken it the few examples to illustrate that point. Here if you see it I have taken the same type of a lattice it is an oblique lattice, two dimensional lattice in to which I am taking a only as an asymmetric motif and put keeping it here.

Though it as a 2-fold rotation now it becomes as if it has got an only 1-fold rotation correct. Now you look here it has a 2-fold rotation associated with it, the motif which has been kept and the axis of that motif which has been put 2-fold rotation axis and that of the lattice that match. So, because of that the crystal exhibits 2-fold. And here it is a 2-fold and to which of motif with a 4-fold symmetry is kept, but still get what it will exhibit is only the 2-fold symmetry. Here it is I am putting a 3-fold around a 2-fold, because the crystal a lattice has got a 2-fold symmetry. I put a motif which has got a 3-fold symmetry. With the axis of the motif match, but between two and three there is nothing common in that symmetry elements. Because of that this will exhibit now only in 1-fold; you understand that.

So, what we have looked at is crystals and lattices we have looked at it. What all the symmetries which are associated with the lattice we have discussed. And depending upon the symmetry of the motif which we place it, what all associate in what all symmetry elements which are common, not only they are common which are matching with the symmetry elements at a specific point where we are putting that motif that is going to decide what will be the symmetry which the crystal will exhibit, is this clear. This is the bottom line of this entire discussion so far. If you look at the international union of crystallography table the way these various two dimensional point groups are represented.

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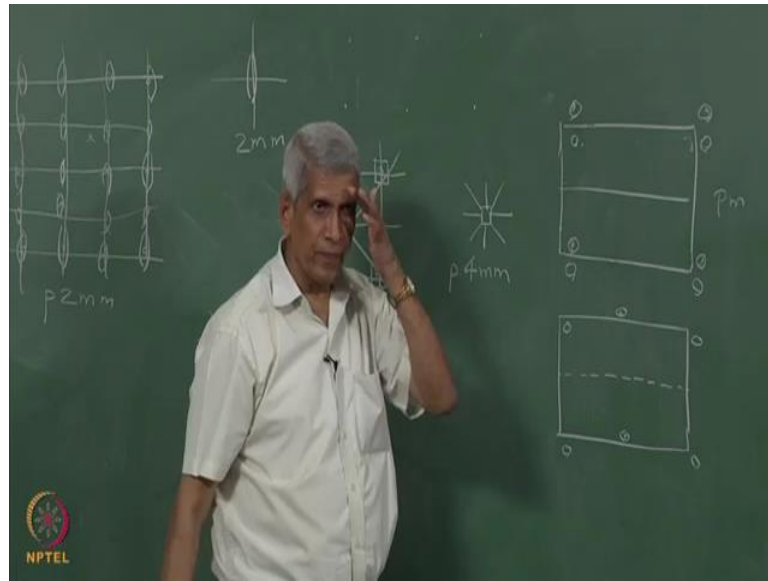


When we try to put motifs around each of these point one it will be just showing what is the unit cell shape; this is how it is going to be; this is for p 1. And we are putting a motif at one point that it will represent a motif this is just a symbol which is being the circle is a symbol which is being use to represent a motif. If we keep it at any particular point at a identical position we keep it, this is a crystal which will be there. This is called as a general point. That is where we put it the motif which does not contain any symmetry that point is called as the general point.

And here at this lattice if you see these are all the symmetry elements which are associated with it, but we are essentially putting motif at one particular point, so correspondingly 1 will come here by 180 degree rotation. This is how exactly the general point which is going to be there. If you look within this unit cell always two motifs are going to be there, is it not, because this also will satisfy a 2-fold rotation. Similarly if you take a mirror which is going to be there on one axis, if we take here, since the mirror is only one single mirror is there. So, essentially this symbol which is being used that is circled with a (Refer Time: 41:04) that is what the international crystallography table they use it that represents that it is a mirror image. So, this is how it will be done.

What is essentially interesting is that here that is the mirror is there that mirror image when we take it if we give a glide also; that is half a translation doing it then what will happen for this point the mirror image will come here, because what is being done is that you take it from here translate it and then take a mirror, then translate it take a mirror, then these type of structures can also exist, is this clear.

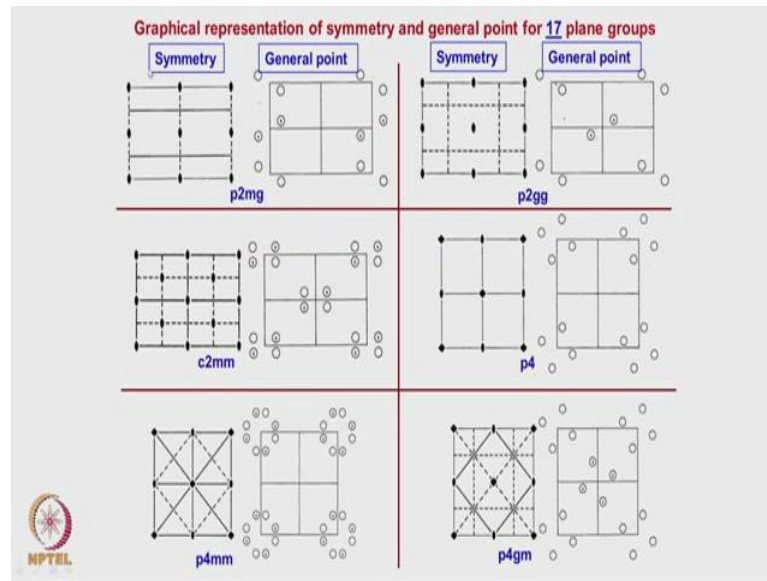
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Essentially what we do assume that the mirror is here; so for this point the mirror is, this is pm just a mirror is there. If the same structure this dash plane if you use is to represent the glide plane. Now if you see it in this structure what we have done it from here, from here to here is the lattice translation vector. We have shifted it by half and then take a mirror image. Again shifted it by half that is translated by half is strength and then taken a mirror image, so it will come back to this position. These types of structures are also possible in crystal structures.

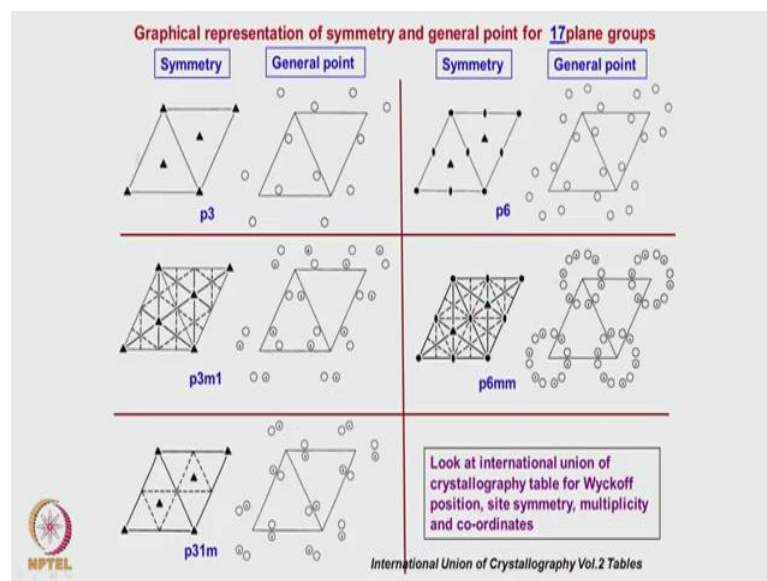
So, this is another type of lattice in addition to mirror the glide also gets added to it. Then the number of two dimensional groups which we can have turns to be 17.

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That is where you can see that only wherever somewhere mirrors are there mirrors also get translate. In some cases the glide is inherently a part of the mirror then we do not run. In some cases the glide can be generated like in this particular case. This type of crystal structures are also there, many of the molecules have this type of structures are there. So, essentially this you can go through it later through these slides or the books which I have mentioned where these structures are explained in detail. But generally in those books this is the graphical representation.


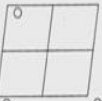

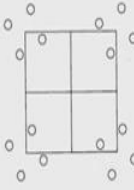
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One is the symmetry which is represented on the unit cell; another is the position of the asymmetric motif where around each lattice point is represented that is called as a general position. These are all the two things which are represented. And in addition to it another information which is important is that if we have to construct a crystal structure at two dimensional structure, if we go from what all the coordinates when we do this symmetry operations; for any particular how we transforms that information is also required.

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Examples of plane group representation in IUCr table

Oblique	p1	p1	1	Multiplicity/ Wyckoff letter/site symmetry	Co-ordinates	
				1 a 1	x,y	
Square	p4	p4	4	No:10	Multiplicity/ Wyckoff letter/site symmetry	Co-ordinates
				4 d 1	x, y -x,-y -y, x y,-x	
				2 c 2	1/2, 0 0, 1/2	
				1 b 4	1/2, 1/2	
				1 a 4	0, 0	

Site symmetry - point group symmetry associated with a site in the unit cell



That information is given also given in the international union of crystallography. Like here what happens is that you see that this is a oblique lattice two dimensional lattice only an asymmetric motif is kept at any particular point and what is being given is that something called as a Wyckoff position that is the symmetry associated with these 1-fold and the coordinates are just x y. To this what will be the coordinate of this one? By a lattice translation operation if you do it in this direction you will be adding by 1 0 0 if you add you will be getting it. In this one that is 0 1 0, like that in any direction in 1 1 if you add in this direction. Like that we can find out what will be the coordinates at which the motifs have to be placed that we can find out.

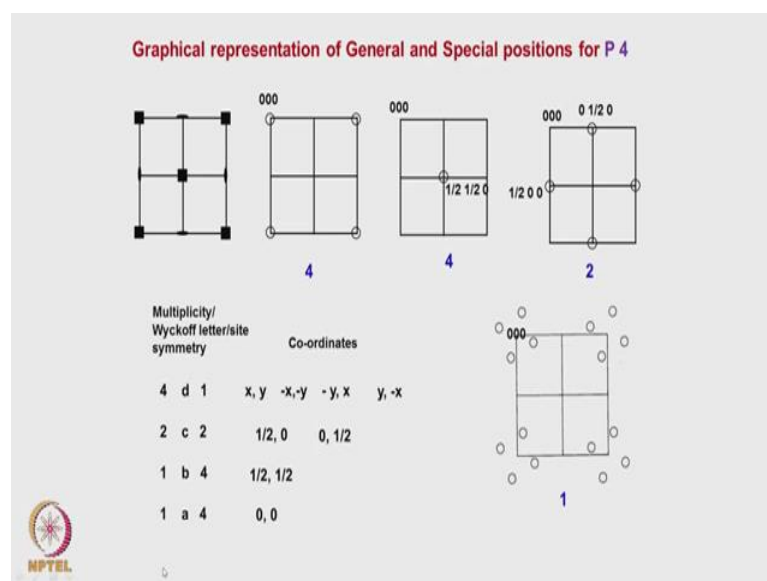
By here if you see it this is a square lattice. In this square lattice we have a 4-fold rotation is there and a 2-fold is there, but there is no mirror. So, what all points which we have? There is one point here which has a 4 mm symmetry, I had shown just some time

back that in this point has got a 4 mm symmetry this point also has got 4 mm symmetry, this point has got 2 mm symmetry.

So, that is what is being shown. That is if you see one what is essentially is being shown is that the 4-fold symmetry; that means, that if I keep an atom at this position 0 0 by lattice translation the atoms at all other points could be generated. That is essentially what is being shown here, the multiplicity is one here. And if you see at the middle also you can put one, then also it will satisfy the full symmetry of the lattice; that is another point. Instead of putting an atom at this point I can consider a square lattice infinite lattice. Put atoms at these points at the centre of that lattice points, then also it will exhibit the same symmetry of the lattice will be exhibited crystal can happen. Or I can put it at this point, if I do that the positions where I can do it is half 0 that in this case x is half y is 0. Similarly, 0 half in this it can be done.

In these two points also if I put there is also exhibit the 4-fold symmetry. And then general point, anywhere you put it not at any of the special lattice points if you put an atom then also the 4-fold symmetry will be satisfied. That is if we have an atom, this is the lattice which is there what all the various ways in which or what all the various positions where we can put the atom and still satisfy the symmetry of this particular crystal. This itself is I am showing it in another way. This is one I put it around 0 0 by lattice translation vector.

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Next one we will come at another lattice point all lattice points we have to keep an atom. And if you look at these four once by satisfy of 4-fold symmetry: they satisfy a 4-fold symmetry correct. If I put one at the centre here instead of putting it there and like that one will come here, another will come here, another will come here, all the lattices then also a 4-fold symmetry satisfy. We look here put at these two position by taking the lattice translation symmetry one point will be generated here, another will be generated. Though this is the lattice which we considered atoms are put at these positions now this also as a 4-fold symmetry. So that way also we can fill up the lattice and this is where we are putting an atom at a position which does not have any symmetry associated with it, then we have to keep it like this then you can see that this also satisfies a 4-fold symmetry.

But what is the difference which you see between all these? Here the number of lattice points per unit cell is one, here also the number of lattice points; the number of atoms per unit cell is 1 here; here the number of atoms per unit cell is 1. What happens here; 2, here 4. So, depending upon where you put it the number of atoms which will be required to generate the specific lattice changes and that is dictated by the symmetry which is associated with it. The points which have got the maximum symmetry of lattice the 4-fold symmetry then we require at only 1, that is what that multiplicity in this table which we represent it gives out.

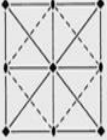
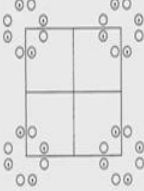
And here the multiplicity is 2 in a general one shows the full maximum number of atoms which will be required, if you put it at the general point to create the lattice. But all the way we are creating a crystal by all these methods; the various methods which I have adopted we are generating a crystal, but it is having a symmetry which is that same; crystal has got the same symmetry.

If you have any questions you please do stop me and ask me, that is very a important. And that is what essentially is represented. Now in these points what is being given the coordinates of each of these points? If you take x y it will turn out to be $-y$ x , then $-x$ $-y$ y $-x$ this is going to be the coordinates. If these are all the coordinates of the point for a general transformation we can find out the matrix which is responsible for it also, you can relate. That way also we can represent the lattice translation we can represent the symmetry.

There are many methods of representation. But this table is very important, because if you understand this table and how the structures come this could be utilized to construct any crystal structure. That is what we use from international in a crystallography table to generate and draw different type of crystal structures, is it clear.

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Examples of plane group representation in IUCr table

Square	p4mm	p4mm	4mm	No:11
				
		Multiplicity/ Wyckoff letter/site symmetry	Co-ordinates	
		8 g 1	(1) x,y	(2) x,ȳ (3) y,x (4) y,x̄ (5) x̄,y (6) x,ȳ (7) y,x̄ (8) ȳ,x̄
		4 f .m	x,x	x̄,x̄ x̄,x x,x̄
		4 e .m	x,½	x̄,½ ½,x ½,x̄
		4 d .m	x,0	x̄,0 0,x 0,x̄
		2 c 2mm	½,0	0,½
		1 b 4mm	½,½	
		1 a 4mm	0,0	
		Special:		
		no extra conditions		
		no extra conditions		
		no extra conditions		
		hk: h+k=2n		
		no extra conditions		
		no extra conditions		
		Symmetry operations		
		(1) 1	(2) 2 0,0	(3) 4 ⁺ 0,0 (4) 4 ⁻ 0,0
		(5) m 0,y	(6) m x,0	(7) m x,x (8) m x,x̄

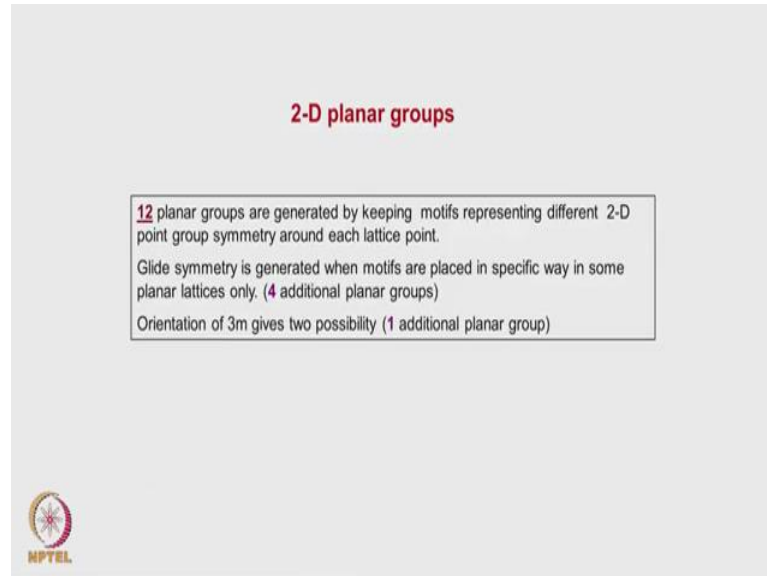
Here I have taken; this is a lattice symmetry is 4 mm. Now I am taking a one with a 4 mm symmetry. Here if you look at it a mirror is also attached to it each of the lattice point here.

Now, the number of special points that is these points which have got some symmetry associated with it they are called a special points. Each point has got some called as a sight symmetry right; what is sight symmetry is at this particular sight it has a 4 mm symmetry at this particular sight it has a 2 mm symmetry because with respect to a neighbours if you try to look at it positions where they are what is the symmetry which is shows that is called as a sight symmetry that is what is being. That sight symmetry is also a sub group of the main symmetry element of the lattice, is this clear?

And in addition to it they give also for the different type of what all the conditions under which the reflections will be absent or present all those conditions are also mentioned in this table itself. This table is a very useful. This contains lot of other information with a crystallography. But to construct a crystal structure this particular table which gives the

coordinates and the Wyckoff positions of the various special and general point is what is really necessary, is this clear.

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2-D planar groups

12 planar groups are generated by keeping motifs representing different 2-D point group symmetry around each lattice point.

Glide symmetry is generated when motifs are placed in specific way in some planar lattices only. (4 additional planar groups)

Orientation of 3m gives two possibility (1 additional planar group)



So, if we do that we will have totally around 17 planar point groups are going to be there.

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Details of plane group symbols

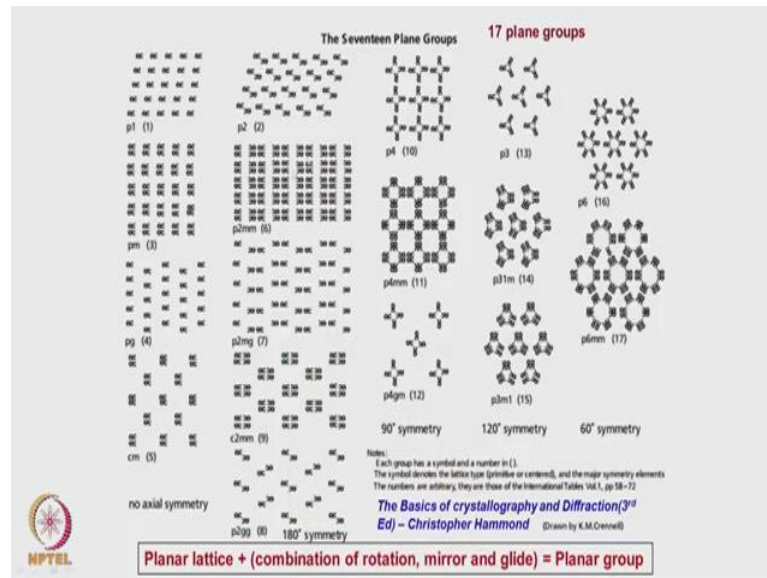
- p1** - 1 fold symmetry (P111)
- p2** - 2 fold rotation along z-axis and 1 fold on other 2 directions (P211)
- pm** - mirror plane perpendicular to y or x axis (Pm11 or P1m1)
- pg** - glide plane perpendicular to y or x axis (Pg11 or P1g1)
- cm** - centred lattice; mirror plane perpendicular to y or x axis (Cm11 or C1m1)
- p2mm** - 2 fold rotation along z-axis; mirror plane perpendicular to y and x axis
- p2mg** - 2 fold rotation along z-axis; mirror plane perpendicular to y(or x) and glide plane perpendicular to x (or y) axis
- c2mm** - 2 fold rotation along z-axis; mirror plane perpendicular to y and x axis
- p2gg** - 2 fold rotation along z-axis; glide plane perpendicular to y and x axis



Now, we have come to an end. So, I have done it is that when we say p 1 1-fold symmetry actually it has to be written p 111, because along x axis 1-fold symmetry y axis is 1-fold symmetry z axis is 1-fold symmetry, because we use some coordinate

system to represent it with respect to that, but generally a short symbol is use to represent as p 1; this also I had given.

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This is taken from that book a Hammond's book that using r as an asymmetric one then what are the types of crystals which can be constructed two dimensional crystals with different space groups. We can have distinctly only 17 which is possible.

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Two dimensional lattices, point group and space group

System and lattice symbol	Point group	Space group symbols		Space group number
		Full	Short	
Parallelogram	1	<i>p1</i>	<i>p1</i>	1
<i>p</i> (primitive)	2	<i>p211</i>	<i>p2</i>	2
Rectangular <i>p</i> and <i>c</i> (centred)	<i>m</i>	<i>p1m1</i>	<i>pm</i>	3
		<i>p1g1</i>	<i>pg</i>	4
		<i>c1m1</i>	<i>cm</i>	5
		<i>p2mm</i>	<i>pmm</i>	6
		<i>p2mg</i>	<i>pmg</i>	7
Square <i>p</i>	4	<i>p4</i>	<i>p4</i>	10
		<i>p4mm</i>	<i>p4m</i>	11
		<i>p4gm</i>	<i>p4g</i>	12
		<i>p3</i>	<i>p3</i>	13
		<i>p3m1</i>	<i>p3m1</i>	14
Triequangular (hexagonal) <i>p</i>	<i>3m</i>	<i>p31m</i>	<i>p31m</i>	15
		<i>p6</i>	<i>p6</i>	16
		<i>p6mm</i>	<i>p6m</i>	17

A. Kelly and K. M. Knowles, Crystallography and Crystal Defects, 2nd Ed., John Wiley & Sons, 2012

This is also another way in which that same thing is being represented. This is taken from the Kelly and Knowies book. One can go through this and understand it. Essentially

all are the same, only in this case of 3 m there are two positions are there: that is 3 m 1 and 3 1 m. This I will not discuss about all these finer details, because I just wanted to give you a flavour of what all the types of symmetries which are associated with it, how this can be used to construct the various types of lattices and understand; because the aim of doing x ray diffraction or electron diffraction or neutron diffraction.

One of the main aim is to find out the crystal structure for which looking at the symmetry of the pattern which is especially the two dimensional pattern is what we get it and how to go about an it look for which one should understand the symmetries which are associated with the lattice it is very much necessary. The earlier people use to work on mostly metallic systems, now it is not just metallurgy it is on material science where people work on all types of ferroelectric materials, piezoelectric materials, various types of photonic materials, where they have different types of crystal structures are there and people are doing extensively electron microscopy so one should be able to looking at the diffraction pattern one should be able. And all diffraction patterns are two dimensional patterns. So, the types of symmetries which it can exhibit these are all the types of symmetries and these are all the five types of a two dimensional lattices which it can found.

What I will do is I will stop here, it is already time. You will have class now right; some of your class is there stop here. In the next class we will; from most of the information which is necessary has been told then we will talk about what all the other additional symmetry elements which are necessary for a space lattice that we will consider. We will stop here now.