

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

Lecture - 03
2-D Lattices

Welcome you all to the second lecture on Defects in Material. In the first lecture, we had covered about 1-dimensional lattice. In the second; in this present lecture, we will talk little bit about the 2-dimensional lattice.

(Refer Slide Time: 00:41)

Two dimensional Lattice


Arrangement of 1-D lattice at a periodic distance in a direction non-collinear with the 1-D lattice, 2-D lattice can be generated

△ △ △ △ △ △ △
△ △ △ △ △ △ △
△ △ △ △ △ △ △
△ △ △ △ △ △ △
△ △ △ △ △ △ △
△ △ △ △ △ △ △
△ △ △ △ △ △ △

Examples of 2-D crystals

.P .P .P .P .P .P .P .P
.P .P .P .P .P .P .P .P
.P .P .P .P .P .P .P .P
.P .P .P .P .P .P .P .P
.P .P .P .P .P .P .P .P

How many types of arrangements we can have in lattice and crystal ?



The first thing which you have to look at it is how can we construct a 2-dimensional lattice; like we have like crystal, we have considered as some motifs which is arranged in a periodic fashion, if you repeat this motifs in the second direction because most of the motifs has been shown as periodicity in the y direction, in the x direction if we keep at some particular distance and also as a particular angle if we keep them.

Then various types of 2-dimensional lattices could be generated. I had just shown some 2 examples of it and in the second one of; some lattice points associated with the motifs also. What are the different types of if we consider only the lattice points that we generate a 1-dimensional lattice, what all the different types of lattices which we can generate? Let us look at it.

(Refer Slide Time: 01:26)

Two dimensional periodic structure

Oblique P lattice

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

$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2$

$\vec{R} = n_1 \vec{a} + n_2 \vec{b}$

$\vec{R} = u \vec{a} + v \vec{b}$

All lattice points have identical environment. Lattices are infinite.
Lattice size is so large that surface effects can be neglected.
Any two primitive vectors can be used to generate unit cell. (unit cell not unique) Generally one chosen is that which exhibits the maximum symmetry of the unit cell

Primitive and non primitive lattice

Here what is being done is that we have the 1-dimensional lattice which is there. It is the 1-dimensional lattice is kept at regular intervals in the x direction, but inclined at an angle with respect to the x axis, when this is being done we are able to generate if we look at is where type of a parallelogram which repeats itself. These parallelogram if you look at it, there are various ways in which this lattice itself could be represented 1; once we fix our coordinates of the lattice like fixing the coordinate at this particular position once the coordinate has been fixed at this particular point. And at the origin of the coordinates is fixed and this is the i x coordinate are the a coordinate and the b a coordinate using the vector notation, we can write it as \vec{R} is equal to $n_1 \vec{a} + n_2 \vec{b}$, \vec{R} as I mentioned if you use a v w to represent the number of times they repeat in the x and y direction, we can write it in the vector notation as \vec{R} is equal to $u \vec{a} + v \vec{b}$ into b.

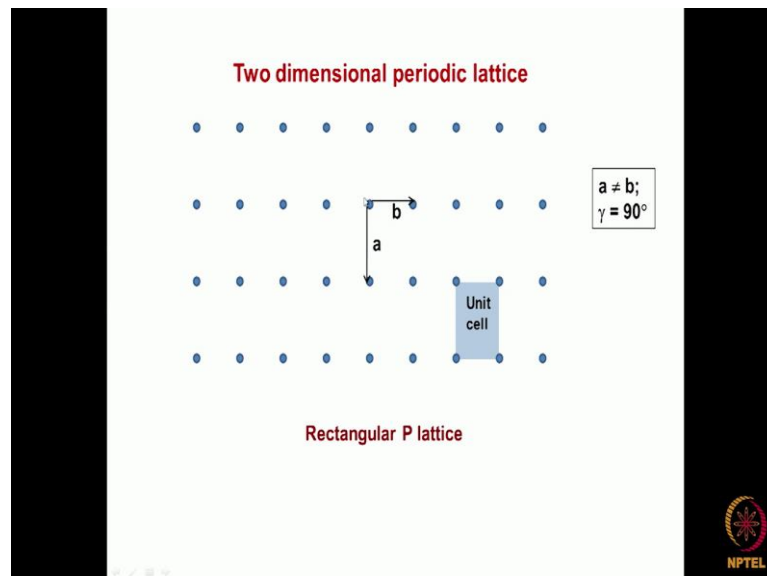
And another way in which it can be represented is that the area which is being covered by this unit cell if you look at it, this can be kept adjacent to each other and this way also it repeats itself and another important aspect which you used to see that this unit cell; how many lattice points are present per unit cell, if you look at its only one and is it the only way the unit cell can be constructed? No, if you look at it here this is another type of a unit cell which repeats itself. This is another way in which a unit cell is generated which repeats itself. So, the unit cell is not unique, we can have any type of a unit cell,

but what is important about all this unit cell is that area of the unit cell remains the same and only 1 lattice point per unit cell is being present.

So, these types of lattices are called as primitive lattices. What we do to generate a primitive lattice is used the shortest translation vectors in two directions and the directions which are not parallel to each other. And similarly we can generate non primitive lattices by generating a lattice of this particular type and here the number of lattice points which are being present is essentially 2 lattice points which are being present, here if you wanted to represent it with this vector R ; if you are trying to represent. This lattice you find that all the lattice points will not be represented using this vector notation this is the mathematical way of representing the lattice.

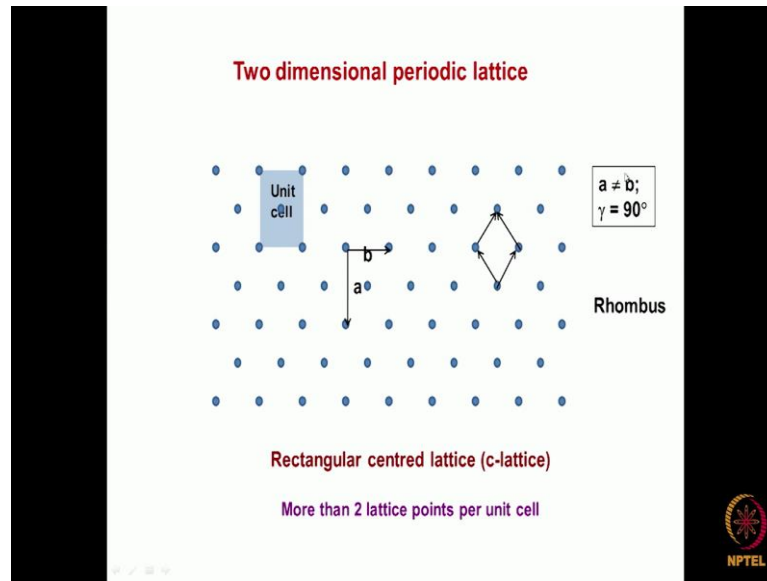
So, in the primitive lattice only, using this vector all the lattice points can be generated using this 1 single expression. Generally as I mentioned earlier, the lattices are infinite lattice points are. So, large than the surface effects can be ignored and most of the time you will notice that we choose not only a primitive lattice in many cases we use a non primitive lattices there is a reason for that the reason essentially is that we choose the lattice which shows the full symmetry of the crystal structure under consideration.

(Refer Slide Time: 05:23)



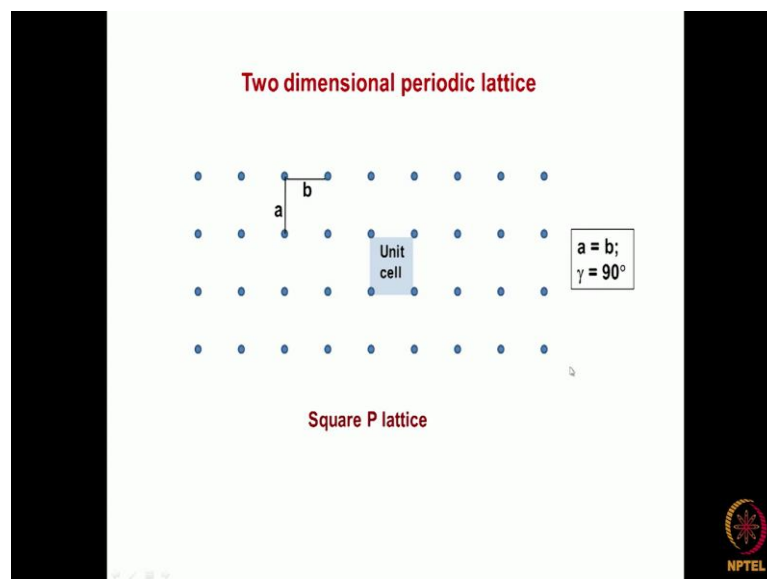
This is another type of a lattice where if you look at it the angle between a and b the to access is 90 degree, but a and b are not equal to each other this is a rectangular lattice.

(Refer Slide Time: 05:39)



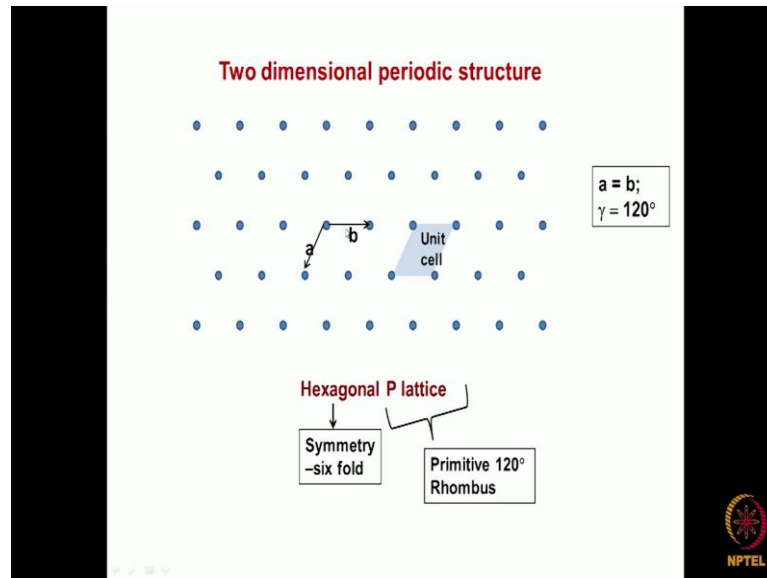
Similarly, we can consider another lattice where we find that there is 1 more lattice point in between. So, this is called as a centered lattice here again the a and b access the lengths are not equal, but that angle between them equals 90 degree.

(Refer Slide Time: 05:56)



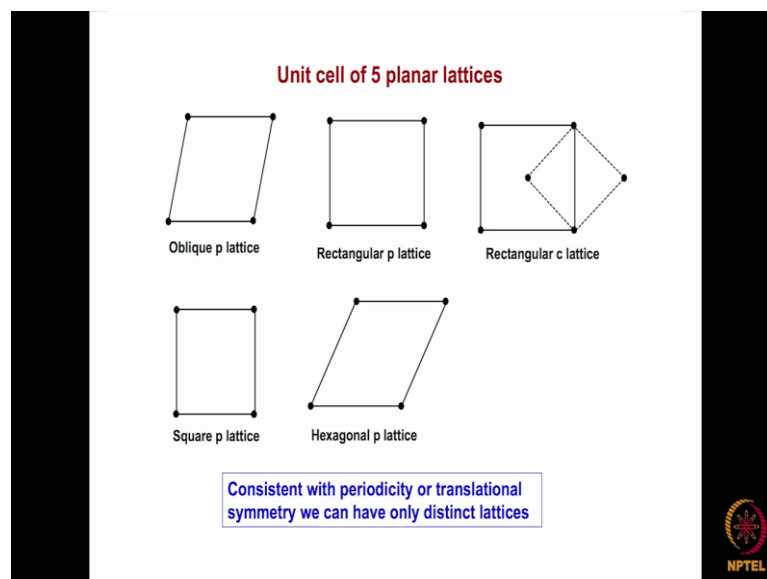
Then we have a another type of a periodic cell where a and b ; the length of a and b are equal and the angle between them is also 90 degree this is then that is a square lattice and then angle between a and b when it is equal to 120 degree and a equals b then be generate essentially like hexagonal lattice.

(Refer Slide Time: 06:08)



So, essentially if you look at it, what are the types of lattices which we have for can be generated by keeping 1-dimensional lattice Adjacent to each other maintaining periodicity in two directions?

(Refer Slide Time: 06:21)

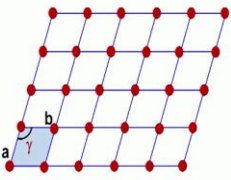


Maintaining a periodicity along the x as well as the y axis we have only 5 types of lattice planar lattices are possible these 5 planar lattices of this nothing but in geometry we have studied essentially what we can have is a parallelogram, a rectangle, a rhombus, a square and the hexagon.

(Refer Slide Time: 07:09)

Two dimensional crystal structure

Motif on or around a lattice point generate crystal structure



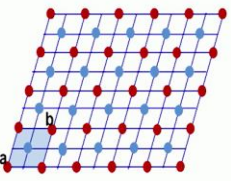
One atom per unit cell

$$\vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2$$
$$\boxed{R = n_1 a + n_2 b}$$

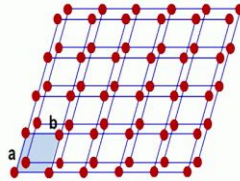
R = translation vector in the lattice
a, b = primitive translation vectors

$$\boxed{\text{Area of unit cell} = a b \sin \gamma}$$


Unit cell not unique



Two different atoms per unit cell



Two atoms per lattice point



These are all the basic 5 planar lattices which possible in these planar lattices if you try to put an atom are the motif around each of the lattice points then we can generate 2-dimensional crystal structures you are seeing it here assume that 1 atom has been put around and put on top of each of the lattice points, now we are able to generate a crystal with 1 atom per unit cell.

You look here, what we have done it is that at the center of this each of this unit cell and another type of atom has been placed here. So, if you look and this one, we have 2 types of atoms which are being present, but what is the motifs which is getting generated? If you look at it, these 2 together can be considered as a motif and a lattice point can be generated anywhere that mine gets repeated itself. So, the unit cell dimensions if you look at it they remain that same. So, in this particular unit cell we have two different types of atoms per unit cell is there, but still if you look at the lattice this is again your primitive lattice. This is another example where you can see that the same type of atom is being present, but in this particular case we have essentially 2 atoms per lattice point, but this again is a primitive lattice area under the unit cell can be calculated by finding out the magnitude of the axis times the sin of angle between the axis.

(Refer Slide Time: 08:59)

Definition of symmetry

Symmetry is a type of *invariance* - the property that something does not change under a set of *transformations*.


From Wikipedia

Symmetry Elements in 2-D lattice / crystal

Periodic arrangement of atoms can be described in terms of symmetry elements. Symmetry arises because of groups of atoms or lattice point repeats in regular way to form a pattern

Symmetry operation in 2-d lattice:

Translational symmetry	Rotational Symmetry
Reflection symmetry	Inversion (nothing but 2-fold rotation in 2-D)
Glide	




Before we go further into this one, as I had mentioned and given some idea of what the symmetry is let me talk about what is the type of symmetry which how symmetry is defined mathematically symmetry is defined as a type of an invariance that is it is invariant the property that something does not change under a set of transformations the transformation could be either rotation translation our reflection whatever be the operation it brings you to a position which appears as if it is the same as the original position.

What are the types of symmetry elements which we can have in 2-dimensional lattices? One like what we mentioned in the case of 1-dimensional lattice, in 2-dimensional lattice, we can have a translational symmetry, rotational symmetry, reflection symmetry and inversion which is nothing but a rotation and a glide we will go into a detail shortly, but what we should remember is that in 1-dimensional lattice, we have only one type of a rotational symmetry only a 2 fold rotation.

(Refer Slide Time: 10:14)


Symmetries around 2 – D lattice



In addition to translation, this lattice exhibit, other symmetry elements

- Translational symmetry
- Rotational symmetry
- Reflection symmetry
- Centre of inversion
- Glide

Rotational symmetry not consistent with translation




$n = 360^\circ/\theta$

$xyz \text{ transforms to } x' y' z'$

For only rotational symmetry
n fold rotation is possible

$X = AX'$

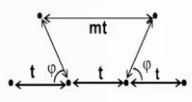


Let us look at what are the different types of other symmetries which are possible in 2-dimensional lattice. Suppose we assumed that we wanted to find the symmetry around any point which is not consistently like this is a lattice which I am showing it here around this lattice, if I take any point here and this point, if I rotate it by some arbitrary angle this the entire lattice will move and come to an another position which is distinct from the earlier one so; that means, that it is not consistent with translation that type of a symmetry if you look at it infinite symmetry which is possible around a point.

(Refer Slide Time: 10:59)

Rotational symmetry in 2-D lattice

A crystal or periodic lattice is said to possess n fold axis of rotational symmetry if it coincide with itself upon rotation about an axis n times, each angle of rotation being $(360^\circ)/n$. Each rotation by $(360^\circ)/n$ brings it to a position where it is difficult to identify it from the previous position.



$$mt = t + 2t \cos \varphi \quad m = 0, \pm 1, \pm 2, \pm 3 \dots$$


$$\cos \varphi = \frac{m-1}{2} \quad \cos \varphi = \frac{N}{2}$$

Determination of rotation axes allowed in a lattice

N	cos φ	φ (deg)	n
-2	-1	180	2
-1	$-\frac{1}{2}$	120	3
0	0	90	4
+1	$+\frac{1}{2}$	60	6
+2	+1	360 or 0	1

Restrictions on rotation because of consistency with translational symmetry

Rotation consistent with translation is 1,2, 3, 4 and 6 fold



But if we look for a symmetry which is consistent with translation there are some certain restrictions are there. These restrictions, we can easily find out how exactly it is been this year looking at this figure; in this figure, if you look at it that is the lattice vector here the lattice point here and the lattice point is here is rotated by an angle t where the translation periodicity is t .

So, this generates a new point; one here and another new point here, if it is consistent with the translational symmetry; the distance between these 2 points should be again you have multiple of the translation vectors that is what is it turn us empty. So, this empty is nothing but t plus 2 times $t \cos \theta$ and if you do all the mathematical operations then we can find out that the number of rotations which are possible which are consistent with translational symmetry is 1 fold, 2 fold, 3 fold, 4 fold and 6 fold; these are all the only type of translation symmetry; rotational symmetry which is possible which is consistent with translational symmetry what is the other type of symmetry which we talked about which of you mentioned earlier also is a reflection symmetry.

(Refer Slide Time: 12:23)

Reflection symmetry

By this symmetry operation, the object is brought to a position which is similar to reflection in a mirror (enantiomorphic image is formed)

Easier to visualize with motif

Reflection symmetry (Mirror)

Reflection in a mirror

$xy0 \rightarrow x-y0$

Mirror on x-axis

$X = A X'$

Inversion symmetry

Equal to 2 fold rotation for 2-D lattice

$xy0 \rightarrow -x-y0$ for 3-D

$X = A X'$

Find out the transformation matrix for these operations

So, in reflection symmetry if you put a mirror in front of an object, the mirror image will be generated on the other side of it. So, where can we place that mirror if it is like here it is a 1-dimensional periodic lattice which is being shown, the mirror can be kept either halfway between the lattice points or it can be kept on the lattice point itself these are all the 2 options which we have for keeping the mirror symmetry. How can we represent

this mirror? This is essentially basically the trying to understand qualitatively how a mirror symmetry is generated, but mathematically when we look at it, essentially by this operation of the symmetry there point which has got some coordinates x, y, z , it gets repeated and generates new point.

What should be the coordinates of those points that is given for a mirror reflection if we consider around the x axis, where the mirror plane is lying on the x axis then it will be $x, y, 0$, if the coordinate of this motifs then it gets repeated to $x, -y, 0$, y had chosen 0 because that in a 2-dimensional lattice, it is only the x, y plane. So, the value of z becomes 0 otherwise if you consider 3 dimension, this will become x, y, z turning to $x, -y, z$. This can itself can be also represented in the form of a matrix form where x is a column vector x, y is a and x' is the new vector column vector; no, x and a is the transformation matrix which transforms from 1 coordinate system to the; another coordinate system.

This way mathematically we can find out by an; our symmetry operation using the specific transformation breaking matrix which is associated with it that all the coordinates of all other positions could be generated. Similarly for if it is an inversion symmetry which is equal to a 2 fold rotation, if you considered here, it is a x, y turns to $-x, -y$ and for a 3 dimensional 1 its x, y, z will turn to $-x, -y, -z$ like I mentioned for a reflection symmetry, we can write a similar expression transformation expression for transforming from one coordinate that is how the coordinates of that other lattice points could be generated using the transformation matrix associated with the inversion operation.

(Refer Slide Time: 15:04)

Reflection / Glide symmetry

By mirror symmetry operation, a random point xyz changes to $x-yz$ when the mirror plane is perpendicular to y axis (xz plane) and passes through origin. Depending upon the co-ordinates of mirror plane, appropriate sign change will occur for reflected points.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Glide is mirror plus translation
 Mirror plane is represented by a line
 and glide plane is represented by dashed line.

$x, y, z \rightarrow -x, y + \frac{1}{2}, z$; glide on y direction

In addition to these symmetry elements, another symmetry element which comes like which mentioned in the case of 1-dimensional crystal is a glide symmetry.

The glide symmetry essentially as I mentioned earlier is that like for this the motifs are shifted by a distance some particular distance are t by 2 and then it is reflected and again you shifted by another t by 2 again you reflect it then one can generate your particular type of a pattern this is called as a glide this is something like when we walk on this beach sand our body itself is across the body that is a mirror symmetry associated with it.

So, when we walk that our right leg and the left leg; as we move the periodicity is from right leg how much the first position to the next position which it takes, but half the distance is the one where that left leg comes. So, this is a perfect example of glide symmetry. So, as I mentioned the glide symmetry this can be represented by this sort of a transformation if it is a coordinates are $x y z$, this changes to minus x ; y plus half to z and the this coordinate transformation takes place only for glide when it is taking plus on why there glide is present in the y direction.

(Refer Slide Time: 16:40)

Symmetry elements for 2 - D lattice

- Rotation consistent with translation
- Reflection consistent with translation (Mirror)
- Reflection plus translation (Glide)

Point group symmetry

NPTEL

What are the types of symmetry elements for 2-dimensional lattice which we are saying? One rotation consistent with translation reflection consistent with translation and reflection plus translation glides.

(Refer Slide Time: 16:59)

Point groups

If the translational symmetry is disregarded, the remaining symmetry elements (rotation, reflection and center of inversion) consistent with translational symmetry can be arranged into distinct groups and each group is called a point group. The operation of these symmetry elements pass through a single point and this point remains unmoved.

The planar point groups consistent with 2-D lattice are 1, 2, 3, 4 and 6-fold rotation and reflection. Their combination consistent with translation give rise to 10 point groups.

Why point group study important ?

Macroscopically measured properties like thermal expansion, electrical resistivity, elastic constants, optical properties show a symmetry and can be understood without reference to translational symmetry of the lattice. The rotation, reflection and inversion are called macroscopic symmetry elements since their presence can be confirmed by macroscopic experiments.

NPTEL

These are all the type of point group symmetries which are present for a 2-dimensional lattice. Essentially the same thing is being defined in this way that if we forget the translational symmetry, then the remaining symmetry elements; rotation, reflection and the center of inversion consistent with translational symmetry can be arranged into

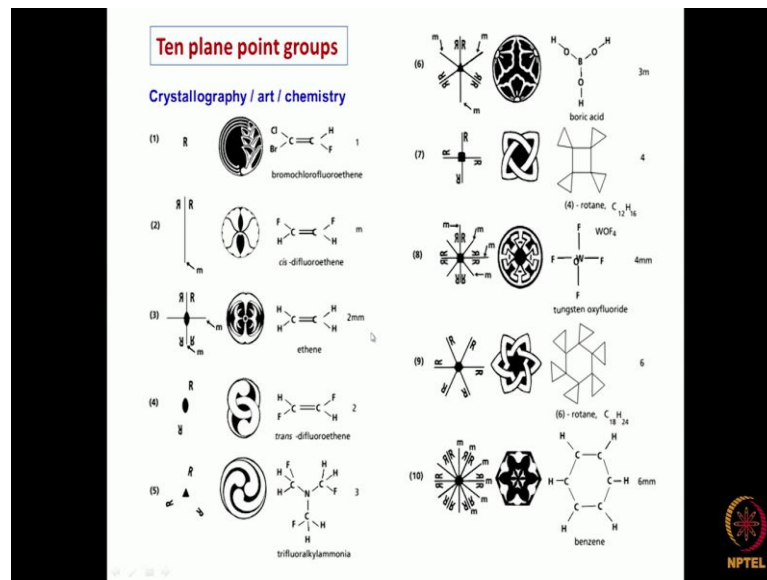
distinct groups and each group is called as a point group. What are the rotational symmetry elements which are possible 1, 2, 3, 4 and 6 fold rotation and in addition to it reflection is the one which is possible.

So, we have essentially 5 plus 1; 6 types of point groups are 6 types of symmetry operations are present we can choose various combinations of these symmetry operations we can choose and you can calculate how many combinations which are possible out of which we will find that only ten point groups which are present which are consistent with the translation. Why this study of point group is very important because whenever we look at a property of a material, any sample it is the property which can vary for example, thermal expansion, electrical resistivity, elastic constants, optical property, if the crystal structure external a symmetry of the crystals when we look at it, all these properties what essentially is that we can visualize it by macroscopic experiments and look at it and decide how the properties are changing in various directions. Like electrical conductivity, we can measure it at different directions and find out how in which all directions they are identical, which are directions are different.

On that basis, we can find out what all the types of symmetry elements which are associated with this. These symmetry elements when we look at all of them will pass through a point in the case of a intersection of different types of symmetry element other ways if it is only as rotation which is being present only a 2 fold rotation if we consider or 4 fold rotation which is being considered then around an axis it is invariant.

So, because of this; this is called as point group symmetry, the rotation reflection and inversion these operations are called macroscopic symmetry because by simple experiments macroscopic experiments like measuring properties we can identify these symmetry elements.

(Refer Slide Time: 19:50)



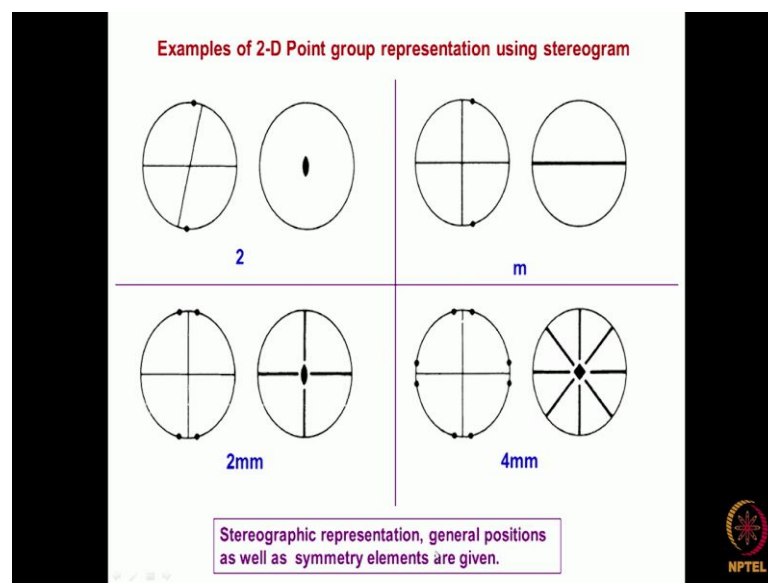
Now, coming back to what all the types of 10; I mentioned that there can be a point group symmetries associated in 2-dimensional lattice what all the point group symmetry which can have which is consistent with the translation periodicity in 2-dimensions when. So, here what I have done it is I have shown taken an asymmetric motifs then in an art form there is different types of motifs which have for asymmetric sanctity associated with it and then chemistry a type of molecules which exhibit the corresponding symmetry like if you take a own fold symmetry this is Bromochlorofluoromethane, this if you look at it; it has got only own fold symmetry otherwise way whatever operation which we do other operations 2 fold rotation it will not be brought back to its identical version the same is true for this particular motifs also for R.

If a mirror is being present then what we do is that the; how it is getting repeated is that R across the mirror there will be a mirror reflection. We can generate, this is the symbol with which it is expressed and amidst the symbol which is used to represent that mirror and if you look at this picture this picture has got around this axis vertical axis we have a mirror symmetry which is being present. So, like difluoroethane if you look at it this as a 2 fold mirror symmetry which is associated within and if you look at this structure; it is not this is a 2 fold symmetry which is associated with it and trans difluoroethane is one which if you look at it; it has a by 2 fold rotation, the hydrogen it will come here. So, we will not be able to make out whether it is the position which we generate new position is

identical with the earlier one know whether it is undergone a transformation or not will not be able to make out hence we say that this has got a 2 fold symmetry associated with it.

Similarly, we have examples for 3 fold symmetry, how exactly and if you look at the center, we are showing what all the different symbols mirror is essentially shown with a line; thick line and ellipses which is being used to show a 2 fold equilateral triangle is used to represent the 3 fold symmetry a square is used for a 4 fold symmetry to represent it and then hexagon is used for representing a 6 fold symmetry, you can go through this slide and you will be able to make out that around your point these are all the types of symmetry elements which we can have which is consistent with a lattice translation because of that this puts a restriction and hence we have only ten plane groups are there.

(Refer Slide Time: 23:04)



I will give you some assignments later, you can go through the assignments and then you will notice it that whatever be the combination you choose finally, turn out to be only ten distinct ones are possible there is an another way in which this is represented this is represented under stereogram.

Now, about the how that stereogram is being constructed, it will come into the next lecture, but I just wanted to mention here that this is something like an stereographic sub projection of what is happening in is 3 dimension are on the on a sphere onto a 2-dimension and the advantage of a stereographic projection is that all the 3 dimensional

angular relationships are being maintained in 2-dimension in the case of in the case of a 2-D lattice essentially it is essentially a projection 2-dimensional projection of a 2-dimensional lattice because of it is much simpler. So, it is essentially a circle which represents the stereographic projection and the central point all the angular relationship which are present between the different lattice points can be represented all the symmetry points by points on the circumference of the circle.

The two ways in which a stereographic projection is represented in international union of crystallography one is a general point how by a symmetry operation, it is getting represented on the stereogram and another is what are the symmetry elements which are associated with the point group representation. These are all the 2 ways in which is being represented in addition to it corresponding to the general point, what all the positions which are possible the coordinates of them that is also being represented that I are not given here, but you can go through the book on international Urethrography for planar groups where you will get all the information.

For example, here if you look at it the mirror which is to be there around this plane that is under y axis a motif which is being present, generally it is represented by a dot on the circumstances this is getting reflected and it comes here and if he what is the mirror symmetry element if you want to represent take a circle and on this same axis as the thick line which is being drawn that represents the mirror. If you look at a 2 mm symmetry here, these are motifs which is there by a 2 fold rotation this gets reflected here.

We can see the position of the motif and now if I put a mirror in this direction; this axis this will get reflected, new positions are generated, but when this has been generated, we can see that it is equivalent to putting another mirror here. If you put it then also these positions will be generated which are identical to each other. So, here now we show the 2 fold rotation which is there at the center and that the mirrors are also being represented similarly for 4 mm, we can represent it that is what is given here.

(Refer Slide Time: 26:44)

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

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)

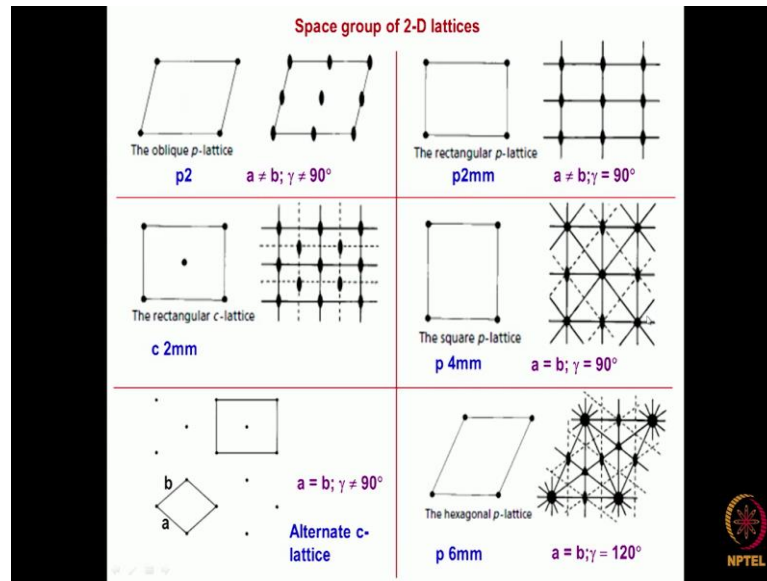
Orientation of 3m gives two possibility (1 additional planar group)



if you look into that the type of point groups which are present 2-D point groups, we have pure rotation which are 5 numbers are there 1, 2, 3, 4 and 6 fold and then reflection and in mirror is 1 then the combination of rotation and reflection if you take it there is 2 mm, 3 mm; 3 mm, 4 mm and 6 mm; these are all the; so essentially 10 distinct our point groups are possible.

So, far we have talked about only point groups these point groups are generated around a lattice point if you put this point group around each lattice point the 5 lattices which we said that we can have in 2-dimensional lattice then what are the type of planar groups which we can generate that is what we will look at it.

(Refer Slide Time: 27:51)



Here it is an oblique that is only one unit cell which is being shown here since it has got only a 2 fold rotation that is around this point which is the origin of the coordinate system if you take it by a 2 fold rotation this point itself will rotate and come somewhere here then this point will rotate it and come here. So, that way this lattice will be generated. So, essentially around each lattice point we have a 2 fold axis which is being present, but once this 2 fold axis if we look at it. So, now, we can notice that around this point there is another 2 fold axis at the center also another 2 fold axis is generated and at the center of the x axis also did another 2 fold axis is generator.

So, by having a planar lattice where we have a 2 fold rotation around the lattice point we notice that there are other positions where either the same symmetry element or some other symmetry element could be generated like in this particular case of a rectangular lattice if we consider here if we notice it we can see that only 2 fold rotation has been 2 fold axis is present on all the lattice points. Now if we look at it, the presence of them has generated another 3 more positions where 2 fold rotation axis is present in addition to it along that lying on the x axis as well as the y axis we have mirror planes which are being present similarly at halfway between gender is in this direction as well as in this direction we have again mirrors are being present.

If you look very carefully by putting motifs are looking at the symmetry around each of the lattice points we can see that at other points also different types of symmetries are

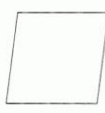
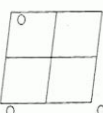
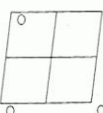
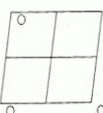
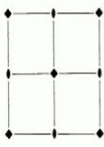
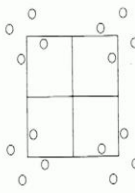
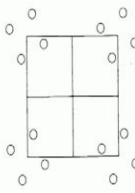
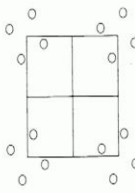
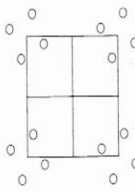
generated here we have a rotation and a mirror and if you look at the square lattice here we can see that these are all the atom points around each of this point we will have a 4 fold rotation which is being present. So, when we put a 4 fold rotation around this point then we can see that at the center also there is a 4 fold rotation is present and if you look at the midway bit in the x axis between the lattice translation vector we have a 2 fold rotation which is present similarly here if we look at it another 2 fold rotation and by lattice translation vectors we can generate the other 2 fold rotations.

So, essentially for this; the symmetry which it has got is a 4 fold rotation then in addition to it along the x and y axis mirror symmetry is there then at passing through this center point we have again mirror symmetry is there then along the body diagonals we have mirror symmetry is present. So, essentially what we have is that the actual symmetry representation which we call it as 4 mm, but if you look at it there are the 4 fold rotation 2 fold rotation then symmetry along x and y axis symmetry shifted from that by some distance and then symmetry passing through the body diagonal not symmetry the mirror passing through the. So, 3 types of mirror symmetries, 2 types of a 4 fold rotation and one type of a 2 fold rotations is possible.


How are these represented in international inverse cryptographic table; that is what is shown in this slide if you look when we try to represent a planar lattice.

(Refer Slide Time: 32:18)

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 2 c 2 1 b 4 1 a 4	x, y -x,-y -y, x y, -x 1/2, 0 0, 1/2 1/2, 1/2 0, 0

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



The lattice can be represented by a unit cell these what essentially is being shown is unit cell which is being shown the angle between the unit cell is not equal to 90 degree, these 2 sides do not have the they are not equal if I put take a motif. Generally the motif is represented by an open circle if I keep this motifs at a point which does not have any symmetry element associated within its an one fold symmetry then what is going to happen is that only by own fold rotation this will repeat itself. So, essentially we will not fold, what are the coordinates of these points? These coordinates of the points could be x y and in the international union of crystallography table. There are 2 things which are important as far as when we wanted to generate the crystal structures 2-dimensional structures essentially what we should know is that what all the special and general positions for the motifs which have to be placed how are they graphically represented these are all the 2 important information which we require.

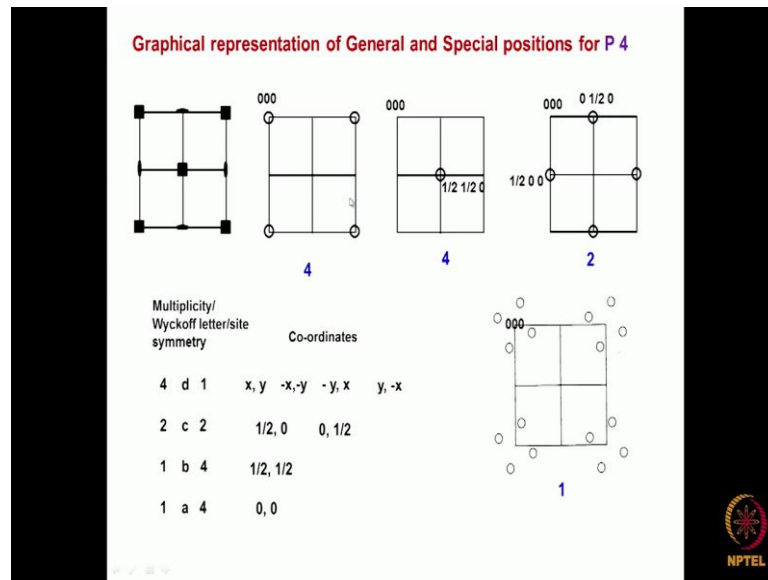
Let us look at a case with a the plane group which has a 4 fold symmetry associated with it only a 4 fold symmetry is present then this is how the graphical representation of the symmetry is given all the lattice points we have symmetry element are the 4 fold symmetry is there at the center of the lattice again another 4 fold symmetry then at the edges at the midway, there is a 2 fold symmetry is percent if we take a motif and put it around any point in this random point at this point if we try to look at it what is the type of symmetry which it will have if I do around this point you rotate. This lattice will rotate and come back to its original position only for 1 fold rotation for all other one they will generate a position which is not identical with the original position.

So, this is called as a general point or the symmetry associated with this one is only 1 fold rotation. We have put a motif around that position and when we try do the symmetry operation this has to be repeated itself by a 90 degree we rotate it we generate an another position then by another 90 degree then by another 90 degree. So, the full symmetry operation is completed now we can see that around each that is point if you put our motifs at a position which is not a symmetry any symmetry or special position than 4 points have to be generated. So, which show only then the crystal will exhibit the 4 fold symmetry.

Now, we can see that around each lattice point we have a 4 fold symmetry if you look with respect to this center again we will see that there are 4 points which are associated with it. So, from this what we can make out is that if the point which is occupied by the

motifs has a own fold symmetry then its multiplicity is 4 four more points have to be generated their coordinates are given in this fashion suppose I assume that this motifs I am trying to put it around this particular point then by lattice translation I can generate the unit cell then the motifs will come at this point this point and this point.

(Refer Slide Time: 36:59)



And this is being shown here. So, now, we can see that this is the coordinate of the origin. So, by putting a motif around these points now we are able to generate. So, what is the symmetry of this point it has a 4 fold symmetry. So, since it has got you know; 4 fold symmetry only 1 lattice point, motif has to be placed around each lattice point and if you look at the number of lattice points per unit cell, it is only one which is required and that it satisfies that condition.

So, in the Wyckoff table if you look at it this is how it is being represented the symmetry around the lattices fine this called as a special position where it has got a 4 fold symmetry there the multiplicity one means that we have to keep only one motifs at that point if you look at this position this position essentially yes got a half of 0 is there the coordinates are in 2-dimensional lattice it will only half, half, half here again since it as a 4 fold symmetry associated with it we have to put only one motif that is what essentially is represented as the multiplicity here if you look at this point this particular point has got a 2 fold symmetry associated with it if you put a motifs around this point the coordinate of this will motifs is going to be 0 half that what essentially is given here and by a lattice

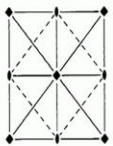
translation we can generate the another which is going to be present on the unit cell and then along this axis is another there is at opposition half 0 your motifs has to be kept. So, by lattice translation vector we can generate the other position of this position of this motif in the unit cell.


Now, if you look at it that number of motifs which are a number of motifs which correspond only to the unit cell is 2 and the way in which these motifs are being placed that satisfies the 4 fold symmetry that is essentially what is being given here is the symmetry around this point is a 2 fold symmetry and what are the coordinates of those points that is being given and then these are all that this is the total two points are supposed to be there that is what is being shown here and general point as I had mentioned earlier.

So, around each lattice point, if you are placing a motif at a point which does not have any symmetry associated with it. So, that is called as a general point then we have we should have 4 points which be generated for each of the motifs this way if you look at it essentially in the cryptographic table they had given the on the unit cell what are the types of a symmetry elements which are present if you are trying to place a motifs around motifs at different points how many motifs have to be placed. So, that the symmetry the full symmetry of the lattice is the crystal is satisfied that information is given. So, if we have this information this can be used to. In fact, generate 2-dimensional crystals.

(Refer Slide Time: 41:13)

Examples of plane group representation in IUCr table

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




This is another example which is being taken where it is we have 4 fold symmetry along with it mirror symmetry is also there that is essentially p4mm here. If we look at it we have one general point and then other symmetry positions are 1, 2, 3, 4, 5, 6, special positions which are possible. So, totally essentially if you look at it the motifs could be placed at any of these particular positions and then we can generate the various types of the we could generate atoms occupying different positions in the unit cell, but having that same type of a symmetry element associated with it and only thing which you should notice is that here when there is a mirror reflection is being present the symbol which is being used is within a circle like comma is being inserted.

(Refer Slide Time: 42:23)

Symbols used to represent symmetry elements in 2-D


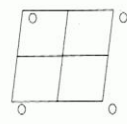
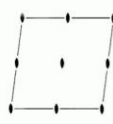
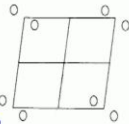
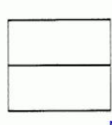
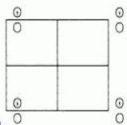
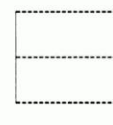
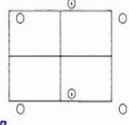
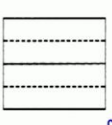
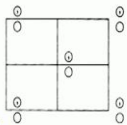
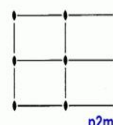
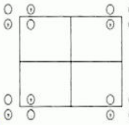
●	2 - fold rotation
▲	3 - fold rotation
■	4 - fold rotation
◆	6 - fold rotation
—	Mirror or reflection
-----	Glide
○	Asymmetric motif
⊙	Mirror image of asymmetric motif




What are the symbols which are used to represent symmetry elements in 2-D lattices? One 2 fold rotation and 3 fold; 4 fold mirror with a line glide with a dashed line and a symmetric motif is represent with an open circle and mirror image of a symmetric motif is represented with a circle with a comma in say.

(Refer Slide Time: 42:45)

Graphical presentation of symmetry and general point in unit cell for 17 plane groups

Symmetry  p1	General point 	Symmetry  p2	General point 
Symmetry  pm	General point 	Symmetry  pg	General point 
Symmetry  cm	General point 	Symmetry  p2mm	General point 

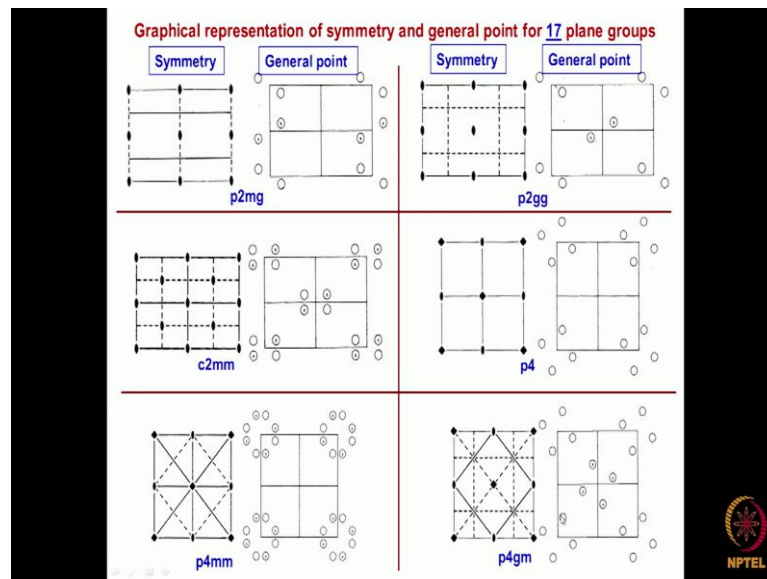


Now, what I have shown is all the seventeen plane groups in 2-dimension how are they represented we show one of the that we show the unit cell and then how if we take a motif and put it in a general point how the motifs are generated that is the only structure

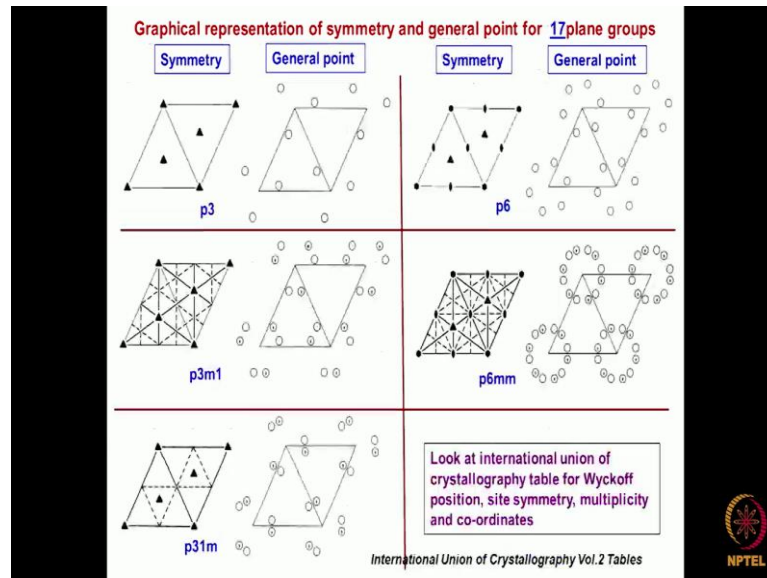
which is being shown. So, this is how oblique motif looks like we put one of the symmetric motifs here.

So, this is how it will appear when it has got only one fold symmetry when the same structure there is a 2 fold symmetry is associated with it corresponding to this there will be an another point which has to be done which is one eighty degree rotation around each of the lattice point this is how it is generated if we look at it, it becomes very clear that is now if we look at it though the motifs are placed around each of the lattice point now symmetry elements are generated here as well as at this point correct and similarly in this particular case where we have considered a mirror which is associated with it here the symbol which is being used that the this is the motif a symmetric motif and that symbol essentially is that with the open circle in which we put a comma that shows that it is a reflected image this way all I will not go into a detail and explain all of them, but you can go through it and find out the all the different types of planar lattices how they are represented here its only a graphical representation which has been shown.

(Refer Slide Time: 44:16)



(Refer Slide Time: 44:27)



In addition to this graphical representation there is something else also is there the coordinates of the various positions are also shown how these coordinates of the various positions are shown that I will tell you if we look at the square lattice $p4$ we can put a motif here at this particular general point which has been placed which is what is shown in that we can put a motif at the lattice point where 4 fold symmetry is there we can put a motifs at the center where 4 fold symmetry is there we can put a motifs at these points also where 2 fold symmetry is there then also we can generate a lattice.

So, there are many possibilities are there all of them are finally, going to generate a lattices though these positions are distinct were motifs are being placed, but all these structures will show the same $p4$ symmetry correct this is what is being given by the Wyckoff position what we call it the positions where they can be present coordinates of the Wyckoff position the site symmetry which are associated with it that table gives all this information like 12 planar groups can be generated by keeping motifs representing different 2-D group symmetry around each lattice point that is one and then the glide symmetry is generated when motifs are placed in a special way in the planar lattice there are 4 additional planar groups are generated then the 3 m group symmetry there are 2 orientations are possible.

So, they give rise to one additional planar group. So, totally we have seventeen these seventeen are represented. So, here what I have shown is just only the graphical

representation of both the planar lattice and the general point the other information which we require are essentially the site symmetry Wyckoff position and the multiplicity associated with in the coordinates of the motifs that I think one can look into the international of crystallography and then that all this information.

(Refer Slide Time: 47:13)

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

NPTEL

And in this particular view graphs what I have done it is whatever what are the types of symmetry elements that is if you mentioned as p one this is how the different that is this one space group are the planar space group.


So; that means, that there is only one fold symmetry is associated with it what all what all the symmetry elements which are associated with this p one is given here p 111 and p 2 is a 2 fold rotation along z axis and 1 fold on the other two directions similarly for various like for p2mm, there is a 2 fold rotation along the z axis and the mirror plane perpendicular to y and x axis. So, like this I had just given explanation for what all the various types of symmetry elements present which are present the same symmetry elements.

(Refer Slide Time: 48:00)

Details of plane group symbols

- p4** - 4 fold rotation along z-axis and 1 fold on other 2 directions (P411)
- p4mm** - 4 fold rotation along z-axis; mirror plane perpendicular to y and x axis
- P4gm** - 4 fold rotation along z-axis; glide plane perpendicular to x and y axis and mirror plane perpendicular to y and x axis. Here designated as P4gm
- p3** - 3 fold rotation along z axis (P311)
- p31m** - 3 fold rotation along z axis; 1 fold rotation perpendicular to x axis and mirror on x-axis
- p3m1** - 3 fold rotation along z axis; mirror perpendicular to x axis and 1 fold rotation along x-axis
- p6** - 6 fold rotation along z-axis (P611)
- P6mm** - 6 fold rotation along z-axis and mirror perpendicular to x, y and u axes

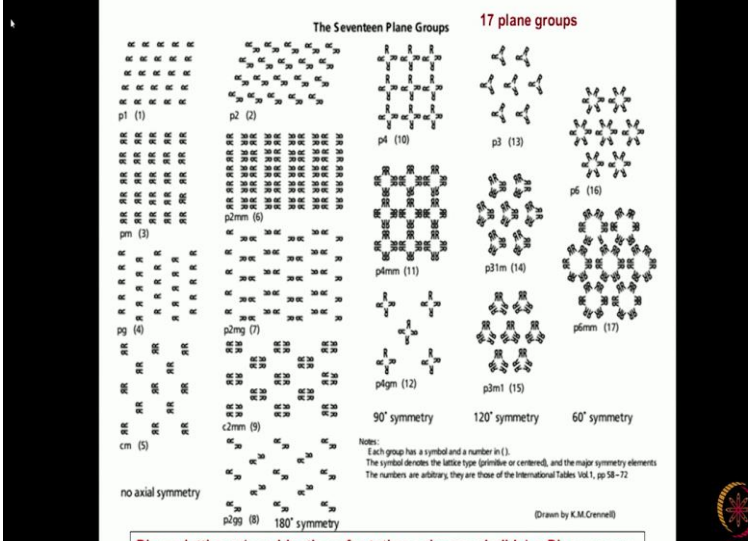
See IUCr plane group table for details



(Refer Slide Time: 48:04)


The Seventeen Plane Groups

17 plane groups



Notes:
Each group has a symbol and a number in [].
The symbol denotes the lattice type (primitive or centered), and the major symmetry elements.
The numbers are arbitrary, they are those of the International Tables Vol.1, pp 58-72.
(Drawn by K.M.Creswell)

Planar lattice + (combination of rotation, mirror and glide) = Planar group



If you try to put a motifs around each of their points the seventeen plane groups which are generated that is being shown here especially here one should look at it that with respect to that coordinate axis which is being chosen x and y in this particular case pm symmetry.

The 3 fold axis is always normal to the plane of the page that is along the z axis and the x axis is in this direction. So, the mirror is along the x axis this particular axis and then if you look perpendicular to each we have only a 1 fold rotation which is being present in

this particular structure if we look at it in this particular that is 3 fold axis remains that same along the z axis, but along the x axis we have only a 1 fold rotation and perpendicular to that the mirror is there. So, these 2 if we look with respect to a coordinate system which has been chosen they are two distinct one. So, they are given as two different plane groups.

(Refer Slide Time: 49:27)

Two dimensional lattices, point group and space group						
System and lattice symbol	Point group	Space group symbols		Space group number		
		Full	Short			
Parallelogram <i>p</i> (primitive)	1	<i>p1</i>	<i>p1</i>	1		
	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>2mm</i>	<i>p2mm</i>	<i>pmm</i>	6		
		<i>p2mg</i>	<i>pmg</i>	7		
		<i>p2gg</i>	<i>pgg</i>	8		
		<i>c2mm</i>	<i>cmm</i>	9		
		Square <i>p</i>	4	<i>p4</i>	<i>p4</i>	10
			<i>4mm</i>	<i>p4mm</i>	<i>p4m</i>	11
<i>p4gm</i>	<i>p4g</i>			12		
Triequangular (hexagonal) <i>p</i>	3	<i>p3</i>	<i>p3</i>	13		
	<i>3m</i>	<i>p3m1</i>	<i>p3m1</i>	14		
		<i>p31m</i>	<i>p31m</i>	15		
	6	<i>p6</i>	<i>p6</i>	16		
	<i>6mm</i>	<i>p6mm</i>	<i>p6m</i>	17		

This is a tabular form in which the various types of 2-dimensional lattices point group space group. There is the full as well as the short symbols for the point group underlying groups and what is the space group symbol which is being given for them and how this is being represented in that international of crystallography table is given in this.

With this I had given some brief idea about the different types of 2-dimensional lattices now we will go into a 3 dimensional lattices in the next class.