

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

Lecture – 04
Symmetry in 1-D Crystals

In the last class, we discussed about stereographic projection. I mentioned that the use of it is that angles are angular relationship in three dimensions is represented in a two dimension. The advantage it has is that like orientation relationship between crystals we can find out, angular relationship between different planes even when we wanted to projection of symmetries that could be done in stereographic projection.

Similarly, when we wanted deforming a single crystal; how the various lib planes are oriented, how they shift from one orientation to another under application of stress; all these things could be determined using its stereographic projection. I will come to that may be later or some of these applications which we will take it up. Whatever I have told in the last class, is just what is basically what is the basic minimum thing which is required to construct a stereogram. And I have told that how the different poles; which are a intersecting the sphere gets projected in two dimensions that is what will be required when we talk about symmetry.

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Symmetry Elements

Periodic arrangement of atoms described in terms of symmetry elements.
Symmetry because of groups of atoms repeated in regular way to form a pattern

Definition of symmetry

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


From Wikipedia

Periodicity can be described in terms of any one of the three types of pure symmetry element or symmetry operation. They are

Translational symmetry

Rotational Symmetry

Reflection symmetry



What is symmetry? What is the definition? He said that symmetry is a type of a

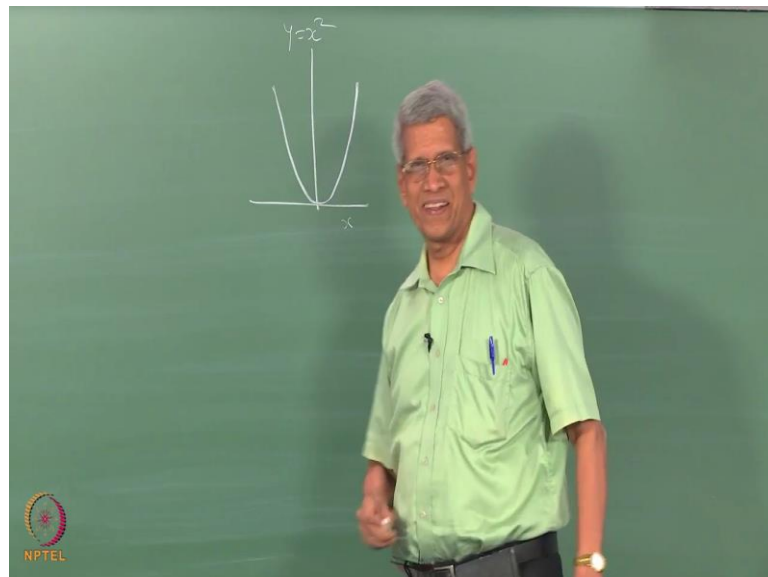
Student: (Refer Time: 01:50).

Invariance that is by application of some transformation that could be a translation or it could be rotation or a reflection or an inversion. We find that the structure looks identical to what it was earlier; that means, that we are not able to differentiate between what the structure was. This sort of symmetry is there even in mathematical equations, Can you tell me an example of mathematical equation where symmetry is there?

Student: Equation of circle, passing through a origin centers origin.

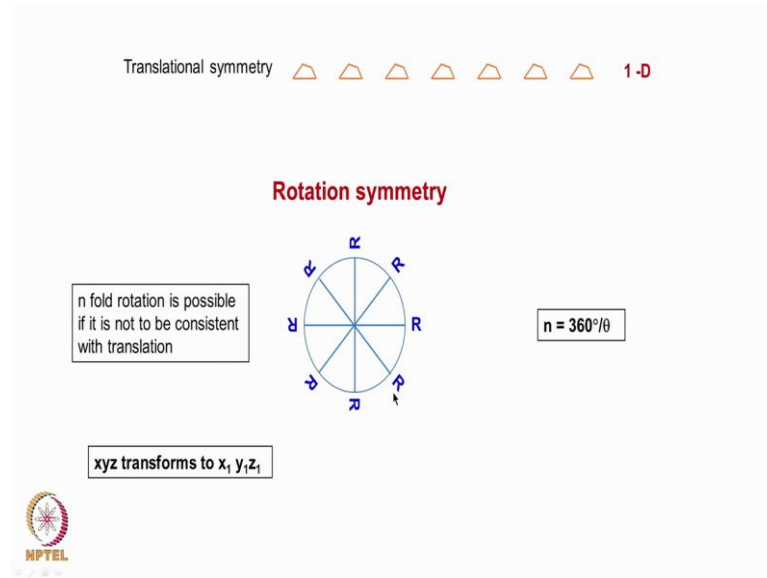
Centers origin; parabola y equals x square, it has a whether x equals positive you take it or you take x to be negative, it does not matter the value of y does not change.

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So, around an axis if this is x ; this is a graphical plot of a parabola; so, what if the symmetry it has; it has got a rotational symmetry around it. You take whatever be the value will be there, so many mathematical equations have got symmetry, when symmetry is described sometimes these equations are use to represent them also. That is not what is part of these lecture, so when we talk of this sort of invariance as far as crystal structure is concerned, there are few types of transformation which we can consider; one is translation then rotation, then reflection, then we can have inversion there are very under all these transformations. If the crystal looks identical then we say that there is some symmetry which is associated with it.

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The translational symmetry one dimensional periodic lattice if you try to look at it like; this one this is it is getting repeated, so there is a one dimensional periodicity is there. Suppose a shift it from here to this position, then it looks identical we do not know whether this transformation it has undergone or not. So, we say that it has a translational symmetry; the other symmetry which we talked about is rotational symmetry. Can you give me an example, where you are played in a toy which has a rotational symmetry?

Student: (Refer Time: 04:50).

(Refer Time: 04:51) when you go round you have seen where the horses will be there you sit on that; that you look at it any where it has got a rotational symmetry. So, there is an axis that is what as shown here; there is an axis around which; what I have done it is taken one motif R and it has been placed at this point, then if you rotate it by specific angle; this R repeats itself; this R if this should have a symmetry which is associated with it having one motif here alone is not sufficient; when we route by a specific angle at all positions that motif should be there and which should be identical with this one, when it is rotated and brought here; that it was you can see here. But here if you see the number of R; which has considered the motif which is considered eight R there correct.

As for as around the axis if we consider, we can have any symmetry associated with it, if you wanted to know what are the positions have this R; that is what I have given here that n fold rotation is possible that is what ever be the value of n; if it is not consistent

with translation, if it is consistent with translation there are some restrictions. Suppose you wanted to find out the position of R, if we go from here to here; this motif, how do we find out? To go from one position to another position, if you wanted to find out what is the way in which we can do it.

Student: Since (Refer Time: 06:43) we can say how much angle it has rotated.

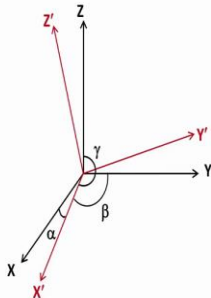
The angle you has rotated, but mathematical how do you transform into it?

Student: Angular displacement.

Angular; this can be done you see a coordinate transformation.

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Co-ordinate transformation



$$\begin{aligned} x' &= x \cos\alpha_{x'x} + y \cos\beta_{x'y} + z \cos\gamma_{x'z} \\ y' &= x \cos\alpha_{y'x} + y \cos\beta_{y'y} + z \cos\gamma_{y'z} \\ z' &= x \cos\alpha_{z'x} + y \cos\beta_{z'y} + z \cos\gamma_{z'z} \end{aligned}$$

$$\begin{aligned} x &= x' \cos\alpha_{xx'} + y' \cos\alpha_{xy'} + z' \cos\alpha_{xz'} \\ y &= x' \cos\beta_{yx'} + y' \cos\beta_{yy'} + z' \cos\beta_{yz'} \\ z &= x' \cos\gamma_{zx'} + y' \cos\gamma_{zy'} + z' \cos\gamma_{zz'} \end{aligned}$$

The same equation can be written using another notation


$$\begin{aligned} x' &= x'_1; y' = x'_2; z' = x'_3 & x &= x_1; y = x_2; z = x_3 \\ \cos\alpha_{x'x} &= a_{11} & \cos\beta_{x'y} &= a_{12} & \cos\gamma_{x'z} &= a_{13} \\ \cos\alpha_{y'x} &= a_{21} & \cos\beta_{y'y} &= a_{22} & \cos\gamma_{y'z} &= a_{23} \\ \cos\alpha_{z'x} &= a_{31} & \cos\beta_{z'y} &= a_{32} & \cos\gamma_{z'z} &= a_{33} \end{aligned}$$

$$\begin{aligned} x' &= a_{11}x + a_{12}y + a_{13}z \\ y' &= a_{21}x + a_{22}y + a_{23}z \\ z' &= a_{31}x + a_{32}y + a_{33}z \end{aligned}$$

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

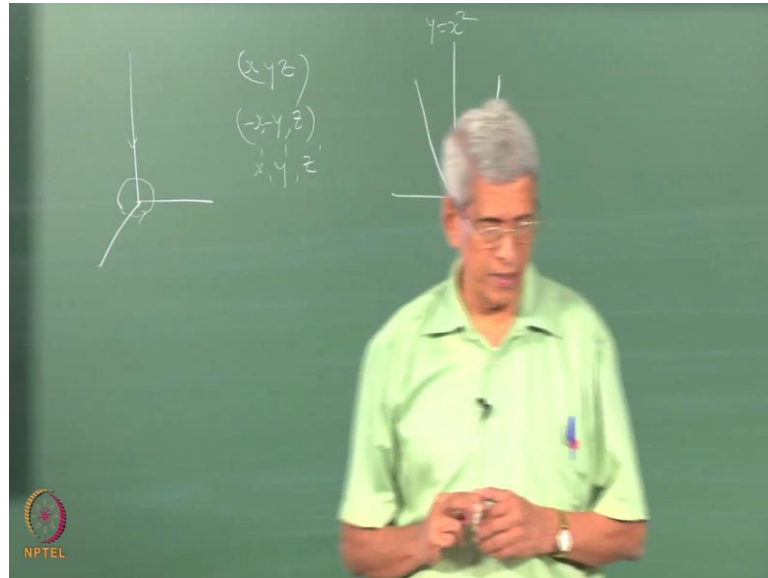
Rotation matrix



Suppose, we take two axis; this is the original orthogonal axis and it is being rotated. If we know the new position what is the angel which it makes like this; X 1 coordinate makes with X Y and Z. Similarly, we can find out what the angle if it makes; the relationship will be that x dash will be equal to x cos; angle between these two, that y cos beta plus z cos gamma. This can be easily proved and verified, so using this set of linear equations, we can find out what is going to be the coordinates; that means, that we have just rotated the coordinate by some angle. This is equivalent to suppose some point is there it has coordinates X and Y; if you rotate that also the same type of a transformation which takes place, it will give the position of the new coordinates.

Similarly, if you wanted to come from the new coordinates to old coordinate; this is the same transformation which normally we write it in this form. Suppose we wanted to find out 1-fold rotation is only there how will you go about and find out.

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Suppose, an axis system which we have chosen only a 360 degree rotation around the Z axis is possible, then what will happened to the axis; axis are all identical correct then what will be the angle which this x dash axis makes with the x?

Student: 0.

0, but with respect to Y; 90, with respect to Z; 90. Now, if you substitute it what will happen here now; this will become X dash will become.

Student: (Refer Time: 09:11).

X; Y dash will become Y, Z dash will become Z; that means, that are identical to itself; that is the way we can find out. This is essentially what is being written in a matrix form we can write it, this transformation matrix where these are all only the cosines of the angle which are involved the matrix. The same transformation; suppose we think that it is essentially a 2-fold rotation is there, then what is going to happen; if a 2-fold rotation is there intuitively what you can think of; that is if it is x, y and z is the point after rotation; it will become.

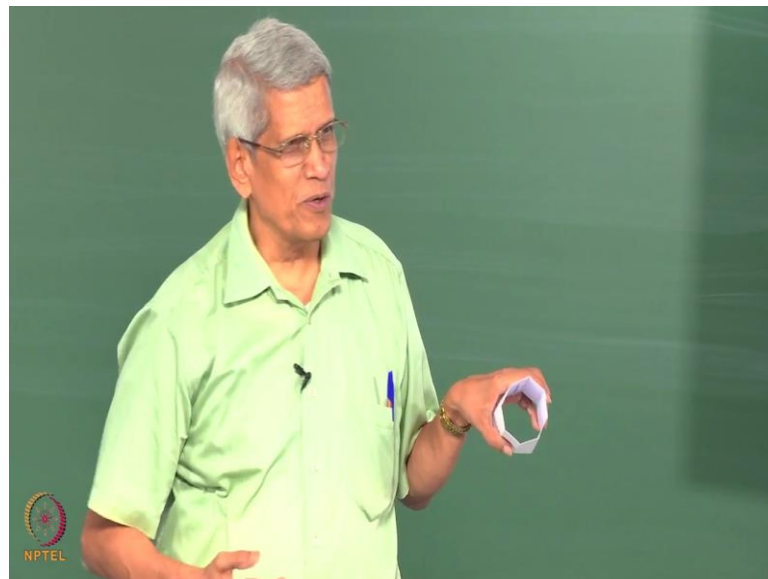
Student: Minus (Refer Time: 09:57).

Minus x minus y , z ; is it not that is 180 degree rotation if we do that with respect to any point x , y , z ; z remains that same because we have rotating around z axis. So, this will come back to this opposite side, so x and y would have changed z is remaining that same. Now, we know what is going to be the angle between that new axis; suppose this is we call this as x dash, y dash, z dash then we can find out angle between them; when you know the angle of rotation.

So, this expression essentially tells about any angle of rotation which we can make it around any axis, this is the most general formula which we can use it to find out the co-ordinates of a point which are related by a symmetry operation of rotation, Is it clear? Yes?

Student: (Refer Time: 11:10).

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See; you see this has I got a symmetry associated with it; what do you mean by symmetry? A point corresponding to it, there is another point which is there. Suppose the coordinate of this point is x , y ; what will be the co-ordinate of this point?

Student: (Refer Time: 11:34).

Minus x minus y; this by intuitively you can tell, what we have done it is since it has a symmetry associated with it; if I rotate it by 180 degree, the point which was there earlier as come here. So, its new coordinates is minus x, minus y; how do you find out that co-ordinate? By using the transformation; that is either we can keep the axis fixed and from rotation from one to the other we do or essentially it is equivalent to; if we rotate the axis around the z axis by 180 degree that also will give you the same equivalent results, that is the way we can find out mathematically.

Because in many books these all values are given the International Crystallography Table, these values are readily available. But this is how it is generated; this is the matrix and in any co-ordinate transportation, which involves rotation where that origin remains that same.

Student: Sir.

This is the sort of transformation.

Student: (Refer Time: 12:39).

So, this way suppose we taken angle of 45 degrees, the rotation of the axis around z axis or any of the axis, then we can find out what will be the coordinates of the various positions which when we give a rotation of 45 degrees, it will be essentially 8-fold rotation; what will be the position of each of the point, their coordinate we can determine; that is what essentially I had just given the transformation matrix here.

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Rotational symmetry

A random point xyz is transformed to xyz by 1fold rotation
 A random point xyz is transformed to $-x-yz$ by 180° rotation.
 Using appropriate transformation matrix co-ordinates of point generated by a particular symmetry operation could be determined.

xyz to xyz by one fold rotation $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$ Transformation matrix

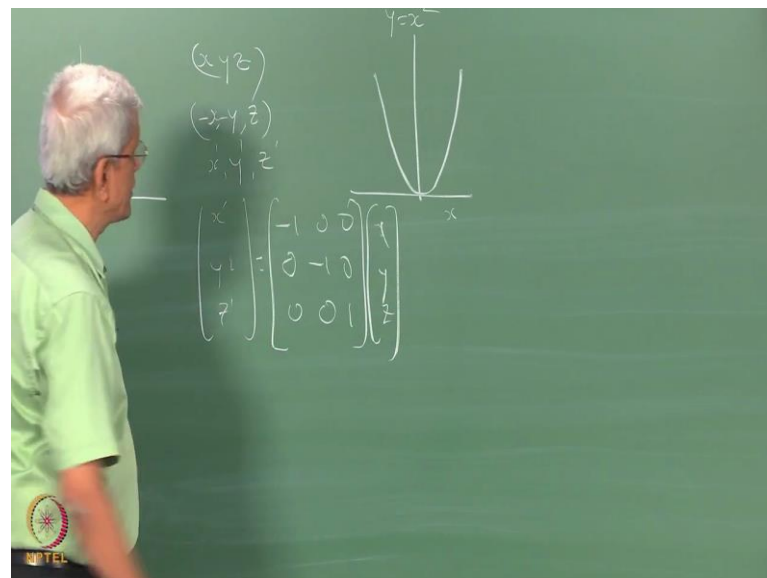
xyz to $-x-yz$ by the rotation around the z axis $\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$ Transformation matrix

One of 4 fold rotation changes xyz to $-yzx$ around z axis (anti clockwise) $\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$ Transformation matrix



If you have an only 1-fold rotation, this is a sort of a transformation rotation matrix which we will have.

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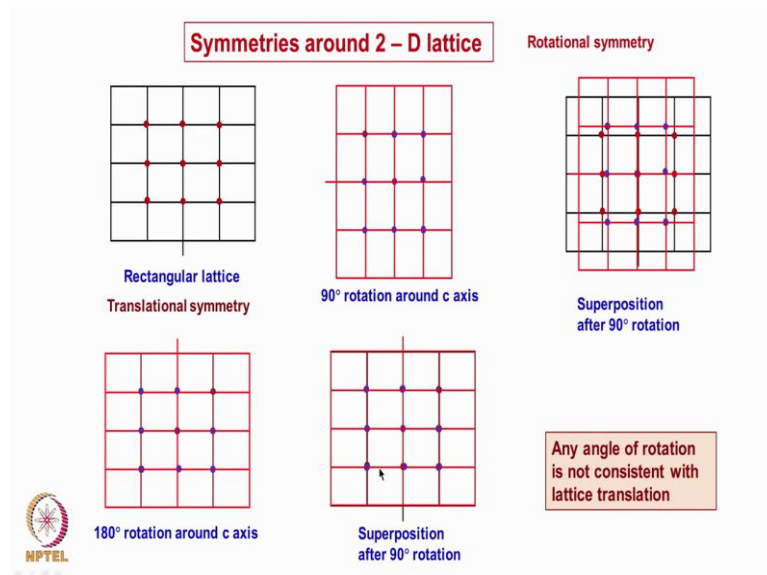


If, we have a 180 degree rotation then if the matrix is; so, if we take that it will turn out to be the co-ordinates will become minus. Similarly, if it is a 4-fold rotation is the operation which we are performing, this is the sort of a matrix which will come. So these things slides I will; no in fact, I want you people to work out all these things, then you will understand much better you just listen. So, for what you have considered this only

just how to go about and find out the co-ordinates of different points when we are doing a rotational symmetry operation and this is around any axis which we are considering it. Quite often when we have a lattice, if we are looking at around an axis a rotational symmetry; that symmetry should be consistent with all the lattice point or translation also.

Because after the rotation, every point should come back and should be coinciding with another point, then only we can say that the structure is in an identical position it has reached; that means, that the rotation should be consistent with a translation; just I have taken a rectangular lattice.

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This lattice I had just rotated by 90 degree; this is how it looks like, I had just shown this projection. So, that this tells that there is a rotation which has been given to it. Now, if I try to superimpose these two; one on top of the other, you find that the lattice point positions are atom positions do not match at all correct; that means, that this 90 degree rotation is not consistent with this lattice.

I have rotated this by 180 degree that is why we can see that this position which was there which was here initially, now has come back on to a top. Now, if I superimpose these two structures, now you see that they are matching perfectly well. So, 180 degree rotation for this particular crystal structure is consistent with translation correct; that means, that in crystal structures when we consider, all angle of rotation is just not

possible, does not give us symmetry; that is rotational symmetry for any angle of rotation is not satisfied for periodic lattice.

So, what we will do is that; what are the type of symmetry elements or rotational symmetry which are possible in two d lattice which we will try to look at it.

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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	$\cos \varphi$	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

This I explained in the previous class, that essentially what you do it is you take a lattice; each of this lattice point we rotate it by an angle phi, we assume that it comes to another lattice point. So, if they reach another lattice point these distances should be an integral multiple of t; that is what we have taken. So, this is going to be nothing, but t plus 2 t cos theta; for any value of m, can be any value which it can take; that means, that cos phi will turn out to be this angle tend to m minus 1 by 2 or the cos phi equals n by 2 m minus n 2; we can take it to be n, but we know what is the value phi can take; minus 1 to plus 1; that is the maximum value which it can have.

Student: Cos phi.

Cos phi.

Student: Minus.

Now, cos phi can have minus 1 to plus 1; that is phi can take value from 180 degree to 360. Now, what are values of n for which these are possible that is what is given in this

table? It immediately turns out that 1-fold, 2-fold, 3-fold, 4-fold and 6-fold these are all the only rotation which is consistent with translation. Whether it is two dimensional lattice or a three dimensional lattice, the rotational symmetry only these which a crystal can have a periodic crystal; is it clear?

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Reflection symmetry

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

Like reflection in a mirror

Reflection symmetry (Mirror) { | }

$xyz \rightarrow x-yz$ $X' = A X$

Mirror lying on x-axis

A is the transformation matrix for reflection

$$X' = \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} \quad X = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

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

Find out the transformation matrix for these operations

Suppose, we consider a reflection because that is also another type of this one, so and which we can there is a mirror symmetry which it comes. Many crystal lattices; it can so happen that one can have molecules which are sitting a different lattice points, there is a (Refer Time: 18:53) have some mirror symmetry associated with it because of which the lattice itself can have; a mirror symmetry associated with it.

This is just an example of an objective which we have taken, put a mirror it is getting reflected. So, this mirror also how do we represent mathematically that is if we choose the co-ordinate system; such that this is x axis as I mentioned this is y axis and z axis is normal to it, so along these x axis that is on the x is z plane mirror if we keep it; then what will happen that.

Student: (Refer Time: 19:35).

For a point xyz; the x will remain that same, y will become minus y, z remain that same. So, this is how the transformation will take place, this can be written in the form a column matrix. Then this is going to be the transformation matrix for reflection, this is

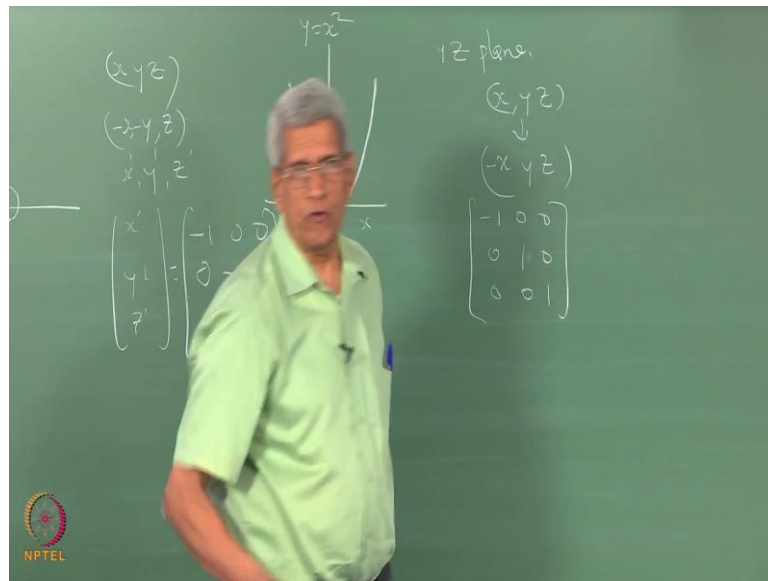
around the mirror lying in the xz plane; the mirror can be along the yz plane also; if it is lying on the yz plane; What we will have?

Student: (Refer Time: 20:26).

With a coordinates of the z it will turn to?

Student: Minus x .

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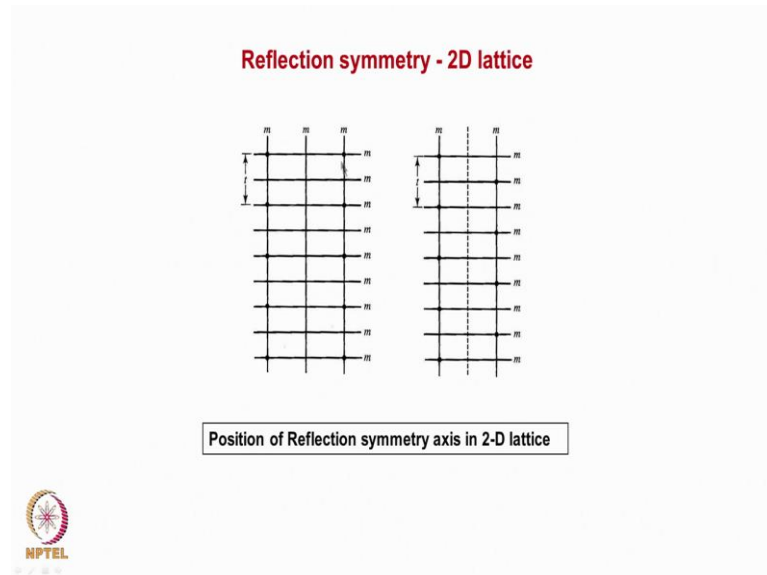


Minus x y z ; this is how it will turn; the transformation matrix will be this is what it will be. So, using these transformation matrices; we can find out the position of the coordinates; that means, that if you know the symmetry element which are associated with a crystal and if we fix a co-ordinate system on any point, we can find out using the mirror symmetry what are points or what are positions in which; the lattice should be there if it is we are looking at the symmetry of a lattice or if we are looking at a crystal structure, what are positions in which the atom should axis in the crystal that information can be generated.

This will take it up a example later and we will do a some (Refer Time: 21:32) as an assignment. Then here if you see, this is with respect to we have considered only a just an object; looked at the mirror symmetry here we are showing a two dimensional lattice, they are not two dimensional; one dimensional lattice. So, in a one dimensional lattice I can keep a mirror here and then I put a mirror, then you find that or at any point then all

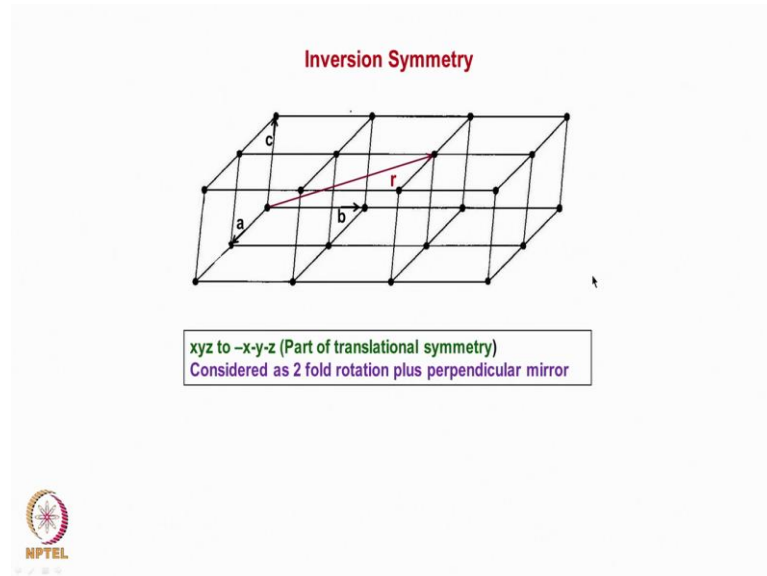
the points will be brought to an identical position. So, this is one position we can keep the mirror or in between that lattice points, at the middle of it if we keep it also; it satisfies the mirror symmetry. So, what we have considered with respect to an object with respect to with only one position.

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But in a crystal, when we keep a mirror on one of the lattice point because of the translation periodicity; we find that there are at other positions also where the same type of a symmetry operation lives the structure unaltered. With respect to a two dimensional lattice if we consider it, there is a mirror which is kept here; that is a mirror which is in these one. Now, we can see that in between there are two types of mirrors which are coming because of the translational periodicity; understand that. Here you can see that is what I had just shown here how it is coming.

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What is inversion symmetry? If we have a three dimensional lattice like here; if there is a any point is here and it is co-ordinates are xyz ; this will transform to, if there is an another identical point which has coordinates minus x , minus y , minus z then we say that they are related by inversion. Inversion also there is a question which arises whether inversion symmetry; is it a pure symmetry operation?

Student: No.

Or whether it is a mixture of him; it is essentially if we do a rotation.

Student: (Refer Time: 23:53).

That is like for this hand if I take; rotate it by 180 degree and then I put a mirror perpendicular to it and take it, then; what it happens? There it is a combination of two symmetry operations; rotation and reflection that gives rise to inversion.


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Point groups

The symmetry elements (rotation, reflection and inversion consistent with translational symmetry) and their combination is called plane point groups.

Many combinations are possible but 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 is unmoved.



Here also we can write a transformation matrix for this operation, so far what we have considered a what all the type of symmetry elements which are possible for a periodic arrangement of crystals, translation symmetry, rotation symmetry, reflection symmetry; these are all the symmetry or a combination of a rotation and reflection is there; rotation and reflection or rotation and translation, reflection and translation or a combination; all are possible.

If different types of symmetry elements are present; suppose there is an axis of rotation axis is there. So, around this axis if I do rotation symmetry; what is it which is going to happen the point on the axis will remain unmoved, all other points gets rotated. So, with respect to a only if; only one symmetry element is there which is a one rotation axis, all the points on the axis remain unmoved; others all shifted. Suppose there is a mirror which is cutting it perpendicular to it, then what will happen? If both the operations are there where intersect that point is going to unmoved; all other points are shifted during the symmetry operation.

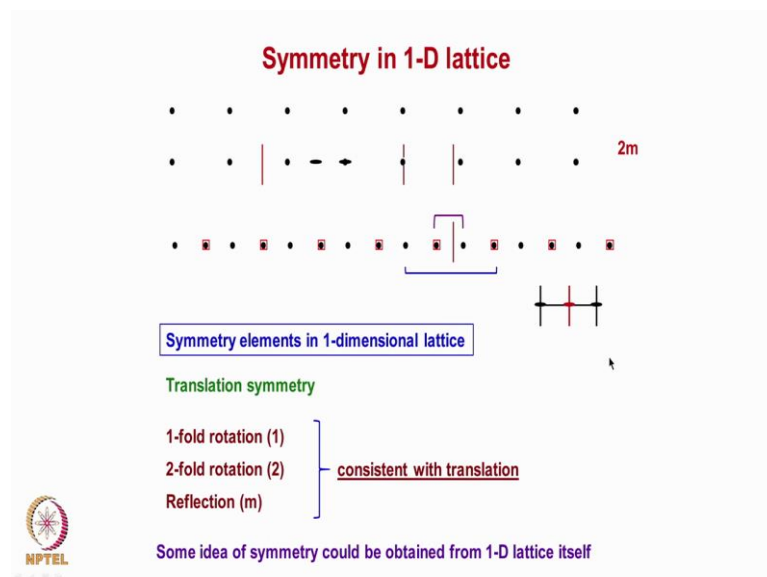
Since one point remains unmoved, these sorts of operations are called as point group symmetry operation. There are other operations are there like screw axis, as well as a glide; where all points are shifted, nothing is remaining fixed. So, this operation point group operation where; that is why this point group operation is called as a symmetry operation, where all these symmetry elements pass through a point single point and that

point remains unmoved and why study of symmetry point group symmetry is important because all the properties of the crystals, externally if you look at it they exhibit a point group symmetry; that is all the symmetry elements pass through the point.

So, whatever the properties which we determine like either magnetic susceptibility or if we are look at the external forms of crystals; what we can see is that whether a glide is there or screw is there we will not be able to make out, but whether there is a reflection is there, rotation is there or inversion is there these are all the things which we can see.

So, they will all be intersecting at a point, so this is called as point group symmetry because that is what we are; that is a property which we measure or we are able to observe. Let us considered the case of a; up to this it is clear? The concept of rotation symmetry, reflection, inversion we have considered and what are the base in which it can be represented the co-ordinates when we do this operation that also we have looked at it.

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Now, let us look at one dimensional lattice; this is just a one dimensional lattice which we are considering it. In this lattice when you look at it; what is the sort of a rotation symmetry which you can think of what do you see here rotational symmetry translation is anyway it is going to be there.

Student: (Refer Time: 28:329).

Only 180 degree rotation correct; that means, that a 2-fold rotation, if I rotate it by 180 degree; it comes to a position which is identical, but when a rotate it again by another 180 degree, all the positions come to a original position which they were occupying earlier that is what I have shown. Now, the come back to an identical position; that means, that one dimensional lattice has got all one dimensional lattice two periodic lattice as got 2-fold rotational symmetry.

The axis is on a point which is on a lattice point normal to the screen or I can take an axis which is mid way between these two points lattice points anywhere; then also if I take a rotation around this point if I take a rotation of this one. Again, it will come back to identical position; so there are two points are there as well as this like that I can; I had just shown as an example these two it could be a very where it is going to be there.

Any of this point if I try to rotate it; looking at this figure we will think that suppose you take it here we rotated to be coming towards this side because by definition lattice is infinite. So, what we are showing it is only a very truncated small form of the lattice correct, so this has got a 2-fold rotation; what else you see other than a 2-fold rotation integrals which we can see in this any other symmetry operation?

Student: Mirror.

Mirror that is if I put a mirror here or anywhere on the lattice point, it will come to an identical (Refer Time: 30:26) mirror reflection or if I put a mirror mid way between lying on the x z plane then also it will be; these are all the positions which suppose you put a mirror here then what will happen.

Student: (Refer Time: 30:45).

See now you see that this when it has rotated this shows the position which it is occupying they are not coming back to an identical position; that means, that there are once a lattice is fixed there are specific positions only at which symmetry operations are possible, all other position the only type of a symmetry operation which is possible is only 1-fold, at this point if I given 1-fold rotation that is 360 degree rotation around, it will come back to an identical position, but there is know the symmetry operation which is possible.

So, even in a lattice when you look at it in two dimensional or three dimensional lattice; once a lattice points are fixed there are specific positions in the lattice on lattice only these points are called as special points, which will come later this what. So, just similar to a unit cell in two dimensional or three dimensional lattice; in one dimensional lattice also from here to here is what the unit cell is going to be correct and these are all the symmetry operations which are going to be there.

So, in this one dimensional lattice itself we have a translational symmetry a 2-fold rotation is there, a reflection is there. So, what are the symmetry elements which it has got? It has got a 2m symmetric; these are all the symmetry elements which a one dimensional lattice has got, these only a lattice which we are consider; suppose we wanted to yes.

Student: (Refer Time: 32:36) rotation and mirror the same operation?

Which one?

Student: So, rotation (Refer Time: 32:43) should be the same operation right? because x y z will become (Refer Time: 32:48).

No any operation which you do, whether it is a reflection any crystal structure; it does mean even in a three dimension, all symmetry operation should be one lattice point to another point, it does not matter whichever be the operation which you perform.

Student: Sir, mirror and rotation are the same operation we like; your x will become minus x in rotation also x will become minus x?

We will just see when we put a motif; as far as the lattice is concerned, the lattice point has got infinite symmetry. Now, what we have to see it is a suppose you put a motif what will happen, so this is just an one dimensional crystal.

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Examples of symmetry in 1-D crystal

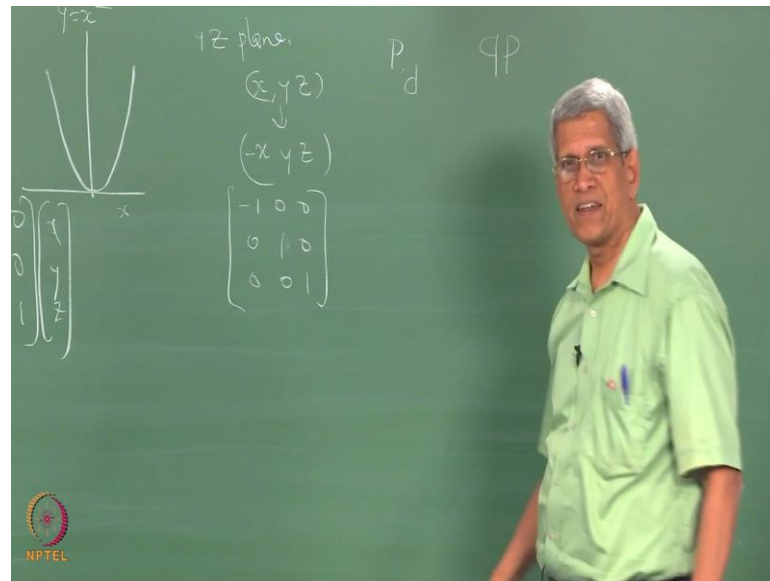
Seven one dimensional group

Now, I place a motif which is a symmetric motif; I choose it to be P as a motif; I place it here and at all positions it has been placed like this; now what is this symmetry which this crystal exhibits?

Student: 1-fold.

Only 1-fold all other symmetry elements are lost; so, the symmetry which is a lattice exhibits is the maximum symmetry which the crystal can have. But generally now you can make out, it is not the; so, once you place motif depending upon the type of motif, the symmetry elements will change. We will come back to it in some cases identical, but in many cases there is a difference between reflection and rotation; though this right hand and left hand look like 180 degree, if both have got identical infinite symmetry, then only it will be; otherwise like here also if you look at it; 180 degree rotation will bring it like this; they do not come to an identical position. If you put an object that is why when you put a motif, you can see the difference.

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Here, what we have done it is; we have chosen a motif this P and asymmetric motif and another around this point if I look at it, there is a 180 degree rotation; there is 2-fold rotation is a symmetry is there. I place this motif around each of the lattice point; now what are symmetry elements which are there; along the x axis if you now try to look at it, there is no symmetry there is y there is only 1-fold z that is around the z axis there is a 2-fold symmetry is associated with it. So, that is how it is that the primitive 112 these (Refer Time: 35:42) here it is primitive all symmetry along all the directions are 111.

Now, you look at here; here I have chosen the motif P; this is mirror related, if I place this motif. Now you see that with respect to the x z plane; that is a mirror others are all 1-fold symmetry. Now, I am choosing a motif at P; it is reflected across this, now what it has P 1 along the y; that is mirror symmetry. In other two axis, there is only 1-fold rotation; here it is along the x axis.

So, these are two different structures; crystals, here now what has happened is there, this has a 2-fold rotation around it and there is a two perpendicular mirrors are there on x and y. So, it becomes mm2, this symmetry if you look at it; around the point all the symmetry elements either intersect or there is one axis of symmetry which is there. So, this is essentially are all point group symmetries; one point remains unmoved.

So, in one dimensional lattice, we can have five types of like space group lattice we considered about we tell that there 230 space groups. Similarly, with respect to point

group if you considered there are five are possible; is that anything else which is possible? That is a glide is also possible, that is if I take p from here to here is the lattice translation vector in this (Refer Time: 37:49) one dimension.

Now if I move it half and take a mirror reflection, it will come to this position, again move it half mirror reflection, so this is a glide. So, now what we have is that around the x axis only 1-fold rotation, z 1-fold rotation a glide along the y axis and there are symbols to represent the glide these called as a b glide on y axis that is why I have chosen these aspects of it will come later, but what we have to understand that this is an another type of a crystal which can be constructed.


The third which we can do it is that we have this one; this is also can be instead of a mirror here in this one; we can have a glide operation then this is shifted by half then reflected again shifted by half reflected, it comes back to original position. So, here there is a mirror along x on the x z plane, then along the y direction we have a or the y z plane there is a glide and then on the around this point, if you consider there is a 2-fold rotation is also there along the z axis.

So, these are all the symmetry elements; here what happens is that all the points are getting shifted because of the glide which is associated with it; this we can call it as equivalent of the space group. So, the total number of equivalent of space group in three dimensional 230 we have in one dimensional lattice we can have seven groups can be there point space groups.

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Important aspects studied




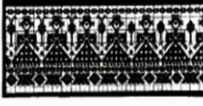
- Lattice
- Motif
- Crystal
- Symmetry
- 1-D Point group symmetry
- 1-D group symmetry (lattice)




So, looking at this one dimensional lattice itself; you have got an idea of how the various symmetry elements come, concept of a lattice, what is the difference between lattice and the crystal some idea you have got it. Symmetry elements like rotation, reflection not all symmetry element you have seen, but some symmetry elements you have seen; glide, you have seen reflection 2-fold rotation these are all the aspect which you have seen; this is just I had given some example.

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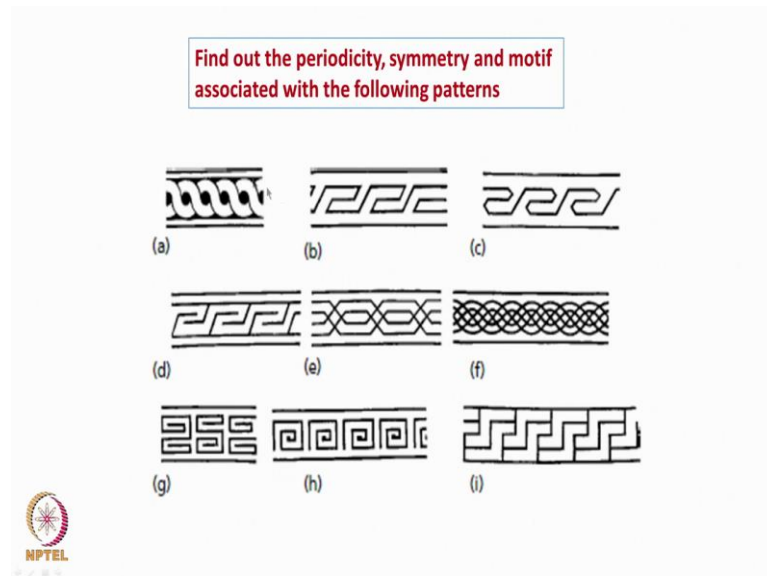
Seven one dimensional groups

$R \ R \ R \ R \ R \ R$	$p111 (p1)$	
$\cdot \underset{B}{R} \cdot \underset{B}{R} \cdot \underset{B}{R} \cdot \underset{B}{R}$	$p1a1 (pg)$	
$\cdot \underset{R}{R} \cdot \underset{R}{R} \cdot \underset{R}{R} \cdot \underset{R}{R}$	$p112 (p2)$	
$ R \ \bar{R} \ \ R \ \bar{R} \ \ R \ \bar{R} \ \ R \ \bar{R} \ $	$pm11(pm)$	



These are all from all the border the same if you look at it, there are some symmetry associated with it; one dimensional symmetry is always there. Here this is one which as an only 1-fold rotation is there, this is an another structure this will look go to any cloth shop and look at all the sarees are border, which we have you try to find out what symmetries are associated with it (Refer Time: 40:57) so, various type.

(Refer Slide Time: 41:02)



Here I had given some patterns, you can try to find out what are types of one dimensional symmetry, which is associated with it; that will give you how to identify; that is to identify the symmetry first thing what we have to do it? Because so far what we have done it is we know a lattice, we are taking a motif and trying to generate it.

Now, we are come to a reverse problem; we have a pattern which is there, periodic pattern. Now we have to identify what is the motif which is their first and then how the motif gets repeated then we try to identify then we will be able to get what are symmetry elements which are associated; that is what actually the real problem is always correct

I will just mention briefly about two dimensional lattices and then we will stop. So, far what we considered is only a one dimensional lattice, what are symmetry elements which are associated with it and we saw that five point groups crystal can be there and space group crystals if we considered in one dimension, there are seven are possible. Let us try to look at what all types of point group symmetries which we can have with respect to two dimensional lattices.

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Point groups – 2 D crystals


The symmetry elements (rotation and reflection consistent with translational symmetry) and their combination is called plane point groups.

Many combinations are possible but 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 is unmoved.

10 distinct plane point groups only exist for 2-D lattice / crystal

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 plane point groups.













Like we considered the point group because they are on the every point here also; like the symmetry operation rotation, reflection or an inversion; these are all the operations which will intersect will leave some points or an axis or a plane unmoved.


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Ten plane point groups

Crystallography / art / chemistry

(1)  1 bromochlorofluoroethene	(6)  3m boric acid
(2)  m cis-difluoroethene	(7)  4 (4) - rotane, C ₁₂ H ₂₄
(3)  2mm ethene	(8)  4mm tungsten oxyfluoride
(4)  2 trans-difluoroethene	(9)  6 (6) - rotane, C ₁₂ H ₂₄
(5)  3 trifluoroalkylammonia	(10)  6mm benzene

The Basics of crystallography and Diffraction(3rd Ed) – Christopher Hammond



Suppose we take a motif R; what is being shown is this is taken from this book; Christopher Hammond book on crystallography it is a very nice book edited by International Union of Crystallography. You take a motif R; what symmetry which it has? Only 1-fold rotation; that is why we call it as an asymmetric motif, other than 1-fold

rotation it does (Refer Time: 43:15) any other symmetry, this is also a figure which you see this is taken from an art you can go to an art museum also look at it, many of the drawings which are there they have this type of symmetries are associated with this various symmetries one can understand.

This has only a asymmetric and this is another the molecule which is being shown; which I were talked about in the first class, it has got only 1-fold symmetry which is associated with it. So, in various works of like you can always see that is symmetry is a manifestation of nature, but symmetry does not become nature is only a manifestation and if you take R and put a mirror if gets reflected. So, you can see this structure here this is difluoroethene, this has got only a mirror symmetry which is associated with it and similarly, here if you see it; it has got a mirror two perpendicular mirrors and a 2-fold rotation is there.

So, you can see that 2mm, then this is a 2-fold rotation is there; this is a putting a asymmetric motif around this axis if you see; when it comes here. So, similarly you can see a 3-fold rotation here this is then you have a 3-fold and a mirror then how the structures will look like that is for boric acid these 3m symmetry; here just a 4-fold is there for these structure; this is one of the I think rangoli is which people draw the various shapes this has 4-fold.

Here you can see that it has 4mm symmetry, then this is a 6-fold then here it is 6mm then plane point group because we know that rotational symmetry; 1, 2, 3, 4 and 6 are possible, and then mirror is another one because in two dimensions we cannot have an inversion because a space lattice is required. So, that become seven then a combination of this can be taken, so when we take the combination 2mm is one which it comes, 3m is one comes 4mm, 6mm if we add all together there are we have 10 types of plane point groups are possible.

These different point groups can be represented in different methods because whatever I talk about here, that is exactly there same way it is then for a three dimensional lattice also.


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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

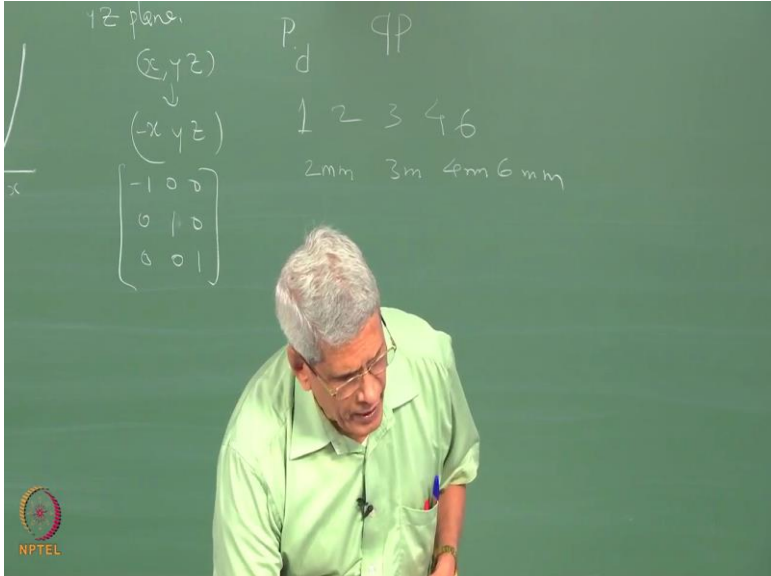
- (i) by means of their Hermann–Mauguin or Schoenflies symbols;
- (ii) by means of their stereographic projections;
- (iii) by means of the matrix representations of their symmetry operations, frequently listed in the form of Miller indices (hkl) of the equivalent general crystal faces;
- (iv) by means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



International union of crystallography tables

One is by like a symbols which we use 1, 2, 3, 4, 6; then another is a combination of 2m.

(Refer Slide Time: 46:06)



yz plane
 (x, y, z)
 \downarrow
 $(-x, y, z)$
$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

P, d, CP
1 2 3 4 6
2mm 3m 4mm 6mm

2mm, 3m, 4mm, 6mm like that, then the other is there is a Schoenflies symbol is there I think that is the symbol which there is c 1, c 2 like that then d they (Refer Time: 46:33) there are many ways in which it is represented, that is another method mostly people who work on a material chemistry; chemistry people they use not Harmon Magnum symbol, they essentially use that shown place type of a symbol.

Then a stereographic projection in with which it can be represented also all this symmetry, that I will show that. Then each point when we do a symmetry operation, equivalent points are generated in the lattice; those points with they are co-ordinates we can represent them, co-ordinates of the point that is one way. The another is that using the matrix transformation, the co-ordinates of the points, will have the type of translate specific transformation matrix for each of the operation of transformation with which we can do that or we can draw actual crystals and look at it also.

These are all the various ways in which we can represent it. Like different symmetry elements which we have looked at it, I will give us assignment to work out for different structures, how the points are generated that when you do that it will become much clearer to you people how the symmetry elements. We will stop it here now.