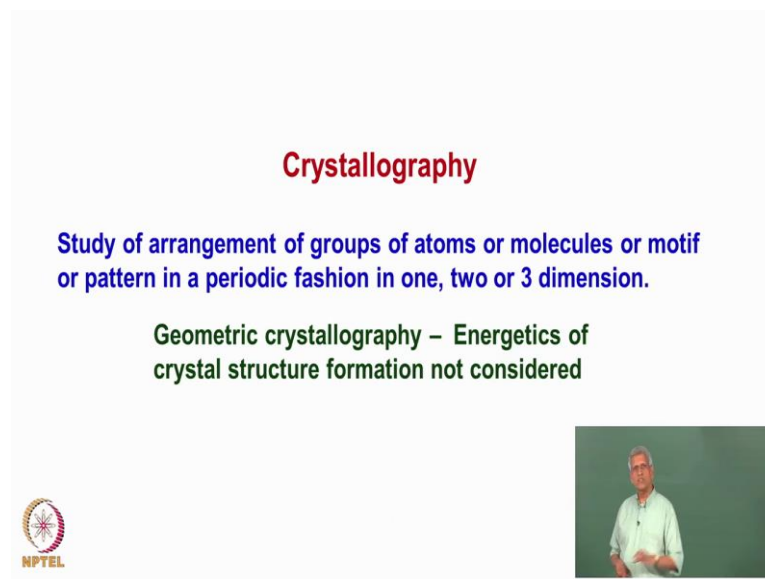


Electron Diffraction and Imaging
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Lecture – 01
1D-2D-3D Lattice

Welcome you all to this course and Diffraction and Imaging. Today what I thought I will try to cover is how to construct different types of crystal structures or lattices. You might have studied about a crystal structure of various materials like FCC, BCC (Refer Time: 00:40). How are this crystal structure is really constructor, is there any rule governing this construction of this lattices. If you understand that then it is easy to construct any type of a crystal structure are you understand why particular type of a structures only are possible; that is what will try to look at it.



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Crystallography

Study of arrangement of groups of atoms or molecules or motif
or pattern in a periodic fashion in one, two or 3 dimension.

Geometric crystallography – Energetics of
crystal structure formation not considered

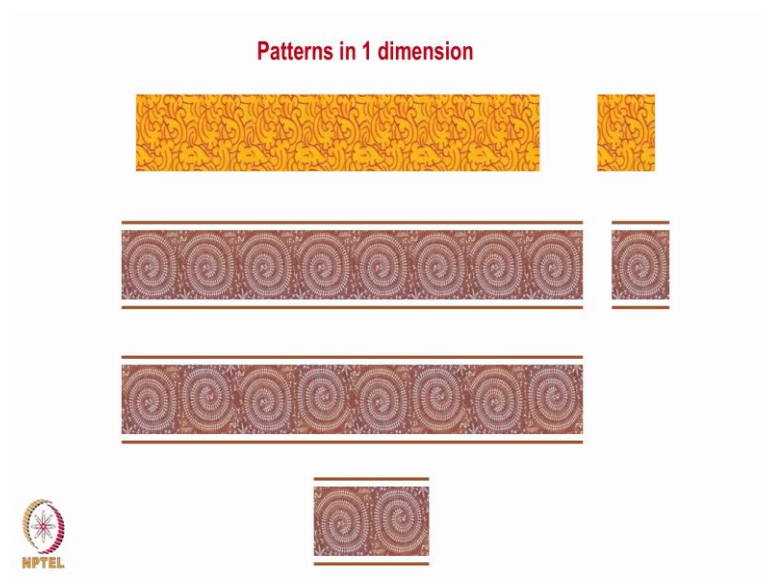
What is the basic definition of a crystallography? Crystallography is nothing but study of arrangement of atoms in a periodic fashion, it could be an atom, it could be a motif, an asymmetric unit or it could be a group of atoms which constitutes a molecule. There are various types of. This could be in one dimension, two dimension, three dimension. This you might have studied also there are periodicity of various dimensions are possible. In fact, one or two dimensional periodicity, this part of the studies extensively used in fashion technology, especially in textile, printing, then flooring which is being put, the

different types of the scenes which are created, for all of them the same crystallography which mathematician have developed that is being used to represent also to generate different types. In fact, softwares are available with which one can generate.

But one thing which one should always remember is that the crystallography which you study right, different types of crystal structure that called as geometrical crystallography. The reason why it is called as a geometrical crystallography is essentially is that this study tells what all the various types of crystal structures which are possible. It never talks about which type of a crystal structure which element or which type of crystal structure a particular element or a particular material will take. There are n number of possibilities are there.

Suppose we take aluminium: we normally find aluminium takes an FCC structure in the solid state, but why cannot it take a BCC structure. That cannot be answered from crystallography. That comes from the energetics of it that decides. So, here what we talked about it is supposed we take some particular element or a material, if you has to arrange itself in some period fashion, and that too having some specific property then we can tell that these are all the possible types of crystal structures to which this material if it forms. This type of property which (Refer Time: 03:24); actual energetics will decide which crystal structure it takes.

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Let us start with a one dimensional; just have taken some pattern. Looking at this pattern can you tell there is any periodicity in this, what is the sort of periodicity which you see

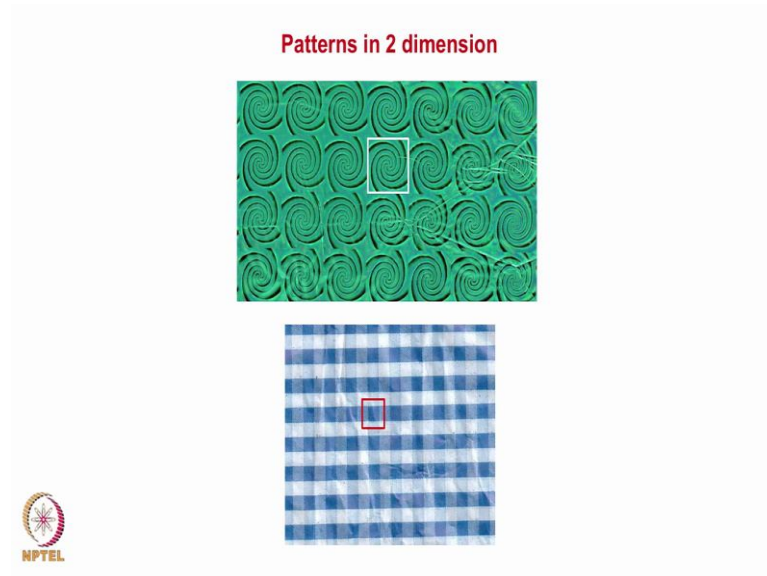
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It is a linear one. So, this is the particular type of a motif which gets repeat itself. When you look at this type of a structures like if I look at your shrug or a look at mathai shrug everything has a periodicity associated with it correct. There is a pattern which gets repeated itself, all the cloths which we are everything has a pattern which in it this pattern could be an symmetric pattern or it could be asymmetric pattern, but this pattern repeat in some periodic fashion.

What all the types of periodicity? Infinite numbers of patterns we can have, but still they can have only one type of a periodicity. That is what we will understand go through. This is another type of a pattern; it is also an asymmetric pattern. Here it is easy to visualize it because you can see what the motif which is getting repeated correct. The other pattern you have to it is not that easy to make out which is the pattern which is getting repeated. What part of the pattern is getting repeated?

You look at this pattern what do you see between the top and the bottom; these two patterns two are getting repeated. That is also periodic pattern one dimension periodicity, but one thing which you can see here is that if you look at the motif which gets repeated this motif itself also has got some symmetry associated with it. It is an 180 degree rotation is associated with it correct. So, that is why I mentioned that the motif could be an asymmetric motif like the one which is given in the top or a motif could be like this, but it is all have only one dimensional periodicity.

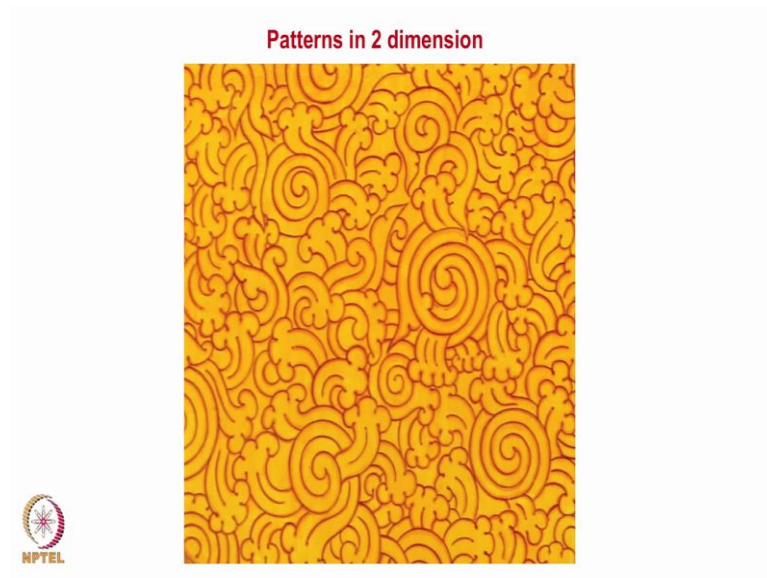
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And here I have just showing a two dimensional pattern. Here also is there anything common between them between these two, both are two dimension other than that actually look both of them they have a square type of lattice which repeats itself, here also a square which is arranged here also it is essentially a pattern which repeats itself. We are not able to make out this difference because most of the time our brain is confused by the pattern which we see. When we see a pattern we do not see the periodicity.

How we can overcome this? Each of this motif which gets repeated if you present it by a point, and then forget about the motif you can tell the this motif which represents, then it gives a better visual appeal and we will be able to recognize the type of symmetry which it has.

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This is another pattern which you can see, but here actually it is a asymmetric motif; it is only the one which is expanded.

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1-dimensional lattice

Pattern which repeats itself in the design is called **motif**.
Motif could asymmetric or could be having some symmetry.
It could be single atom or groups of atom or molecules

Each repeating motif is denoted by a point called **lattice point**.
Underlying periodicity in the design is described by **lattice**.
Lattice point is defined to have zero dimension. Lattice has infinite length
The shortest translation vector of the lattice is called the **lattice parameter**

Crystal structure = Lattice + motif
Crystal structure = Lattice + Basis

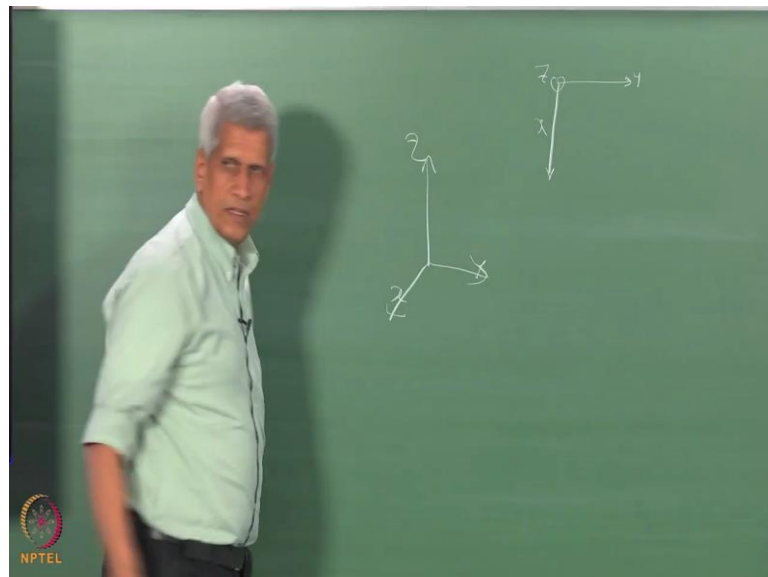
$R = n_1 a$ $R = ua$
u or n1-integer

Here what I have done is essentially showing the same pattern. Now, I am represented by a dot; this dot represents each motif. Now if you look at that the dot you can see that there is some particular periodicity with which the dot gets repeated. To this dot you can put any type of a motif, then when you put different type of motif we say the different types of the motifs are there, but actually the periodicity with which gets repeated it is

almost the same. And another one which I have done it is that I have just shown here axis in crystallography there is a convention which is followed to represent the axis that one should always be quite clear about it.

You might have seen in books the different way in which crystal structures are represented. Most of the times I find that from memory, most of the students try to draw what is drawn in the book, why is that particular fashion in which the crystal structure is represented. There is some meaning to it following some names which we will come when we talk about stereographic projection, but as far as choosing the coordinate system is concerned that one some convention is follow. The convention essentially is that from top to bottom is where always the x axis is represented.

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Then left to right y axis is z axis is normal to the board. This is the representation which is always followed in all books on crystallography, that any book which you read one should know that this is a convention this is followed and one has to follow this convention also when drawing figures. This throughout the lectures I will be following the same convention. Normally you might have seen that whenever we draw crystal structures in three dimension we wanted to give a perspective representation, how do we do? We generally try to draw this is x this is y this is z this is how we represent. Essentially this is a distorted form of this representation, x is always from top to bottom, y is from here then the z when it has to represent when it is stilted this will also be

coming on that screen. Otherwise when these two are in the plane of the board then this has to be normal to it. That is so most of the books they represent the access system.

Now, we can see that it is essentially only the dots which represent each of the motifs. This dot we call it as a lattice point. So, it is a mathematical form of convenience with which we are trying to represent different types of motif which are getting repeated by a point. And the spacing between the adjacent we represent as the lattice parameter or the periodicity of the lattice. So, this could be a motif, this could be a group of atoms or it could be a single atom which are residing at the lattice point all these possibilities are there.

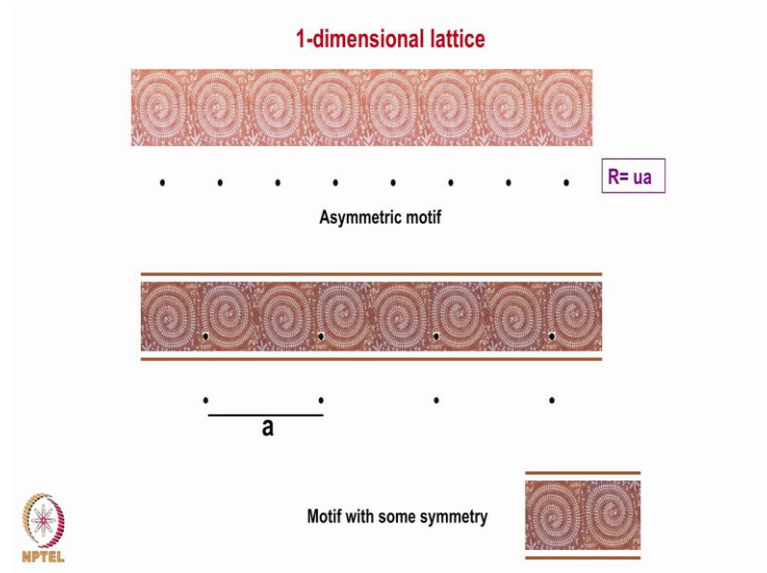
So, today most of the class I will be talking only with respect to the lattice, because the lattice is the one which represents the periodicity with which the pattern is getting repeated. Generally, if we have to represent this lattice mathematically how will you do. It choose a coordinate system, once a coordinate system has been chosen from point then this distance if it is a the vector r will represent some n one into a we can represent it which will be the vector or in many books you will find that r will be represented the n in u into v u v w will be the directions which are the number of repetitions which are taking place in those directions x y and z that is use to represent the lattice correct is this. So, far it is clear.

Generally, the lattice point which we assume, we assume that it has a zero dimension and the asymmetry is infinite that is the one assumption under which we are doing all this generation of this pattern. We will see the consequence of it, if these points have different types of symmetry associated with it. If it has an infinite symmetry a circle we can use to represent a lattice points, it will be a circle. In a three dimension it will be a sphere which has a zero dimension. That is how we represent the lattice point.

So, crystal structure the way we can construct is that crystal is a real material. The lattices are to represent the units which get repeated you are representing it by a point. So, that lattice plus the motif put on top of them that represent the crystal structure. Lattice itself has got a periodicity. Similarly the motif itself also can have sometimes periodicity, sometimes this can have associated with some symmetry also lattice also can have symmetry. We will talk about it little bit later about the symmetric.

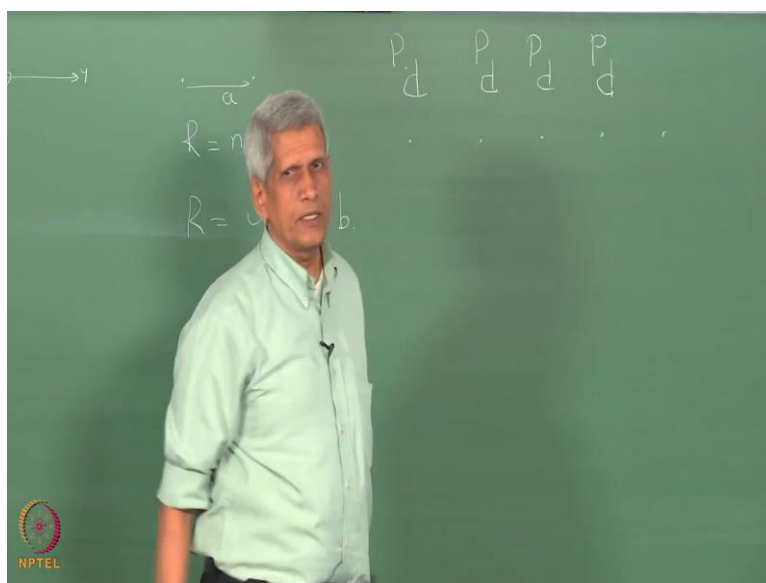
So, the combination of the symmetry of the lattice and the symmetry of the pattern which is put at around each of the lattice point that put some restrictions and the number of types of crystal structures which we can have.

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Here the motif which we have chosen is an asymmetric motif. Here if you look at it the only difference is both are one dimensional lattice correct, but the lattice parameter is different in these two cases; that is the only difference between these two lattices. But only difference here is that in this case the motif itself got some symmetry associated with it.

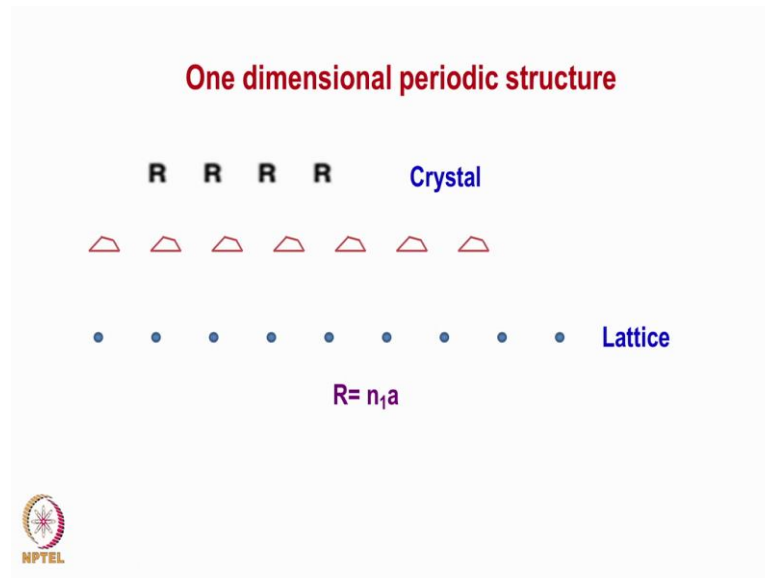
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The same thing how I can represent it is that suppose I use a letter P. The other one will be 180 degree rotation it will P like this. This will come to later, this is how if you look at a pattern this is the way the pattern will be the represented, is it clear.

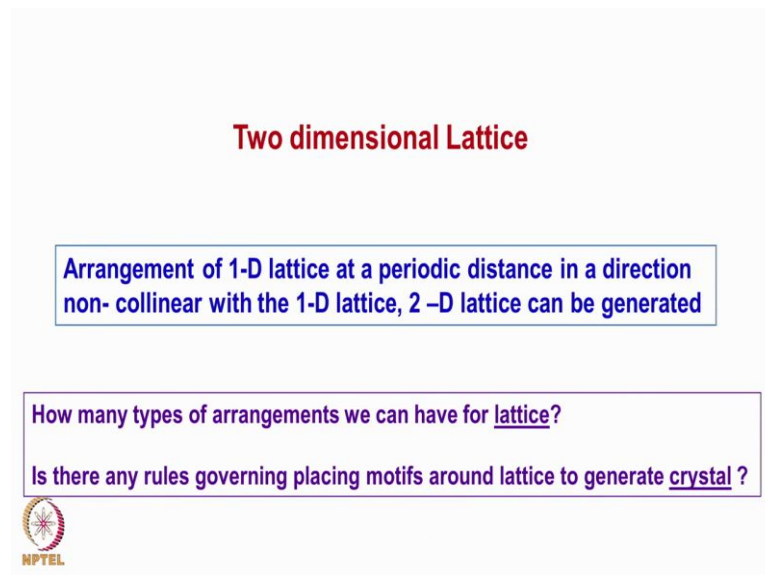
So, here motif has also got some symmetry associated with it. That is what it happens in many real systems. An asymmetric motif if we look at molecule; that is bromo, chloro, fluoro, ethene is one which is an perfect crystal asymmetric molecule. Whereas when we consider many of the atoms; atoms we assume that they have an infinitely symmetry associated with it.

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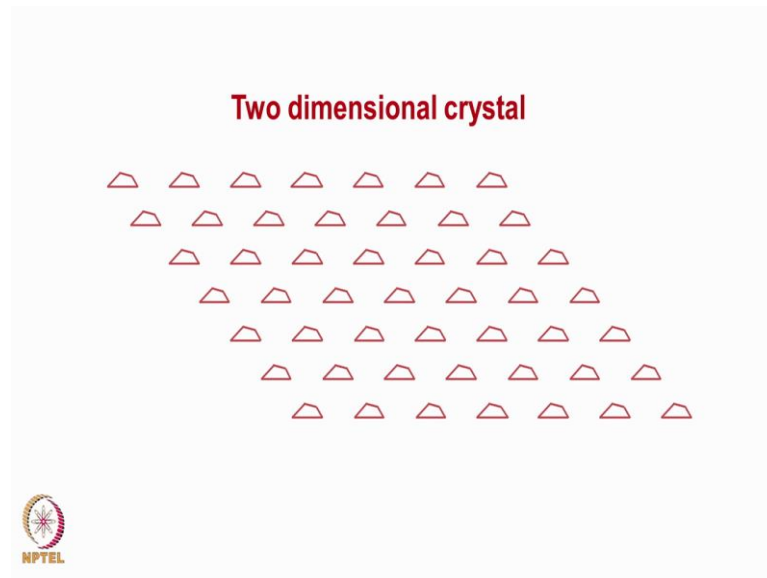
Now let us look at; here what I had just shown is an example of a few periodicity in one dimension and as well as the how it can be represented with the lattice.

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From this one dimensional lattice that is only one type of a lattice periodicity in particular direction one row. Suppose we have to construct a two dimensional lattice, how many types of lattice we can construct, any idea? Five types, because you have attended the last class. Others, anybody can justify it (Refer Time: 15:28) not you.

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How exactly we can do it is that this is only a pattern which I am showing it. This pattern we can now; the same pattern we can keep it here, but in this direction if you look at the x direction it is kept at some angle with respect to x axis at a particular distance. We repeat it like this and if we keep it we generate one type of a pattern. This is a two dimensional lattice. There are many ways in which we can do it. I can do it by putting it just straight down, that is one way we can do it. And then I can keep this distance as well as the periodicity in this direction the same or different, then I can generate and another type of a lattice. So, this put some restrictions, this we will see how many we can have.

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Two dimensional periodic structure

Oblique p lattice

Unit cell is not unique

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

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

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

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

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

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

Tiling

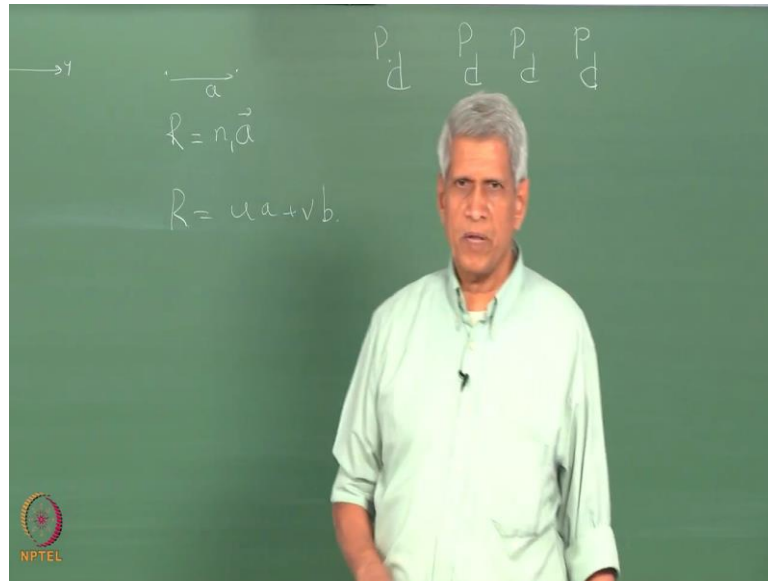
So, before going into the details we will look at some basic definitions the lattice. In this two dimensional lattice, this is the two vectors which normally used to represent the lattice. They should be non collinear. Generally those having the shorter translation vector which we using, but that is not the only way it is represented there is symmetry is the one which is some consideration which comes into is the picture, representing the lattice.

Here if you look at it this is a and this is b, translation vector. We can have the unit cell in this particular way, this particular way also all this unit cells if you look at it; all of them have only one lattice point per unit cell. And all of you might have study only just I am starting from the beginning and going ahead for the sake of completeness. So, this we call it as a primitive lattice.

So, the first thing is that the lattice unit cell is not unique to any lattice; that nothing like a unique unit cell which you can choose any type of a unit cell which we can construct. Then if you look at any lattice point it has got identical surrounding around it correct. So, that is another property of a lattice that all lattice points will have identical surrounding. An ideal lattice essentially is infinite in dimension so that the surface effects can be ignored, because surface is a discontinuity. Only in real crystals the surface effects have be considered and the properties are different, but when we consider a lattice we consider lattices and infinite lattice so that the surface ignore.

Then here if you see we have a lattice which is different type of a lattice. This contains two atoms per unit cell, this we call it as a non primitive lattice. There are many instances like body centered face centered all, we use only non primitive lattices; we will come to it later there is essentially that. Generally we use a unit cell which represents the full symmetry of the lattice. So, in this case what we take as a condition is that a and b lattice parameters are not equal, the angle between them is also not equal to 90 degree. This lattice is called as an oblique lattice.

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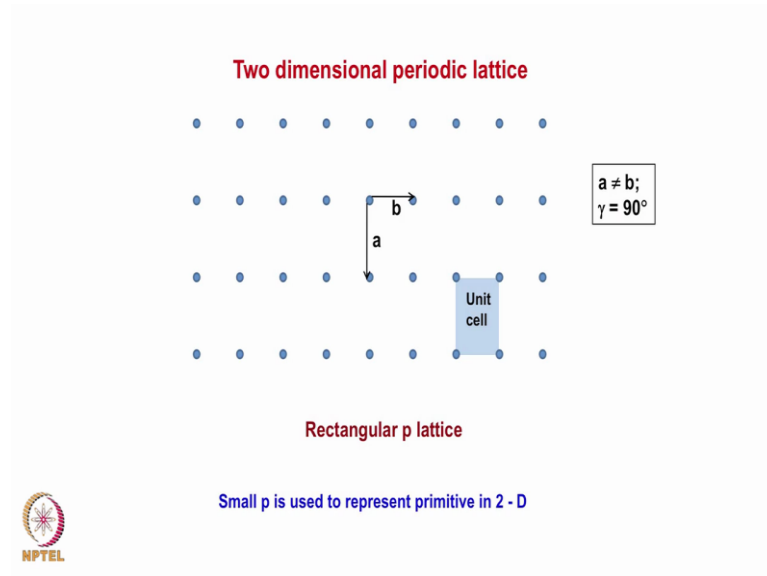


In this type of lattices we will be representing the vector R v; this is the way we are representing. Any lattice point can be represented where u and v are essentially integers it would be positive or negative; they cannot be fractions, that is only thing which you should remember, is this clear. That is exactly what I have told that we choose a lattice which represents the full symmetry, because immediately from symmetry only we try to identify it.

Why are we looking at these types of two dimensional lattices? Is that when you study diffraction when you take electron diffraction pattern all are two dimensional patterns; what are the types of patterns which we can have that will become clear when we go through this slides; then another way in which these lattices can be represented, which we call it as a tiling. Essentially, if you take a unit cell like this we can keep adjacent unit cells unit cells adjacent to each other and do a space filling correct. So, this is one particular shape which does that and space filling can be completed.

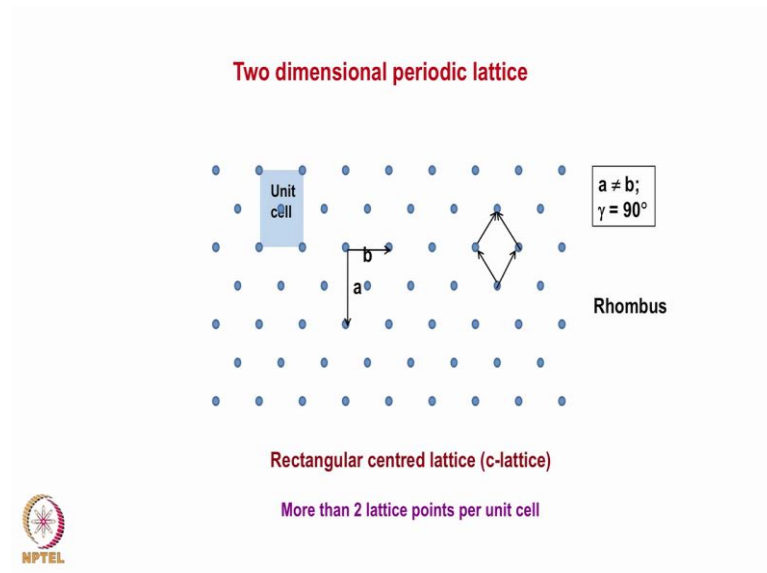
This you might have seen that when people put this rangoli, they put dots which is essentially in some period fashion. Then either the dots are connected or some figures are made around each of the dots to create various types of pattern. That is a lot of science behind it. Though people do not understand it, but I think the mind it is what doubt; that is why we are there able to generate various symmetric as well as asymmetric patterns.

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You see here, this is another way in which from a one dimensional lattice we can generate a two dimension, because each one dimensional lattice is kept just below the other. And the distance a and b are not equal. So, this lattice is called as the rectangular lattice.

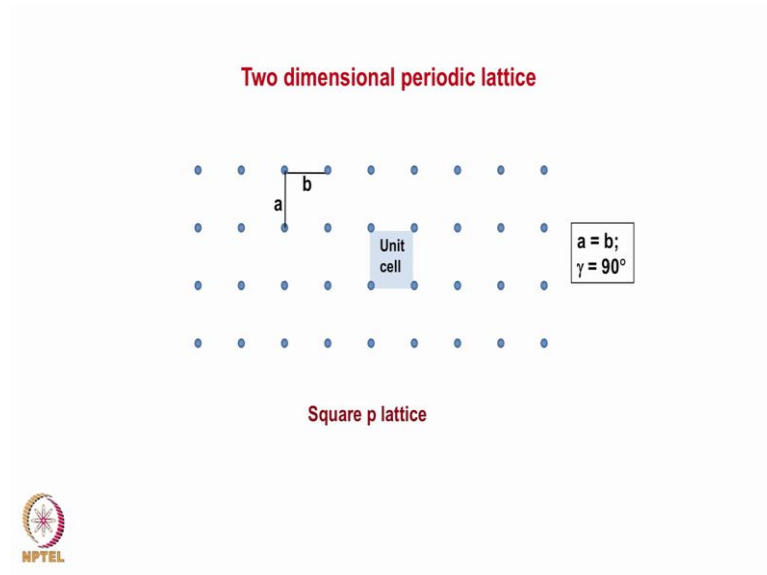
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The other way in which we can do it is that in one lattice is kept here another is kept here one dimension, in between at the centre of it you keep the next one; this way if you try to arrange it. We get a lattice which is called as a c centered lattice or if you look at it

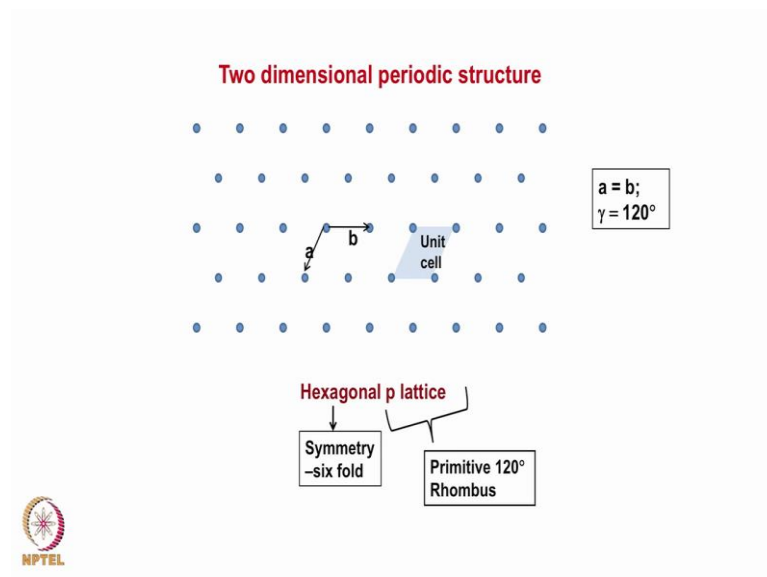
because c centered lattice is a non primitive lattice, because this one atom is there at the centre. If you see here this is essentially nothing but a rhombus is a primitive lattice, because every lattice is a primitive lattice.

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If you take a equals b and the angle becomes 90 then we get a lattice which is a square lattice.

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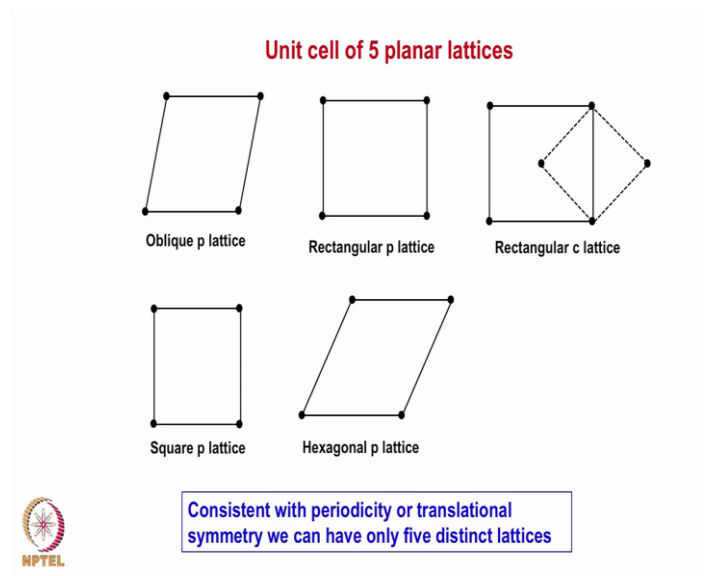


And if a equals b and the angle becomes 120 degree we generate hexagonal p lattices p lattice which has a 6-fold symmetry as well as it has a 3-fold symmetry also associated

with a rotational symmetry associated with it. These are all the only types of two dimensional periodic lattices which we can have. This we have studied in geometry all these names; parallelogram, rhombus, rectangle, triangle, square, so that is all it is. We are never understood we are never told that why these are all, these are all the shapes which we can have. And these shapes are all periodic once. If we take quadrilateral that is also but quadrilateral it is a periodic correct, it is not the periodic shape.

Any diffraction pattern you get it in two dimensions even with x ray or with the electron beam used to generate, the diffraction pattern should have symmetry corresponding to one of this. From those patterns finally we try to find out what is the type of a crystal structure which the material has got. That is what the essentially I had shown here.

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These are all the 5 lattices. And periodicity which we see here this is also called a translational periodicity; not a translational symmetry. We talk about symmetry; the first symmetry which we will see in any material if it is periodic is translational 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

Inversion symmetry is not considered as unique one since it is a combination of rotation and reflection



What is symmetry? That question comes is that how do you define a symmetry. Symmetry is something like a type of invariance; that is an operation which we perform that brings you to a position which is identical to itself because from the end position and the initial position there are no differences.

So, in a lattice which is repeating itself like this; if I shift it from here to here in an infinite lattice it comes to a position which is identical to itself. So, we are not able to make out that we have made it undergo transformation. So, this called as translational symmetry. Similarly we can have another type of symmetries which are: one is a rotational symmetry, another is a reflection symmetry is also another type of symmetry. Then inversion is another type of symmetry which we can have round a point.


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Symmetry Elements in 2-D lattice / crystal

Periodic arrangement in 1, 2 or 3 dimensional space 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:

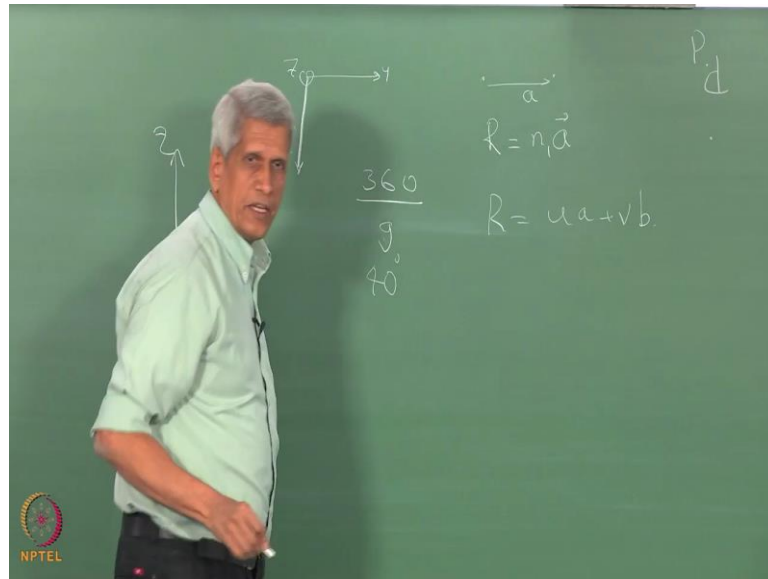
<u>Translational symmetry</u>	<u>Rotational Symmetry</u>
<u>Reflection symmetry</u>	<u>Inversion (nothing but 2-fold rotation in 2-D)</u>



So, in a two dimensional lattice if you consider this if we take this case itself we have a around this point. If I take an axis perpendicular to it, rotated by 60 degree, all the atoms will come to position which is identical to itself, will not be able to make out that the rotation has been performed. But suppose we are able to identify a tag each of these lattice points unless we do 60 degree rotation then only each lattice point will come back to original position. So, this sort of an operation we call it a rotational symmetry.

Similarly, if I put a plane here, anywhere here, I have a mirror image of each of the side and the lattice positions are now identical to each other then. So, this is which we call it as a this has got the reflection symmetry also associated with it. But is there any rules governing the symmetry, if I take around any axis if 360 is divisible by any number n.

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That is I had given n equal and if I take it will be 40 degrees. If I rotate it 9 times a point I will be able to come back to original position. But as far as around a point this is possible, but whether if further is a translational symmetry is associated with a two dimensional lattice is it possible to have this sort of a symmetry or not. There are some restrictions are there, not all rotations are consistent with translational symmetry. That how many of them we can have, is from this slide which one can understand.

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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

Here what have done is that taken a lattice, this is the translational periodicity. I have rotated this by an angle ϕ here and rotated this by an angle ϕ this point and it has come to assume that come to another lattice point matching with it. Then this distance if I tried to see, since these are two lattice points it should be some integer times the periodicity. That is this turns out to be empty. This empty will be equal to this t plus the rotation 2 times it has been rotated $2 t \cos \phi$.

So, this will put a restriction on $\cos \phi$ should be equal to m minus 1 by 2 that m can have any value 0 plus minus 1 and all these values are possible, but what is essentially important is that now this $\cos \phi$ if you look at it this is n by 2 it turns out to be because m minus n is taken to be n . Then what are the values which we can have, the $\cos \phi$ can have a value 360 degree 1 rotation, it cannot exceed that. So, if we take that as a criterion then the values which n can have which will give raise to is 180 degree, 120, 90, 60, and 360, or it is 1-fold, 2, 3, 4 and 6-fold rotation. It will natural consequence it turn out to be only these are the rotations which are because here the condition which we have put it is that is consistent with the translation symmetry.

So, with translation symmetry these are all the only five types of rotations which are possible, other rotations are not consistent with it. We can have around it symmetry like this any angle, but in a lattice only these six types of rotational symmetry only is possible. Then another is a reflection. And you should remember here that in this also the translational symmetry we should, this we consider it around an axis correct; around one point we are considering all these translational symmetry.

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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)

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

$\{ \quad | \quad \}$

xyz → x-yz
Mirror lying on x-axis

X' = A X

A is the transformation matrix

Find out the transformation matrix for these operations

Here if you look at it, this is a reflection; that is the right and left handed our whole body also has got externally if you look at it that is a mirror symmetry which is associated with it. And here a linear periodic one dimensional array is being shown. Here if you look one fact which becomes in quite clear is that I can put a mirror on any of this lattice point, it will get reflected. In addition to it in between the lattice point at the middle also we can put a mirror that also gives raise to the same mirror symmetry.

So, there are two positions of mirror symmetry is there in this lattice. What are shown here is essentially only a with respect to a mirror, but in a lattice when you consider not only at one particular point there are some points other than the lattice point also where the sort of symmetry it can exhibit this, is this clear.

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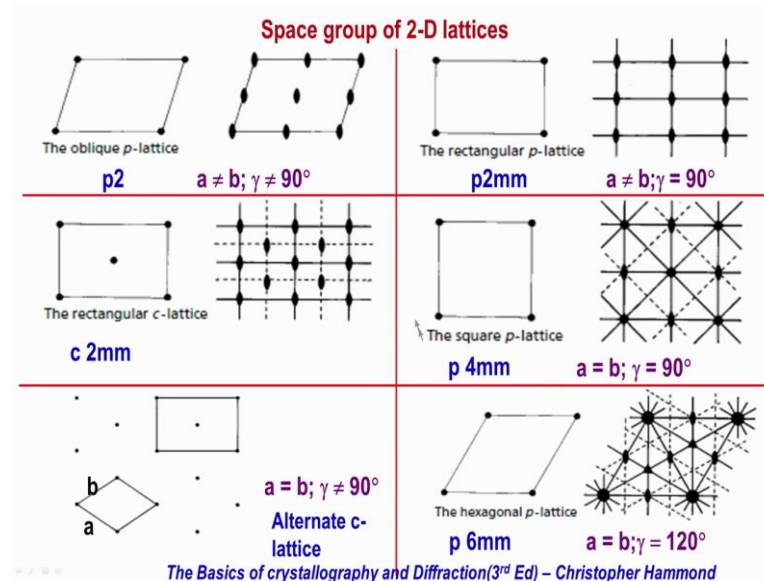
Reflection / Glide symmetry

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.

I will come back to all these mathematical things later I talk about it. Then another type of symmetry which happens also is this is called the glide. Like when we walk on the beach sand that right and left leg both of them are mirror symmetry of each other, only thing is that with a periodicity half of the distance between the leg which we keep it that half the distance is with which that is as if like here what is being shown its an r. This or this is periodicity here, but if I repeat it by half the distance and take a mirror reflection it will come here. Again move half the distance and take a mirror reflection it will come to this point. This is how it gets repeated itself.

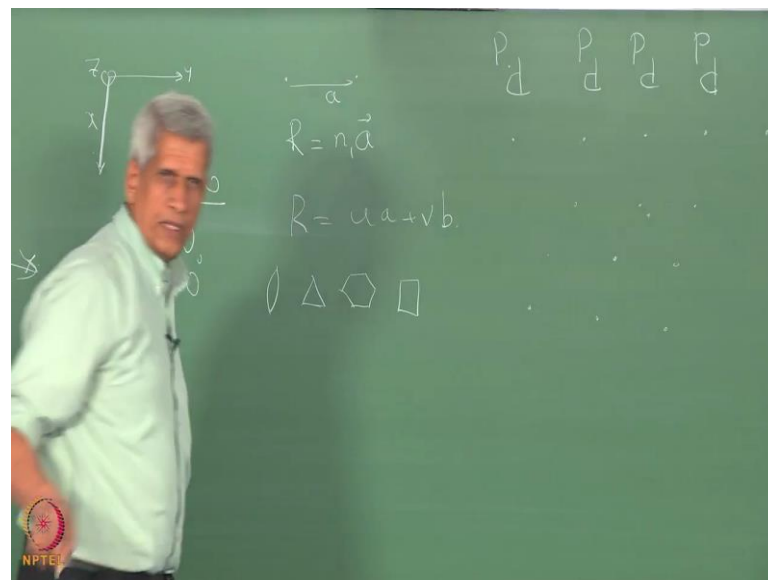
This is around this lattice points we have, but this automatically generates another glide symmetry plane halfway between. Essentially in crystals we can see that because there is a translational periodicity is associated with it, it gives raise to some points also other than the lattice points where some additional symmetry elements can come. That is what the message which I wanted to convey.

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Here what I had just come back again to the 2-D lattice. If you see this is the primitive p lattice.

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In this lattice around the centre if I rotate it by 180 degree this point will come here, this point will come here; 180 degree rotation is there. Similarly, I can take any point as the centre will have that 2-fold rotation, but if I take a point here also around this point also I can have a twofold rotation. Similarly here also I can have a twofold rotation, here also I can have that is what is essentially is being shown. So, once some basic symmetry

element is associated with the lattice point this only just showing the unit cell. In the unit cell there are other positions also different types of symmetry elements are present. These points in crystallography generally they are called as within the unit cell when they are called as special points.

These given in the international crystallography so one should know. But if I choose here instead of it supposed I choose a point here and put the axis and try to rotate it by 2 fold, will I get a this one the pattern will not come identical. That is only at the lattice point are at the middle of it, that is middle of the x and the y axis (Refer Time: 32:22). Only these points where they show that 2-fold symmetry, any other point if choose an a axis it will not show any symmetry it will show only one fold symmetry that you have to do a 360 degree rotation to come back. These points are generally called as general point or these are called these points with no symmetry, is this clear.

Like here if you see a rectangular lattice, now we have some mirrors also associated with it. There are various types of this I will come back later about it. But what I wanted to tell you essentially is that consistent with the lattice there are some symmetry elements which are associated with it both are; so 2-fold essentially represented by this symbol 2-fold rotations. If it is a 4-fold rotation it is generally represented by a fill square; 6-fold essentially with the hexagon it is represented; 3-fold will be represented a triangle. These are all the way 2-fold is essentially represented this way this rotation axis. And the mirror generally is represented with a solid thick line; that is what essentially is being shown here.

And then this line which is being shown is essentially a glide. For the purpose of today's lecture I am not going into a detail of it, but this I will explain later.

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Generation of 3-dimensional lattice (from 2-D lattice)

Follow the same method that was followed to generate 2-D lattice from 1-D lattice

Stacking of a layer of plane lattice on top of another layer at points corresponding to the symmetry of the bottom layer or otherwise, three dimensional lattices (Bravais lattice) can be generated.

Illustrated with examples

From a hexagonal plane lattice, trigonal, hexagonal and cubic lattices can be generated

From a square, tetragonal and simple cubic Bravais lattices can be generated

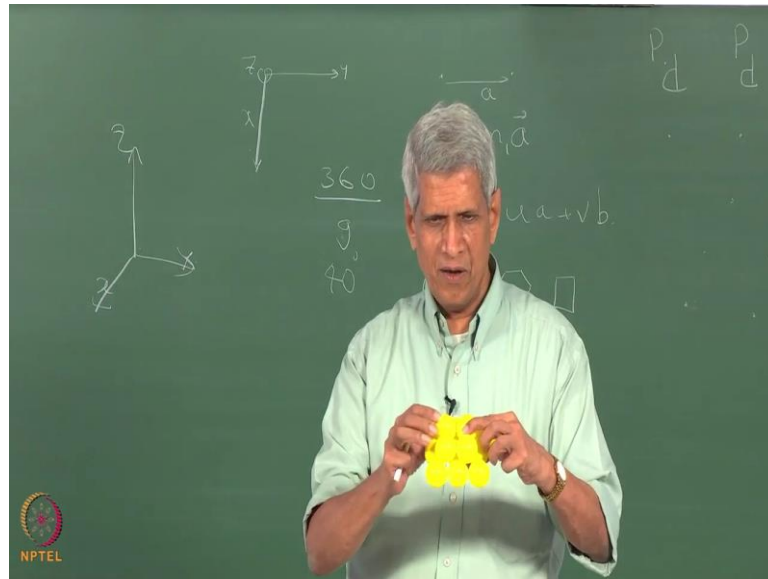
From a rectangle and centred rectangle, different orthorhombic Bravais lattices could be generated

Because today's lecture I just wanted to concentrate only on construction of lattices from 1, 2, 3. So, so far what we discussed is essentially from one dimension how two dimension can be constructed. We have seen that there are only five types of two dimensional lattices can be constructed. Suppose we have to construct a three dimensional lattice, what should we do, then this periodic lattice which is their two dimensional lattice. We stag them one on top of the other, then we can construct a three dimensional lattice. But here also when we try to stag them one on top of the other. Is there any sum how many lattices we can construct is it infinite.

Student: 14.

14 ways lattices are only possible. You can choose any type of a pattern and do it. This I will I think the first time when I took the class I asked all the students to take straw and make it and they made it. And better than what I expected they could do. I will expect all of you to form into some groups and try to make it will be very nice. We will learn a lot then whatever you learn in the class I can show you a very simple example here.

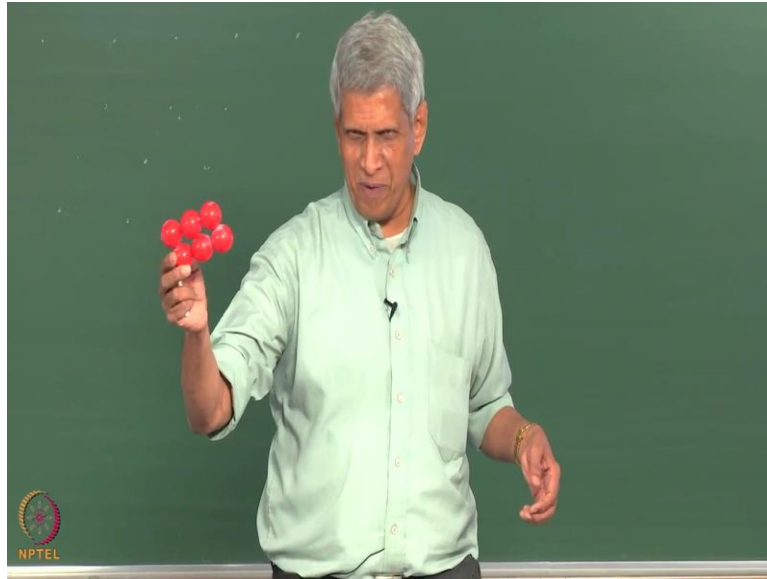
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You take this; this is a square lattice, if I put this one on top of it one on top, and another one on top of it if I put it this is one at the middle another square lattice has been kept I am just putting an atom which is essentially the same square lattice repeat itself so this comes on top of it. So, this is if it considered as an a type of a lattice and if it is a plane and b stacking and this will be an another a stacking a b a b a b. If you look at this one a equals b and c will be around root two time, so it essentially a tetragonal lattice.

The same lattice if I keep one on top of the other what I do I create a simple cubic lattice. So, depending upon how you keep one on top of the other various types of lattices which you can the space lattice can be generated. This is what I want you people to do.

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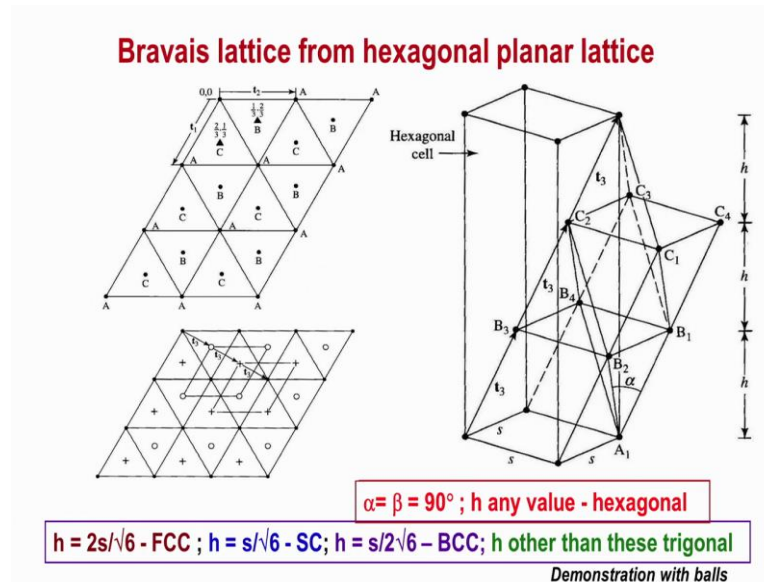


This is essentially another one; it is essentially a parallelogram type of a arrangement. Here also you can keep one on top of the other and you can generate various types of lattices. Here if you look at it this is a hexagonal lattice. In this hexagonal lattice if I keep it at one particular a position and this on another position which comes on top of it, the third one which I keep it if you see 1 a b and c if I keep it. Now this is also an FCC lattice cubic lattice. If I keep this in a position instead of it here if I keep it like this, now these become a hexagonal lattice. These are all only hard sphere models which had kept it so there at the particular ratio. By changing this separation here, if I keep it instead of not touching keep it like this a b and c if I keep it on another this becomes a rhombohedral.

Depending upon what the height at which I do if I can gets simple cubic, we can create BCC, we can create FCC. And if I keep this one just on top of each other it is a simple hexagonal lattice. So, various types of lattices can be made from these two dimensional lattices by arranging one on top of the each other. This arrangement could be that is here what I have done it is I kept one on top of the other over a symmetry point. I can do it in another way; like here on top of it if I keep it becomes simple cubic. Suppose I shifted little bit like that and do it what happened, this a face becomes a parallelogram, then it may become a triclinic structure.

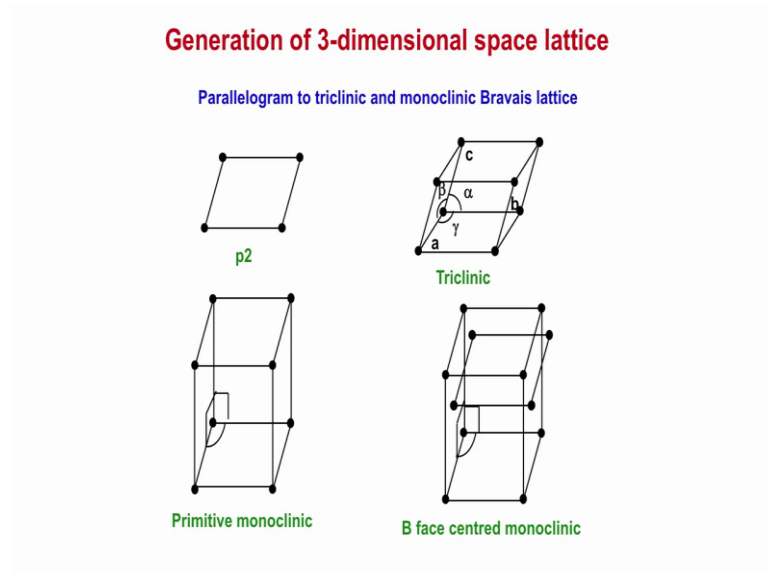
Essentially by arranging two dimensional lattice one on the top of other various types of lattices could be generated. And we will just show some sequence which is being shown here.

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Here it is a hexagonal type of a lattice; a lattice on top of which a b lattice is kept like what I had shown here. And then c lattice comes on top of a and b that is exactly the sequence. Then on top of which a lattice come. Depending upon the height at which these are being kept; if the separation between them is s and the height h is equal to $2s$ by root 6 it can become an a FCC. If the height becomes a s by root 6 it becomes a simple cubic. The height equal s by 2 into root 6 then it becomes BCC. If the height h is other than this it becomes trigonal. If it comes on top of one another then it becomes a hexagonal. And all types of lattices are possible.

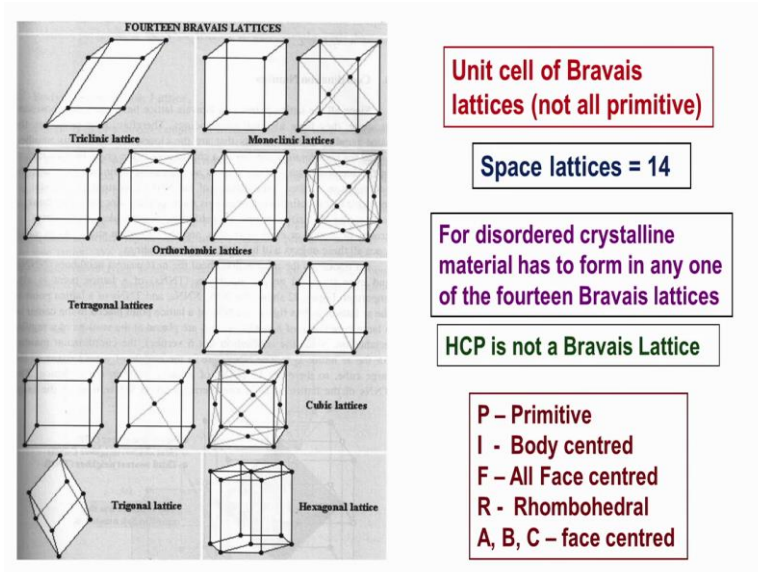
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Similarly, another example is being shown, this is a parallelogram; this parallelogram which has a not equal to b . I keep another one on top of it, but it is not exactly. If I keep it exactly on top of it at some height then it will become a monoclinic structure, but with respect to the bottom one if the top one is shifted the little bit someway, it will create a triclinic structure. Here in between if I put one more layer that is what it creates the base centered monoclinic structure comes; that is one face is centre.

So, essentially where are we keeping it? Either at a point which has some symmetry associated with it other point where there is no symmetry is there, we are trying to keep these two dimensional lattices on top of the each other. Then the total number of lattices Bravais lattices which we can generate. This is essentially showing the structures, but I will just come back.

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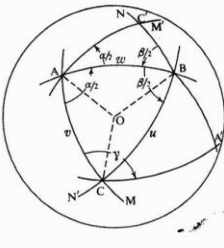
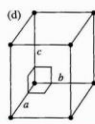


These are all the only 14 Bravais lattices are possible. What were the infinite number we can try; that is you have 5 two dimensional lattices, you can have various array way in which you can arrange it, then you can take the number of combinations which we can try- 5 times, what were the (Refer Time: 44:36) you take it how many what will be the number. But finally, when we say that only 14 are going to be there; that means that this also based on some symmetry consideration.

So, generally what is being told about these lattices is that these are all based on a equal to b not equal to c alpha equals beta equals gamma that is the way it is being written in most of the books this is how you might have studied. But it is not based on that, it is based on actually symmetry. In crystallography language a not equal to b actually means that a necessarily not equal to b; that means, that a can be equal to b as well. So, if the symmetry which says whether it is monoclinic or triclinic or whatever is the structure and it is not the lattice parameters. That one should always keep it in mind; that I will come with some example later how it happens.

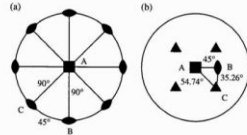
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Combination of rotational symmetries

Angle between
symmetry axes and
rotation angle for
symmetry operation


Stereographic representation



tetragonal Cubic

Table 1.2 Permissible combinations of rotation axes in crystals

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



So, when we keep this type of two dimensional lattices one on top of the other generally we have seen with respect to either on lattice point or the middle of it this will have a 4-fold symmetry we know that. Suppose I keeps one on top of the other and if I look at some other angle also there may be some other rotational symmetry associated with it. In a three dimensional lattice if I try to located it there may be many symmetries which are possible in different directions. If we try to look at all those symmetry elements then try to look at. Then what is going to have this is what essentially is being this is essentially a problem which becomes of a spherical trigonometry. If we give one rotation in one direction and in three dimensions finally that rotation should be consistent with the translation so that the position of the lattice should be lattice point should become identical with the earlier one.

When that is being done it is like this. If there are access we find that in a crystal only 2-fold axis are there; that is three directions 2-fold access only we see nothing else. Then each 2-fold axis is 180 degree then angle between this axis will turn out to be 90 with respect each other and that gives raise to an a orthorhombic structure. Similarly, if two 2-fold axis we find the crystal and then in another direction we find 3-fold axis; 3-fold rotation axis, then the crystal turns out to be essentially trigonal why I am telling it because when you look at the diffraction pattern is the one which used to find out the crystal structure.

Then you have to look at symmetry; suppose I take a diffraction pattern in one direction and diffraction pattern, in another direction with respect to some angle it gives 2-fold symmetry. In the third direction if I take it if it gives only 3-fold symmetry. By looking at these three diffraction patterns I can immediately tell that this crystal is a trigonal crystal, you understand that. That is where it is useful.

So, there is some sense to learning all these things. There is the reason for learning all things this way if you consider 2 2 and 4 gives rise to tetragonal. That if 2-fold, 2-fold and 6-fold is there it will be a hexagonal type of a lattice; 2 3 and 4 it will be a cubic lattice. These are all the way it is going to be 2 3 and 3 it is going to be again a cubic.

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

System	Symmetry	Conventional cell
Triclinic	No axes of symmetry	$a \neq b \neq c; \alpha \neq \beta \neq \gamma$
Monoclinic	A single diad	$a \neq b \neq c; \alpha = \gamma = 90^\circ < \beta$
Orthorhombic	Three mutually perpendicular diads	$a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ$
Trigonal	A single triad	$\left\{ \begin{array}{l} a = b = c; \alpha = \beta = \gamma < 120^\circ \text{ or} \\ a = b \neq c; \alpha = \beta = 90^\circ, \gamma = 120^\circ \text{ or} \end{array} \right.$
Tetragonal	A single tetrad	$a = b \neq c; \alpha = \beta = \gamma = 90^\circ$
Hexagonal	One hexad	$a = b \neq c; \alpha = \beta = 90^\circ, \gamma = 120^\circ$
Cubic	Four triads	$a = b = c; \alpha = \beta = \gamma = 90^\circ$

*Rhombohedral unit cell.
*This is also the conventional cell of the hexagonal system.

So, in this particular transparency if you look at it that classification is based more on these symmetries. Triclinic if you take it, a triclinic crystal will have only 1 1 fold rotation that is nothing else will be there. Crystal structure will not have any other symmetry other than translation. Translational symmetry all lattices will have. Then if you look at monoclinic: monoclinic will have only one 2-fold rotation around an axis and that is the only symmetry element which is presented that. That is the minimum symmetry element which is present; you can have more than that also. But the minimum is if it is there then we say that this is monoclinic.

If along three directions which are perpendicular to each other if there is 2-fold rotation axis is there; only 2-fold rotational symmetry then it is going to be essentially an

orthorhombic structure. If a crystal has got only one 4-fold rotation and there could be anything else other than that then that is the tetragonal structure. Suppose a crystal has got only a 6-fold rotation then it becomes hexagonal. Suppose a crystal has got only one 3-fold axis rotation then it becomes a trigonal or rhombohedral. Suppose we have four 3-fold axis is present making some angle between them then it becomes a cubic system.

The difference between cubic and trigonal is essentially that in trigonal there is only one 3-fold axis, cube we have four 3-fold axis are there. Like for this cube if we take it has along all the four body diagonals there is the 3-fold axis is there. Suppose I try to stretch it along one body diagonal then what will happen is that only one 3-fold axis will be there where we have stretched it, all other 3-fold axis will vanish. Then it becomes a trigonal structure, is this clear. Yes.

Student: There any correlation in a b c and x y z?

A b c and?

Student: X y z crystallographic axis.

X.

Student: X y z and a b c are.

No, x y z generally we use to represent the axis. Here a b c represents what are the directions around which these symmetry elements are existing. It could be any it can coincide with the x y z need not also. Like for example, if you take a cubic structure the 3-fold rotation it is being given with respect to b; that is essentially along 1 1 1, but the coordinate system which we choose for cubic is along x y z does not match with that. Whereas, the 4-fold which you see that will match with one of the other; this I will come to explain later what is the similar, but it need not be the same.

Whereas in the case of a orthorhombic structure the 2-fold rotation matches with that of the x y z axis, then no need for it. This is essentially what I had given here also, these are all the various types of. But what is essentially important is that one should remember that all the classification into seven crystal systems is based on what is the minimum symmetry which can have. Then one is that in the case of cubic we can have a primitive

that a simple cubic, body centered and then we can have face centered. These are represented. Yes.

Student: Sir, why centered square is not (Refer Time: 53:08) 2-D dimension.

Which one?

Student: Centered square we have centered rectangle right c centered.

Centered square if you take it, it becomes another square.


Student: Centered square become another.

Another smaller square with a by root 2 as the lattice parameter, so it is symmetry is square symmetry only; you understand that. It is the symmetry which dictates.

(Refer Slide Time: 53:19)

Seven crystal systems, Bravais lattice and symmetry

System	Bravais lattices	Axial lengths and angles	Characteristic (minimum) symmetry
Cubic	<i>PIF</i>	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	4 triads equally inclined at 109.47°
Tetragonal	<i>PI</i>	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	1 rotation tetrad or inversion Tetrad
Orthorhombic	<i>PICF</i>	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	3 diads equally inclined at 90°
Trigonal	<i>PR</i>	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$	1 rotation triad or inversion triad (= triad + centre of symmetry)
Hexagonal	<i>P</i>	$a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	1 rotation hexad or inversion hexad (= triad + perp. mirror plane)
Monoclinic	<i>PC</i>	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta \geq 90^\circ$	1 rotation diad or inversion diad (= perp. mirror plane)
Triclinic	<i>P</i>	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$	None



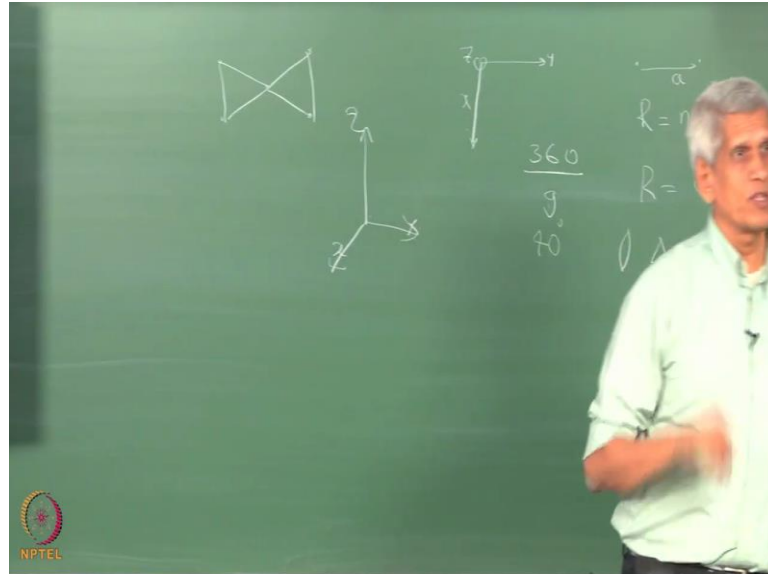
So, essentially all the classification of crystals and crystal structures lattice structures and all are based on symmetry. What is the type of symmetry which it has got on that basis we grouped up.

Student: Triangle (Refer Time: 53:46).

A triangle if you take or if you take an isosceles triangle it is going to be different; it will have only 2-fold symmetry, it will not have a 3-fold symmetry. Though we call it as a

triangle, symmetry wise if I join two isosceles triangles it will become a centered in two dimension it is a centered rectangle it will become.

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That is if I can right these how it is going to be, but this will have 2-fold and not a 3-fold. 3-fold rotational symmetry will be exhibited only by an equilateral triangle. But the same equilateral triangle has got when we are a space filling is taking, because the space filling also has to take place with all these kinds. Then when that happens it will have a hexagonal that 6-fold symmetry associated with it. I will come back to a crystal structure later.

So, what I just wanted to tell is that starting from a one dimensional periodic lattice we can construct only five types of two dimensional periodic lattice. From these five types of two dimensional periodic lattice only 14 types of unique three dimensional lattices could be constructed. Around each of these lattices either one dimension or two dimension or three dimension we can put motif around them, satisfying some symmetry conditions is a reflection symmetry or rotation symmetry or a combination of these symmetries when we do that; that can generate real crystal structures can be generated. That there are some numbers are available; like only 70 two dimensional space groups can be generated. In three dimensions we can generate only 230 space groups those restrictions come. This we will discuss it in the next one or two classes.

So, essentially here I just told about construction of the lattices from one to one to two, two to three dimensions; is this clear? If you have any questions please do ask and get it clarify.

Student: Sir, in quasi crystal 5-fold symmetry is possible.

Which one?

Student: Quasi crystals.

Quasi crystals has got a 5-fold symmetry. Yes.

Student: (Refer Time: 56:32).

Essentially quasi crystal is not a periodic lattice. Many of the material in nature show a 5-fold symmetry which is there, when we talk about point group symmetry I will tell you what it is going to be. It can have 2 m, mirror symmetric is possible in quasi crystals; 2-fold symmetry is possible 5-fold symmetry is possible this is the combination which will show

Because so far when we talked about here a tiling which is with respect to a tiling which fills the complete space; if it do a tiling model quasi crystal essentially is a particular type of which is a 5-fold symmetry. In that tiling if I put one quasi crystal this one regular pentagon and keep another on top close to each other there be some gaps which will be there; that will be essentially a rhombuses which will come. So, generally this filling is called as a fat rhombus and the lean rhombus, because the angle between them will be different; that is two types of one rhombus can be like this, another rhombus can be thin type specific arrangement of which this tiles fill the lattice.

A earlier to the start that the periodic arrangement is with respect to translational periodicity, the quasi crystal does not have a translational periodicity. But it has a symmetry 5-fold symmetry is possible, but periodicity is not possible; understand that is basic difference between these two structures. But generally when we talk of periodicity we talked with respect to one dimension, two dimension and three dimension; the one which appears as a two dimension which is periodic as I look at it we talked about reflection right with respect to a plane mirror. Suppose we take a concave mirror and

look at it in that space how will it look like it will (Refer Time: 58:41) distracted it will not (Refer Time: 58:53) does the periodicity.

So, when you go to higher dimensions depending upon which space we are looking at it, when we are looking at a normal Euclidean space this is how the periodicity is define. When we look into other space; similarly the structure which does not show any periodicity that is if we look through a crowd mirror you will see that it looks us periodic, but in reality that never periodicity. So, essentially all these periodicity which will look mathematically when you try to definite it is with respect some frame of reference which we choose it, depending up on that there are going to be changes.

That is why when diffraction pattern in quasi crystals people try to interpret it which I will towards the end I will come to. Then they have their thought that only in the fifth dimension or sixth dimension we can have periodicity that is the way it has been worked out. So, what is periodic or not periodic in, because normally we are able to visualize it only in dimension which is up to three; but mathematically we can define any dimension we can attach to it. And such a way when we try to process it we find that I think it is in six dimensions or five dimensions, it is being grouped at.

We will stop it here.