Defects in Materials
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Lecture - 04
3-D Lattice

Welcome you all to today's class, the last 2 classes, we have covered one dimensional lattice and then how to constrict over from 1-dimensional lattice; 2-dimensional lattice what are the symmetry elements associated with it; what are the types of crystal structures which we can have, are planar groups which we can have. Today we will talk about how to generate 2-dimensional lattice; from a 2-dimensional lattice, how to generate a 3-dimensional lattice, what are types of a point groups and space groups which are associated with these lattices.

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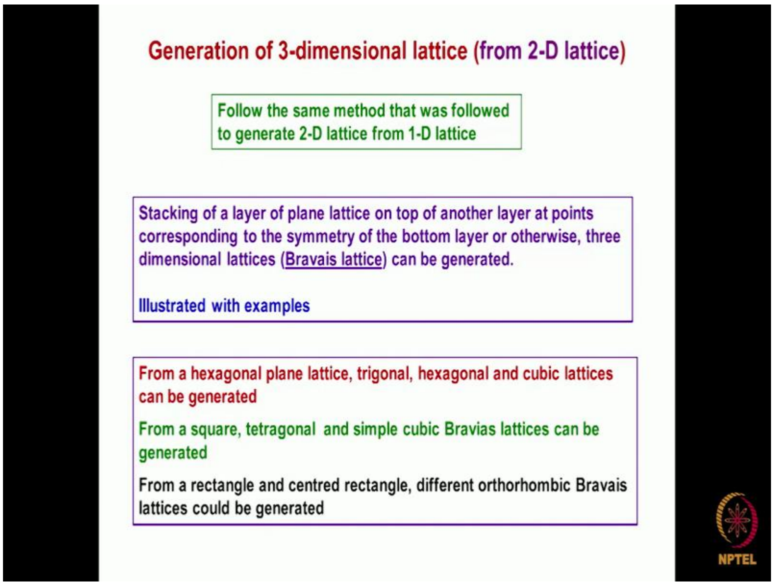

We have to follow the same procedure which we have done for generating the 2-dimensional lattice from 1-dimension that is take a 2-dimensional lattice keep it on top of one another at some particular angle or some specific positions with respect to the lattice which is kept below and try to generate a lattice and see how many types of lattices which can be generated, but there are many positions we can keep it, one lattice on top of each other, but the distinct number of space lattices which will generate are only 14.

We will take a few examples and illustrate how this is being done, one I will take with respect to hexagonal lattice and how different types of lattices could be generated, the other example which I will take is essentially a parallelogram that is oblique lattice and from that what are lattices which could be generated.

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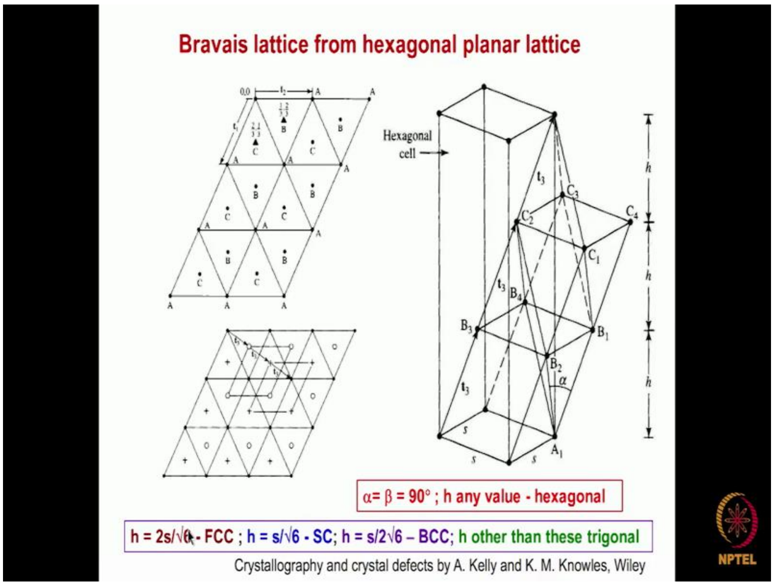

What are types of; how we can generate a Bravais lattice from hexagonal lattice, we will consider what are we done here we essentially this if you look at it, it is a hexagonal lattice, one lattice is what is where the lattice points are marked as a this is the hexagonal lattice in which if you kept an another lattice on top of it, the lattice points which it can come is that this lattice can be called as the B lattice which is kept at this particular position that is on a hexagonal lattice if I consider it, here this is one particular position where the next layer can come or this is an another position where the next layer can come if you keep at this particular position B layer position and the next layer on C layer position and the third layer if you keep it, it will be kept on this one A B layer, C layer then the A layer will come.

So, this is how the layering sequences that are first layer, second layer, third layer, 4th layer. So, if we consider it, this way we can generate a space lattice can be generated while depending upon the distance which we choose it from here if we consider it this distance it is called as s here and then at what height the next layer is being kept depending upon that various types of lattices can be generated. If we keep the B layer at a distance which is h is equal to 2 s by root 6 then this stacking sequence will generate an FCC lattice, if we keep the B layer and all the successive layers at a distance which is h is equal to like s by root 6 then we can generate a simple cubic.

If we keep the distance between the layers such that h the height is equal to s into s by 2 into root 6 then we can generate your body centered lattice if we choose a value of h which is different from any of this value then we can we generate a trigonal lattice. Now you can understand that using the same hexagonal lattice at what positions that is the stacking sequence is A B C - A B C type of a stacking sequence, but the height at which these lattices are this each of planar lattice is being kept with respect to one another we can generate either trigonal simple cubic or body centered or face centered Bravais analysis can be generated if we keep on top of an A layer and another A layer we generate h hexagonal lattice. So, all the all these lattices could be generated from just a 2-dimensional hexagonal itself.

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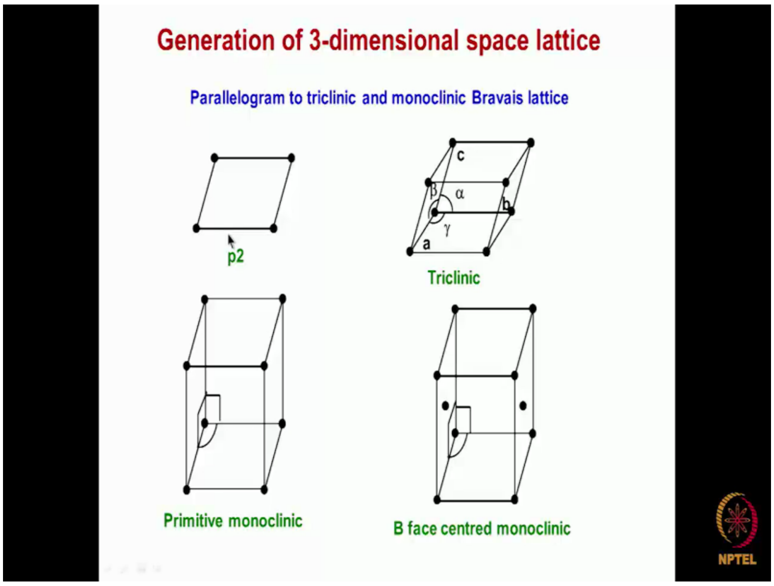

Suppose we take a lattice which is an oblique lattice its nothing but a unit cell is a parallelogram, if we keep this parallelogram one just on top of the another then what we generate and keep the distance such that it is not equal to neither the translation vector A nor the translation vector B then what we generate essentially is nothing but a monoclinic lattice. If we keep the next layer so that this lattice point is at some position the projection of it at some position which corresponds to a random point in the lattice and the lattice parameter in that direction is not equal to neither a and b, we generate a triclinic lattice. And if we keep these lattices in such a way that we kept at some particular one the next lattice, but at a position which is halfway on the x axis just above it then this is you can see that this the next layer which is being kept and then the third layer which is being kept is right on top of a the first layer if you repeat it like this now what we have generated is a face centered monoclinic lattice.

So, by keeping either at symmetry points or at random point we can generate different type of lattices, but finally, if you try to look at how many lattices which we can generate there are going to be only 14 these 14 lattices are represented here.

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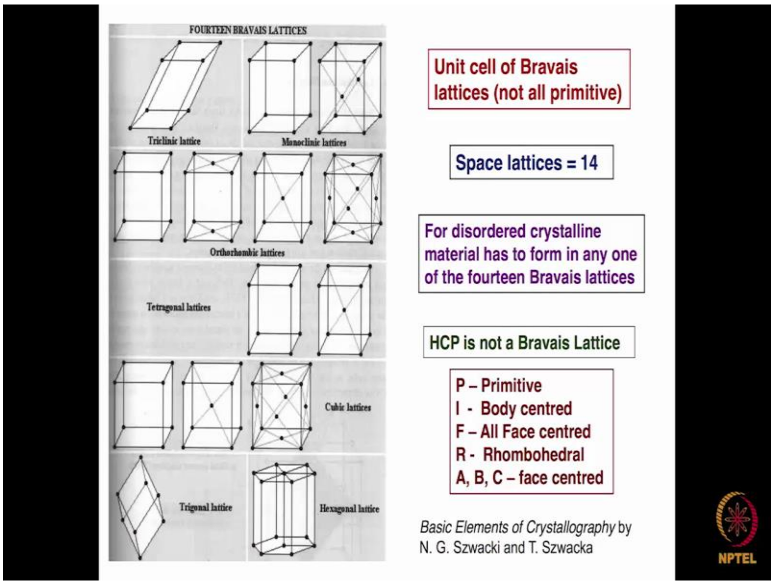

So, generally the way these lattices are represented is with respect to a B and C the lattice parameter and with respect to a angle between them actually that is essentially a consequence of the type of symmetry which is associated with these lattices strict classification is on the basis of symmetry that is if we take triclinic it has no symmetry associated with it if we like monoclinic it has one 2 fold axis rotation axis if you take at orthorhombic perpendicular to each of the axis there is a 2 fold axis if you take triclinic there is only one 4 fold axis which is there if we look at a cubic systems there are 4 3fold axis which are present if you take trigonal there is only one 3fold axis hexagonal is one which has got a 6 section hexagonally has got one 6 fold axis.

So, essentially what we have now is the seven crystal systems which we call it is based on these types of symmetry these are all the minimum symmetries which will be associated with these crystal systems they can have a maximum symmetry that will come to later what is the maximum symmetry which we have and we should always remember that hexagonal close pack system is not a Bravais lattice Bravais lattice is only hexagonal it is a one which contains 2 atoms 2 lattice points per unit cell hexagonal close pack lattice and the symbols which we use here are primitive lattice is represented by P I for body centered F for face centered R Rhombohedral A, B, C for the different face centering, but all are capital letters which are used unlike in the case of 2-dimensional lattice.

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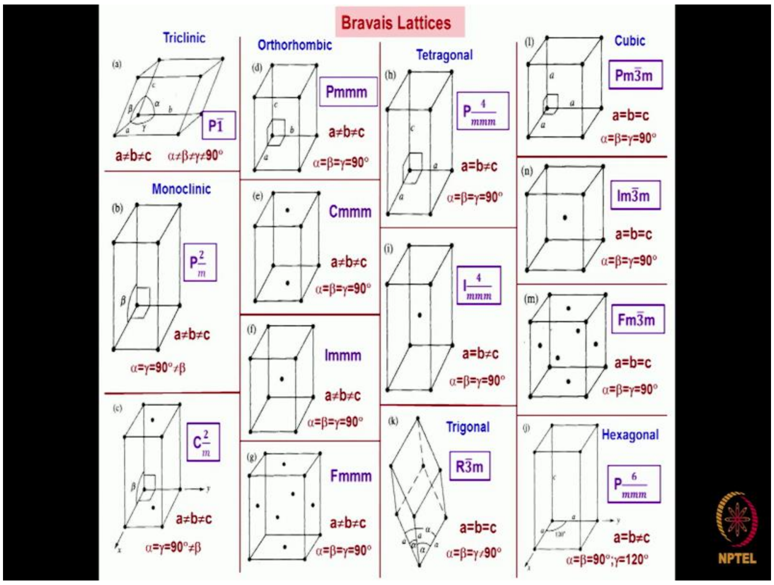

In the next slide, in this particular one all the 14th Bravais lattices are being shown what x i have try to show here is that in addition to the this one bodies the space group symmetry which is associated with this I will come back to it later what these space group symmetries are, but essentially what the P represents is what is the type of a lattice which we have and what are the symmetry elements which are associated with it that is what it represents generally the lattices as I mentioned earlier exhibits the full symmetry of the lattice the maximum symmetry will be exhibited by all the lattices that way here all the maximum symmetry which is associated is exhibited.

One thing which one should always remember is that earlier case when we considered how if you put a motive around different planar lattices we are not able to we are able to join only uniquely some of them that is if we put your motive asymmetric motive around whether it is a square lattice or whether it is a rectangular lattice we generate only an 1 fold symmetry. That gives an indication that irrespective of the value of A and B they the symmetry is the one which besides the; what type of a specific space group which it has.

On that basis that when we write a not equal to B not equal to C it does not mean that it is not equal to a necessarily not equal to B not necessarily not equal to C that is what in crystallography term it means not equal to is does not mean not equal to necessarily not equal to it can be also.

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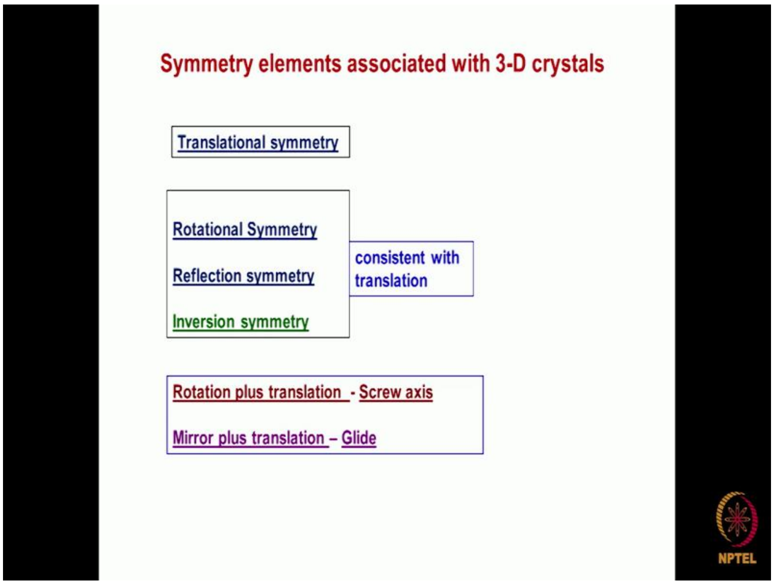

So, now let us look at what are the types of symmetry elements which can be that is before going into the details we will just list these are all the symmetry element and then we will try to see how go into a details about the symmetry elements they are one translational symmetry element will always be there with any lattice, then we have a rotational symmetry element which we have already seen, what are rotational symmetry elements? Reflection symmetry element which we had seen it in addition to it here we will have an inversion symmetry element also will come then in addition to this, this is all with respect to consistent with translation, but we are considering it around a point in addition combination of rotation and translation combination of rotation and reflection combination of rotation and inversion all the 3 are possible they will also we can consider cases. So, these are all the cases which we look at it.

In fact, the combination of rotation plus translation gives raise to screw combination of rotation and translation gives raise to screw axis reflection and translation gives raise to glide reflection and translation will give rise to one is a glide which you get it then the other is a rotation and translation gives a screw axis then rotation and a reflection perpendicular to the rotation axis if we consider that will give rise to an inversion we will complete later.

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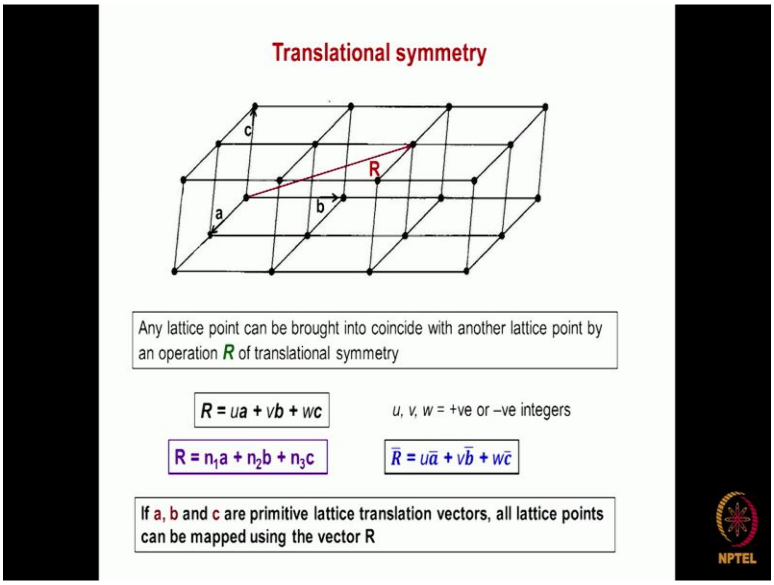

In this particular slide we have just shown the 3-dimensional unit cell which is essentially a like a triclinic structure and any vector in this can be represented by a vector R is equal to u into a plus v into b plus w into c where u v w are the integers and a, b, c represents the translation symmetry this way in the vector notation all the lattice points can be generated by taking various combinations of u, v and w and what I have shown here is that various types of this one because different types of notations are used different ways it is represented in the books about the rotational symmetry I had already explained how this rotational rotation consistent with translation put some restrictions on the type of a rotations which are possible. So, I will not go into the detail.

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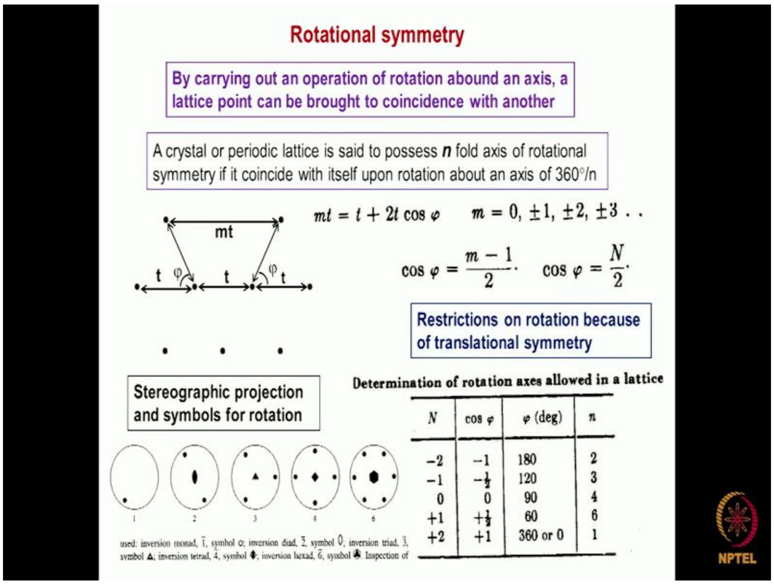

But in this slide what I had shown is there how they are represented on the stereography projection I had just given a brief idea without going to a detail anything about the stereography projection.

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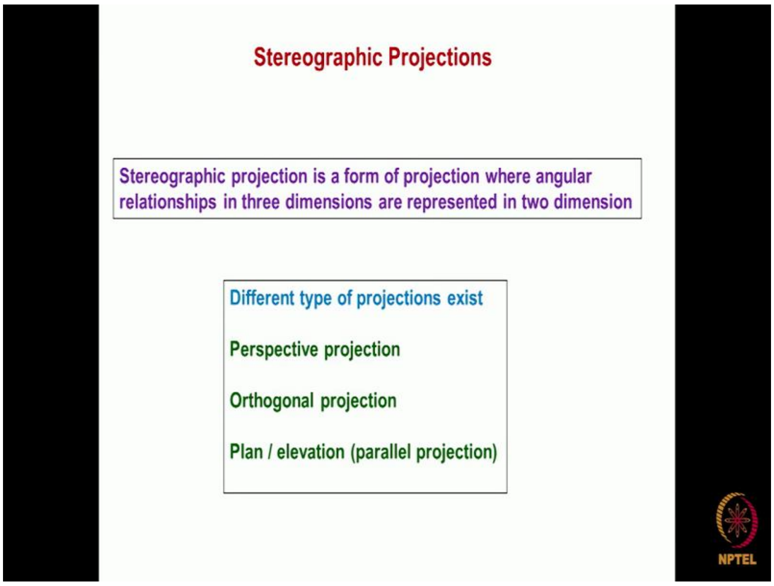

But that I will do it now what a stereography projection is how important it is because when we have to represent in 3-dimensions what we would like to do is that when we talk of symmetry angular relationships have to be specified or the angular relations that be shown on 2-dimensions because 3-dimensions we can view it, but when we have to put a projection it is always in 2-dimensions we deal with how do we go about and do it there are various types of projections are there the simplest is a perspective projection in a perspective projection we can see it, but the distance unless we give more information we do not know how far an object is far away in a stereography projection is a projection where it is from the angular relationship in 3-dimensions could be represented in 2-dimensions here I had just given what are the applications of stereography projection.

One in the crystallography for may showing angular relationship between different planes and directions we can use stereography protection in x ray diffraction when we have to represent texture we require it in electron microscopy different orientation of crystals their planes and directions between different interfaces when we wanted to find out orientation relationship in all these cases, stereography projection is important then when we reforming a single crystal, how the different slip planes are rotating, all these information, we can get it using a stereography projection because there it is at a 3-dimension, what is happening?

But we wanted the same angular relationship to be projected in 2-dimensions. So, that it is easy to do the calculation what is a stereography projection the way in which we can understand it is that you take a sphere in a sphere as we know for a globe when we consider there are latitudes longitudes are there or we can have it similar to that we can have it in a globe we assume that there is nothing else is there fix the coordinate system at the center x y and e z coordinates are fixed and then what we do is that take a point which is on the surface of the sphere with respect to the e z coordinate it makes an angle theta are the e z coordinate we considers the pole and if you look at the if you view this from the other end of the pole from the south pole.

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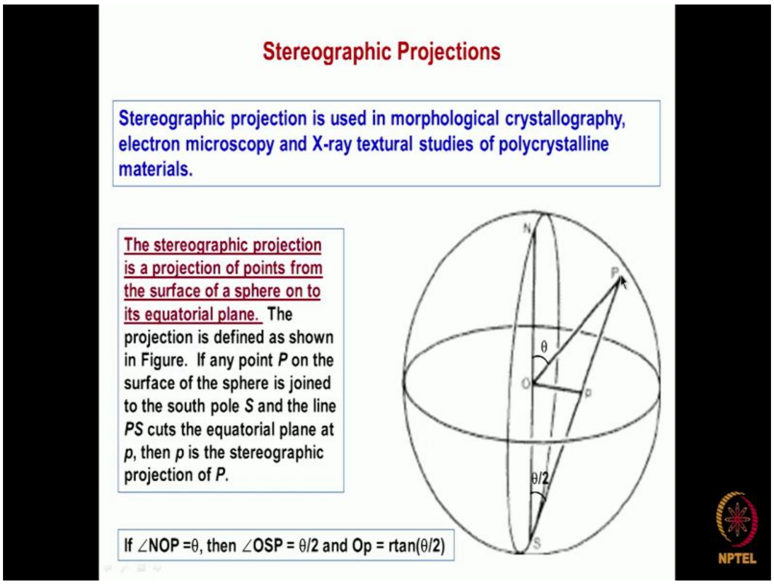

The ray which connects our eye to this pole cuts the equatorial plane at some particular position. So, this distance O P if you look at it on the equatorial plane, it is given by the formula R is the radius of the sphere into tan theta by 2, what the angle which this point P makes with respect to the s (Refer Time: 18:07) axis. So, essentially using this relationship all the points which are there on the sphere can be represented on the equatorial plane. If this point P rotates around this pole making an angle theta it will be a circle and the projection of it will be nothing but this O P will take a rotation you take it a circle. So, it will generate a circle.

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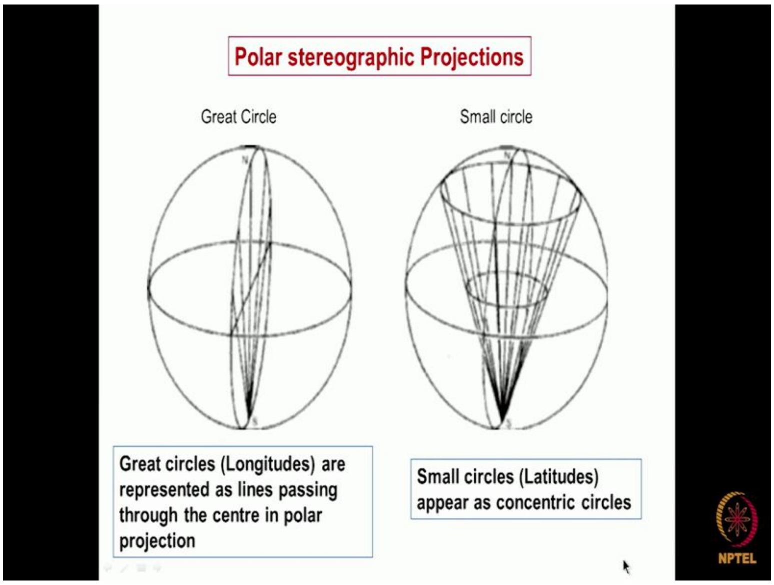

Similarly, you take this particular this one longitude this longitude all the points on this longitude the final projection will be nothing but it will be a line passing through the center this will be clear from this particular slide this slide here. If you look at it these are called as the great circles are nothing but in the geography if we look at it we call it as the longitude this longitude, essentially you can see that all these projections pass through the center and this is a line which passes through this is nothing but a diameter and these circles which are the latitudes their project, it has a concentric circles if you assume that on the surface of the sphere we have marked at every 1 degree 2 degree or 5 degrees.

So, some specific angular separation latitudes and longitudes and then view it from the south pole then how will it look like we will be generating projection this projection is called as the polar projection.

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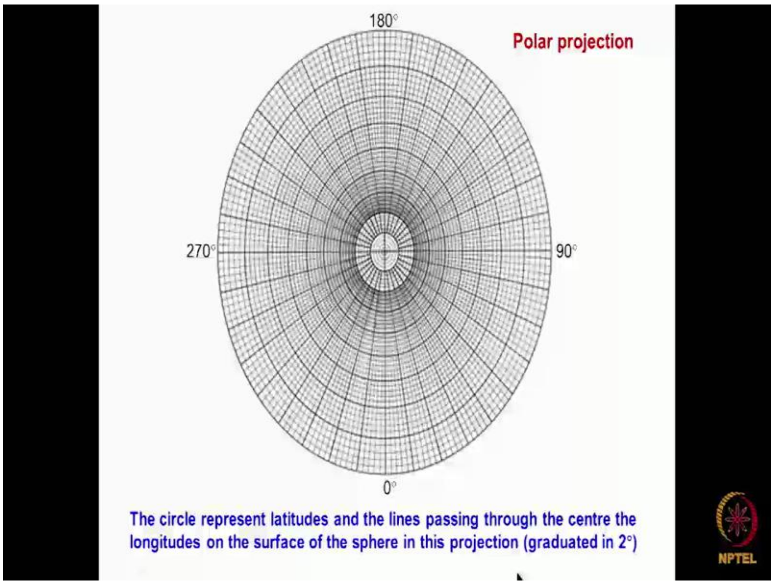

In this projection if I consider this particular one it makes an angle thirty degree these are latitude which it represents. So, if I take any particular position, if I fix the coordinates x y and this will be the normal to the screen is there e z coordinate now we know that if I mark a particular position, I know what is the position of this on the surface of the sphere. So, essentially all the angular relationship in 3-dimensions are projected in this 2-dimensional (Refer Time: 20:19) we essentially for stereography projection this is the polar projection which is used this is, but only thing which is important which we should and which we should note is that if we consider.

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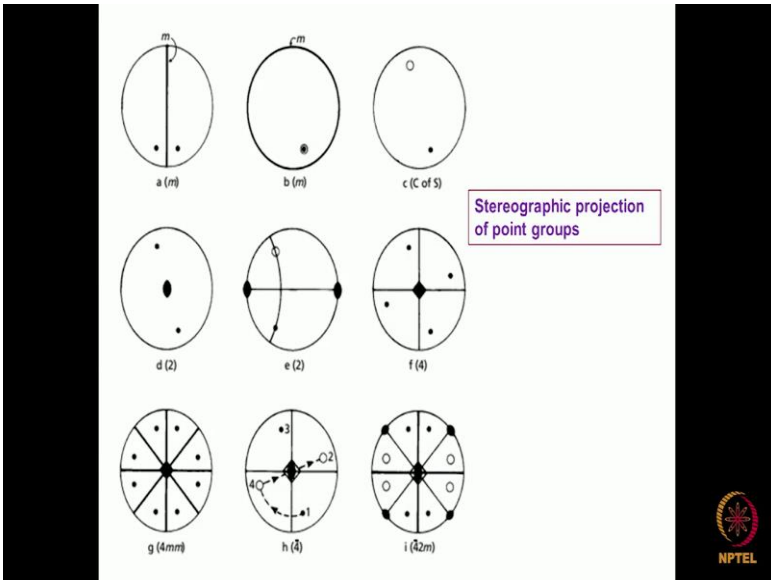

In this particular projection if we consider any point on the sphere if it is on an equatorial equator where will it get projector it will get projector onto the circumference of the equator correct, if it is going to be anywhere on the top hemisphere the projection will be inside the circle equatorial plane. So, that is essentially and when we consider in a space lattice if we consider any planar directions it is going to be in 3-dimensions. So, anything that is in a 2-dimensional lattice when we considers only the equatorial projection which you have to consider that is why the motifs are always placed on the circle here since it is a 3-dimensional case the motifs are all kept right inside the circle.

So, if you take a motif like this here if a mirror operation is there we put a mirror along this x axis then it will be getting reflected and this is how the mirror will be reflected in a 3-dimensional projection in a 2-dimensional projection this point would have been put here and this point would have come here that is all the difference is mirror perpendicular to it if it is there. Now we can see that the circumference of the circle is made thick to show that this is a mirror if it is an inversion operation that is the points on the upper hemisphere invert it through the center it will come into the lower hemisphere.

So, anything which is on the lower hemisphere when we show in the projection the closed circle represents always motifs on the upper hemisphere and the open circle shows motifs on the lower hemisphere. So, in an inversion operation this is how it will take place and if it is a 4 fold rotation. Now we can see that a motif which is being kept here a 4 fold rotation this is how in a stereogram their various types of rotation and reflection and inversion symmetry operation could be are rotation and a mirror which is perpendicular to it all these can be represented all the examples are present here in this slide.

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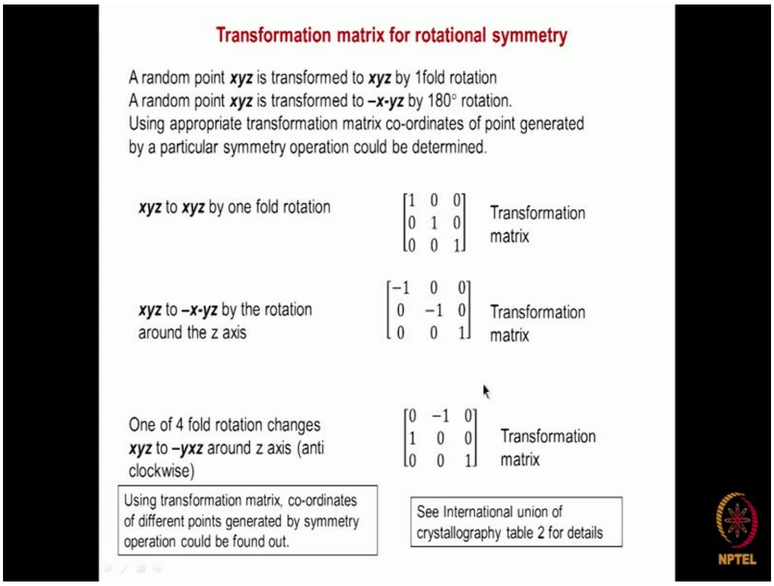

So this is about a symmetric representation, but when we have to find out the coordinates associated with any one of them all the motifs which are generated if we are given a coordinate x y z, we should know what is the transformation matrix which is associated with it each of this symmetry operation and then we can find out because of using the formula which I had given earlier, in the last class one can generate various types of a a points. All the corresponding symmetry related points could be generated whether it is for a rotation or whether it is for a reflection or whether it is for inversion here for different operation, this is for a 1 fold rotation, the matrix.

This is the matrix which will be there if it is one which is a 2 fold rotation then this is the type of a transformation matrix which we will using; if it is a 4 fold rotation that this is the sort of a transformation matrix which you have to (Refer Time: 24:22), but on also we have to define that whether it is a clockwise rotation and anti crosswise rotation that is also very important with these what we have looked at it is what are the various types of rotations which are possible and how they are represented.

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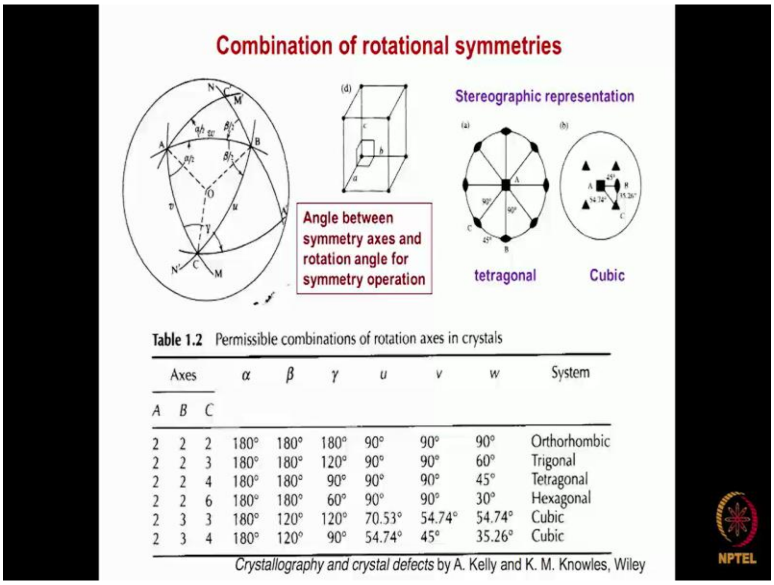

Now, can we have a combination of this just the rotation itself axis suppose I take a 2-dimensional 3-dimensional lattice like for example, I have taken a orthorhombic structure in this along each of this axis along this axis or along this axis or along this axis all these axis we can have a 2 fold rotation. So, what is being done is that if I represent a 2 fold axis on the surface of a sphere because this is the origin o.

So, around this direction or around this direction around this direction along 2 directions I find out some sort of a rotational symmetry what is the third direction in identify an another third direction where what is the type of symmetry which exists these are all the combination of symmetry elements which are possible. So, if I take that is 2 and 2 and then you find the some other direction I find the 2 fold rotation then what is going to happen is that between the 2 axis which have 2 fold rotation all the axis each of them taken separately 2 at a time we find that angle between them is ninety degree and then that structure is orthorhombic.

Suppose the 2 operations it is there in another direction you find that a 3fold then the crystal system becomes their trigonal one then the angle between the 2 axis 2 fold will be ninety degree and the other one is turning out to be 60 degree this way various combinations are possible on that basis we can have different types of crystal structures also this is one way in which various types of crystal systems could be classified. So essentially, what means that these are all the unique combinations, which are possible by combination of just rotation alone?

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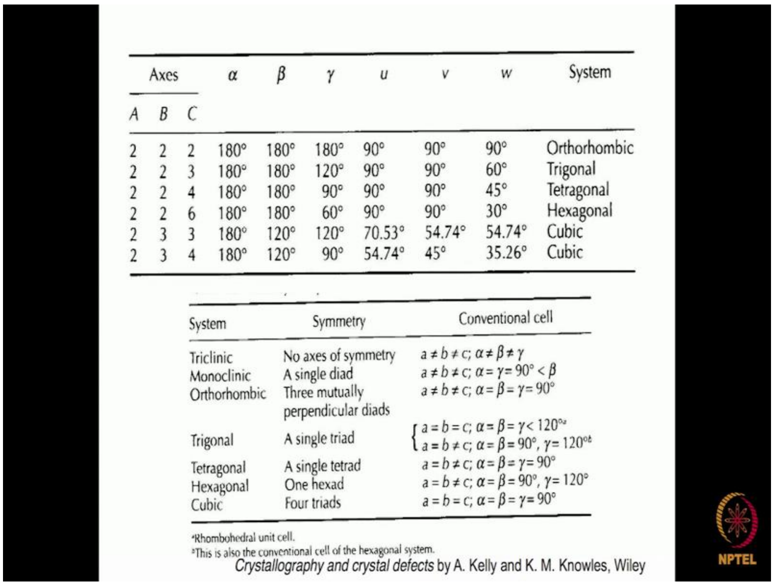

Axes			α	β	γ	u	v	w	System
A	B	C							
2	2	2	180°	180°	180°	90°	90°	90°	Orthorhombic
2	2	3	180°	180°	120°	90°	90°	60°	Trigonal
2	2	4	180°	180°	90°	90°	90°	45°	Tetragonal
2	2	6	180°	180°	60°	90°	90°	30°	Hexagonal
2	3	3	180°	120°	120°	70.53°	54.74°	54.74°	Cubic
2	3	4	180°	120°	90°	54.74°	45°	35.26°	Cubic

System	Symmetry	Conventional cell
Triclinic	No axes of symmetry	$a \neq b \neq c$; $\alpha \neq \beta \neq \gamma$
Monoclinic	A single diad	$a \neq b \neq c$; $\alpha = \gamma = 90° < \beta$
Orthorhombic	Three mutually perpendicular diads	$a \neq b \neq c$; $\alpha = \beta = \gamma = 90°$
Trigonal	A single triad	$a = b = c$; $\alpha = \beta = \gamma < 120°$ [a] $a = b \neq c$; $\alpha = \beta = 90°$, $\gamma = 120°$ [b]
Tetragonal	A single tetrad	$a = b \neq c$; $\alpha = \beta = \gamma = 90°$
Hexagonal	One hexad	$a = b \neq c$; $\alpha = \beta = 90°$, $\gamma = 120°$
Cubic	Four triads	$a = b = c$; $\alpha = \beta = \gamma = 90°$

[a] Rhombohedral unit cell.
[b] This is also the conventional cell of the hexagonal system.

Crystallography and crystal defects by A. Kelly and K. M. Knowles, Wiley

Now, in this particular slide, what I had shown here is essentially that the different crystal systems based on how they are defined based on symmetry and what is the minimum symmetry which is necessary for this Bravais lattices and also the for a conventional cell if we consider what are the relationship between the angle between the axis and the translational vectors this all of you have studied also earlier itself you are very well aware of it.

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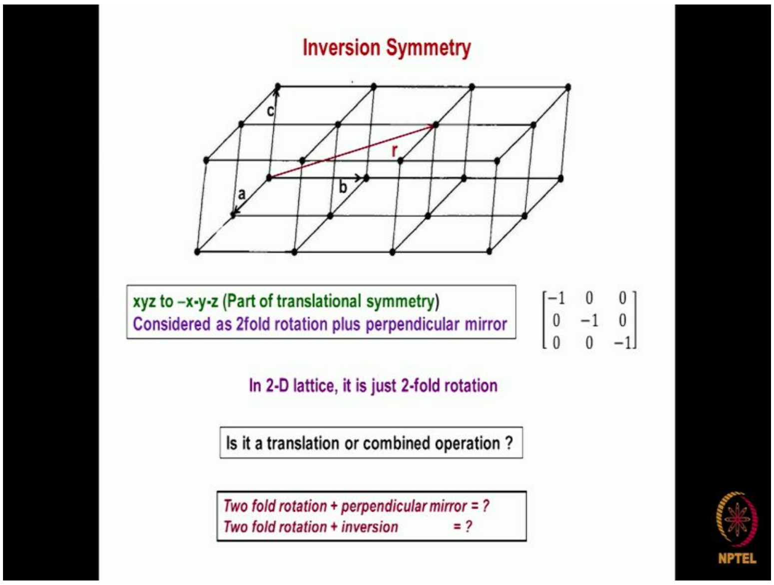

Now, about reflection I had already explained. So, I will not go into the details, now let us look at the inversion symmetry so far, I am not talked about the inversion symmetry there is if we take with respect to the unit cell where or the crystal lattice if you take any point r by an inversion the r will become minus r. So, the all the coordinates will become the x y z will become minus x minus y minus z. So, for this the operation the transformation matrix which will be is this particular type of a transformation matrix which has to be used.

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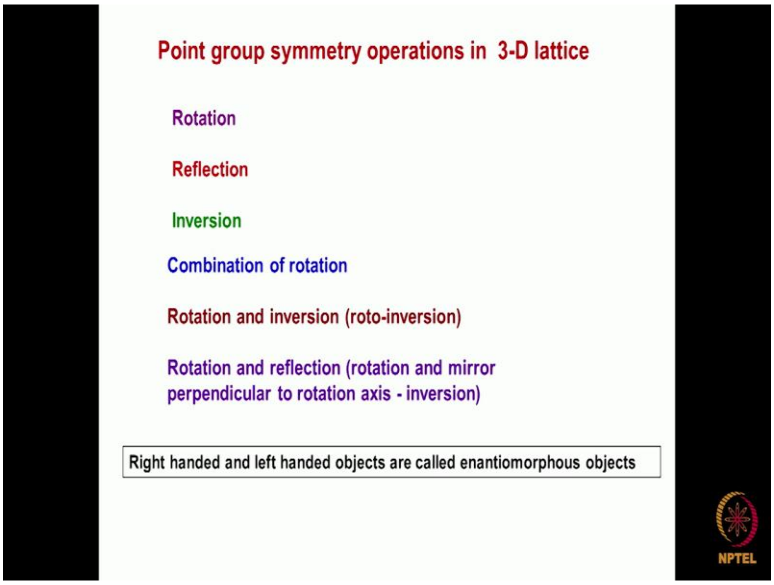

So, essentially if you now look at it, what are the types of point group symmetry operations which are there in 3 D lattices rotation which you have considered reflection which we have considered inversion is one then we can have a combination of rotation its possible then rotation and an inversion, we can take that combination rotation and reflection also we have considered right that is either that rotation axis is there the mirror is a reflection is parallel to it or perpendicular to it that combination can be chosen then we can have a rotation and a reflection that is rotation and a mirror perpendicular to rotation axis that gives rise to inversion that is why sometimes inversion is called as is it a new operation or is it a combination of 2 operations of a rotation and reflection then in these things what we have to look at it is that if we take only a rotation what is going to happen is that.

Suppose I take this object by a rotation it will come like this it will go like this always it creates one particular type of an object that is if I take a right hand I rotates it like this all the directions its only the right hand gets rotated, but during this rotation operation right hand motif can never become like a left hand reflection and inversion of the operations where that enantiomorphic structures where the by this operation the right hand is generated into a left hand operation this has some significance.

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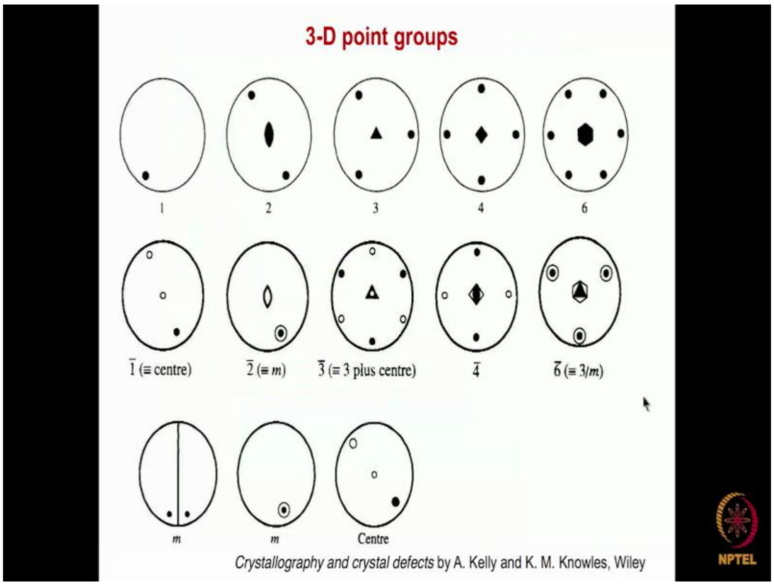

In the behavior of the material which I will not go into the detail because that is not particularly for the defection material one does not have to bother about it.

So, as I have mentioned using stereography projection, we can represent it, here all the basic symmetry elements especially the point group symmetry elements or. So, the combination of a rotation reflection and inversion and Roto inversion these together constitute the point group symmetry. So, this can be represented in a stereography projection in this it is for 1 fold and then 2 fold that symbol which is used to indicate that it is a 2 fold rotation and the 3 fold rotation we can see that a motive which is being placed here that a 3 fold rotation it generates like that various symbols are being used.

I will not go into details of any of these symbols because a internet in our crystallography table if you look at it all the symbols are explained very nicely and in many of the books which I had mentioned earlier also in those books also all these symbols are explained essentially what we can make out is that these are all the just pure rotation and this corresponds to Roto inversion this layer and this layer if you look at it, it is mirror which is parallel and the another is perpendicular then this is just a simple inversion.

So, these are all the basic operations and various combinations which we can choose of all of them then you can imagine how many combinations which we can have generate many, but how many distinct ones finally, we find it like in the case of 2-dimensional lattice we did the exercise then we find that only ten are going to be there point groups correct plane or point group similarly here it is going to be only 32 distinct point groups are possible.

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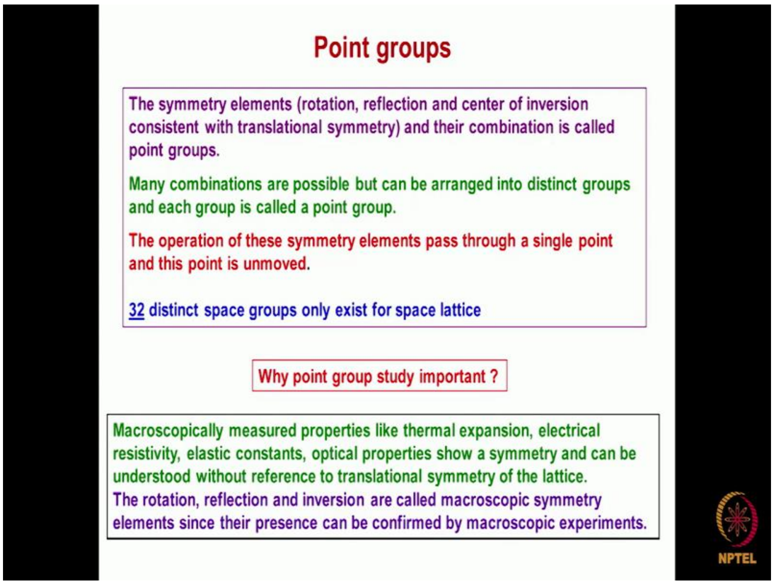

So, essentially what is point group is essentially the various a symmetry operations like rotation reflection and center of inversion consistent with translational symmetry and Roto in the and their combination Roto in the combination is called as a point group symmetry many as I mentioned many possibilities exist, but distinct ones are only thirty 2 why do we require a study of this point group symmetry or why it is very important this is because when we look at the properties of the material change in different directions are on different surfaces.

If you look at it, if a crystal grows you find that it grows with some particular morphology earlier all the point group symmetries where found out by looking at the morphology of the crystals similarly electrical conductivity thermal expansion all these are and different directions can change depending upon the crystal structure they are related to a point group symmetry how experimentally we can find out is by measuring these properties in different directions we can determine what are symmetry elements are associated with it are essentially the point group symmetries can be done, but the space group symmetry if we look at it which involves others like a screw axis which I will come shortly it is going to be externally. It is very difficult to see because it is only associated with that only a translation which is very. So, the translation it will not shows a change in property in a particular direction.

So, what is important is that study of point group symmetry is important because that gives information about the properties in various directions in crystal structures in short what we can have is that 32 point groups symmetries just the combination of all the symmetry elements which consider they are eleven are there Roto inversion gives another 5, then combination of proper and improper rotation axis, if you consider altogether, another 16 so in short 32; our generator.

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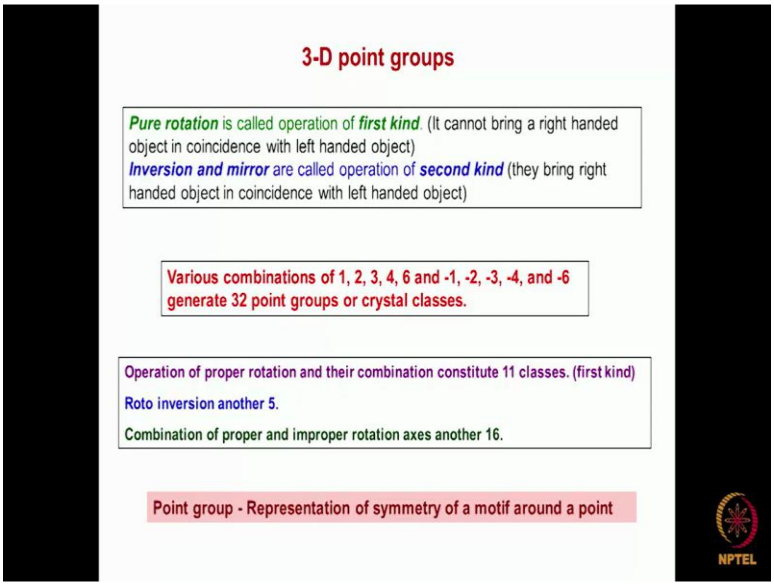

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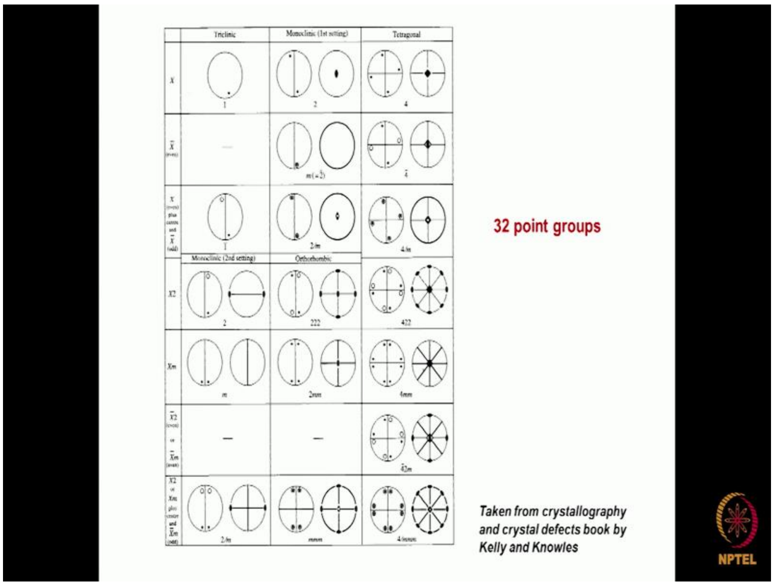

In this slide, I am just showing how they are in a stereography projection, they are represented, I will give some assignments, one can work it out how to generate given the point group symmetry which is given how these a stereography projection they are generated the how they look like then one will understand, how this has been generated actually and presented in various books.

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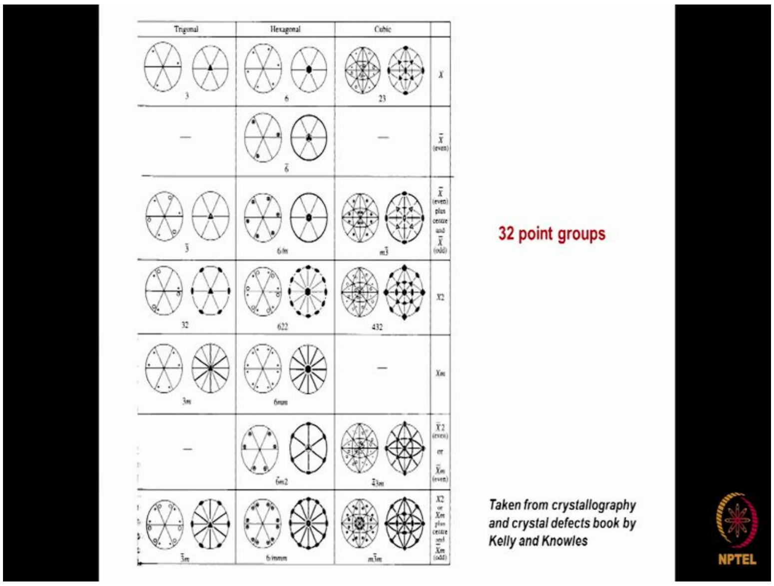

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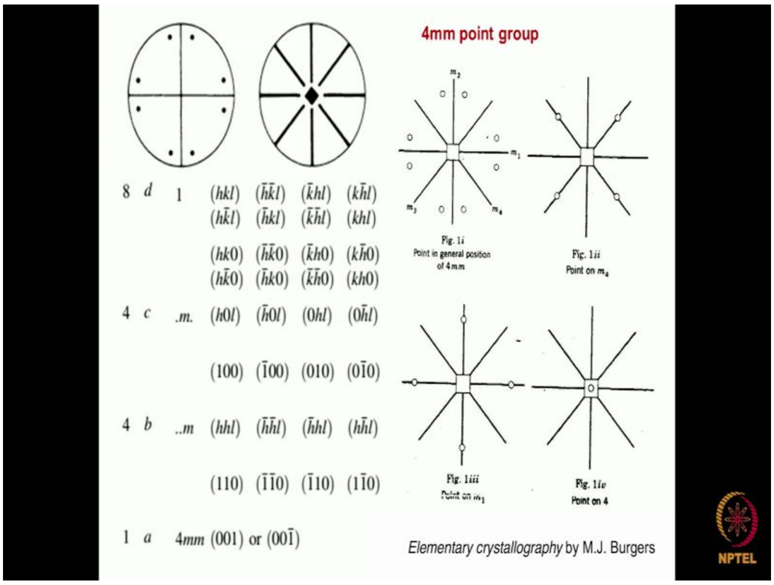

Now, we will be going to the international in our crystallography table if you look at it one a stereography projection which is being given this is the case which is considered is

4 mm point group. In this particular one in addition to giving this position of the motif the general motif what are other positions if the motif we keep it also the same symmetry element will be a can be represented like for example, if I put one at that center that has got a 4 fold symmetry.

So, I do not require 4 motif to present them only one at the center is good enough that is how what is being essentially explained here like the way I explained earlier for 2-dimensional lattice here also what is the side symmetry associated with it then the Wyckoff position and the multiplicity corresponding to the particular side symmetry and here it is not represented in x y z, it is given in terms of a planes because most of the symmetry elements earlier pin when the plane groups point group symmetry if try to look at it some directions we are looking at it the planes which are perpendicular to them that is what its being represented.

So, the symbol which is used to represent is planes then in this side what I had shown it is that for the general one position exactly if we put one motif around it how the other motifs will be generated for this particular point group symmetry one 4 fold rotation which is taken here that is this point is rotated from here it comes here then from here now from here to here to here to here it comes and then what we do it is that put the symmetry elements mirror symmetry you consider it, then you find that that gets reflected. Suppose on the symmetry axis on this if I place it only 4 points have to be placed here, still that 4 fold symmetry and mirror all the symmetry elements, if I place it around this axis the symmetry element mirror symmetry elements which are there then I have to place at only 4 positions if I place it at the center only at one position.

So, this is essentially what is being given one this is corresponding to general this is corresponding to one mirror this is corresponding to another mirror how the various planes will come this is corresponding to the third one 4th one.

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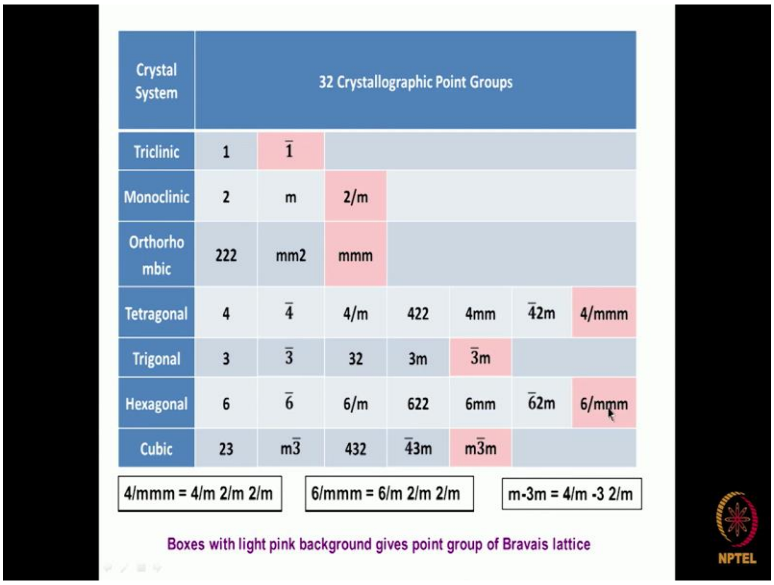

Crystal System	32 Crystallographic Point Groups					
Triclinic	1	$\bar{1}$				
Monoclinic	2	m	2/m			
Orthorhombic	222	mm2	mmm			
Tetragonal	4	$\bar{4}$	4/m	422	4mm	$\bar{4}$2m	4/mmm
Trigonal	3	$\bar{3}$	32	3m	$\bar{3}$m		
Hexagonal	6	$\bar{6}$	6/m	622	6mm	$\bar{6}$2m	6/mmm
Cubic	23	m$\bar{3}$	432	$\bar{4}$3m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

These various 32 crystallography point groups, they correspond to seven crystal systems which are there we can route them. So, triclinic has got one and one bar monoclinic if you look at it is 2 m and 2 by m. These are all the point groups which are associated with it, in this if you look at here, what is essentially is being given here is the minimum symmetry elements in this side, what is marked with the pink color shows the lattice which will have the maximum symmetry elements, that is how I have just identify marked it.

So, trigonal will have 3, but if you take us the trigonal as a lattice it can have 3 bar m that is if we have a crystal at least you should have a one 3 fold axis is it clear and then another is that here some symbols are being when we use m 3 bar m this is essentially is a short form it actually corresponds to 4 by m 3 bar and 2 by m then the next question comes is that what is the convention which is being used to represent these symbols is there, any convention which is being followed otherwise we do not in one case we triclinic use only one monoclinic we use 2 here 3 symbols are being used in which directions are where which the direction along which the symmetry operations are performed.

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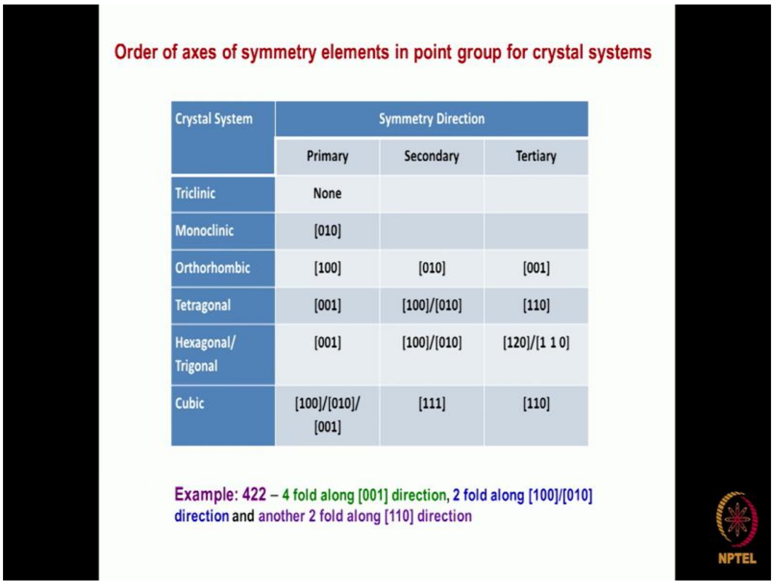

And that is given in this slide, triclinic if you look at it, we do not have any symmetry operation there is nothing like a primary or a secondary if you take monoclinic always that 010; the B axis is chosen, further show the 2 fold symmetry which is present there, orthorhombic if is see A, B, C, all have got a 2 fold.

So, essentially what it represents is these are all the symmetry along various axis when we say 2 mm; that means, that 2 fold along the a axis that is primary is a then secondary is mirror along this direction then another is along this direction mirror. So, that will be. So, 222 and here if we look at it tetragonal 001 is shown along the primary 1. So, the first letter represents a 4th then the next one represents a secondary that is what is the symmetry along 100 or 010 and the third one the third letter represents symmetry along 110, direction like cubic if you see it again that on the primary one represents the symmetry which is along the x y are z axis and the second letter represents the symmetry along 111 direction. And the third letter represent a represents the symmetry which is along the 110 direction if you take 432; that means, that 4 fold along any one of the A, B or C axis and 3 is along the 111 direction and the 2 fold along 110 direction.

So, from this one very clearly understand how what is the sort of coordinate system which is being used to represent the various symbols which are given here for the 32 point groups.

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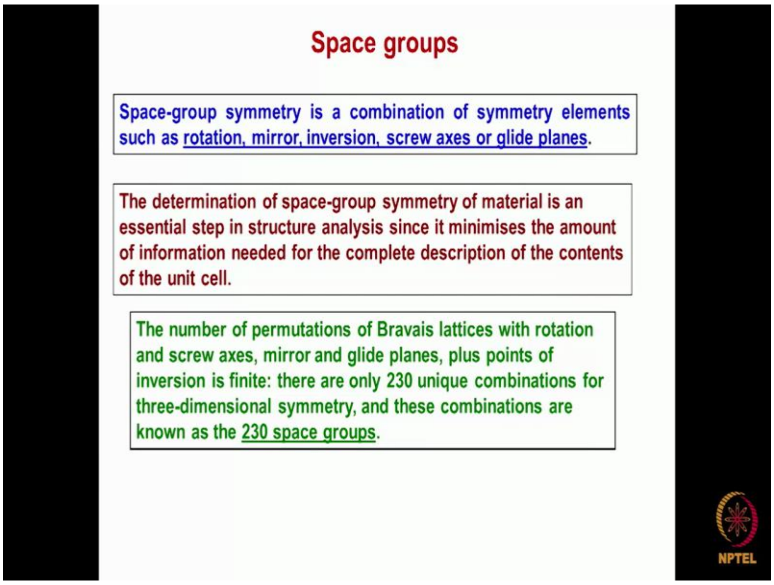

Having looked at this 32 point groups and their representation, how it is done in stereogram if you try to generate a space group what we have to do it is that point group is around a point which we are considering it space group with that around the lattice if you are trying to put motifs having this sort of a point groups around each of them what are the distinct types of a crystals which could be generated with having specific symmetries associated with them is there here again the combinations if we try many are possible distinctly finally, we find that only 32 space groups are possible.

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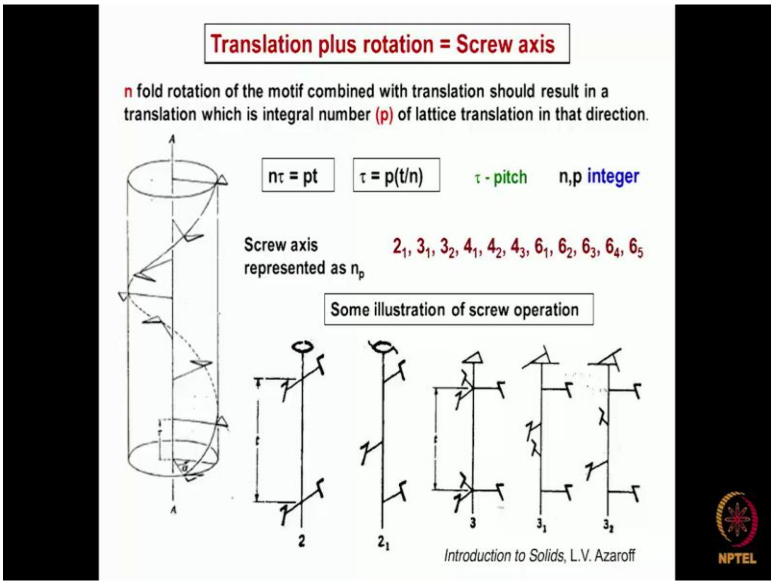

We will not be going into all of them, but before going into them. So, far we consider only point group if we consider as a lattice or what we have not done is that we have considered between rotation and reflection which is consistent with translation, but we are not combined in translation we can combine rotation and translation. And we can combine mirror and translation if you do it in the lattice they generate some special symmetry elements. For example, if we combined rotation and translation it generates a lattice which we call it the symmetry which it generates is called as the screw axis correct.

For example, here if we look at it example if you take this is a 6 fold, you know that 6 fold means that 60 degree rotation has to be given and then a translation by some vector or some pitch you that is you rotate it and then translate it along the screw axis by some vector of magnitude you take tau or a pitch which is tau. Then after n rotations we should be able to come back to original position what is the position which well be coming it could be either equal to the lattice translation vector if it is t or it could be some multiple of t that is what essentially return n rho equals P into t this is equivalent to; like a example which we can think of in real life is spiral staircase when we go on a spiral staircase that is a pitch with which its being the staircase it rotates and finally, afterwards it will be coming back to original position again it rotates correct.

So, depending upon the how many times it gives we have different types of combinations which are possible one here the pitch which is taken is if we take one sixth of the lattice translation vector for a 6 fold, but after every rotation by 60 degree we move it by one by 6 of t. Then we find that after 6 rotations and a in combination with that translation. We will be able to come back to identical position original lattice point we are able to reach it, but it has been shifted by a lattice translation vector that is how it can be done.

So, this also if you take a 2 fold rotation its possible in a lattice because this is not possible in a point group, but it is in a space group when we consider positions of atom these sort of translations this sort of symmetry is also possible if it consider for 2 fold there is only one is possible 2 1; that means, that 180 degree rotation and translation by t by 2 3 fold, if we consider it there is 120 degree rotation and a translation then another 120 degree rotation. So, 3, it can be 3 1 or 3 2 there are many combinations which are possible because I do not want to go into a detail of this one because if it has to be done it should be done in a separate crystallography class where all these things could be explained at length, but essentially these are all the symbols which are being used.

So, in this slide we can see that if it is just a mirror which is their 2 fold we can see that it is a 7 which is getting just reflected this is how at different lattice points the motifs will be kept. Now if we look at a 2 1 rotation, this 1 is rotated by 180 degree, it comes here another rotation and a translation it is brought to that point similarly for 3 fold 3 1 as well as 3 2 how a motif will be rotated and translated around the screw axis it is depicted in this figure from this we can I understand that the 3 1 and 3 2 1. It will be a clockwise rotation and a translation another is an anticlockwise rotation and a translation both of them this is the difference between these 2 though the pitch remains that same the angle of rotation is also the same, but the sense in which it is being rotated is different.

Glide if we consider it this has mirror plus translation which is their glide is nothing but a mirror plus translation I had already explained glide, but what is essentially important is that if the glide is along the a axis the symbol which is being used to represent in the crystallography table is a and the translation which is associated with the glide is a by 2 B (Refer Time: 48:44) it will be B by 2.

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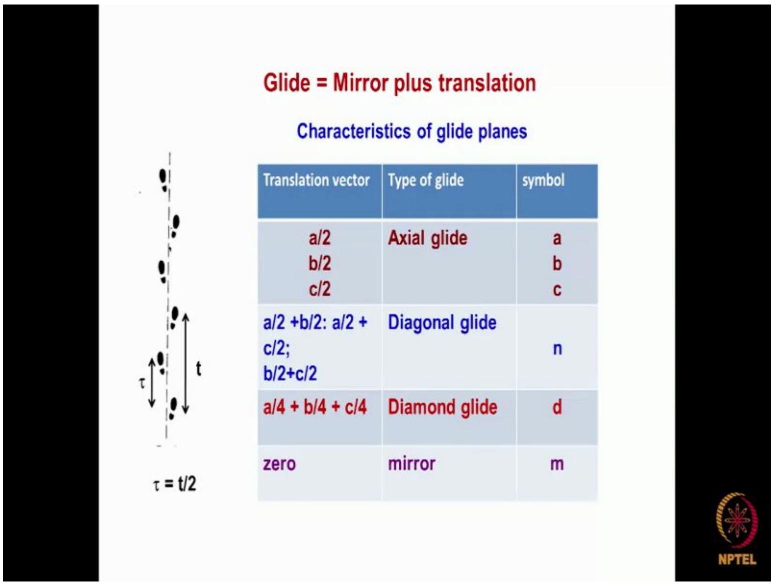

Translation vector	Type of glide	symbol
a/2 b/2 c/2	Axial glide	a b c
a/2 +b/2: a/2 + c/2; b/2+c/2	Diagonal glide	n
a/4 + b/4 + c/4	Diamond glide	d
zero	mirror	m

Similarly, we can have a glide along the face diagonal are on the body diagonal which is called as a diamond glide, if there are no translation which is involved then it becomes (Refer Time: 48:57) a mirror operation, all these various types of operations and symbols what is the translation vector associated with different types of glides is given in this transparency.

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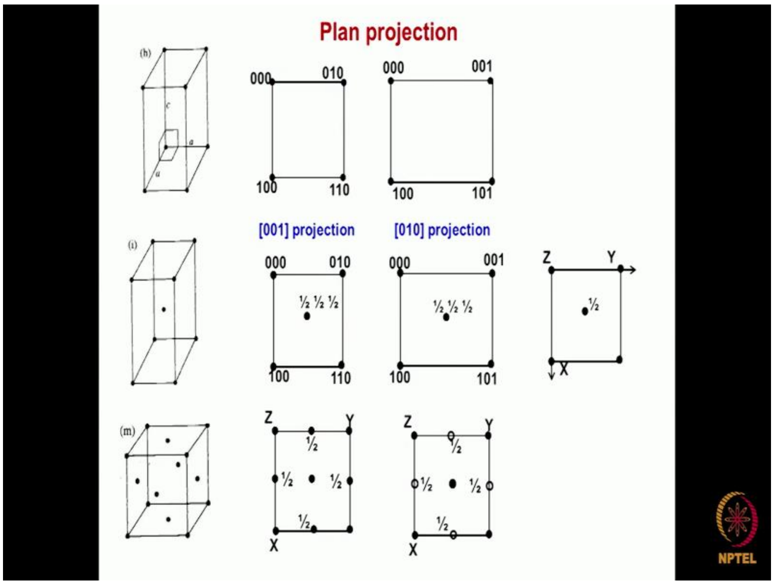

So, far what we have considered is different types of symmetry operations which are that is glide and screw which are symmetry operations which involve either rotation and translation or reflection and translation now like we have represented in planar lattice how do we represent all these symmetry elements. So, first what we have to do it is that some projection will be required suppose we take the example of an orthogonal the example of a orthorhombic lattice how are we going to present orthorhombic lattice if you look at projection of one particular plane that completely does not represent the orthorhombic lattice right at least 2 projections are minimum required to complete it if it is a cube one projection is good enough.

So, mono depending upon the type of crystal structure different projections are required graphical projections are required to show that this is what essentially is the planar lattice corresponding to that in a particular direction correct are the units corresponding planar unit cell that is essentially what is being when we represent it how are we going to show at, what position they are going to be there, and so that is what essentially is being shown here. Like if we take in this particular one where it is nothing but a tetragonal lattice. In this particular tetragonal lattice the projection if we see in this plane which we show the atom at the next plane will be projected to the middle and the next plane is essentially identical to this one.

So, this can be represented as having coordinates half, half, half are in this projection it can be just shown at all these x y positions are there only that z position is half this way also it can be shown. This is what is being generally used these sort of projection in the case of space group symmetry when we represent it. Now just let us have a look at the different type of how it is a space group is presented in the international union of crystallography table.

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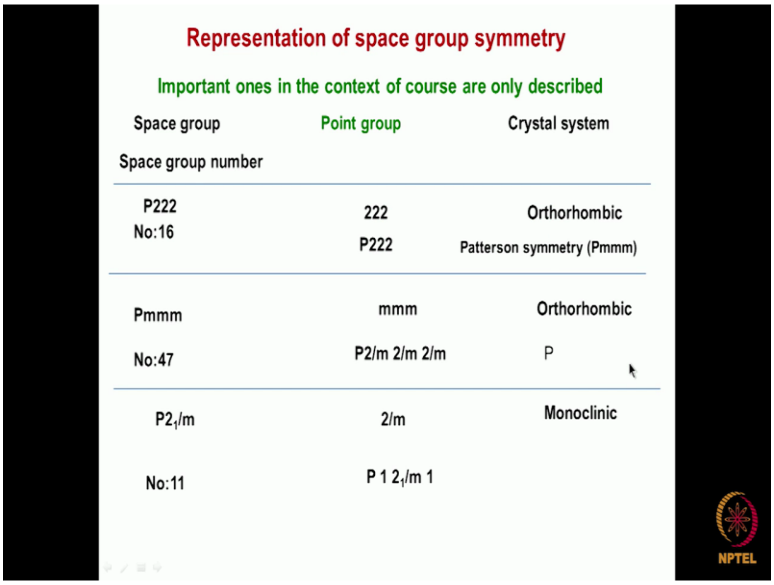

One, if you look at the table at the right hand side, they will show what is the crystal system then what is the point group symmetry which is associated with it then the show symbol also will be shown which I have not just shown here, because that is the symbol which we see the; this particular type of a space group symbol is essentially is the one which is now conventionally adapted in crystallography, but still people who use crystal chemistry they use the (Refer Time: 52:24) symbol because that is one easier to work with when we consider it as different group symmetry operations.

Then that one number is given this gives the; what is the space group number and then what is called as a Patterson symmetry which thought something about that diffraction it is something related to a diffraction symmetry these are all the information which is being given.

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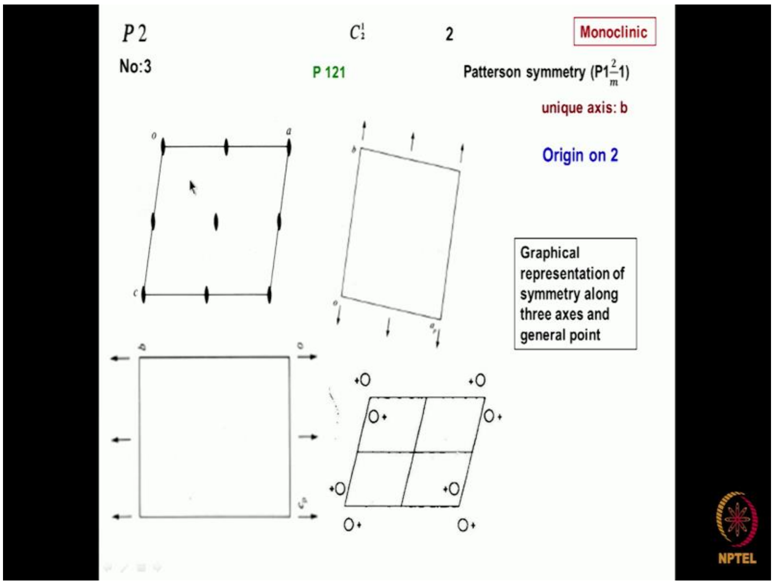

Then next what is the information which is being given is essentially the unit cell and this is the unit cell 1 projection and in this projection the what are the symmetry elements this is for a P 2 means that only 1 2 fold rotation is there and the detail symbol if you look at it P 2 is 121. That means that along x axis 1 fold rotation, 2 fold is along the y axis and 1 fold along the z axis.

Now, this is the and then it is being marked 0 to a this is that the x direction and this 0 to C B direction is perpendicular to it in this specific case and then not only this is being shown in the other 2 directions also how the units cell looks like and the symbols which are associated within, because this symbol which is being used is represents that there is a screw axis and generally afterwards you show a unit cell how the atoms are place in this particular case. Since it is only one fold axis is there the origin could be chosen anywhere if different symmetry elements intersect origin gets automatically fixed like if only 2 fold rotation is there where do you fix the origin; arbitrarily we have to fix it. So, essentially the origin is fixed and done that the projection of that the; a unit cell is being shown.

Now, when you place a motif, the motif is placed where is it being placed? At some position above it; that is why it is being shown O plus, plus indicates that it is at some particular value it is (Refer Time: 55:02) above this plane of the unit cell and from here by around this axis is a 2 fold rotation. So, what is going to happen is that it gets 2 fold rotation and these said it comes again o plus this is how the general position is being shown this is how the graphical representation which is given for a monoclinic lattice.

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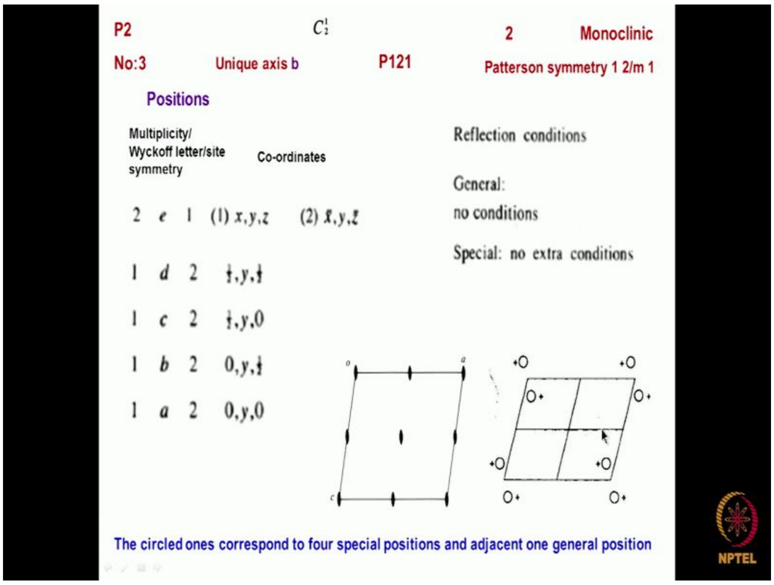

Then as we can see here there are many symmetry elements which are associated with it what are the symmetry elements which are this point has a one unique symmetry this is another one this is another one this is another one because from this point to this point it is a lattice point. So, that is the identical, but these are all the new symmetry elements which are generated in the unit cell. So, we can put atom or the motive is at this position and this position or at this position. So, essentially that is what is being shown one this corresponds to 0 y 0 is its being placed on this axis and another is 0 y half, half position, this is corresponding to here and this one corresponds to no, this is.

Student: (Refer Time: 56:22).

These position and this corresponds to 1 at the; and this corresponds to coordinates where the motifs are being placed with respect to a general point. So, this is the table which is very important for constructing the crystal structures along with it we should know what the lattice parameters are if this information is available we can construct the complete crystal structure.

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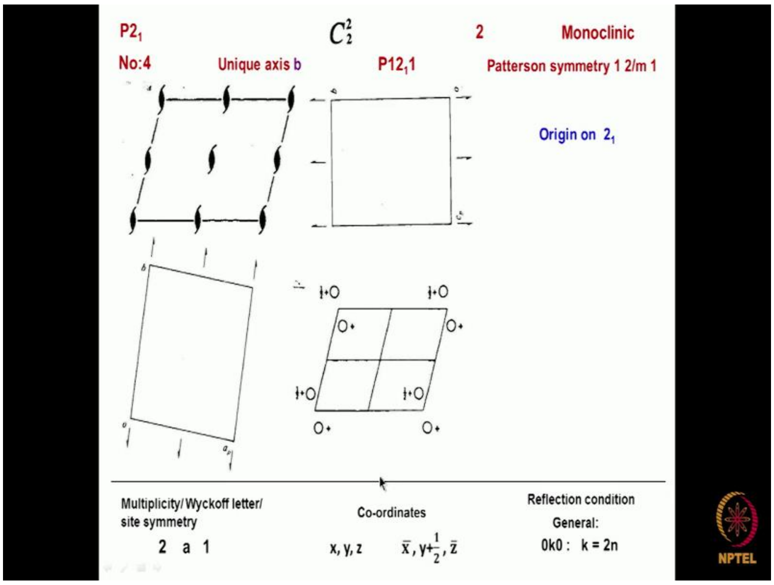

If we consider in this one that is a screw axis also is possible that 2 instead of a mirror rotation associated with there can be a translation. So, it could be a screw axis then the symbol which is being used is this particular symbol again if you look at the symmetry elements which are associated with it. It is an identical type of a symmetry element which you see it. And in this particular case the symbol which is been general point that is at where there is no symmetry is associated with it if you put a motive at a height, some height y then after 180 degree rotation it will come at a position that, but it is shifted up by plus half that is exactly what is being shown and then the coordinates. If you see it here we can generate represent the coordinates this correct.

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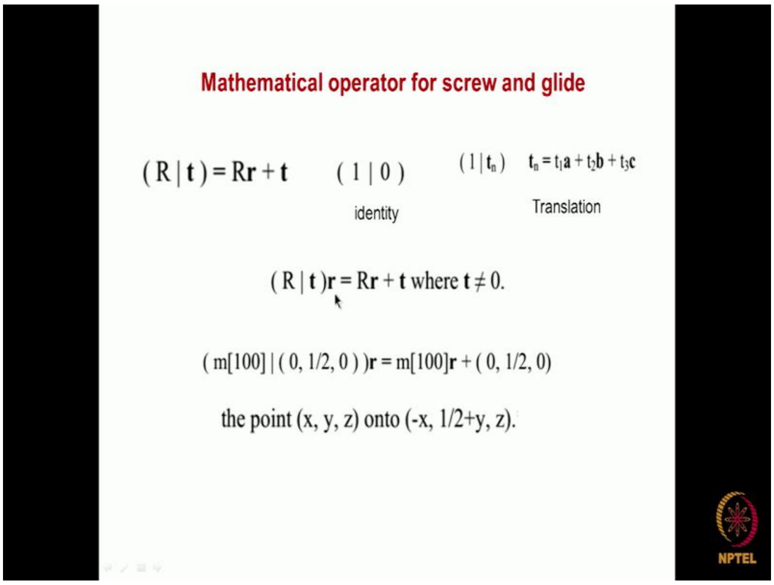

These coordinates also there is another representation in which it is being done in crystallography table I will not go into the detail of it.

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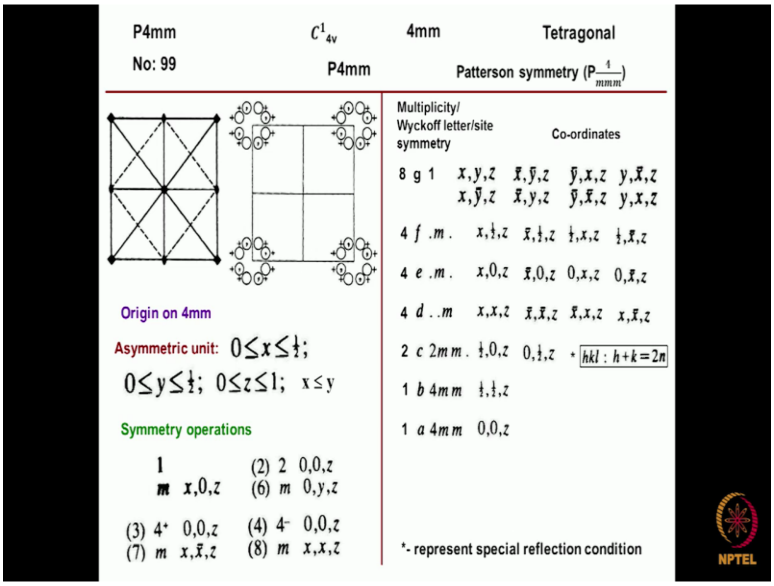

Now, let us look at a P4mm, here it is a 4 fold symmetry, 2 mirrors are also associated with it, the way in which it is represented is that these are all the positions of a 4 fold symmetry lattice points then here we have 2 fold then mirrors which are there the motifs, these are all points if we keep your motive at this particular point it is lying on a mirror. So, it is called a special position if you put it here it has a symmetry which is 2mm. So, this is a special point. And if I put a motif here it is lying at a general point. So, each of the position what will be the coordinates that is the information which is given in this particular table.

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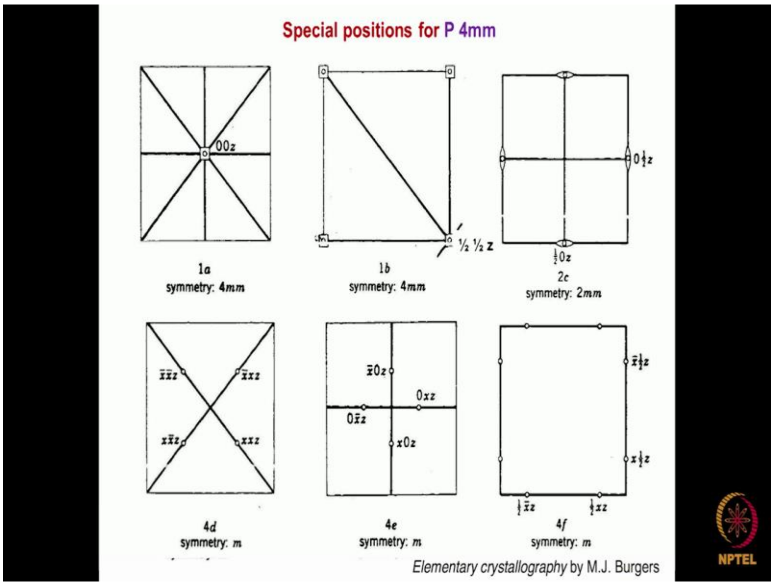

Using this table and essentially here again like as I mentioned for 2-dimensional lattice what are the various positions at which the motifs will be kept for different associated with different symmetry elements.

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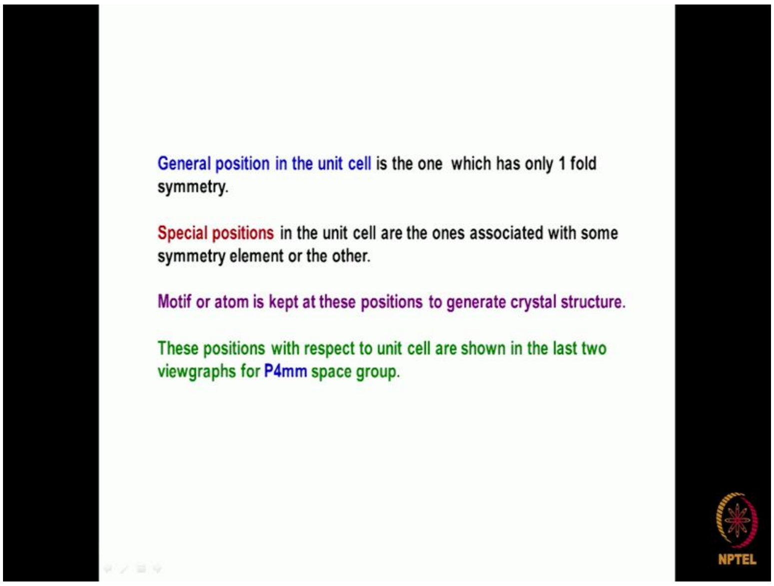

So, in short if you look at it, the general position where we put it has got 1 fold symmetry, the special positions in the unit cell, there we have many symmetries which are associated with it, depending upon that the multiplicity will change. So, the crystallography table if you look at it, the graphical representation shows the unit cell, associated with all the symmetries associated with it and then a general position which is represented. Then in addition to it in another table all the positions of the special positions and the general positions are also given. So, the later part of that information is what is necessary for constructing a 3-dimensional crystal this I have explained it with a few examples, but when we have to look for in the actual crystal structure, all these things have to be specific positions have to be considered.

In the next class we will take some examples and explain how different types of structures can be constructed using the information which is given in the space group table.