Defects in Materials
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Lecture - 05
3 - D Lattice – b

Welcome, you are in the last class we have covered about symmetry in three-dimensional lattice. What we will do is we will have a recap of what has been done some of the significant points then we will go ahead. So, what I am planning to essentially is to consider the point group 4 mm. 4 mm the way in which it can be represented or the way in which these are presented in the international union of crystallography is using stereographic projection.

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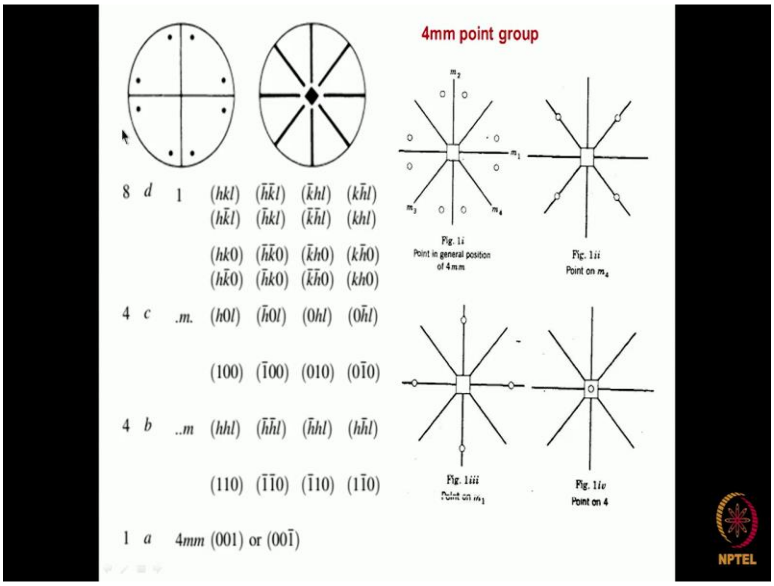

In the stereographic projection essentially what is being done is a circle which is being shown which is a equatorial plane and to which the poles are getting projector. If you take any one of this pole you around this axis if you give A around Z axis A fourfold rotation this will by 90 degree it will come here, another 90 degree rotation it will come here, another 90 degree it will come here. And if you apply a mirror a cross X are wider any one of the diagonal.

Let us see along the X direction we place a mirror then this point gets reflected here correct that is this point gets reflected here, from here this point will get reflected here, this point will get reflected here, then this point will get reflected here. So, already we have all the reflections that is the operation of 4 and a mirror 8 points have been generated. And if I put a mirror across this also it is essentially the same thing this operation is a redundant. So, all the symmetry elements which we can see whereas this point been put this point is been put at a position where there is no symmetry associated with it.

There is an another way in which the same stereographic projection can be shown and which is being shown in inter diagonal crystallography is by showing only the symmetry elements which are associated with it now, if you look at it there is a fourfold rotation is there. So, fourfold rotation is represented with the square which is at the center the mirror is shown as a thick line. So, this line represents mirror along Y axis with represents mirror along X axis and when this has been done if you look at in these 2 directions in this direction as well as in this direction are the another 2 additional mirrors have been created that is exactly what is being shown.

So, we can show the same symmetry elements either by showing just the symmetry elements which are there on the stereographic projection all the symmetry elements are we can show the position of a general point, because in a general point also all the symmetry elements have to operate upon it to generate the full position of the equivalent position of that point which has been placed at the general position right the same thing is being shown here around a particular point how it is getting different positions are getting generated.

Now, suppose I put this point not on a general point suppose it I put it on a one of the symmetry point here then what happens then by mirror A cross it, it will be reflected here where here mirror a across this it will be reflected here these points also has got a fourfold rotation and the mirror is also there. So, all the symmetry elements we have been, but the number of points are now for the same along 110 plane when a mirror is being kept its being shown instead of putting the point on general point are these special points. If I put it at this one which has got the maximum symmetry at the center then I require only one point, because around that point all the symmetry operations leave that point in variant. So, only one point is good enough to show the full symmetry.

So, what are the position of these points are the planes normal create that is being is what is shown in this one. So, this shows the symmetry at which the point has been placed that is where only one fold symmetry is there are no symmetry and then 8 equivalent positions will come and if you put it on any symmetry element that symmetry element has got how many mirror, because reflects from one to the other. So, its symmetry is 2. So, 8 by 2 only 4 points are required. So, the positions of the 4 planes are being shown in this case also again only a mirror we put it. So, it becomes 4 here if you look at it 4 and; that means, their. So, it is suffered. So, it becomes 8. So, you divide it that is only one point is required to represent the full symmetry.

so where exactly the point can be placed to generate all the symmetry is given in this table a similar table will be given in space group diagram as well like what has been given for fine this is a point group representation 4 mm, because we are only around the point which we have considered now as I had mentioned earlier there are 32 point groups are there, they are distinct point groups. So, this way the way it has I had shown earlier we can take any general point on a stereogram and generate equivalent points, if you do that by these symmetry operations we will be generating points are stereograms which are distinct from one other only 32 are going to be there any other combination of the point groups what all the point groups which are there in a material are a point groups which are possible in a three dimension.

Basically, the operations are onefold, twofold, threefold, fourfold and sixfold mirror and roto inversion of that and their combinations that is of this 32 point groups have come these point groups depending upon the type of symmetry elements which are associated they are classified into 7 crystal systems.

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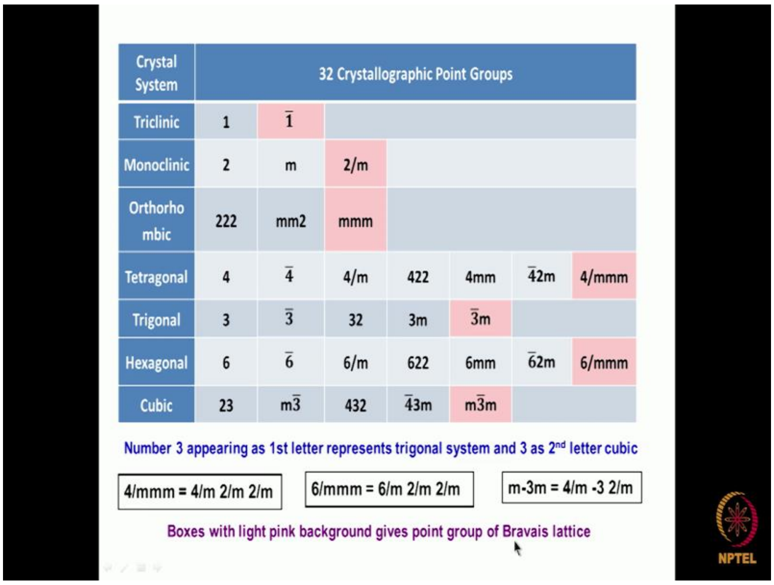

Crystal System	32 Crystallographic Point Groups						
Triclinic	1	$\bar{1}$					
Monoclinic	2	m	2/m				
Orthorhombic	222	mm2	mmm				
Tetragonal	4	$\bar{4}$	4/m	422	4mm	$\bar{4}$2m	4/mmm
Trigonal	3	$\bar{3}$	32	3m	$\bar{3}$m		
Hexagonal	6	$\bar{6}$	6/m	622	6mm	$\bar{6}$2m	6/mmm
Cubic	23	m$\bar{3}$	432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

So, if we look at it the point group which is being shown on the left hand side corresponds to a minimum point group which the system will have the point group which is shown on the right hand side that is in the background which is pink whatever you the color you call it that shows the maximum point group symmetry of the crystal. So, lattice always shows the maximum point group symmetry. So, the ones one bar is the maximum point of symmetry for a triclinic for a monoclinic lattice. If you look at it the point group which will be 2 buy m orthorhombic structure the point group will be mmm like this we can see it correct.

Another important thing you have to see it is that the threefold rotation comes in trigonal as well as in cubic and here we can do that here, we have written as 3 2, we have put it as 2 3 there is some convention, which is being followed the convention is that if the threefold rotation has been put as the first letter in this three letter representation which is fault we are following it for a representing point group then it is a trigonal. If the threefold rotation is put at the second position then it is always a cubic system right. And similar to that some of the form symmetry which are shown here are not the full symmetry like here it is m 3 bar m for cubic it is given. Actually the full symmetry operation is essentially 4 by m this m it corresponds to 3 bar and 2 by m; and if you where it is being written by tetragonal 4 by mmm it corresponds to 4 by m 2 by m and 2 by m.

Student: (Refer Time: 09:09) cubic m 3 by m for a cubic lattice.

Cubic lattice.

Student: M 3 by m.

M 3 by m is a convention which is being used to represent the maximum symmetry element the details of it. If you look at it what are symmetry elements are there 4 by m minus 3 2 by m the question which arises is forget about that structure itself why be use only 3 symmetry elements which are being used that is the first question right which comes into the main if we look at a crystal which is tetragonal 4 fourfold rotation. The fourfold rotation contains fourfold rotation, twofold rotation, and one fold rotation.

These are all the symmetry elements, which are present in this case when we try to represent it we represent only with you if its only rotation which is available what is the maximum rotation which is their only that is used to represent similarly, if it contains a combination of rotation and the mirror then we may have like 4 mm, if you take it 4 mm.

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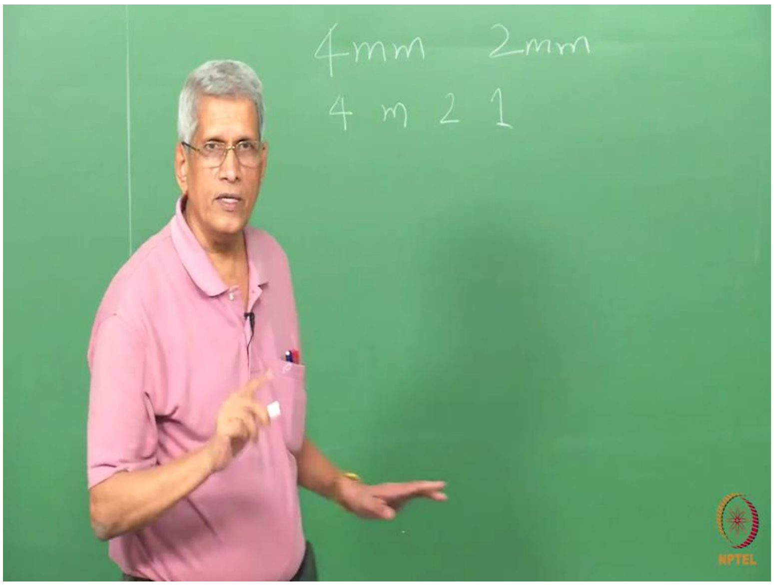

If you try to take it 2 mm is going to be there fourfold rotation mirror twofold rotation onefold. All these symmetry elements are going to be there, we can say that this entire thing combination is going to be there as the symmetry element one way to represent it, then it becomes very untidy and it is very difficult to understand then a convention which is being followed is a what are we should represent to tell that these are all the basic symmetry elements which if we operate upon it upon the system almost the full symmetry can be generated that is the way it is a convention which is being followed.

So, when it is written as m 3 bar m essentially this means that actual symmetry is 4 by m that is why I mentioned that one should, that one should when we put that 4 by mm for tetragonal its actually 4 by m 2 by m and 2 by m that is along and where we use 3, because in 3 directions are used because in a space, if you have to represent 3 directions have to be used what are the 3 directions which are being used there again a convention which is being followed, because I have not talked about it which direction is being followed now.

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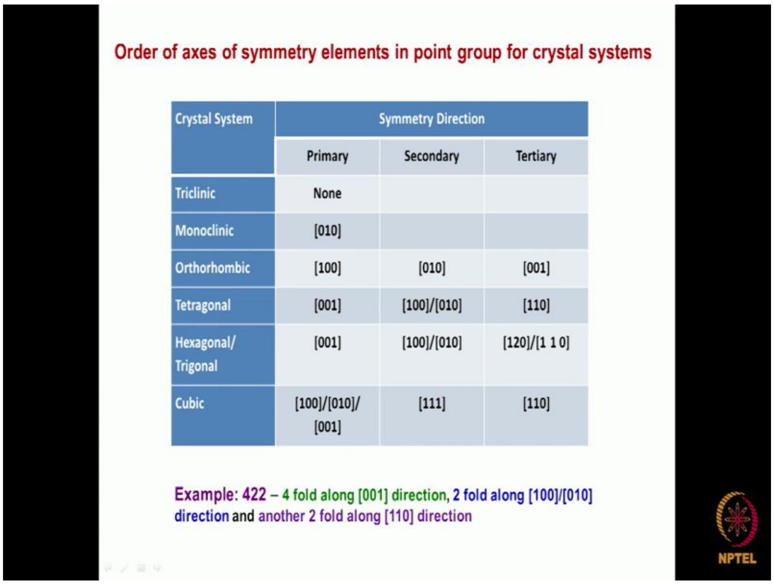

In this table I give that that information is given triclinic that is 3 letters are being put 3 symmetry elements are being written right these primary means the 1st one secondary is the 2nd one tertiary is the 3rd monoclinic 0 1 0 is chosen as the b axis that is what is being represented as the 1st letter.

Let us take orthorhombic if we take it to 2 2 2 mm 2. These are all the 3 symmetry elements which are there. So, the 1st letter shows twofold symmetry along 1 0 0 axis then two fold symmetry along 0 0 1 axis twofold symmetry along 0 0 1 0 axis correct all the 3 letters, if you take tetragonal then the first letter represents fourfold is symmetry along 0 0 1 is a direction, then the another one is symmetry along X or Y direction the 2nd letter, the 3rd letter represents symmetry along 1 1 0 direction this is a convention which is being followed to represent it only. If we understand this convention we know what the rule is which is being followed, then only we can do all this symmetry operations correct.

So, similarly for cubic the 1st letter represents along 1 0 0 or 0 1 0 or 0 0 one what is the symmetry operation which is present the next letters represent symmetry operation along the body diagonal, then the next one represents the symmetry along 1 1 0 direction. Now, it is clear how you can correlate it and then try to find out there are different symmetry elements.

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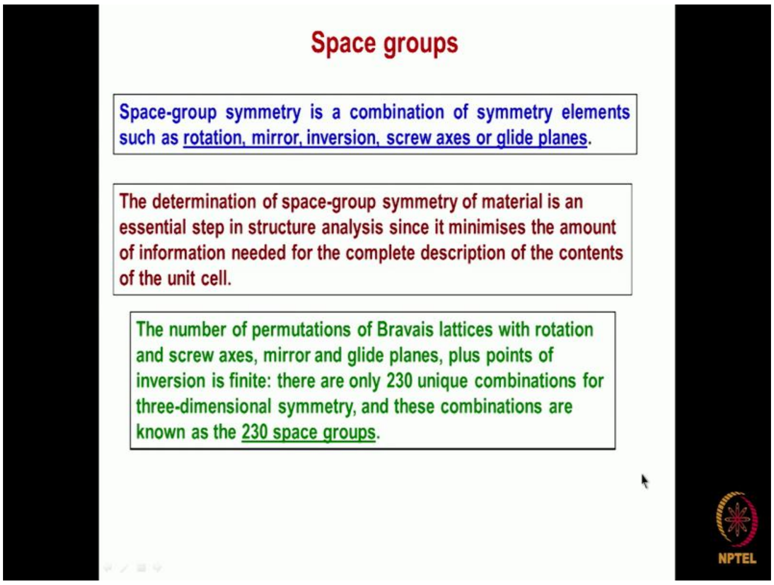

Then I mentioned also about space groups, what do we do in a what is a space group? Space group is nothing, but a combination of various point group symmetry operation alone are together, then if it is acted upon on different lattice points what is the type of symmetries which are generated on the basis of the type of symmetry which are being generated we find that distinctly there are 230 groups are possible that is when we generate these space groups essentially what we are doing it is this is being done around the lattice. That means, that now we are generating crystals what are different types of space groups which we can have for crystals are with what all the types of symmetry which crystals can have only two hundred and thirty types which we can have.

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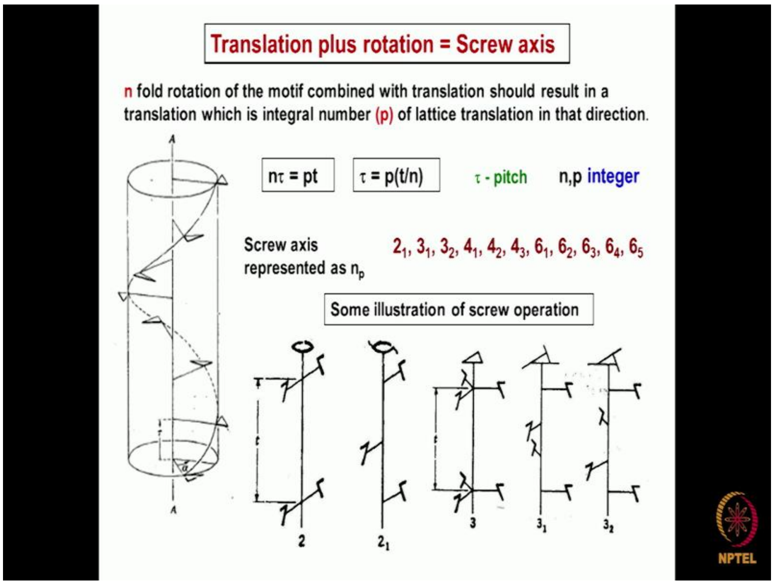

Now, we will look into some of these symmetry elements I had explained in the last class about the screw axis screw axis is like the glide which I had we had represented it in the 1st lecture now, what we can do it is that from one point to another point like when we go from here to here this is a one a symmetry motif and its starting from here and along this axis it has a sixfold rotation is there if it is just a sixfold rotation around this direction itself although motif would have been there then an identical point would have come where all the sixfold all the motifs would have been placed there in many structures especially in chemistry organic chemistry. You can see that from this position to this position. When it moves the motif is placed at different positions, but it is rotated and there is a translation is also there.

So, from this motif to an identical position it comes and some particular translation that translation could be a multiple of the lattice translation vector, it need not be one translation vector. It could be a multiple also these sort of symmetry elements which are arising in the lattice is called as screw axis this for a twofold rotation. If you consider we can have only one screw axis can be there and it is represented as 2 1 the 1 represents that how many times it is repeated 3 1 if we put it is essentially 3 times it is repeated, but the pitch will be 1 by 3 from this we can make out of the lattice parameter other translation in that direction translation vector in that particular direction.

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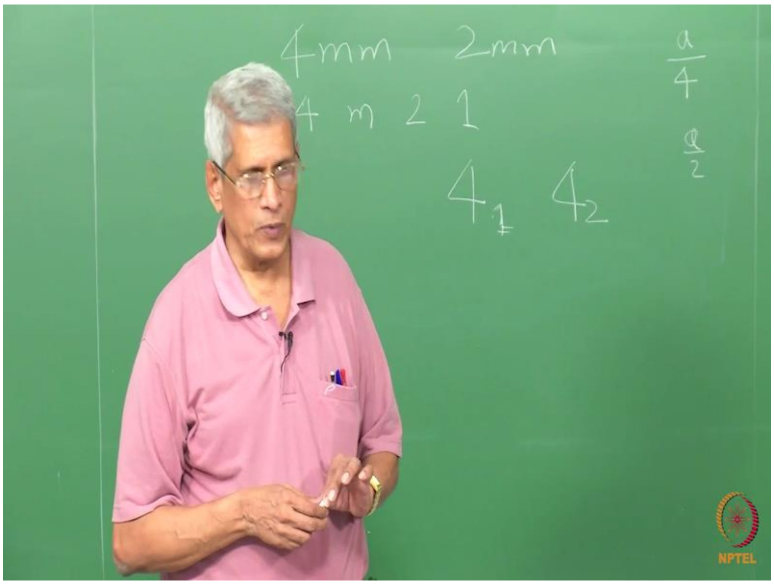

That is if you take fourfold 4 1 means that if a translation vector in the direction is a then the pitch which after every rotation it makes will be A by 4 correct and if we mentioned this is 4 2 which means that the pitch is going to be A by 2, but the rotation is 90 degree when 90 degree you are rotating it, but translating it by A by 2 that is what essentially means this way we can have this much number of additional symmetry elements are possible, but this is because here, we are combining a translation and the rotation.

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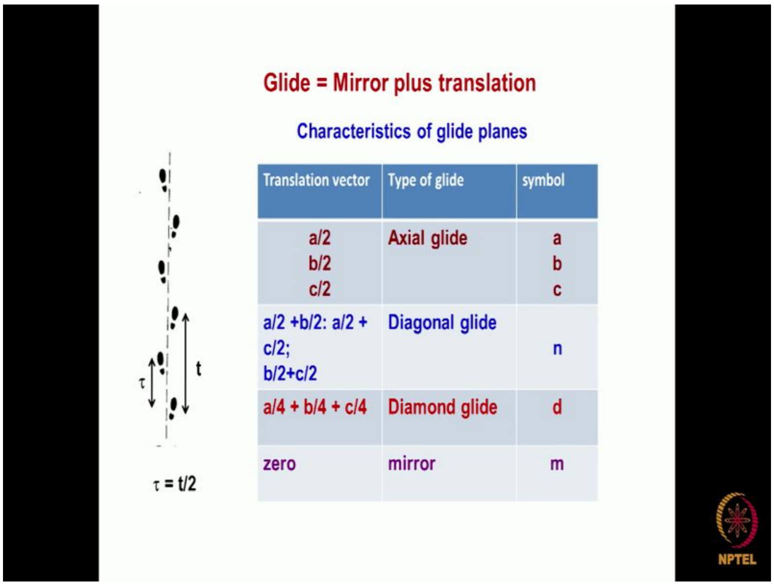

So, similarly, this also had mentioned earlier about the glide. So, if you look at the what all the glide axis which we have a glide B, glide C, glide and then along the face diagonal we can have a glide that is called as a represented by a symbol N, then which I have we have can have a glide along the body diagonal then it is designated as B then what will be the translation vectors that is also being given.

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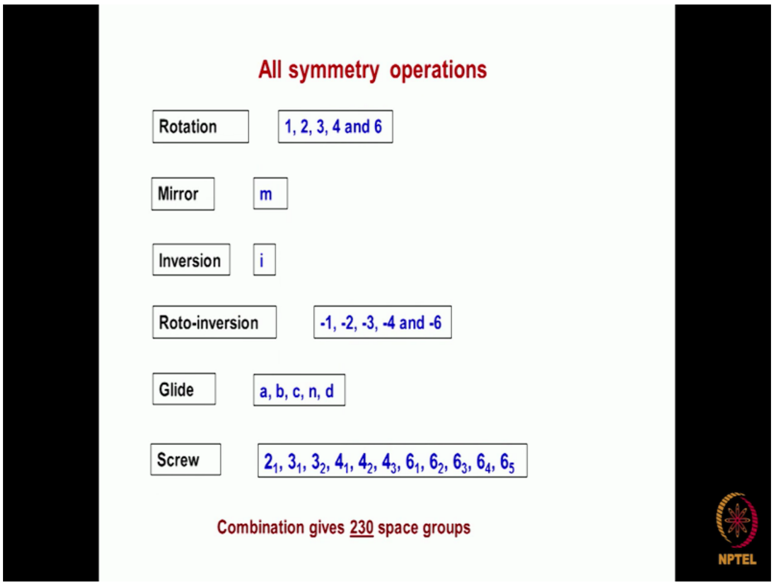

So, now if we look at it what are symmetry operations which we can have in a 3 dimensional space groups 3 dimensional lattice one rotation symmetry, we can have you can have a mirror symmetry all the rotations inversion we have a roto inversion then we have A glide, A, B and C and N and D then there are these are all the types of screw axis now, if we can see a combination of these various symmetry elements what are the distinct types of distinct goals which will be found that number is only 230 ok well

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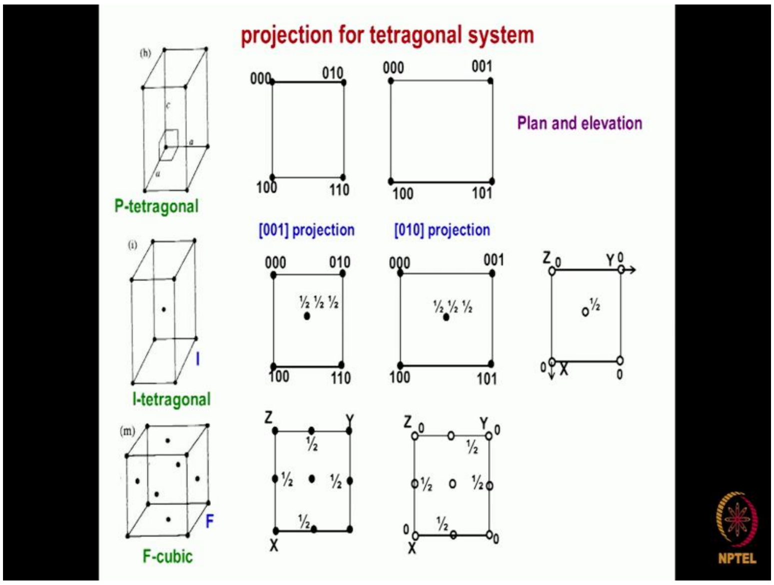

When we look at international union of crystallography table are any crystal structures in 3 dimensions. If you have to represent it how do we go about and represent 3 dimensional structures representing it directly like that and drawing a figure of a cube or a tetragon tetragonal structure and then trying to mark the symmetry elements is going to be very difficult to understand it correct as for as point group symmetry is concerned you found a way out by using a stereographic representation here the only way it can be done is that like in what we do in engineering trying.

If any 3 dimensional structure has to be represented, we take the plan and elevation like if you take a monoclinic structure are a orthorhombic structure a plan and elevation if you take it and put projections of all the symmetry elements which are presented different positions it can be represented that is what essentially is being shown like you take this case of a body centered tetragonal lattice in this one. This is at position which is half half half. So, I can represent this by a square that is what essentially it is being done. I had just mark the axis also and this 0 means that it is at the 0 layer or 0 position, then this position at the middle is just put here and put half what it half means is that with respect to this layer it is at a half position upwards this is the one way in which it is being represented.

Especially, when we have a glide axis and all the glide or screw axis comes into the picture we find that atom are shifted from one plane to an another position, then this sort of representation as we use to represent them and we know that in a crystal as we have looked at it earlier the crystal itself can be identifying the pattern, which is repeating itself are the motif we can generate a lattice points and thus smallest the 3 3 lattice translation vectors we can identify, then we can construct a unit cell that unit cell itself can be assumed to be repeating itself to generate the 3 dimensional lattice, that way also we can look at it.

So, this 3 dimensional unit and since it is repeating, if you find out what all symmetry elements which are associated with that then, we have got complete information about the symmetry element how they are distributed within the complete lattice we have that information, because applying a translational symmetry we can generate all of them correct. So, that is essentially what is being done.

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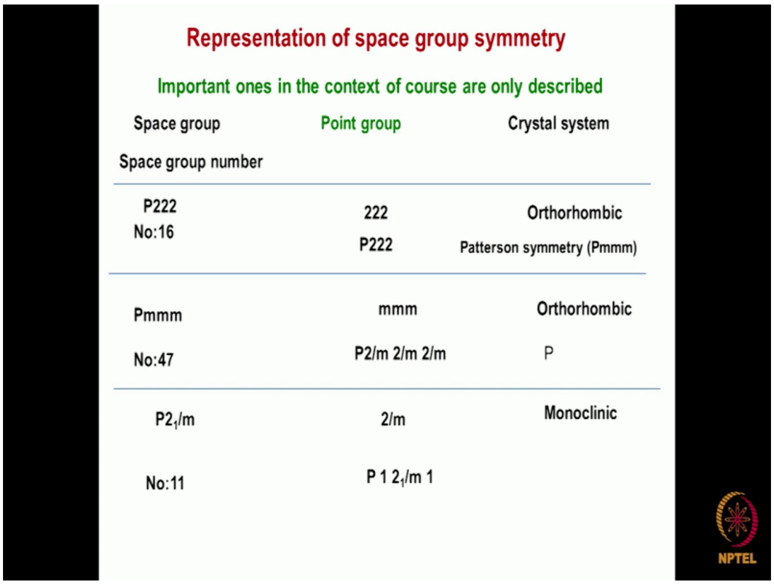

If you look at the international table of crystallography the information which they give is that the first is; what is the crystal system that information will be given at the left and I have shown it here for 3 structures. So, each page is an orthorhombic structure and this shows what is the point of symmetry which is associated with that lattice and this is the a space group symbol. When we put the space group symbol what we have to do it is that whether it is primitive or it is body centered or tetragonal this symbol will change P if it is a body centered it will be I 2 2 2, if it is face centered it will be F 2 2 2 like that it will come correct and then here a detailed of the various symmetry elements are being given for the orthorhombic structure and then this number 16 is given number 16 means that some few pages it is being represented in sequence 1 2 2 and that it is being represented.

So, this is given as the 16th figure representation like here, if you look at this particular structural orthorhombic structure the point group symmetry mmm space group symmetry P mm the number is 47 and this is the details of the space group symmetry P this m means the 2 by m 2 by m 2 by m this is all acting along each one of the A B and C access correct for orthorhombic structure. So, essentially this gives complete information about the crystals whatever is required what is the type of system all this information is given similarly, this is for a monoclinic I have taken where it is point group symmetry is 2 by m, because you know that this glide and screw they are associated with translation they are not called as point group symmetries.

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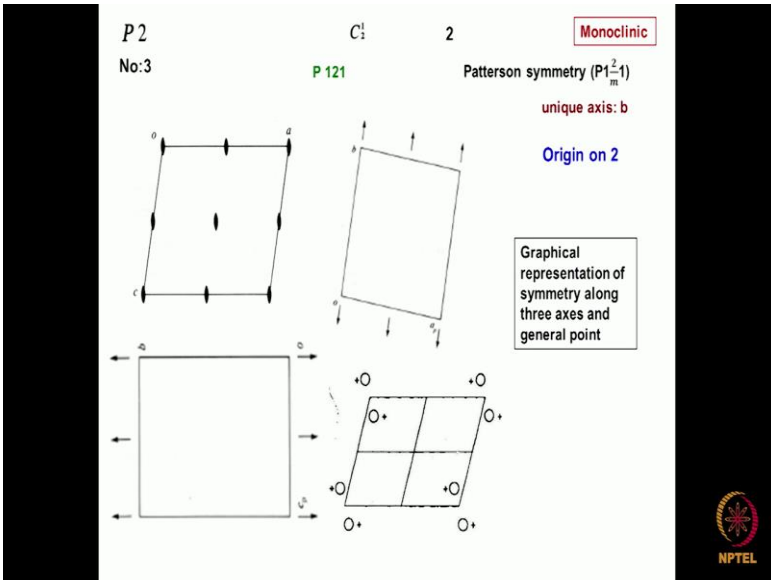

After giving all these details like what is being given for A I have taken the monoclinic structure P 2, because triclinic does not have any symmetry.

So, I thought that I will just take a monoclinic structure; that means, a twofold rotation is going to be there correct this is the A axis, this is the C axis, this is the B axis, and along the B axis only the twofold rotation is B axis is perpendicular to a figure that is twofold rotation means that it can be represented by a symbol the ellipse then around this lattice point also we should have identical around this point and this point it should be there that is if I put a motif this is what we have shown the projection of the lattice along 0 1 0 plane.

So, on this plane now if we see this is layer at a general position your motif is being shown the international union of table of crystallography the motif is being shown as A open circle as metric motif and the plus means that since this has got only 1 symmetry axis the coordinate is not fixed where to take the origin can be taken arbitrarily from that point there is a reset direction are the here it is in the Y direction is where the motif has been placed.

So, that is why it is put as plus sign then if you do a twofold operation this will get repeated itself here, it will come and on the other set and; that means, that around this twofold here is twofold here, it is twofold in this shows that how the mode when the motif is being placed the crystal is being generated all the atom positions in the crystals are being shown are the pattern position is being shown.

But now if you look at it in this particular position at the center now, that is a twofold axis has come now one which has come here another which has come here right. So, then there will be correspondingly here as well as here. So, other positions also twofold rotation has been generated correct these twofold rotations. If we look here what is essentially important is that though this is the in 2 dimension the unit cell which we are representing it. If you look from symmetry point of view this is the lattice by doing a symmetry operation, we can generate the full unit cell itself.

So, when we have to work and any system if you know the symmetry which is associated we can go to the cell which is much smaller than that, that is from here to here if we move within this cell anywhere it is going to be a onefold rotation that is I move from here to here in some direction at some particular point I find that I cross a symmetry point. So, this is what it is called as an asymmetry unit I will come to it later and explain this is how graphically the positions are represented. So, I here it is a general position when I put a atom I allowed to put a another atom here to represent as well I can put an atom at this position this position and this position also in generate the lattice correct I can put an atom at this position and generate a lattice or I can put an atom at this middle also and generate a lattice or I can put an atom at this position also generate lattice there are many possibilities axis.

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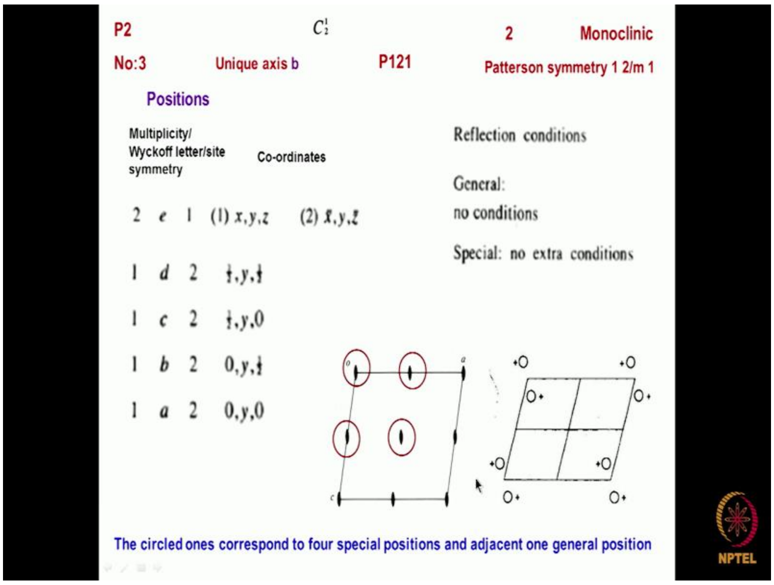

These are all the possibilities we are given in this positions where general position as well as the special positions are given this is the information which is very much necessary to construct crystal structures.

So, for the general position where the symmetry is onefold the position if it is X Y is Z is there by a twofold rotation it will go to X bar Y is Z bar that is the position which will be generated for the other point when one point this is an equivalent position which you are generated by symmetry related. Other position like if I consider it as the center here the center here what is the symmetry which is going to which again a twofold symmetry. So, the number of atom position which will be required is only one and that is given by this position 0 Y half.

Student: (Refer Time: 29:38)

No, if you consider this 1 0 is along the X direction 0 Y directions some distance which you have more no just a minute here what essentially is that Y is along they said that direction right. So, if you consider that this is 0 a direction 0 is a direction half Y direction. That means, A this point I can put one here are this point if I choose it then it is going to be this particular version gives where the atom could be placed other motif could be placed and here it is going to be half Y half.

So, all the symmetry points if you place it these are called special points any one of them we can keep it and generate the lattice. So, these are all the options which are when we have the unit cell when we know the symmetry which are associated at different points then by putting atoms or motif at some of the symmetry points are on a general point in short means that anywhere within the unit cell what are positions atoms are to be generated. So, that the structure will show twofold symmetry right, this is what essentially is being shown the various points.

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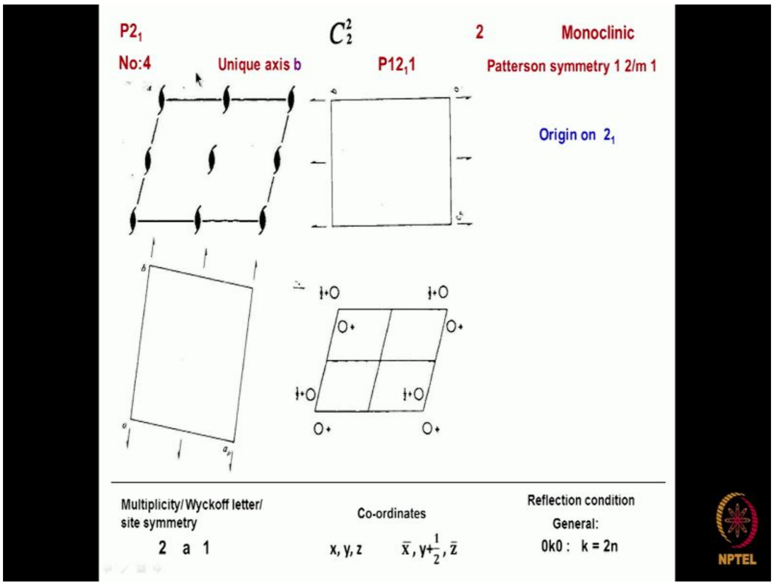

Here what is being done is there in a monoclinic lattice if it is a instead of two it is a 2 1 that is a screw axis is present then this is the symbol which is being used to represent screw and in this case also we can find out how the atom positions are coordinates of the positions we can find out here there is going to be only one position which will come I not go into the detail in this one, because I will explain it with an another structure there is a way in which mathematical operator which is being used for representing screw and glide this is called as a Seitz operator.

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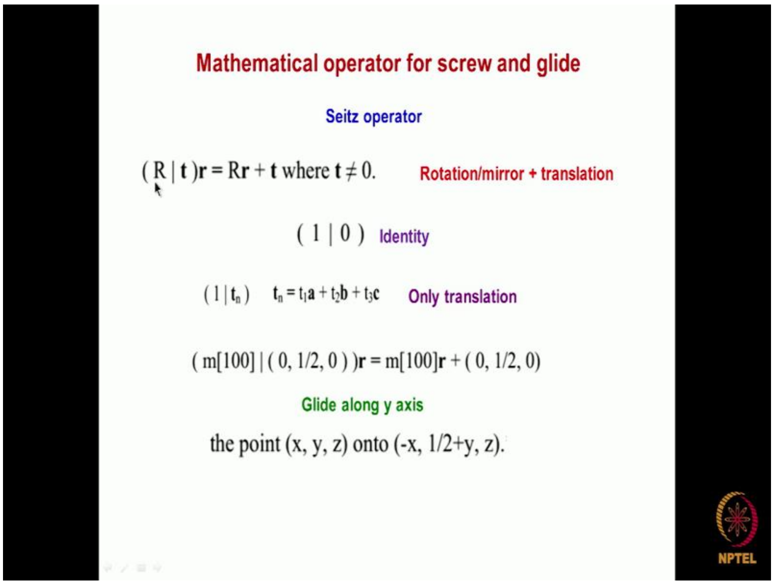

What is it (Refer Time: 32:00) done it is R T this is how it is being shown what it means is that the capital R represents the point groups symmetry operation this T represents the translation operator. And this is being done on any point if you do that it will be equal to R into R plus T the translation this shows how that given one position we can generate the equivalent positions.

Suppose, this R is going to be an identity operation the translation is 0 means that what it happens we are out whatever we do it is in the same point right that is how it is called as an identity. Suppose, identity is there instead of 0 this translation is T N means that in some direction. That means, that only translation is being performed like here, if we put a symbol m 1 0 0 and then the symbol which is being used is that what is the glide which is going to be there this means that mirror which is acted upon first you generate that position to which you add the glide one then you get the coordinates of the other equivalent positions, this is how it can be done.

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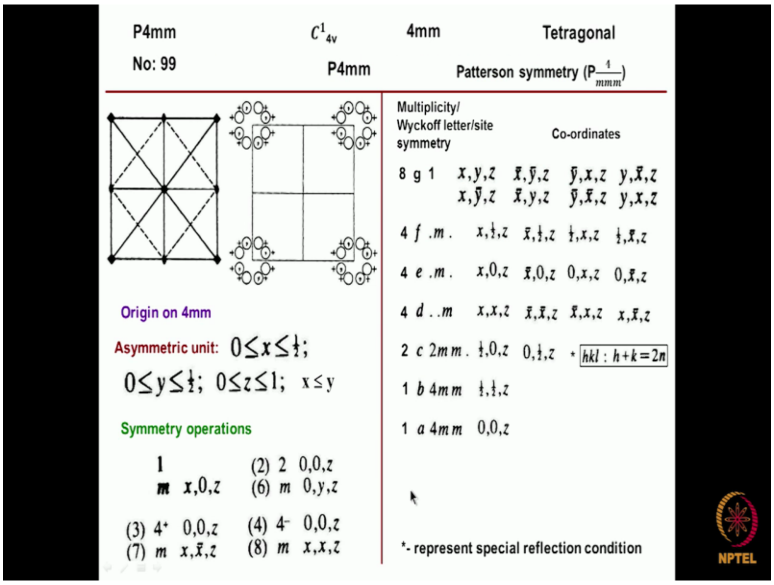

Now, this is the structure which will take up, because we talked about the point group symmetry 4 mm. now, we let us look at a crystal which has got the space group symmetry that is a primitive lattice we are taken to the simplest case to consider P 4 mm. what are the symmetry elements which are there in the unit cell a very lattice point will have a fourfold symmetry correct at the center another fourfold symmetry will come then on the edges at the center that is going to be a twofold symmetry.

Then, if you look at it across this axis if you put a mirror when we will have a mirror symmetry along this also along body diagonal also mirror comes correct and then along these 2 axis also mirror is going to be there 3 types of mirror are going to be there then this generates what is called as a glide what is it glide essentially, if I take a point here like this were an atom has been put it is translated by this distance. And then, I take a mirror of it across this direction it will be generated then again I translate it by the same distance half of body diagonal and then again take a mirror it will coming into this point.

So, that is why here when we look at this particular structure as a consequence of putting of atom and different positions that glide is inherently generated in some structures the glide comes separately inherently they do not they have not present and if you put an atom around any particular position random position we are putting an atom then, when we do the full symmetry operation then all these 8 positions will be generated here that is this is what it is 1 2 3 fourfold rotation then we take a reflection, because the reflection is generally the symbol which is used this within the circular comma is being used.

So; that means, that 8 positions are then. So, everywhere you will have an 8 positions which are going to be there now, what is essentially important is that around this is the origin around the origin, if I am moving it at a random position, if I am putting a motif what is the space within which I can move the position before cutting across any symmetry operation that is what the a symmetry unit represents that is within this triangle.

If you look at it anywhere if I move it there is no symmetry element I will be crossing it if I reach at this Y direction Y value greater than half I will be crossing it here if I move it, but what is the value which X can have, because this is the diagonal na. So, at any particular value the X should always be less than Y when at X becomes Y I will be where the point it will be X becomes Y will be on the body diagonal that is a mirror point it has again It is a symmetry point it has reached.

So, asymmetric unit is essentially the using this as symmetric unit and applying this symmetry, we can generate others that is this will becomes very important when we do many calculations even on computer when you wanted to do some calculations what you have to do it is look at the symmetry then the symmetry dictates what is the lowest structure on which we have do the calculation then using the symmetry operation quickly we can replicate all are them and generate the full structure exactly the same thing is being followed here also and then these are all the symmetry operations which are what are symmetry operations we have when we say 4 mm onefold rotation is there, twofold rotation is there, 3 types of mirrors are there right then 1 fourfold rotation and the positive direction as well as negative direction.

So, total 8 symmetry operations are possible and if you try to put atoms and positions. Now, we consider atom are a motif as a general position. We can put it at any of these special positions also if you try to put at special positions how many atoms will be required or how many positions the motif should be kept that is what the information which is being given here like here, if you look at it what is the symmetry associated with it 4 mm at this center fourfold there is a 4 mm symmetry. If you look here it is a 2 mm symmetry then what are the positions it has to be kept all these information is given this is the table which is extremely useful to generate crystal structures.

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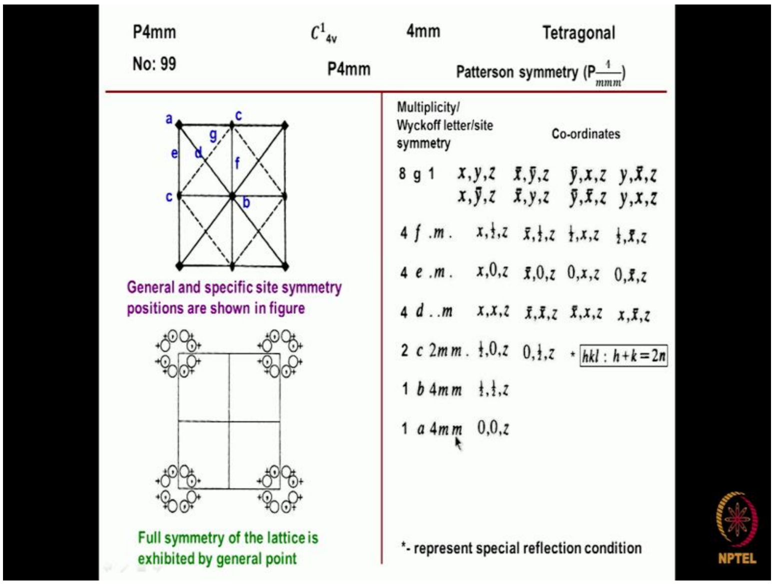

Now, let us look at it to the little bit more detail in these what I have done it is the same figure I had taken it I had shown that what is here represents there is some way to represent this symmetry elements supposed 2 symmetry elements are there 4 mm A 2 different position how do you differentiate. So, the Wyckoff come out with and that you see really label them A B C D like that. So, that will distinguish them. So, that is what essentially is being done then how many equivalent points are there that is only 1 in the case of 4 mm. So, that is what it is being shown and where is the B is this position C is going to be this position D is going to be these 2 E is this mirror F is going to be this mirror G is anywhere within this one we can take a point right that is where it is a general position.

so here you will look at it in the table if you see within multiplicity Wyckoff letter and the site symmetry that is in the unit cell at different places if you look at it the lattice has got some particular symmetry which are associated with it at different positions we can put atom at general position R at specifically anywhere it can come we are talking about we are placing an atom there. But actually, what happens is that the depending upon the type of interaction atoms the type of atom which are being present they will try to occupy preferentially some positions we are trying to look at it what are the possible positions which we the atoms can occupy in the lattice correct.

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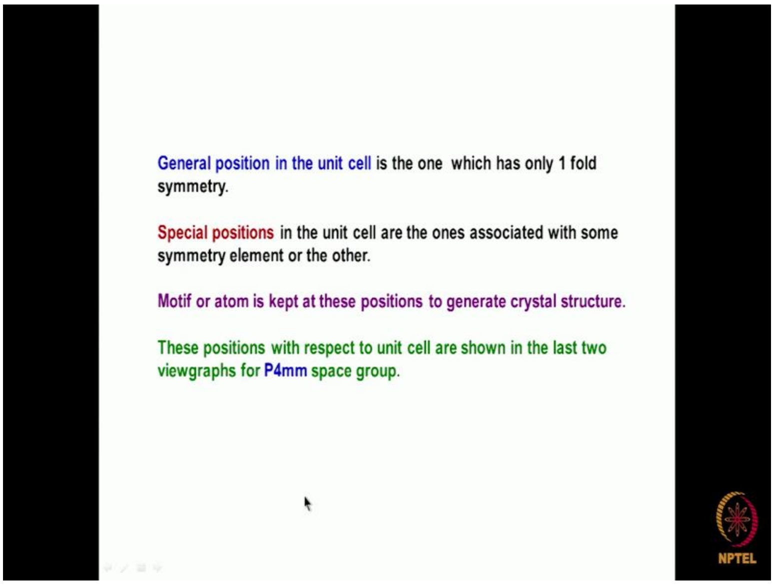

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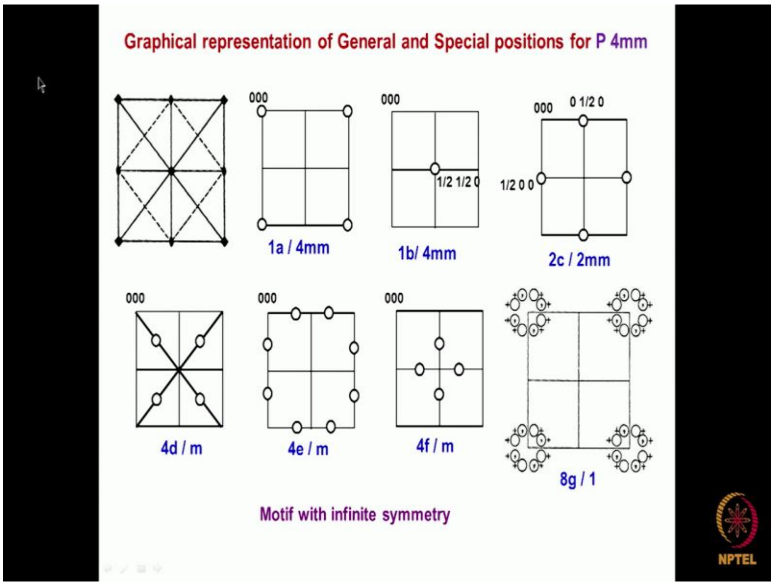

So, here what I have shown it is what all the possible positions if we are trying to put an atom it can occupy. Suppose, I put an atom only one type of an atom is being present and assume that that it is an atom is as circular one or spherical one. So, that we can consider that it has got an infinite symmetry associated with it, we can place it at this position. If you place it at this position by translational symmetry, when we place it at origin this position this position and this position will be generated. So, all these positions live.

So, if we keep it there now, this structure will have the full symmetry will be there 4 mm symmetry correct 1 atom we can keep it here with respect to origin which has fixed instead of it I can put the atom at this body diagonal that is if I keep it here no sorry if I keep it at this particular position then what happens then also only one has to be kept here by translational symmetry will be able to generate another one. Will come here where their centers of other unit cells. So, that way also it is generating the full fourfold symmetry will be there, but within the unit cell only at one position we have to keep it.

Suppose, now, we are trying to keep the atom not at these 2 positions we are trying to keep it at this symmetry point then I like to keep it here and here by translational symmetry these 2 will be generated now you look at this in this unit cell this has a fourfold symmetry along this this has a mirror all the symmetry elements are going to be there correct, but how many positions we have to keep it on the unit cell 4 positions correct that is true with respect to an another this one, here 4 has to be kept, but this 4 have to be kept at these positions the body diagonal and in this particular position here what we are keeping it is 1 is kept here and another will come 8 positions will come, but essentially equivalent how many will be contributing to the unit cell here again only 4 will be there, because the face are shared by 2 correct and here again if you look at it within the unit cell 4 now this is also. So, all of them satisfy their symmetry which is 4 mm symmetry, but the pole place where we are keeping the motif at different places.

But the number of atom which are required is changing here it is 1 only 1 position is here, 1 position here, 2 have to be required in the unit cell, here 4 have to be required if we keep it at a general position, 8 position, because you see that within the units are 1, 2, 3, 8 are there. So, 8 I equivalent positions atoms have to be kept then only if we keep anything in a general position to satisfy this symmetry other 8 equivalent positions are there where also the motif as to be kept that is the only way we can generate; so all possibilities axis one.

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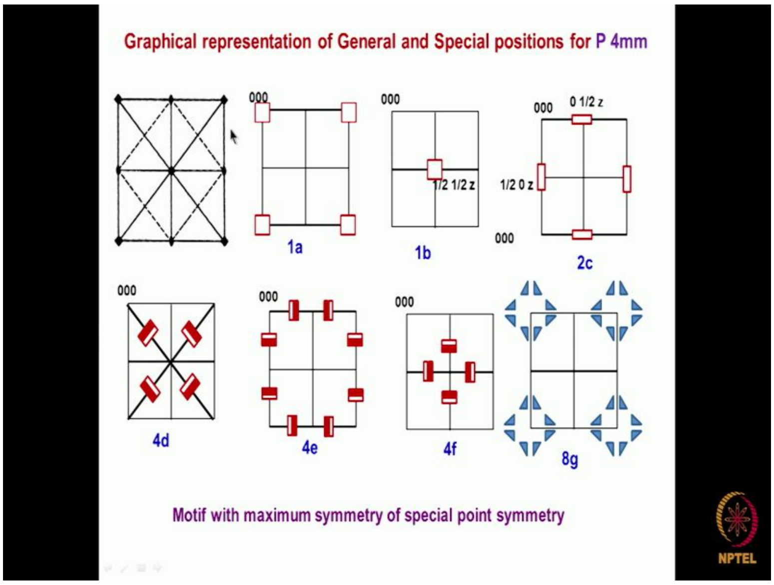

Now, let us look at what sort of a suppose the motif is not an atom which does not have an infinite symmetry it has some finite symmetry then where will we keep it that is if it has a fourfold symmetry the motive which we are trying to generate the lattice as the crystal has got a fourfold symmetry. It can be kept in this position or these positions are at this position only these two options are there right, because those positions the symmetry which is therefore among symmetry. If I keep it this position or this position it has a 2 mm symmetry. That means, that the motif itself should have a 2 mm symmetry should be associated with it. Then this shape of the motif gives a twofold rotation and a mirror is also there, then if this is the way if you keep it now you can see that again a fourfold symmetry is satisfied.

In this particular position if I try to keep it where mirror is there the motif should have a mirror associated with it otherwise this if we keep it in this particular fashion 4 mm symmetry is being satisfied here this is the way in which it will come it will come if you take an asymmetric motif if you try to keep it then this is the way the motif have to be kept to satisfy the full symmetry from this we can understand that there are various positions in which atom could be kept and the number of atoms which are required to be kept on different positions also changes from 1 to 8 in this particular case

Student: (Refer Time: 45:19).

Yeah.

Student: Should motif also have a mirror symmetry (Refer Time: 25:24).

The 2 C also has got a mirror symmetry which is associated with it, it is inherently there, but it is not explicitly clear that is why I do this diagram to show it.

Student: We can have this same thing.

There are some structures which you can have a twofold rotation, but need not have a mirror right that is the only reason why a do it is to show the distinction that now this has got a mirror is also associated with it. In fact, the same thing could have been put here also correct suppose we assume that there is only one type of an atom is there we know the lattice we have to put an place the atom at different any lattice point either at a special or general and generate the lattice energetically.

What will happen? It will try to choose the position where the symmetry is maximum. That means, that minimum energy is required or the number of atoms which will be required is only one. So, the two options which are available now is either in this one or this particular one correct only these two positions it can choose correct others are going to be energetically it is more atoms. So, it is not a probable one that the way which can be chosen, but geometrically anything it can choose, because if you do not consider energy correct.

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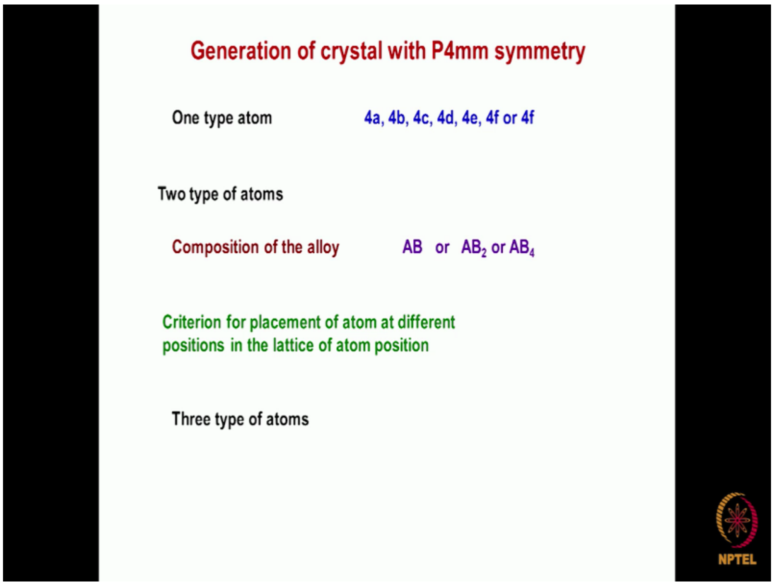

So, that is why I had given all the positions it can we can put that atom in any position and generate the lattice it will have the 4 mm symmetry suppose you assume that there are two types of atoms are present and then atom A and B and the sociometric is AB if we fill all the a position with this particular type of an atom lattice position then what is the option B has. Because, since the sociometric is being maintained if it comes to this particular side the number of atoms per unit cell for both of them is 1 is the only option which is available it will choose that position. Or suppose, we are given told that this is the sociometric of the alloy and this is the space group symmetry which the crystal has got then now, we are able to find out which positions the atom should be placed correct we can consider that result structure from this information looking at this space group table is it clear.

Suppose it is a b two the sociometric, but still this symmetry has to be maintained as 4 mm then what is the option which we have now, the 1st atom could be placed in these positions correct the 2nd atom could be placed in these positions these are not only positions which are available B atom could has to be placed here are the A atom could be placed here and the B atom could be placed here this also possible, because for the a atom there are 2 possibilities axis, B atom the possibilities only this which is defined. Now, which position these atoms will take depend upon the type of bonding which is being present. There are many various ways in which it can consider it, but geometrically A can occupy either this particular position or this position; B can occupy this position although sociometric is being maintained correct.

Student: (Refer Time: 49:18).

2 be A atom, because 1 atom will come here another will come here. The others are generated by translational symmetry.

Now suppose it is AB 4 still maintaining 4 mm symmetry, then the options which we have is A atom can occupy this position or this position. What are the positions which B atom can occupy? Either this or this one or these one; three choices are available that will give rise to A B 4 sociometric will be given. Now which position they are going to occupy how to find out that is the gain where X ray diffraction has to be used to; find out what is the type of bonding, what is the radius of the if it is especially ionic material ionic material it is much simpler because you can consider each of the cat ion or (Refer

Time: 50:19) as an earth sphere. So, that that if they come close together they cannot interpenetrate it and from the size itself we can find out what should be roughly the lattice parameter that way we can find out where exactly they will come other ways in the case of a metallic sample it is going to be its not that easy to tell which position, but we have to do some calculations to find out which will be energetically favorable.

But this gives the options which are available only one of these positions it can come. That is the A atom has these 2 options B atom has these 2 options. Which combination is going to work? Now at least we have narrowed down using this (Refer Time: 50:59) we control the these are all the positions where it can come correct this is the advantage when we know the symmetry what are the symmetry elements which is associated with it. So, what they had given is that the criterion for placement at atoms at different positions that depends upon the energetics rights.

So, that the overall the energy is being lowered that is the criterion which will be set out of the possible geometrical possibilities, which we have that we have to find out suppose there are three atoms are there then also you can try to find out like here if we take the three atom case A atom can occupy this position, if B atom occupy this position, it will be AB 2, if C atom occupies these positions, then it will be a B to C 4 for will be the composition of the ally right from this I think you have got a fair idea of how at different places one can place atoms are suppose, I tell that this is the space group symmetry, this is the sociometric of the ally.

Now, you can find out which are positions that which atom has to go. So, that the symmetry will be maintained this is how this table are you can understand that using this table if we are to construct a crystal what we require this parameter alone is not sufficient that is parameter is required all those aspects of it what all other things which are required and how we will go about and constructing it we will talk about it in the next class. So, essentially what we have covered today is starting from point group symmetry of a particular point group symmetry we have considered the how the space group generates that what are the special and general positions, how atoms have to be placed around this general positions are special positions, what sort of symmetry which should be associated with it if we are placing a motif around these positions. All these details we have looked at it.

We will stop here.