Electron Diffraction and Imaging
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Lecture – 07
Understanding IUCr Tables

Welcome you all to this course on Diffraction and Imaging. In the last class we have discussed some aspects of space school symmetry, today we will discuss it a little bit more further, and how we can use this space group symmetry table and the diagram which is given; the international union of crystallography table to constructs crystal structures because finally, that is the main aim of the table.

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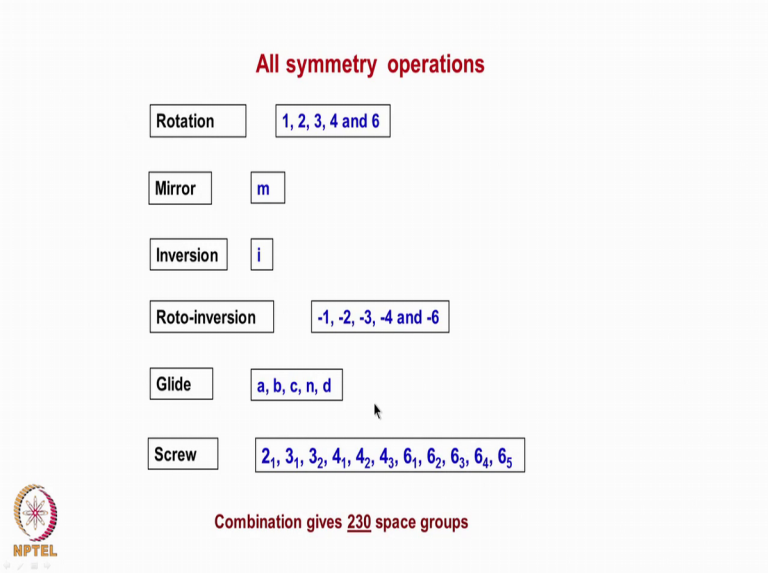

So, any lattice if we consider and in which when atoms or molecules have been put at some specific positions then we call them as crystals correct the type of symmetry elements which this crystals exhibit depend upon what position these molecules or the motives occupy in the lattice correct.

So, the symmetry elements which we have considered are rotation symmetry which a lattice can have then mirror, inversion; roto-inversion, these are all the symmetry elements which are crystallographic point group symmetry elements, correct that is these symmetry elements pass through a specific point. So, any lattice point if we take it what all the symmetry element which we will be crossing through that point that is what we

are looking at it given by these symmetry elements in addition to it in a space group in a space group or in a lattice we can have a screw axis as well as glide the type of screw axis and glide we have discussed it in the last class, these are all the symmetry operation which are possible in a crystal.

When these symmetry operations we combine them with a lattice essentially what are the lattices; the Bravais lattices are there; the Bravais lattices essentially when we look at it there are 7 crystal class systems are there, they are again determined by the type of symmetry element which are associated with the crystal lattices. In addition to it even among the Bravai's lattices like orthorhombic FCC they have a primitive orthorhombic we can have a body centered orthorhombic we can have a face centered orthorhombic like that there also some top classifications are there these what we call it as a space lattices then we combine all these operations together the number of distinct crystallography groups which we can have turns out to be 230.

Essentially if just a point group symmetry operations how many are there point group symmetry operations 32. If these point group symmetry operations if we try to put it on a crystal lattice then the number of space groups which we can generate are 73 and in addition to it, there are another 100 and 57 space groups are coming their coming because each of the axis like if we take us a rotation axis in a space lattice we can have just a rotation axis or instead of the rotation axis we can have a screw axis is also possible correct similarly instead of mirror we can have a glide is also possible.

If we take these symmetry elements also into consideration then the total number of space groups turn out to be 230 then another thing also which you should understand is that the number of point groups which we have considered are 32, many crystals if we consider inversion symmetry will not be there, but when we measure property of a material the property of the material always exhibits as if an immersion symmetry a inversion symmetry is always there, because of that there is an another classification which is called as a Lavey classification under which we can have only 11 groups are possible point groups this we will complete later, but I am just telling that when we measure or when we try to find out experimentally the symmetries there are some restrictions are there, but that is a way in which these are overcome.

Then we had seen that how the unit cell of a lattice could be represented correct then if the symmetry operations are acting on a lattice if we take any specific particular type of space lattice then we know that this is what the symmetry which it has like for example, what we have considered in the last class this essentially P 4 mm.

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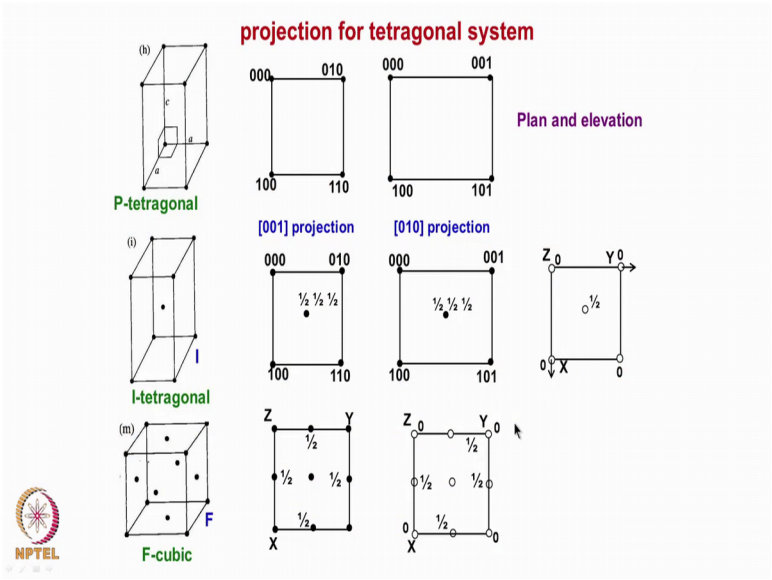

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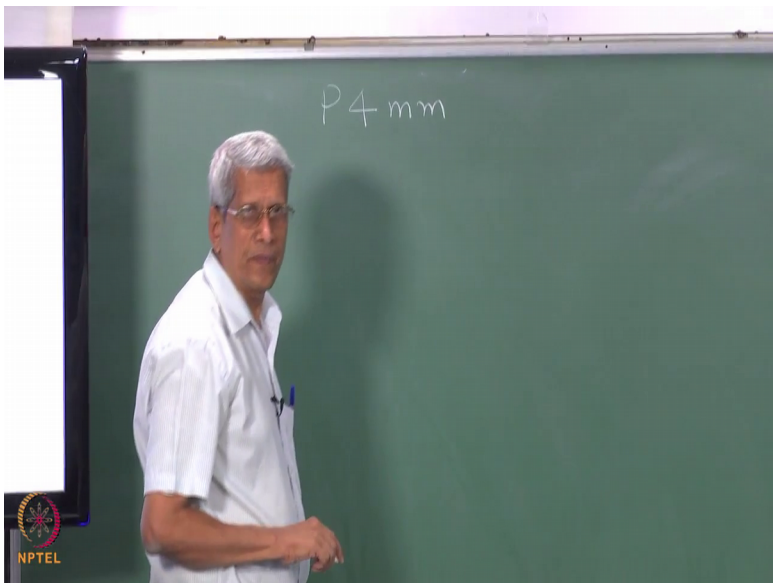

We considered it correct this is the particular type of a space lattice which we considered that is P stands for primitive 4 mm essentially represents the symmetry operation which

is there in these lattice if we look at it 4 mm essentially is a just a point group symmetry correct.

In a space lattice we could have a right plane also can be associated with it then what may happen is that these can turn out to be P 4 m and one mirror if it turns out to be a glide along that direction instead of that mirror then this is the sort of a space group which will be mentioned what essentially is that these are all the classes in which the crystals form.

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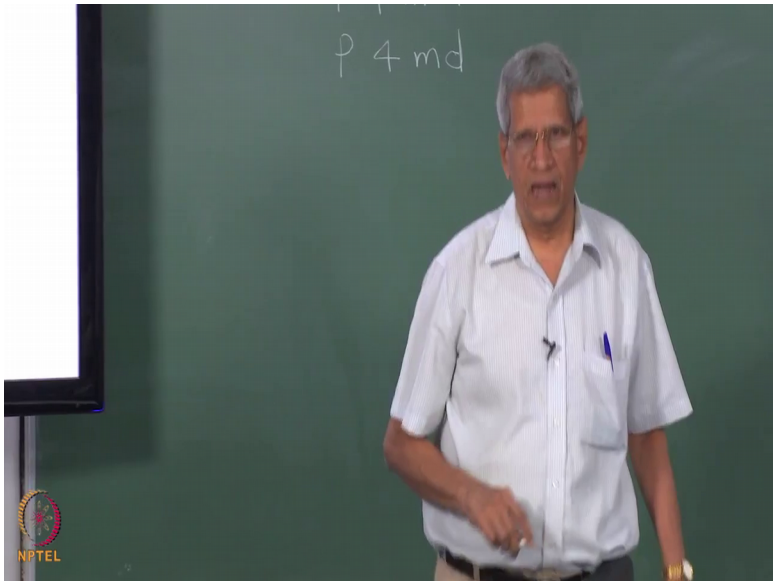

Then we look at what is the type of symmetry elements which are associated with it on that basis all these classifications have been made.

Now, the way we can represent it is one all the symmetry elements which are associated with these crystals can be represented in the projection of a unit cell for this if we construct a unit cell like this like here.

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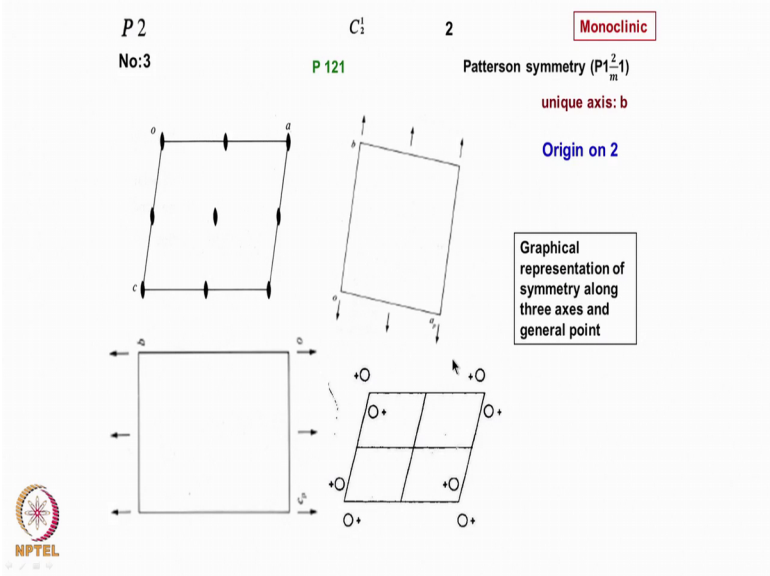

If you see that this is the unit projection of a monoclinic unit is being shown along the b axis where along the b axis 2 fold rotation symmetry is there. So, this is essentially you take this to b; this is 90 degree, this angle is not equal to 90 degree, this is what a monoclinic structure is right alpha equal that is one angle is not 90 other 2 are 90 and this exhibits a 2 fold symmetry.

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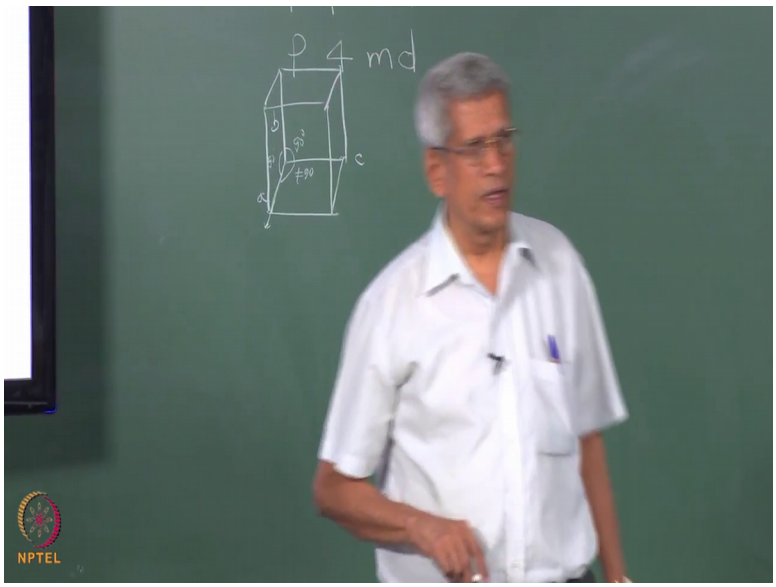

So, this projection if we look along this direction that is the symmetry axis then it will be a parallelogram and in that parallelogram what all positions at which the symmetry

elements are there that is what essentially it is being its shown in this figure correct this is one which is shown in the space group symmetry table looking at that one can understand what all symmetry elements are there at what position this symmetry elements are existing that also all these information is given this is the simplest which one can understand, because the lower the symmetry it is easier to understand though cubic system is the one which is which since we most of the metals crystals in to one of the cubic systems are in HCP we think that that is the easiest from symmetric point of if you look at it I will show you later that is the one which is very complicated to look at it.

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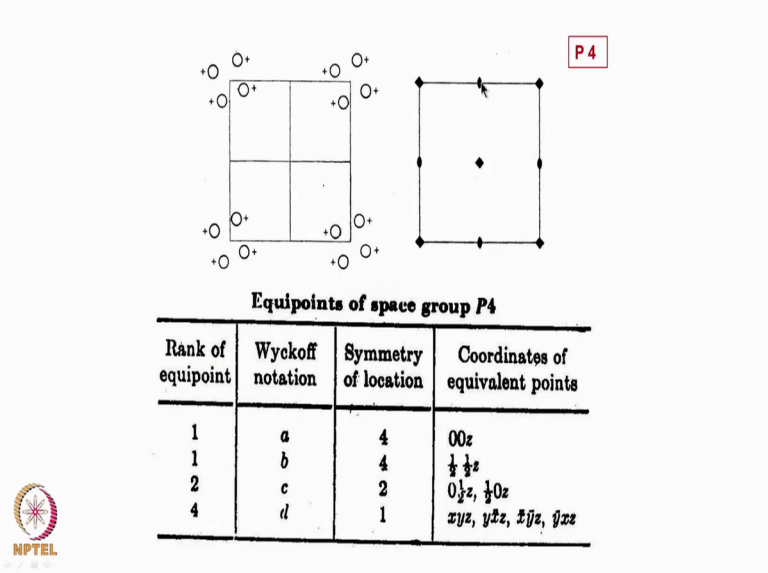

But there are 2 distinct positions are this is one position this is another position because this has only a twofold symmetry that is why it is being shown that if the symmetry is 2 the multiplicity which is word is 2 means that at 2 positions nonequivalent position the motive has to be kept see if I keep a motive here by a lattice translation vector I can generate one from one to from here to here, but unless I keep it at another point also here by a lattice translation vector I cannot generate it.

So, then it will have only just if 2 atoms are going to be there in this lattice it will not have a fourfold symmetry. So, to exhibit the 4 fold symmetry for this you need cell one more position has to be chosen correct these; what it means. So, if a put it at a the motive as position which is essentially at are random point or a general point which has only one fold symmetry that symmetry of the location is one then there are 4 equivalent positions

the atom has to be kept in these unit cell if you see it one is kept here one has come here one here and another one here within the unit cell others are if we can see it is outside of it correct

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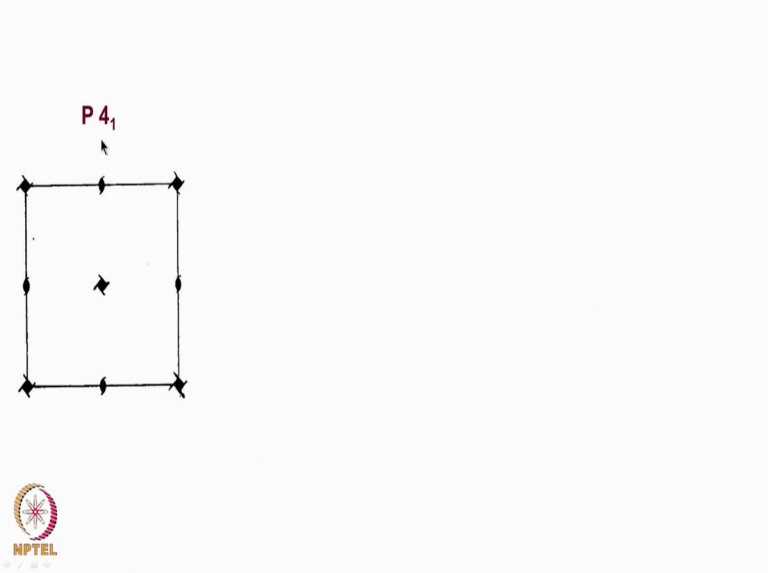

This is the same thing yes I am considering it is a fourfold suppose along the 4 fold let us assume that there is a screw axis is there 4 1; 4 1 screw axis means we have to the translation vector is one-fourth of the lattice translation vector and you displace by one-fourth and give a rotation of 90 degree correct that when you do 4 times you will be reaching the next lattice point and that symbol is shown this way that is essentially for a fourfold we show the symbol like this and on this if we show a symbol like this naturally this symbol means that it is a something like a which is rotating correct like a screw that is what it is that symbol which is being shown.

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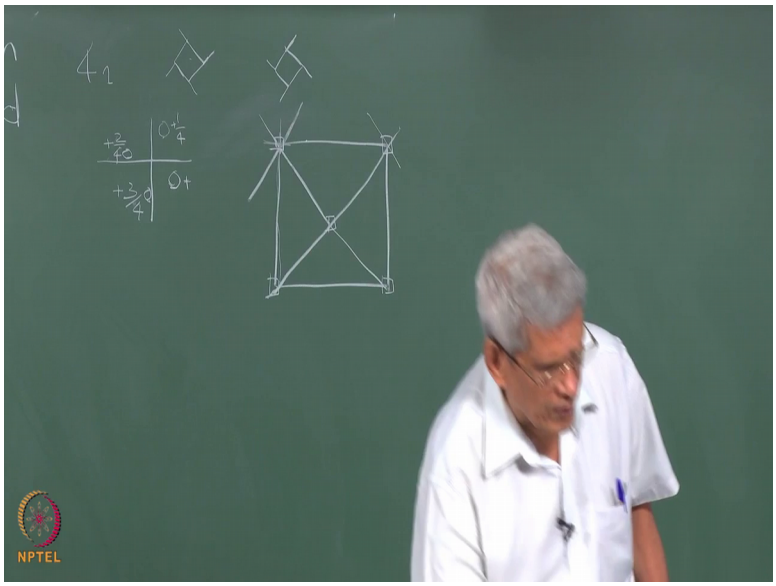

Similarly, here also if you see a screw axis is there 2 fold screw axis is there correct these are if these are all the symmetry elements which are associated with it that is when a fourfold symmetry is going to be there their own each lattice point if we consider it.

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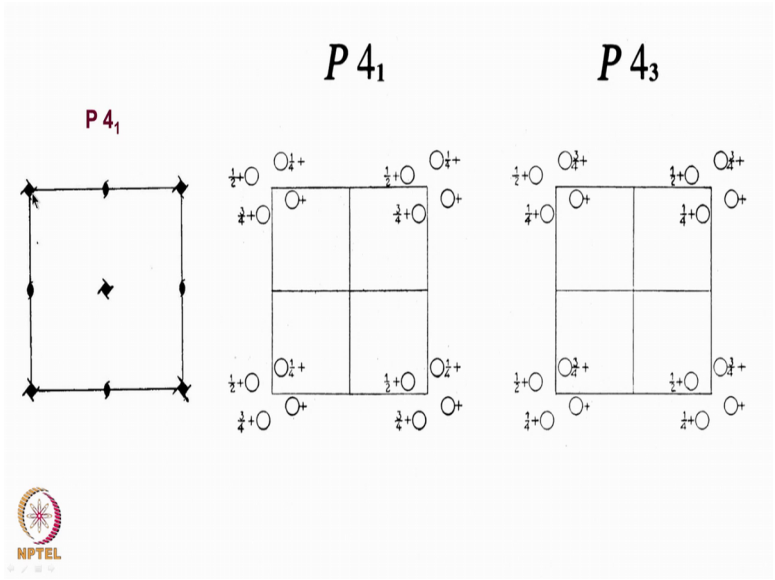

If you put a motive at a general point here 90 degree when we rotate it, it should be lifted by one-fourth correct. So, it will come somewhere here plus one-fourth then again another 90 degree plus 2 by 4 then it will come somewhere here plus 3 by 4 correct then

it will come back again what that represents is your own this axis you assume that this is where the motive has been kept it has been rotated by 90 degree shifted by one-fourth.

So, whichever the position it occupies plus one-fourth it goes up because you should remember that whenever in crystallography we mention the position these are all given in fractional indices. So, that we do not have to know what the lattice parameters are exactly right. So, assume that if lattice parameter is a b c if you take it the fractions of the lattice parameter with which the distances are measured are given.

So, that is; so one-fourth it will come here and another one-fourth if we take it; it will come here right like this and another one-fourth it will come here then after words it will come to this point. So, this if you have to mark it as I mentioned darely here that is if lattice position is at some particular point when we put half or one-fourth; that means, that from the projection plane it is lifted up shifted up by that much of a distance that is exactly what is being shown here and you see between this and this is P 4 3 this is the anticlockwise.

So, this is similar to this what will happen here in this way also we can show what is the other way in which this symbol can be represented both these symbols this one and this one if you look at it if one is clock wise another is an anticlockwise correct. So, these 2 symbols are used to differentiate between clockwise and anticlockwise rotation these are all given in the table you do not have to bother about it these symbol, but I just want you to understand. So, this is how it looks like.

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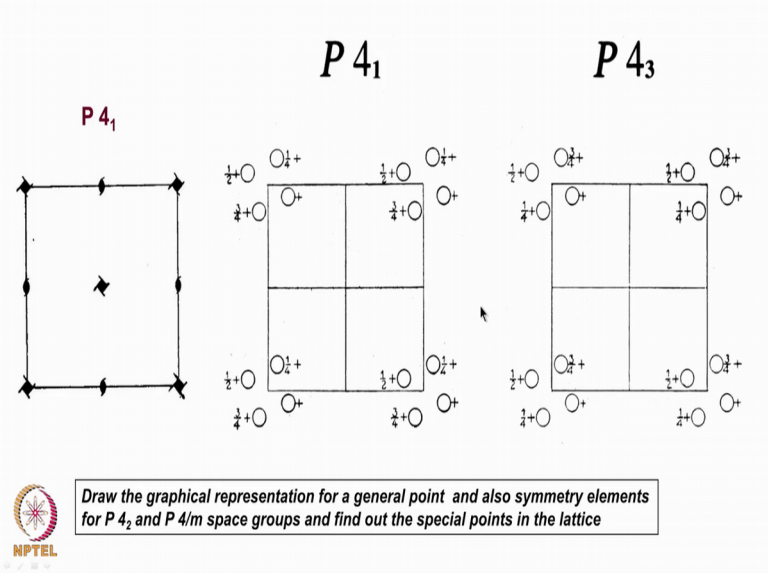

What I want you people to work out is that how it will look like for P 4 2 what sort of symmetry which will be executed by the same logic which you can apply think about it and how the;

Student: Would not P 4 2 become 2 fold.

2.

Student: 2 fold.

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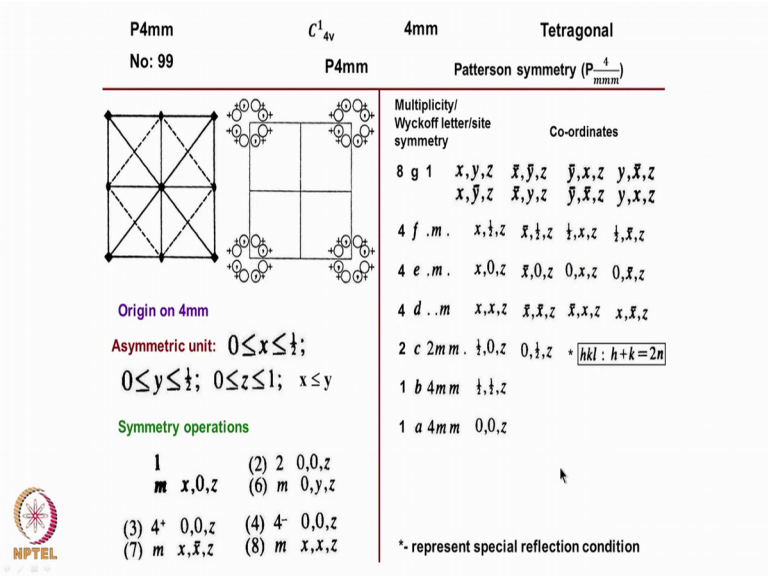

That is a distinct difference is there between this 2 now will just look at if sample has got a crystal has got a P 4 mm symmetry 4 mm is the point group which is associated with the lattice correct.

So, if we take a lattice like this the first thing which you should have is around this direction axis we have a fourfold rotation which is associated with it correct then what are the others symbols then there should be mirror one mirror should be there like this correct another mirror should come like this also right that is what essentiality what is going to be there is it not then; that means, that this is a fourfold how we represent a mirror is this line is made that is the only way this mirror is represented the plane of the paper is the mirror is lying on x is z or y is z plane that line is made thick if the line is thin there is no mirror is associated with it.

There are many ways of representation those symbols you do not bother about it, but now you just look what all the symmetry elements which are associated with it; it has fourfold symmetry at 2 points 2 fold symmetry are there at 2 points correct then mirror is there 2 types of mirrors. So, these are all the positions where an atom or a motive could be kept the simplest case which we can take it is we assume that we are taking an atom and trying to form a crystal having this symmetry then if we put the atom at this point then by translational symmetry this points will be generated or that is one which we can do or we can put an atom at this point also both these points have got the same symmetry which is because here also the full 4 mm symmetry is associated with it correct.

Student: The dotted lines have mirrors in this case.

These dotted lines are glide planes glide also comes in glide as a consequence of the lattice itself it is there dotted lines represent glide plane is it clear see if I put an atom here as I mention if I put an atom around a random point here let us look at the random point at a general point if I am putting an atom here. So, your own this point 4 mm symmetry as we satisfy. So, you take first the 4 fold axis; that means, that one is kept here another has to be kept at 90 degree around it another here another here it should come correct then with respect to this axis we have a mirror plane is also there; that means, at all these atoms which are there this position by mirror they should be reflected.

So; that means, that corresponding to this one here this one mirror that kama represents a mirror corresponding to this one mirror once this has been completed you can see that

that is going to be a mirror here there is going to be a mirror here correct. So, complete mirror symmetry by putting 8 atoms in this fashion the symmetry of the crystal is exhibited. So, we are just put atoms at these positions now the symmetry can be seen, but what is the position at which you have kept it at a general point.

So, suppose we wanted to put it at this particular point then the number of atoms which are required is only one because if you put one atom at this particular point since an atom is got an infinite symmetry associated with that with that this is the point over which all the symmetry elements are intersecting is it not. So, at this particular point it exhibits fourfold rotation mirror all are there since an atom is got an infinite symmetry that also has got all the symmetry elements are there. So, when all the symmetry elements of the lattice and also the motive which we put if they coincide then this is what the common symmetry elements between the motive and the atom which is going to be there.

That is what is being exhibited by the crystal so we require only one to be put there, suppose we put at this particular point one, here there atom which is put around the lattice point then it does not exhibit any symmetry, correct, only a one fold symmetry will be exhibited suppose in a crystal like this I put at only these position like here, like here what symmetry which will exhibit.

Student: (Refer Time: 22:22).

With respect to a lattice the symmetries with respect to a lattice. So, with respect to the lattice has got fourfold symmetry; if I rotate it by 90 degree this points are only at one point which is there in the crystal. So, it does not exhibit the symmetry of the lattice unless other positions also atoms are there is it clear.

Student: Sir, d t exhibits one fold symmetry.

Which one? Only one fold symmetry it will exhibit that is what it turns out to be. So, this is what it says that what is the symmetry of this site this site has got a symmetry 4 mm and since that exhibits the full symmetry of the crystal you require only one atom to be placed one atom or a one motive to be placed at that point provided the motive as got the full symmetry of the lattice then at the center also if we keep take it instead of keeping it at that point if we keep it at the center then also we can do with one symmetry it is there is only one atom has to be kept here.

Suppose we keep it here the symmetry of this point is 2 mm and if you look at it; that means, that one 2 fold is missing. So, the one more point we have to repeat it by symmetry. So, that it will satisfy the complete symmetry that is what these 2 points which turn out to be if we keep at this point at the along the mirror if I keep one at this point at the mirror the mirror has got only a twofold symmetry which is associated with it then the number of point which are required again gets reduced by half. So, 4 positions we have to keep it because out of the total 8 positions for general we have to keep it that is what essentially it represents 4 positions which are going to be there at general point if you put a motive 8 position.

So, the crystal lattice now can be constructed by keeping an atom that is we have fixed a lattice in that lattice the in the crystal lattice atom can be kept either at this position or this position or any of this positions it can be kept and we can construct a lattice having this symmetry P 4 mm is it clear this is what essentially will happen which is the position which atom will actually occupy this is the geometrical possibility looking and symmetry is decided by the energetics.

So, generally what will happen if you are trying to keep a single one atom we take it and if is being distributed what it will try to do is that the position which has got the maximum symmetry always has got the lowest energy also in the lattice. So, that is the position which it is going to occupy. So, conventionally what happens is that like all the crystals of metals we consider like aluminum or copper we assume that the atoms are occupying the lattice points correct.

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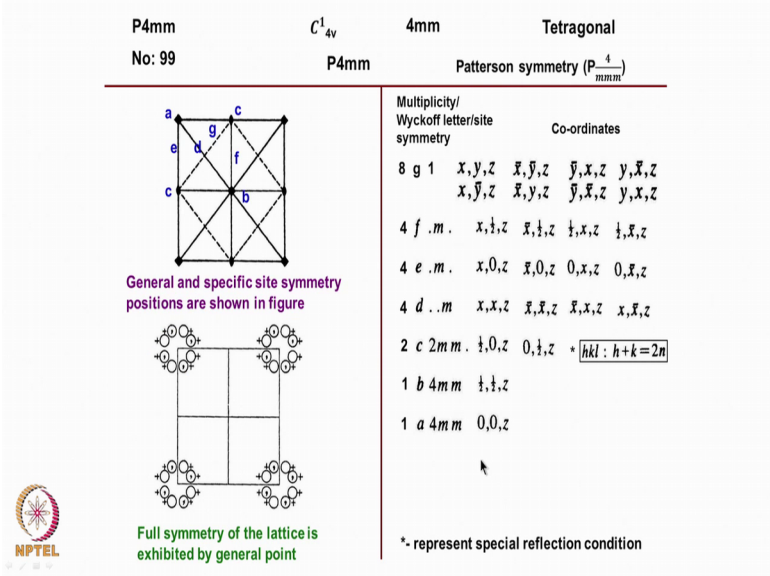

That is how we have studied these are all marked where are these positions are there. In fact, something which is very interesting it is just for the information you look at this point this point this one and the this one if you look at it this a triangle has got a the complete symmetry of the unit cell also.

By doing some symmetry operation if a flip it over it by a mirror I can generate this correct see this full unit cell can be constructed by from this smallest one this is generally called thus the crystallography then there are bodies has the smallest asymmetric unit which is required because whenever we what kind of problem kind a competition you wanted to do it we always try to make the which is the one the smallest unit which has to be constructed. And then applying some symmetric considerations you can expand it and make it the lattice that is the easiest way to do it that is one which conserves the energy also minimum energy consideration always tells that this is the way we have to go here also if we can get this information then the complete information by applying the whatever the symmetry we can generate all the symmetry elements of the lattice

Student: Sir, is it b, c, d, the smallest one.

Which one?

Student: Tan a, b, c, d.

B.

Student: B, c, d or a, c, d half of the triangle.

No, no, a, c, b.

Student: No if you take half of the triangle.

Half a c no, no, this triangle that is this one this one this one this one is what completes that full symmetry that is all which you have to take it.

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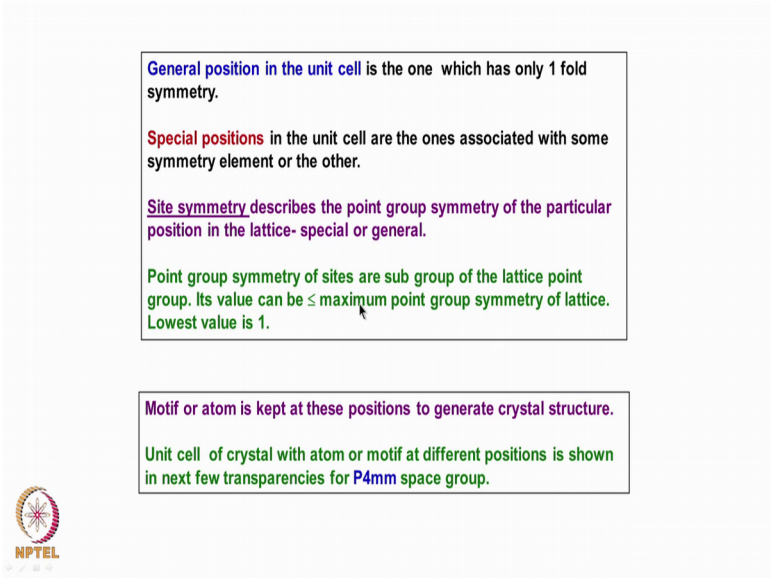

So, these are all the things which have repeatedly told that is general position some special positions are there then site symmetry is associated with each of the position and the site symmetry besides what will be the multiple city of the positions in the unit cell which will be there correct.

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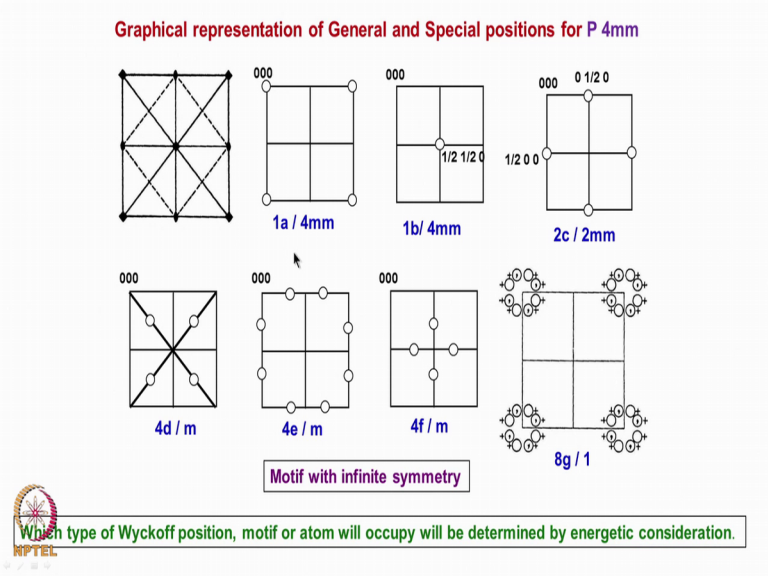

So, this is the same one I had just tried to form that is we put an atom at this position this also if you look at it this has the symmetry 4 mm; I can put an atom with this unit cell here this also shows the full symmetry because 5 lattice translation symmetry if I operate one opposition will come here another will come here another will come here this is going to exhibit the full 4 mm symmetry. Similarly if you put an atom at one of this position another at this position then by lattice translation these 2 translation symmetry when we applied these 2 positions will be generated.

Now, if you look at this; this also has got the symmetry similarly if I put it at these positions also we can generate a lattice having the same symmetry we can put keep the atoms at these positions on the lattice and then also have the 4 mm symmetry at these positions also we can put it have the full 4 mm symmetry or if you put at a general point this is the way the atoms will be put then the 4 mm symmetry these are all the possibilities which are there where atoms can put it, but which position it will take as I mention will be determined by the energy consideration.

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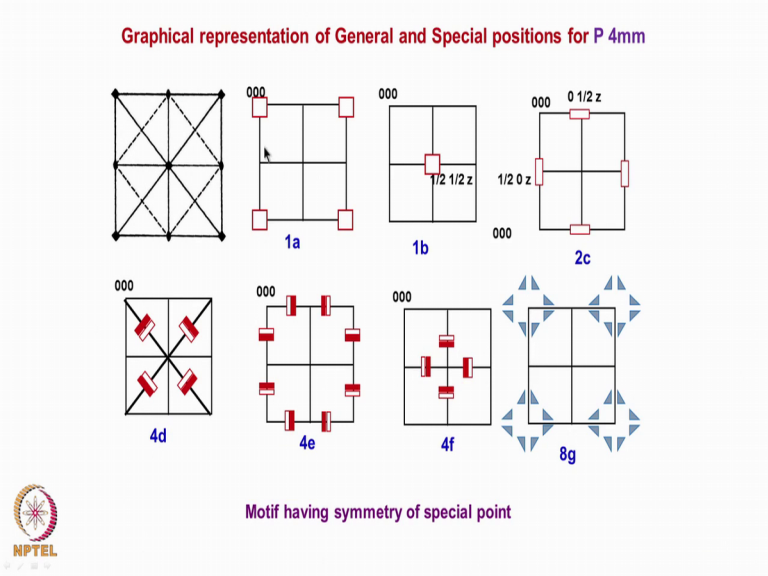

So, if I want to put a motive at this particular position what is the motive should have the motive should have the 4 mm symmetry should be there right that is what I had just shown a motive which is there like this here if I put it at this particular point that motive should have a symmetry, because that is I have chosen a shape of a motive which exhibits their 2 mm symmetry that is what essentially what is being done here an asymmetric point I have put an asymmetric motive that does not matter what it is if I chosen asymmetric point even if I take an atom and put it seems the site in the unit cell has got a one fold symmetry at 8 positions it has to be kept because there is no symmetry element of the motive and the symmetry element of the crystals are intersecting.

So, the common intersection if we look at it is only a one fold between them that is why 8 positions we have to keep in. So, here an asymmetric motive is being taken that is I have just shown and when we keep it around this lattice point this is how it will look like if I put it around this particular point also this is how everywhere if you try to see it within the unit cell how many are there 1, 2, 3, 4, asymmetric 8 are there correct here also 8 asymmetric motives are there here also even though we had kept this around 2 mm symmetry now if you look at the within the unit cell how many?

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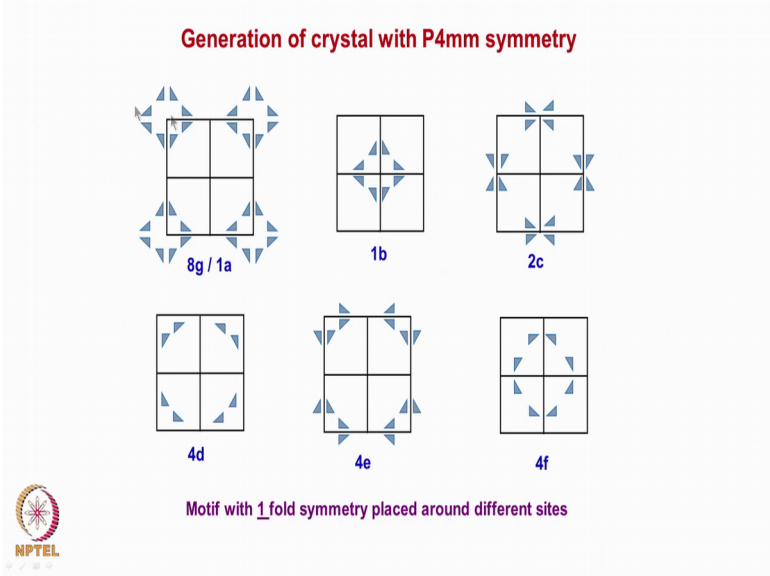

Student: 8.

8 are everywhere you will have they if you look at it they all of them satisfy the 4 mm symmetry that is the crystal symmetry satisfied by the motive. So, whichever configuration you put the motive unless in this specific way they are placed we will not be able to generate the crystal exhibiting this symmetry is it clear that is what I am just showing it see here.

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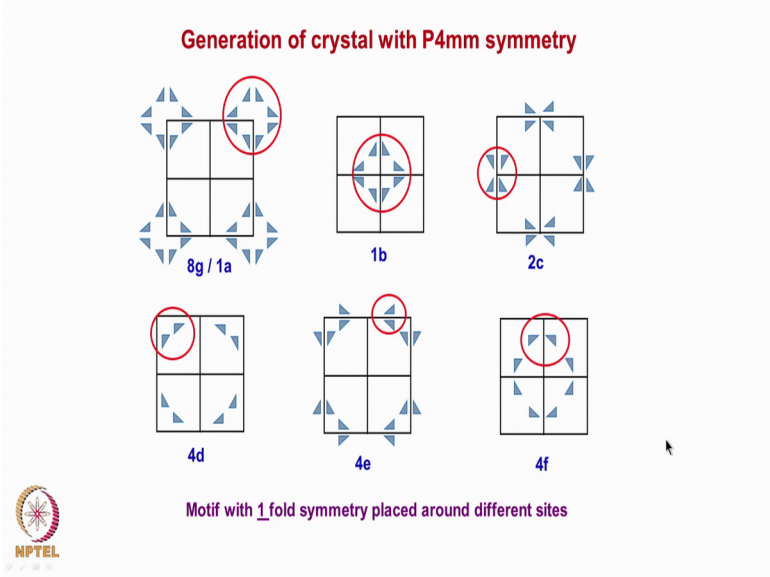

This is an asymmetric motive we have kept the asymmetric motive at a particular point and created the 8 positions. So, that it generates it exhibits the symmetry of the lattice correct.

Suppose I have a molecule with this sort of a configuration exhibiting the symmetry; that means, that it has a 4 mm symmetry associated with it I can put it this position what is the other position in which I can keep it is if I rotate it by 45 degree this also exhibits that symmetric right. So, these are all the 2 positions in which a motive cluster can be kept satisfying 4 mm symmetry you consider this case it has been rotated by a small angle now what is the symmetry this exhibits the symmetry which crystal exhibits.

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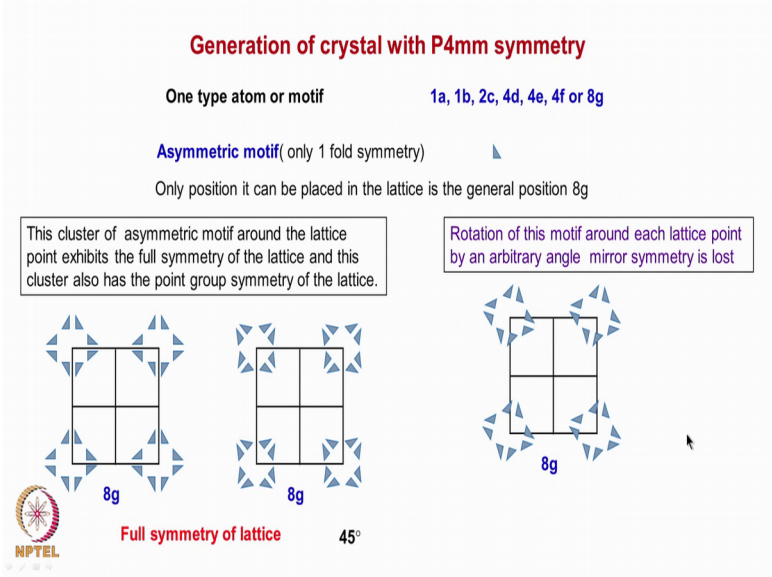


Student: Fourfold.

Fourfold only a fourfold rotation is there.

Student: Mirrors are lost.

Mirrors are all gone though if you look at this cluster this cluster is the same the same cluster of molecule how you place it when you place it because the cluster itself has got a point group symmetry elements associated with it whether the axis of all the symmetry elements matches with the point where we are keeping it with that symmetry element or not at that particular point what all symmetry elements which are common that is the only symmetry element which the crystal will exhibit.

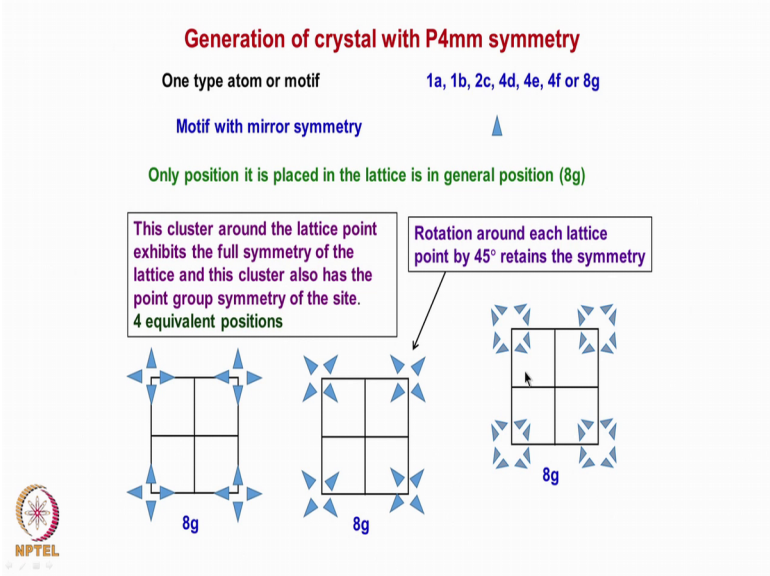
Otherwise in an any lattice you take an atom, atom has got an assume it to be a sphere the sphere has got an infinite symmetry associated with it right if we put the sphere around a rectangular lattice it exhibits only the symmetry of the rectangular lattice correct if you put it around a square lattice it will exhibit the symmetry of the square lattice correct though the sphere has got an infinite symmetry that symmetry is not what is being exhibited, because what is the symmetry element which is common between the lattice and the motive which we are keeping in that the symmetry which the crystal exhibits is it clear here I have taken a motive with a symmetry which is it has got a mirror symmetry is there.

Now this motive because what all the ways in which we can constraint that is what I am trying to explain illustrate it with some examples here if 4 of this motives if I keep it around it correct it satisfies the 4 mm symmetry only 4 motives are required when we chose when we took an motive which has no symmetry associated with it we required 8 right since a motive itself has got a 4 mm symmetry as if associated with it where mirrors symmetry associated with it and we are keeping it in a position such that the mirror symmetry of the crystal.

Student: Matches.

And the mirror symmetry of that motive matches. So, the number of positions at which it has to be kept has reduced to half not 8 it is 4 and the other position where we can keep it is here by 45 degree we can rotate it.

(Refer Slide Time: 35:51)



This I had already explained. So, suppose these motives I tried to put it at a position where the mirror symmetry does not match; that means, that I put the motives somewhere here at this particular point then what will happen 8 motives have to be kept correct though the motive has got a 2 m mirror symmetry unless we keep at a 8 positions it will not satisfy the symmetry of the lattice that is what one should remember.

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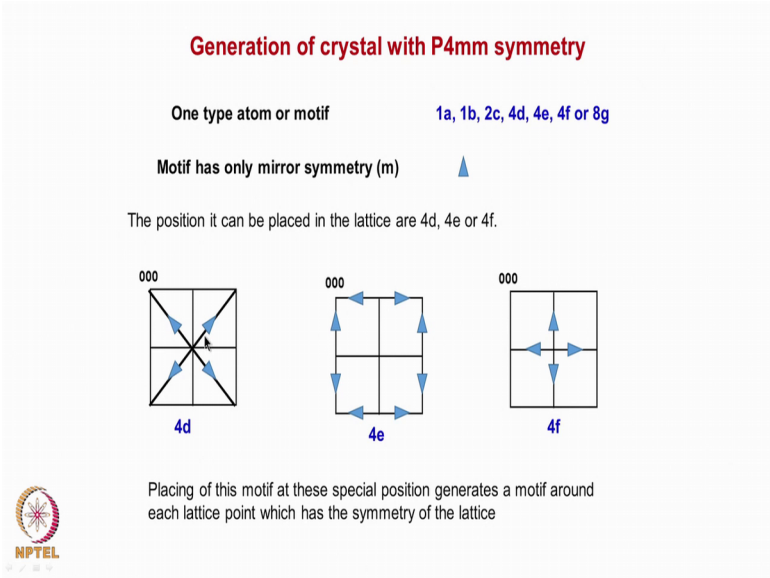

This is for other positions like that Wyckoff positions d that d e are positions and this is the multiple city what is being shown.

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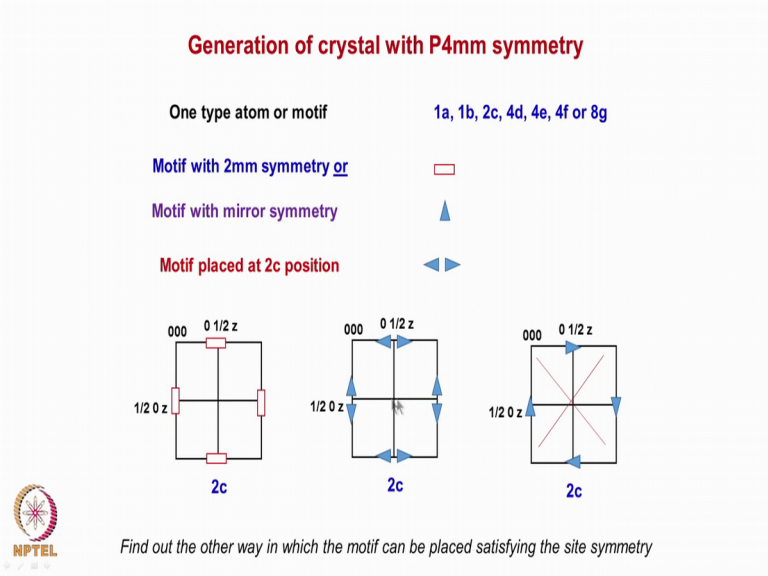

Here if you try to look at it in this one its being shown us it has a mirror symmetry associated with it if we keep it like this; this does not satisfy if you look at it no position is identical these will not satisfy the fourfold the 4 mm symmetry is not there in this; this I will give you some examples which when you work it out you will understand all these aspects.

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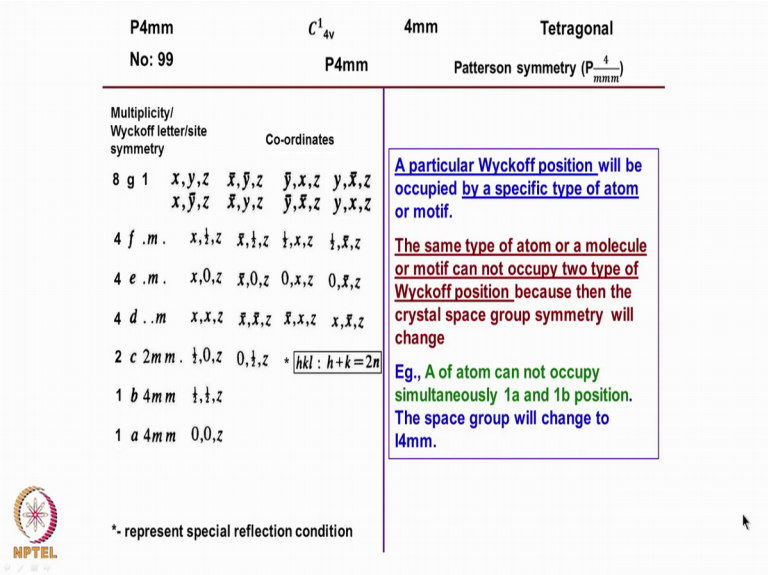

The what is most important part of it is that I mentioned a very ware that when some special position and general position is there in the lattice like here all these positions

which are being given this is one side symmetry another side symmetry these are all the called special positions this is the general position.

Suppose we wondered to put an atom and some position in the lattice and generate the crystal suppose I put an atom of a particular type in these position these position means that essentially I am putting an atom in this crystal one here one here another here and another here then a 4 mm symmetry is satisfied correct is it clear element that is the only position which is possible suppose the same atom I tried to put it in this position you know what will happen that position is also possible after filling it up if I try to put it in that position what happens now what is the symmetry which it will have.

Student: C.

Yeah.

Student: Simulate.

The symmetry is as changed it no more has the same symmetry 4 mm symmetry is not there. So, that is not possible; that means, that only a particular Wyckoff position you can put an atom and fill the same atom cannot be put at an another apposition also if you try to fill it then you find that the structure which we generate the same type of an atom if I put it at all these positions it will be generating a lattice which have some other symmetry now this symmetry. So, one of these positions only you can do it fill it up is it clear that is what I had mentioned a atom cannot occupy simultaneously both one a as well as one b position because then the symmetry of the lattice has changed another is stoichiometry.

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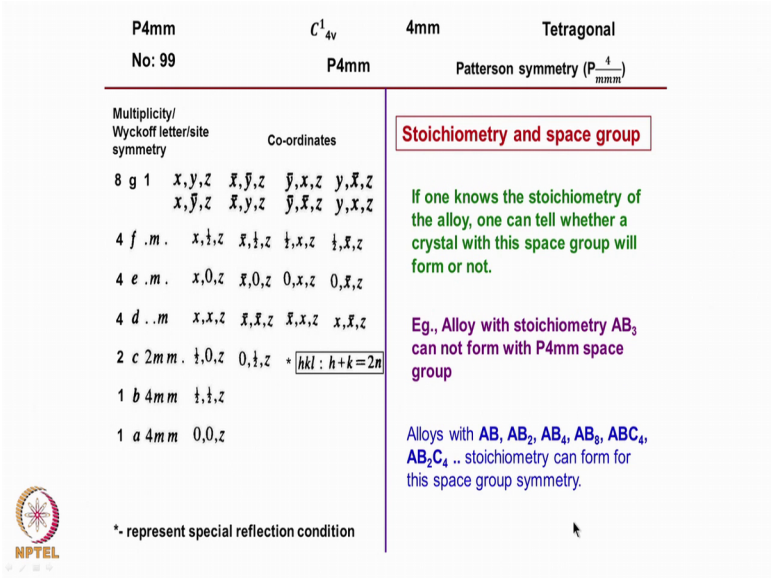

Suppose I put the 2 atoms are there a and b if I put a atom at this position this is where the a atom has been placed I place the b atom at this position this is a and this is b the b atom will also another b atom will come here another will come another will come here these also satisfies the 4 fold symmetry. Now the stoichiometry of the alloy is a b correct this alloy satisfies the 4 mm symmetry right because a atom alone this forms a lattice which satisfies a 4 mm symmetry b atom. If you look at it this as an another lattice similar lattice which also satisfies the 4 mm symmetry these are generally in crystallography, we call it as sub lattices that is e whenever ordering is there each type of atom we can consider us occupying a typical example which we can take it is n i a l if I take nickel and aluminum.

Nickel occupies corners and aluminum occupies center of a cube for this a simple case if we can take it is that a simple cubic lattice if we take all atoms are occupied by a atom. So, its space group is a primitive one correct if the same atom because at the center also will have the same symmetry if you put a atom there what it will happen now it becomes a body center na, it is a different structure that is what I said that symmetry changes. So, that is not possible, but in that position another atom I can put it b atom if I put a b atom in that position then the stoichiometry of the alloy is a b, but the symmetry is like in this case P 4 mm, it will be a simple cubic only that is how it happens by looking at it I can make out that is if suppose I see there an alloy I wanted to have a symmetry which is A 2, AB 2, AB 2 means that what is going to happen is that a atom I fix it this is the highest

symmetry point. So, that is what a atom has occupied and formed a lattice where can the b position can go now.

Student: (Refer Time: 42:16).

It is only going to the face center now in this lattice that is if I draw it a atoms are occupying, I will just put it across to tell the b atom. So, the b atoms now have to occupy only the face center now if you look at the stoichiometry.

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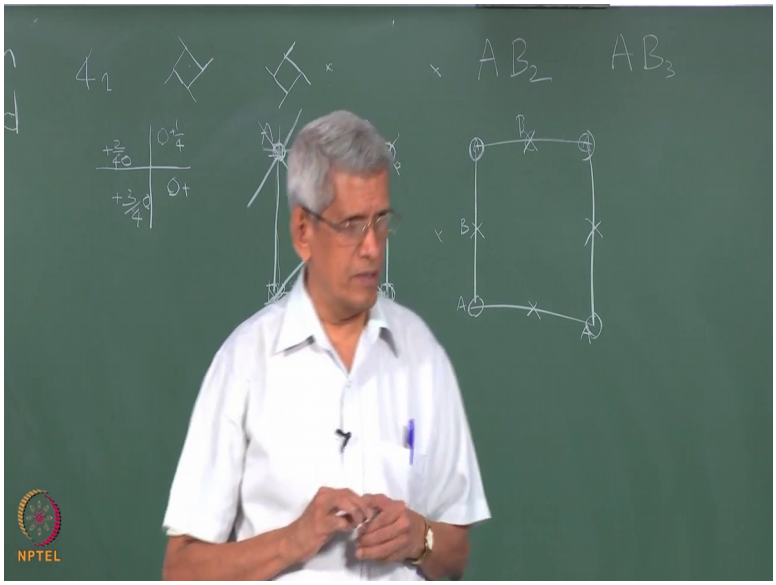

This will turn out to be AB 2, correct that is what here also it says one atom is will be there in the unit cell, it is 2 and in this particular lattice, suppose I wanted to make an alloy with AB 3 that is having the space group 4 mm AB 3 is it possible you look at this table that if we put it is just not possible we can have AB; AB 2, AB 4 is possible AB 8 is possible; a b c; there are various combinations which we can try this are all the ways in which you can build cell is it clear; because this table if you look at it that is a b composition means that one atom can occupy here another can occupy this position; that means, a b is a stoichiometry, suppose in the unit cell what we wanted to have is that not AB; AB means that it is a stoichiometry (Refer Time: 44:08) the number of atoms in the unit cell suppose you wanted to have instead of a this one assume 8; that is A 4 B 4 stoichiometry is a b, but 4 atoms of a and 4 atoms of b as to be there. So, how will we go about now?

Student: We choose.

Then if we choose one this one 4 atoms of a can come in this unit cell and another position if I choose it like this 4 atoms of b will come which we can put it at this position now again the stoichiometry is a b, but the number of atoms per units cell has increased this is what is call it has a molecular formula where is what is the total number, yes.

Student: Sir, you said if a atoms occupy all the 4 corners.

Yeah.

Student: And if it occupies also the center the symmetry is still same right, sir.

No.

Student: Only the structure is different.

No, symmetry has changed the symmetry is always based on which type of an atom which we put it, if the same type of an atom if you put at like that is what I said you take a simple cube in which simple cubic lattice in which you put a atoms at all the corners, what is the symmetry which it has a atom is a showing a symmetry which is a simple cubic symmetry if I put a b atom.

Student: (Refer Time: 45:35).

A atom at the center now what is the symmetry which it exhibits body centered. So, in the space lattice primitive and body centered face centered there are all 2 distinct Bravais lattices now they have changed.

Student: (Refer Time: 45:49) axis in the like the rotation axis and the mirror axis are still the same.

No symmetry how do you define symmetry is defined by whether we have an identical position where it goes. So, if the same atom if you put it the positions are changing if you put a different atoms till the identical position that is how symmetry you have to look from the definition that is how the symmetry changes is it clear. Now, you see that you can make out what all types of a stoichiometry compounds which can form with this sort of symmetry that also we can find out you understand that the power of this table is that

looking at this table we can talk about what sort of a alloy if this is the stoichiometry which a material has got this is the space group symmetry which it has got then we can tell which position atoms are going to occupy in the lattice we can determine looking at this table and construct the crystal structure is it clear. So, now, I have told you about the molecular formula also that is how it is going to be correct, yes.

Student: Sir, atoms sometimes occupy even like alternate tetrahedral voids. So, you can occupy half of the;

See, tetrahedral voids octahedral voids are what essential there that its like this when I fill up a position of an atom on this one the next position which an atom can occupy is what you call it a sub white that also has got a symmetry associated with it I will come back to a crystal structure how it is done then you will understand that this symmetry elements essentially represent what is the position; next position available position which an atom can occupy.

That means, that once this position has been occupied the next available position which has got the lower symmetry is the other one that is where the atom will go if that is filled when we have to put the third atom into it. Now that will look for which is the next available position from the symmetry consideration which is free that is the only position which it can go and the occupy that is exactly what this table also represents this table represents from the symmetry point of view what we have studied is looking at what all the octahedral and tetrahedral voids both are identical from this only that has emerged.

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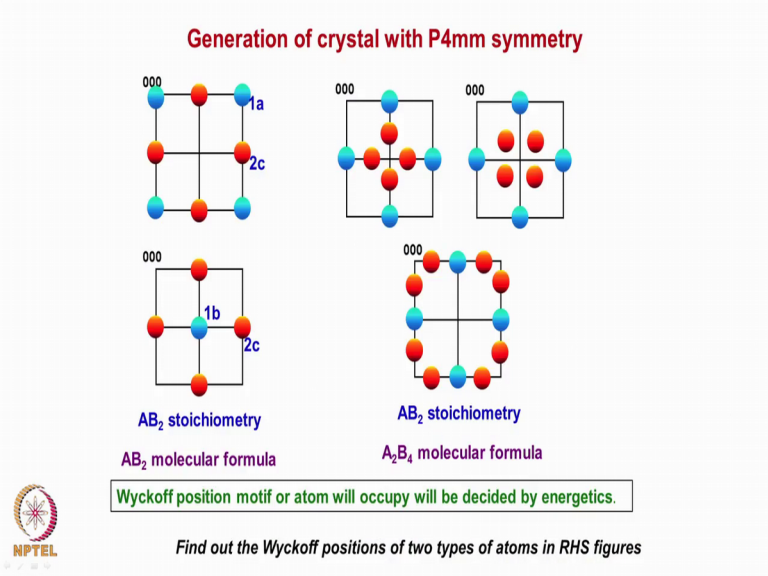

So, here what I have done is taken 2 types of atoms and if you look at this the stoichiometry which I wanted to mention maintain is AB 2. So, which is a position that blue atom occupies all the corners and if the b atoms that is the orange one that occupies all the face centers then this will have an AB 2 configuration correct what is the other way in which it can happen there are 2 possibilities are there the a atom can occupy 4 mm symmetry at the center also it occupies that like here.

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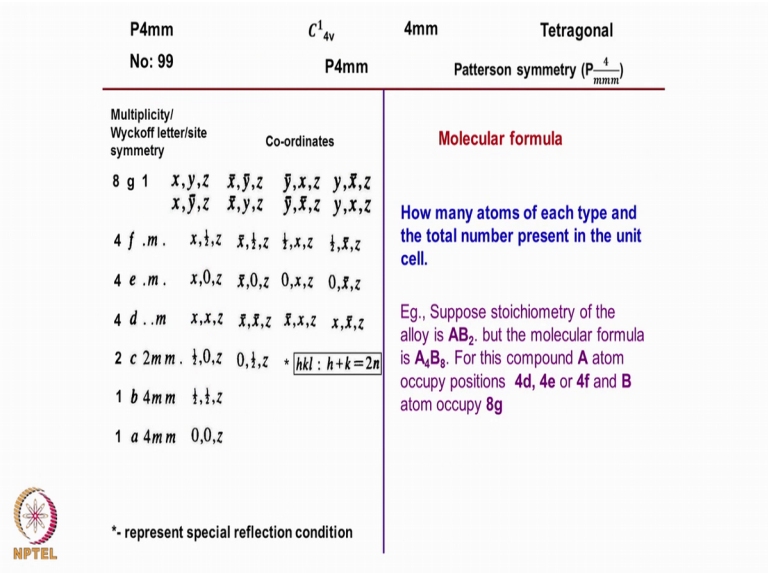

A atom can occupy this position and b can occupy this position or a can occupy this position b can occupy this position these 2 both the possibilities are there correct we are considering both these possibilities, but if you construct the full lattice.

Student: It is a.

Both of them are the same you understand that this actually coming from again a from symmetry consideration now if you look at the next one there the molecular formula is A 2 B 4, but the stoichiometry is if you consider it stoichiometry is A 2 B 2 AB 2 correct. So, there the possibilities which are there are this position or this position this is one combination or this and this another combination or this and this that is a third combination 3 possibilities are there, but all of them will have 2 atoms of a and 4 atoms of b correct that is exactly what we are considering into all these 3 positions

Now, how exactly that atoms have to be there is which one will have the lowest energy configuration for the crystal is will decide which position finally, will be the stable position the crystal will occupy, but what the geometrical crystallography tells is that these are all the 3 options which are available to which it can form now energetics is going to decide which is the position because here you can see that the bound length will be different na. That finally, the bound length is which is going to matter here again you try to draw it and see how it is going to be then you will realize it A 4 B 8 is also stoichiometry B 2, but the molecular formula is different this happens with chemistry also na; CH 2 is there CH 2 N, you can put it they will not be that same that type of a thing which happens here also because that an example which I can tell you is that your studied you about carbide precipitation in stainless steel right what is the type of carbide which it forms.

Student: C r 23 c 6.

C r.

Student: 23 c 6.

C r 23 c 6 here also that same thing which happens.

Student: Here (Refer Time: 52:01).

Exactly like that it will happen.

Student: Here is odd number also.

How many positions which they have to occupy that we have to. So, how many atoms have to be there now in the unit cell that is what you have to be done.

Student: Sir, it s only 116.

Yes, the total number of atoms in the unit cell is 116 for m 23 c six that I will come later and show you the Wyckoff position table then you will understand how it is possible you understand that I will come back to this same example again other one will turn out to be 106 or 108 for m 766. So, not only the structure when 116 atoms are there you cannot put it on a simple just position on the Bravais lattice.

Now the number of positions where they have to be kept the lattice parameter has increased the number of positions where you can keep it like this it is going to happen is it clear because normally we think that when we understand that carbide is essentially chromium carbide is c r 23 c 6, this actually means this only the stoichiometry of the carbide the number of atoms which are going to be there in the units cell is 116 atoms in this ratio it will be maintained this what I wanted to make you then when we understand when we have a table like this the space group symmetry table looking at this we can fill up and tell that this is how the positions which atoms will occupy is it clear.

Student: Sir, the 3 units are there for a 2 b 4 type.

Yeah.

Student: If you fill the fill the whole lattice with.

Yeah.

Student: Many of them as it will generate the same lattice.

You just make out and tell me find out whether it will happen or not.

Student: I think. So, it happens.

It can it can happen; it may not happen, but try to find out and tell me and another also if you see it here these positions some of this positions are fixed positions in fractional indices correct some of this positions I have given x axis (Refer Time: 54:14), right, x axis is said means that if that x has some value y also will have the same value is said as an another value, but what the value of x is not fixed. But from the symmetry point of view it can have any value; x can have any value these are all the things which when we do it experimentally, try to do using either x ray diffraction or electron diffraction or neutron diffraction, try to find out what this values of x y (Refer Time: 54:48) we can find out.

But the symmetry remains that same, but there x y (Refer Time: 54:52) immediately tells you what exactly is the position which atoms occupy correct that is what we get from diffraction experiments that is why understanding these symmetry is important first tells the this is what the structure it can have then when we get the diffraction data then you try to analyze it, because simple structures when we work with FCC based metallic systems it is very simple; all information is available, but when you are working on crystal systems; which have different symmetry or like oxides (Refer Time: 55:30).

These are tough material then you find that one has to find out the version because the charge balance determines at what positions the atoms sometimes it can be slightly off from these positions also is it clear just with this I will stop it.

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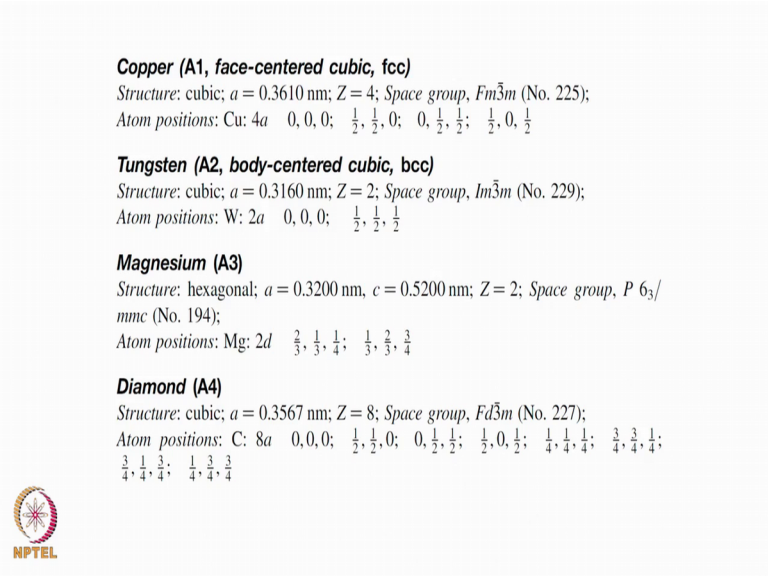

Now, if you look at it how is the information which is available in the literature like copper if we look it into the many of the books which are there appears hand book and all if we look at it; it will copper there are many ways in which these crystal structures are represented a one is one which is being followed then the space group symbol if you try to see it; it is F m 3 bar m these I will come to later and then the number is given as some 2 to 5. This 2 to 5 is the space group number that in that space group if we go we can see it and the structure is cubic lattice parameter is given is Z is 4; Z is 4 means that there are 4 nonequivalent positions are there.

Therefore, atoms have to be there total number of atoms in the unit cell correct and what all the positions a Wyckoff position a means that the maximum symmetry is always for that a Wyckoff of position at the lattice point 4 atoms are there these are all the positions where the 4 atoms have to be there like if you see diamond here; here the total number of atoms have to be 8 space group is f m f d 3 bar m atom positions are 8 a because a position, but 8 add positions it has to be there what all the positions which they should occupy this is essentially the positions which are taken from the table which I had shown we have consider the table only for P 4 mm symmetry, but for all the ones it is given in the international union of crystallography table.

Similarly, for like sodium chloride sodium chloride is a FCC is it not it has 4 atoms of sodium and 4 atoms of chlorine stoichiometry is one iodes NACL, but how many molecule NACL molecules are there 4 are going to be there in each unit cell. So, that is what this number result 4 represents.

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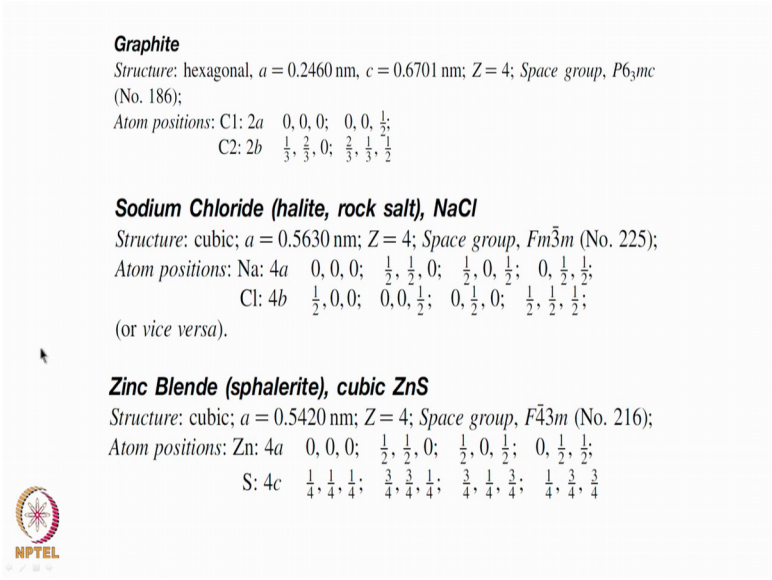

The sodium will occupy a 4 a position that is a position, but 4 atoms chlorine will occupy the b Wyckoff positions 4 atoms are there that positions are also given like this the information are is available from crystal structure data hand book and all these things they give this information these itself could be used to generate data, but suppose we have to find out how to generate a particular type of a stoichiometry with these whether it is possible with these symmetry what all other possibilities which exists.

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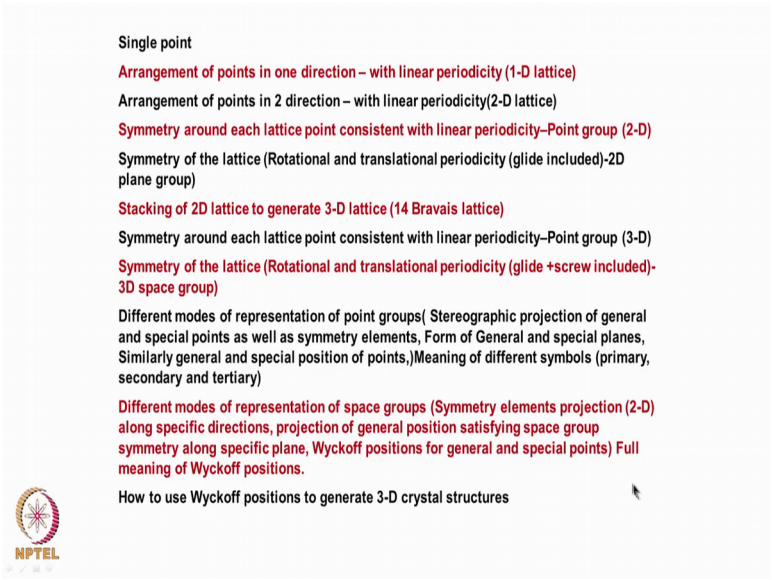

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The 11 Laue groups

System	Laue group	Examples of space groups
Triclinic	$\bar{1}$	$P1$
Monoclinic	$2/m$	$P2$, $P2_1$, $C2$, $C2_1$
Orthorhombic	mmm	$P2_12_12_1$, $C222_1$, $I222$…
Tetragonal	$4/m$	$P4$, $P4_1$, $P4_2$, $P4_3$, $I4$, $I4_1$
	$4/mmm$	$P42_12$, $P4_322$…
Trigonal	$\bar{3}$	$P3$, $P3_1$, $P3_2$, $R3$
	$\bar{3}/m$	$P321$, $P3_121$, $R32$…
Hexagonal	$6/m$	$P6_1$, $P6_2$, $P6_3$, $P6_4$, $P6_5$
	$6/mmm$	$P622$, $P6_122$…
Cubic	$m3$	$P32$, $I32$..
	$m3m$	$P432$, $P4_132$, $I432$, $F432$...

The symmetry of the diffraction pattern (Laue symmetry) does not uniquely determine the space group of the crystal (unless it is triclinic).

Then using this table we can find out what type of stoichiometry and what type of crystal structure can be generated this is what essentially we have considered here.

(Refer Slide Time: 58:54)

Symbols of Symmetry Axes

Symbol	Symmetry axis	Graphical symbol	Nature of right-handed screw translation along the axis	Symbol	Symmetry axis	Graphical symbol (normal to plane of paper)	Nature of right-handed screw translation along the axis
1	Rotation monad	None	None	4	Rotation tetrad	◆	None
$\bar{1}$	Inversion monad	○	None	4_1	Screw tetrads	◆	$c/4$
				4_2		◆	$2c/4$
2	Rotation diad	(normal to paper)	None	4_3		◆	$3c/4$
		→ (parallel to paper)		$\bar{4}$	Inversion tetrad	◆	None
2_1	Screw diad	(normal to paper)	$c/2$	6	Rotation hexad	⬢	None
		→ (parallel to paper)	Either $a/2$ or $b/2$	6_1	Screw hexads	⬢	$c/6$
		Normal to paper		6_2		⬢	$2c/6$
3	Rotation triad	▲	None	6_3		⬢	$3c/6$
				6_4		⬢	$4c/6$
3_1	Screw triads	▲	$c/3$	6_5		⬢	$5c/6$
3_2		▲	$2c/3$				
$\bar{3}$	Inversion triad	△	None	$\bar{6}$	Inversion hexad	⬢	None

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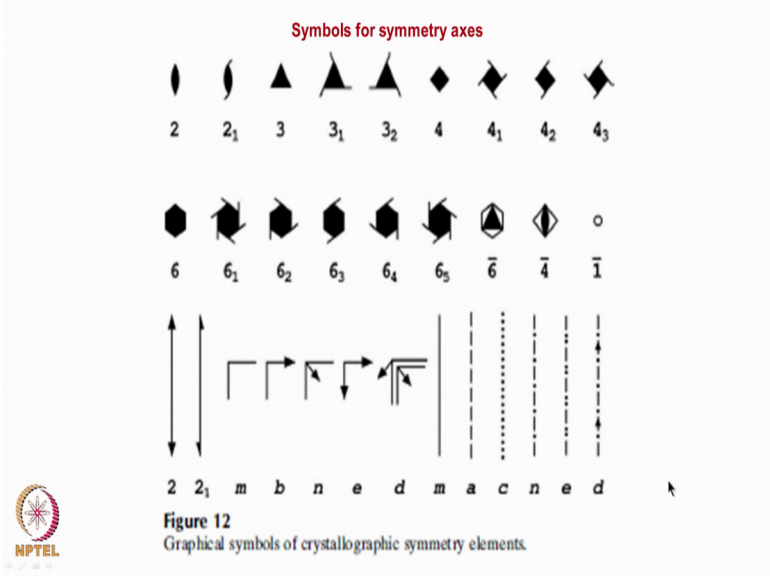

This any way you can see it here I will just not leave it.

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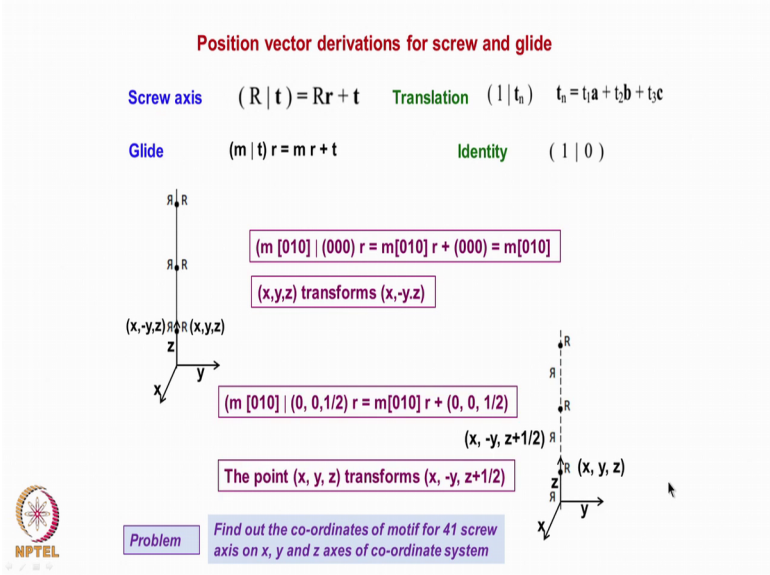

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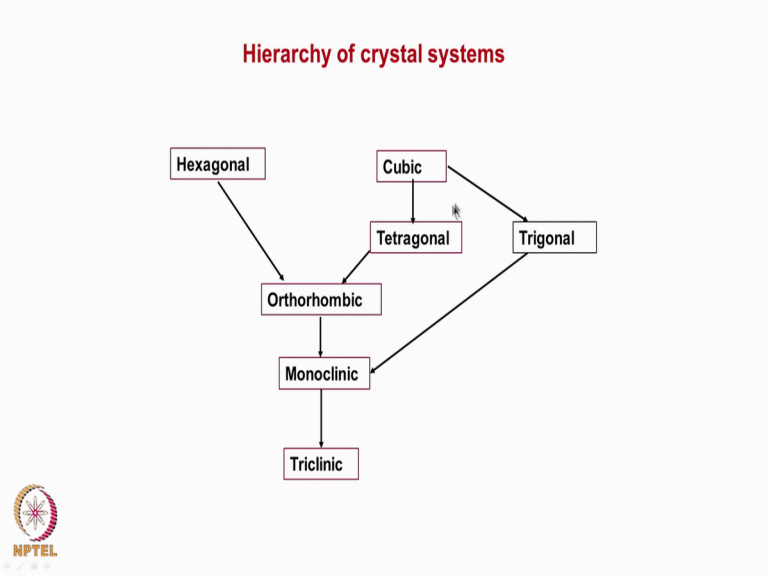

One more which I wanted to show is just the hierarchy of stichio structures. Normally metals form with these are hexagonal or cubic correct most of them metals which form then when a face transformation takes place in a cubic lattice by replacing an atom (Refer Time: 59:20) hexagon by an atom of another type then it can go to only orthorhombic or monoclinic or triclinic from cubic it is to tetragonal or orthorhombic or monoclinic or this one or cubic to trigonal if it forms to trigonal from trigonal it can only go to monoclinic.

So, what is the transformation path when we do some heat treatment what sort of crystal structures which it can form during order disorder transformation that also this table essentially tells us that information suppose in a FCC material an alloy an hexagonal face forms from this you can make out that it is not possible if it has to form only by introducing a defect in the FCC structure you can form the FCC you know that when a stacking fault is formed in FCC it is nothing but the structure of HCP that is the only way we can do it. So, if we can go from one to the other its possible, but that is always by the introduction of some defects in to it without that face transformation can take only these are all the path which are beside that.

So, crystallography when we understand the whole face transformation we can tell about understand from just looking at the basic crystallography we will stop here now.

Student: Sir, then (Refer Time: 60:52) means that hexagonal cannot directly transform to anything it has to go through (Refer Time: 60:56),

If at all a face transformation takes place by a replacement of atom position in hexagonal it will go to only orthorhombic cubic will not come if cubic has to form where defect has to be created in hexagon, but if in a hexagonal lattice if you put some position a atom some position b atom if you try to do it you cannot create an FCC structure.

Student: So.

You will create only orthorhombic or monoclinic or triclinic structure.

Student: Even if like even using stoichiometric 2 dimensional lattices.

Yeah.

Student: While packing in different ways we can only have orthorhombic, monorhombic

Exactly that is 2 dimensional also the same way you have the rule which is there; these for a 3 dimensional lattice.

Student: No, I am saying 2 dimensional hexagonal.

That means, that when you studied diffusional transformation all diffusional transformation how does it take place by an atom coming and replacing it an another position and occupying it in that FCC to HCP is not possible or from an ordered FCC to ordered HCP it is not possible unless and until it has to be through rare defect.

Student: Or shiver or something.

Which one?

Student: What if like shivering something by format at (Refer Time: 62:13).

By when you do deform you are introducing add defect into it that is essentially what it is; right. So, that is what I meant that unless you introduce defect you cannot do that.

Student: Without interrogation defect how do you go about it?

That is if a perfect dislocation is shearing the material you will not be able to generate FCC; HCP in FCC only if the dislocations splits into partial; that means, that we have generated a striking fault which is essentially a defect in the striking sequence; right then only it is possible.

Student: Using pressure also introduction of defects.

Which one; yes, there are many means by which we can introduce defect into a lattice.

Student: Like iron will become HCP (Refer Time: 62:59).

Yes, that that is possible.

Student: So, that is not because of (Refer Time: 63:09).

Which one?

Student: The transformation of (Refer Time: 63:12).

See iron to HCP how does it takes place that face transformation occurs because of what all reasons temperature pressure and the volume change which is associ; and the composition thermodynamically these are all the 4 factors the parameters which are there na is it not thermodynamically. These are the 4 parameters which we consider or entropy that is the another one which will come these are all the terms which are going to be there the face diagram which you can alter it when you are doing it with pressure what is essentially going to happen is that the crystal itself is undergoing not the crystal the atom itself is undergoing some transformations there is by changing the unit cell electronically.

Finally, the energetics when we talk about which type of possible structure which it can come is dictated by the electronic structure of the material the electronics structure is quite often decided by the pressure temperature and all these aspects we can do it. So, there what we are trying to look at it is that by applying pressure when the structure undergoes a transformation to it.

It should have some sort of sort of a shear or hydrostatic pressure it has to undergo some change which will has to undergo that change is instantaneous some of this changes are second order transformations correct, but that will not be stable at room temperature many of them like many of these structural transformations under pressure also we can

do it when we do pressure what is it which we are doing it essentially we are displacing atoms sometimes from their lattice sides correct it is equivalent to being a mechanical deformation.

That is a face transformation can be done in 2 ways: one either by changing by applying temperature or energy to it heat energy or mechanical energy. Mechanical energy also by giving a homogenous shear from one structure to another structure by homogeneously we can transform without introducing any defect it can be done. That is if we take a square by homogeneously differing all these regions we can transform it to this shape, every point is displaced by a particular amount of a shear right. Now it has become a parallelogram it 2 d lattice, his is a face transformation, this is by applying a shear.

This happens under pressure also. Those transformations are homogeneous sash shear. Another is introducing defects into the material that also can happen. The same transformation we can bring it by- suppose I have some dislocation are there like this here which move then also what it will happen is that this is the average shape it we will achieve, but if you look at it critically it will be 1, there may be another which might have. But the average shape if you look at it the shape changes similar to that of a parallelogram.

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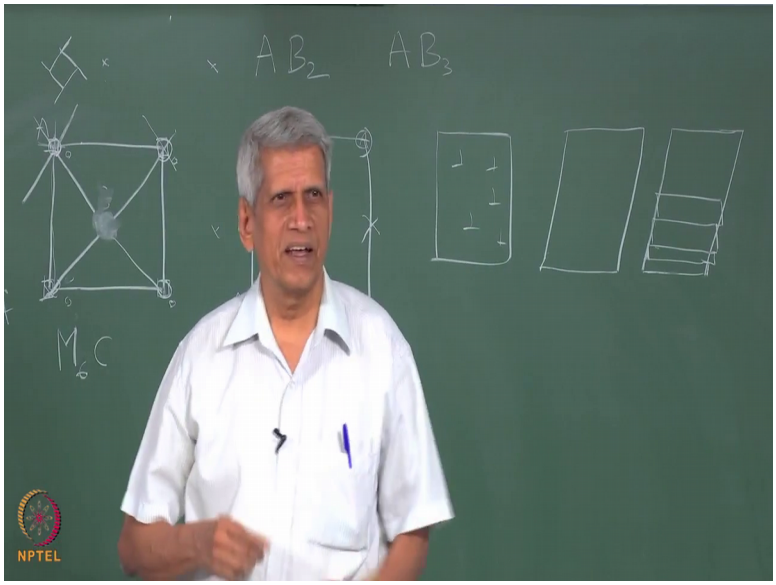

So, by introducing dislocations also we can do it by introducing defect, but another is a homogeneous deformation. Homogeneous deformation which happens under some of

this pressure induced transformation also. But pressure induced transformation essentially lot of electronic structural changes do takes place in the material. That is a different aspect of it you should concentrate. Stop it here.