**Electron Diffraction and Imaging**
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Lecture - 35
Crystallography Revision

Welcome you all to this course on Electron Diffraction and Imaging. So, far in the last few classes we have revised what has been covered about electron microscopy, the basic construction of the microscope it is principle of operation, various modes in which the microscope could be operated like diffraction, imaging and spectroscopy techniques. In fact to characterize a material we require all these three aspects.

The diffraction is one which is required to get information about the crystal structure; the imaging is one which we use to get information about the microstructure, the associated spectroscopy techniques could be used to get composition of the material. As I had mentioned in the first class, we can say that the microstructure characterization is complete then we can get information about crystal structure, then composition then about micro structure ok.

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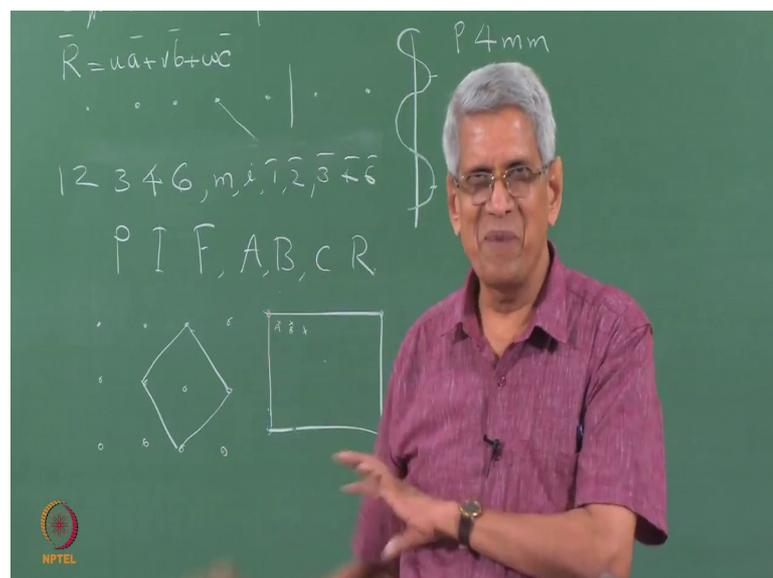
So, the diffraction is the one which gives information about the crystal structure then the question which arises is that what is the information which we seek for about the crystal structure, there are some information which we require what all the types (Refer Time:

01:53). This field where the crystal structure is classified what all the various types in which we can have, this is called as the crystallography. So, what is crystallography? Crystallography is nothing, but study of arrangement of atoms or molecules or motives in one dimension or two dimensions or three dimensions; various dimensions which we can have.

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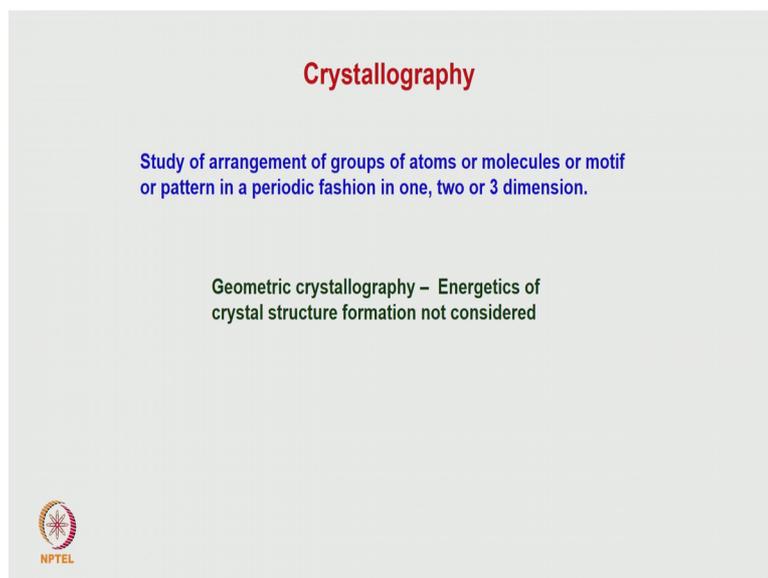
So, what is this crystallography study gives information. It essentially tells given the motif what all the possible choices of crystal structures which it can have. The possible choices it tells, but it never tells suppose I have given a particular type of an atom, what is the type of a crystal structure that specific atom will take, that it does not talk about. But what all the possibilities which are available to it these are all the only possibilities which are there only one of the structures, which it can form that is what this crystallography tells. So, that is why this is also called the geometrical crystallography.

The energetics of it what is the energy which will be gained which it goes to a particular crystal structure that decides which crystal structure, which element or combination of elements will take in actual practice. Then what far we require this out of information that is the geometrical crystallography; because suppose we are given a motif there are various fields in which we require this information. One example which we can take of is this wall design you are given a tile which is a motif how we can arrange it so that different types of designs could be generated.
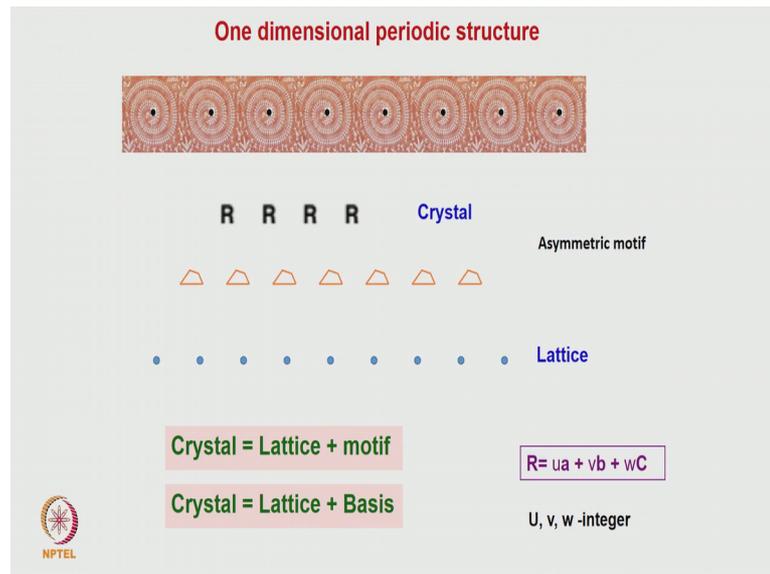
In the case of a floor design that is required, then in the case of textiles we require this sort of information, similarly the same type of information is required in the arrangement of atoms or building blocks of materials or crystals with these are all the area. Then the next question which comes is that can we have an infinite number of arrangements or whether there is some limit on it, yes there is some limit on it all these things which I have gone through, but what I will do is I am just briefly touch up on some aspects of it which I feel one should remember. I am not going through all or I am not telling that this is important what I feel which one should always have some information at his fingertips ok.

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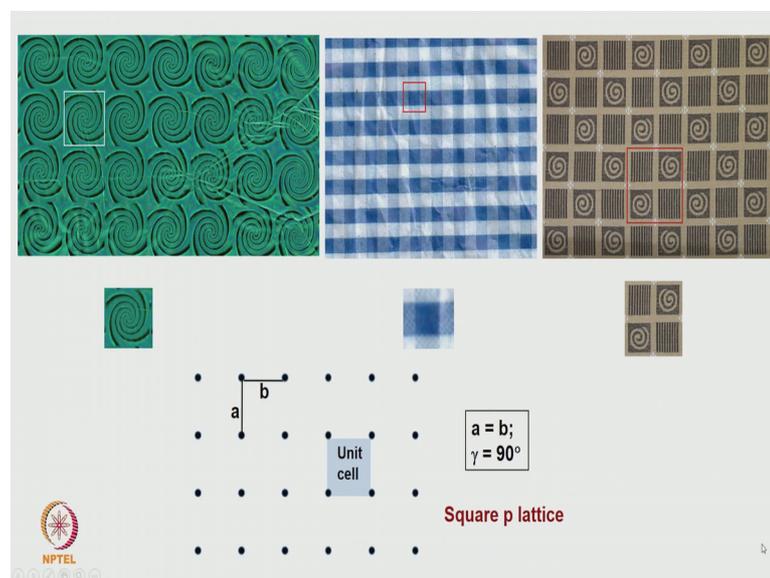
Here what I am trying to show is some various types of designs, this is from a wrapping paper and other is from a cloth and other is which I have taken from a cloth which is put on a sofa, each one of them, if you look at it each looks totally different (Refer Time: 05:00). Is there something which is common between all of them yes there is something which is common.

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One dimensional periodic structure

Crystal

Asymmetric motif

Lattice

Crystal = Lattice + motif

Crystal = Lattice + Basis

$R = ua + vb + wC$

U, v, w -integer

What is it which is common? The common part of it here is essentially in this, this is the pattern which gets repeated, and if you keep that pattern adjacently each other this whole design could be generated.

Here again this is a pattern, here there is another pattern which gets repeated, here I had just marking each of this patterns, this pattern itself has got a fold symmetry. So, I do not talk about symmetry which we will talk little bit later, but as such since yesterday did you know what a symmetry is four fold rotational symmetry, here also fourfold. If you look carefully here you does not have any symmetry do it looks, but if you look carefully it is not. So, if you wanted to and find out what is the underlying lattices symmetry which is associated with it?

The best way is that represent each of them by a point and then try to generate a structure this is that structure which we call it as the lattice. Lattice is nothing, but each pattern or a motif which gets repeated that we represent it by a point, and all of them have got a square type of a unit cell which is there in a two dimensional lattice correct. So, this is what essentially the lattice, on this lattice when we put these different types of motif we generate crystals. So, the number of lattices they are finite and the base of symmetry are depending upon that number of motifs we can have as symmetric motif infinite. So, we can construct infinite crystals.

But if you look at what is the cemetery associated they will fall into some groups a finite group, that is what we see in real practice, this is another example. So, this pattern here is

essentially a pattern which gets repeated, here we can use an asymmetric motif like a latter could be used or some geometric (Refer Time: 07:15) all these things could be represent by a lattice. When we wanted to represent this by a mathematical formula we use a formula like vector R equals u into a, plus v into b plus w into c this a b c are the different code units of the unit cell in three dimensions, u v w are integers once we know this integer values their entire lattice could be generated correct.

And what we considered is a lattice which is non dimensional lattice. So, how many types of one dimensional lattice? Only one type it is essentially with some (Refer Time: 07:56) we can have atoms which can be arranged. Suppose you wanted to construct a two dimensional lattice, there are many ways in which this could be done. That is this thing lattice we keep it up or down at some particular distance periodically and that some particular positions if we keep it like this, then like this keeping it we can generate a two dimensional lattice. So, how many two dimensional lattices which we can generate if we go on keeping it like this. There also there are restrictions this restriction comes from the symmetry which is associated with it.

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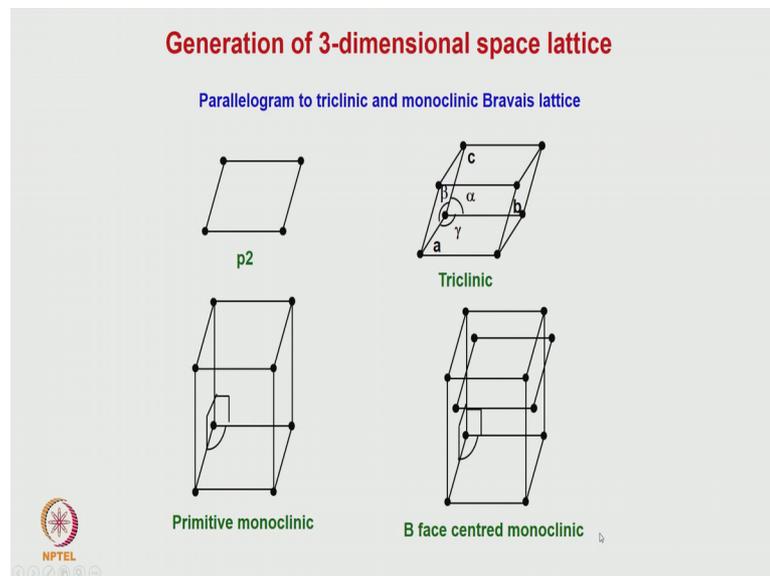
So, there are only five types of two dimensional lattices can be constructed which we have already studied. These 5 types of one is a parallelogram, another is a rectangle and another is a rectangle centre rectangle, which is nothing but essentially a diamond, then we can have a square lattice and then we can have a hexagonal lattice. So, these are all

the five types of these five types of geometrical figures which we can have or the unit cells which we can have, this is also based on the type of symmetry which are associated with this two dimensional lattices ok.

Now if we keep these two dimensional lattices one on top of the other, at some regular intervals at some specific position we can shift it around one lades is there, another you can shift at different position, then if you do that we can generate in principle there are large number of lattices could be generated. That is what essentially is being shown here this is essentially a parallelogram, by keeping a an another parallelogram, but not on top slightly away then we can generate a triclinic structure. If you keep it right on top, but the parameters the c parameter is not the same as a or b, then we can generate a primitive monoclinic or if we keep one lattice here ok.

Then another at a shift and then the next if you try to keep it, then what we can do it is now we can generate a body centered monoclinic like this keeping one on top so many lattices combinations we can generate it. But if you look at all of them what sort of symmetries which are associated with it, then we will see that there are only fourteen Bravais lattices are there three dimensional lattices are possible.

So, though infinite number of lattices which we can consider from the symmetry point of view, only 14 are going to be there, and this is divided into some subclasses like triclinic monoclinic orthorhombic.

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You get tetragonal, cubic, trigonal, hexagonal these are all based on what is the type of a gain and the base of minimum symmetry which is available. So, everything is based on the symmetry principle is being employed, to give this classification to crystal structure. Then which in that there are some subgroups are possible, because the lattice translation vectors will not be able to generate some of the lattice points inside the crystal.

So, that is why they are called as primitive, body centered, face centered, rhombohedral are a b r c face centered this sort of (Refer Time: 11:47). So, in short as far the lattices are concerned we can have only one lattices in one dimensional lattice we already seen it. Two dimensional lattices if you consider there are five types, and then three dimensions we can have 14 lattices which are possible ok.

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

Seven crystal systems, Bravais lattice and symmetry

Now, if you look at these lattices we said that these are based on these classifications are based on some symmetry elements associated with it. These symmetry elements are given in this table; a cubic essentially the minimum symmetry which we draft, four threefold axis inclined at an angle of 109.47, similarly tetragonal has got 144 rotation, this minimum symmetry which is necessary that is how we define that particular class or system, and then the maximum one which tells what is the maximum symmetry which the largest can have ok.

Here we are only given giving a classification with respect to the minimum symmetry triclinic not have any symmetry, monoclinic will have one rotation axis. Once this sort of

a symmetry element has been fixed, automatically the other factors come what is going to be the angle because symmetry essentially involves rotation or a translation or a mirror. So, that immediately tells what is going to be the translation vectors. So, that is why we say that a equals b equal c are a not equal to b not equal to c angle alpha beta gamma. So, this comes from these two these symmetry elements.
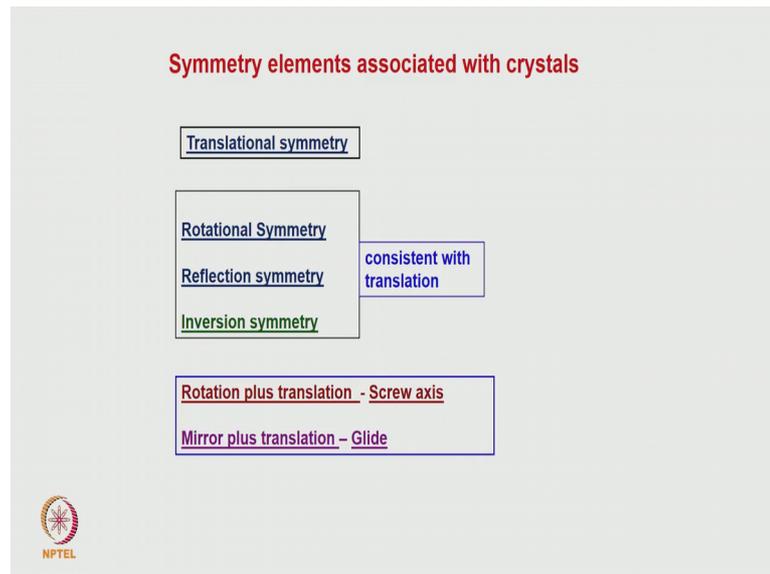
So, when we talk of symmetry what do we understand about symmetry. Symmetry is nothing, but in a mathematical term we can say that there is a mathematical operation which we perform, after the operation has been performed we find that the function remains the same or physically if you see an object like this particular one, I do an operation of a rotation from here if I rotate it by 90 degree, it will come like this around an axis perpendicular to this plane, but if you look at it before operation the operation of rotation and after we cannot differentiate between whether this operation it has undergone or not they look identical surroundings.

So, this is what we mean by symmetry. And symmetry is inherent in nature and the cemetery is the one which makes us spend minimum energy. In copying is a form of symmetry so that only once person has to spend (Refer Time: 14:51) others can just capitalize it like if I take this particular ball, this ball can have an infinite symmetry if I rotate it at any angle you cannot differentiate between the previous position and the present position. So, we say that it has got an infinite symmetry associated with it.

Now, the question comes what all types of symmetry elements which we can have in a material. One is called as a translational symmetry; what is translational symmetry? If I move and in a lattice we defend as one which has got size infinite in all dimensions, we assume that lattice does not have a surface. So, if we move from this point to this point it comes to a point which is identical to it. So, you essentially this points by doing this operation, we are not able to differentiate between the previous position and the present position. So, we say that it has got a translational symmetry which is associated with it.

Similarly, suppose I take an axis perpendicular to it, and then give some rotation to it. By doing that rotation if a lattice point has been moved to coincide with an another lattice point, if either the lattice remains invariant then we say that this is not a rotational symmetry which is rotational symmetry associated with it.

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Symmetry elements associated with crystals

Translational symmetry

Rotational Symmetry

Reflection symmetry   consistent with translation

Inversion symmetry

Rotation plus translation - Screw axis

Mirror plus translation – Glide

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Similarly, we can have a reflection symmetry which is associated with it, like for example, if you consider this one dimensional lattice, if we take this particular plane midway between this then this point gets reflected if we put a mirror, this point gets reflected and comes to identical position.

While doing this mirror operation we can find that again points are all (Refer Time: 16:45) we are able to differentiate. So, we say that the reflection is symmetry. Similarly inversion symmetry around a point if one point is there, just you invert it across origin and if another point exists, then doing the inversion operation it comes to a position which is identical. So, we are not able to differentiate it then we say it has got a inversion symmetry.

So, all these symmetry elements which we have talked about or with respect to essentially an axis or a plane or a point, but what is essentially important here only condition which we tell is that you should be consistent with the lattice which we consider. We are not invoked the translation, but we said that by doing that operation comes to a position which is identical with the original position. So, that is why we always say that these ones which are consistent with the translation, we call them as point groups' symmetry ok.

So, if all these symmetry elements cut intersect at least there is one point which will be invariant, all other points can undergo some movement that point will not that is why it is called as a point group symmetry. Is there any other type of a symmetry element which is

possible? That is since these are all the translation symmetry is associated with it, suppose I have a symmetry which is associated with it along with these I include translation symmetry whatever the cemetery associate it will be moved to this point. So, these rotations are mirror plus these inversions add to it a translation that shifts it correct.

Similarly, we can have another type of a symmetry which is possible, is which we have not considered is what is called a screw axis. That is if we consider a staircase a circular staircase which rotates like this and moves. Suppose you start from this particular point after every step when we take the staircase the step is displaced, but it is lifted up the same type of a step which is been created. So, it moves like this and that some particular number of steps number of small rotation and the step it comes back. So, this is a combination of translation plus a rotation which is given.

But in crystallography the condition which is being put is that not any rotation which you can have, if it has to be consistent with the (Refer Time: 19:35) lattice which is given, then the number of rotations which are possible only that much number of rotations can be given here as well. So, what it will happen is that, that decides how much is going to be the translation plus our rotation this is called as a screw. So, screw axis is one which one can have which essentially a rotation plus the translation.

Similarly, an another one which we can have is a glide, glide is essentially a mirror operation then a shift one side, then again a mirror operation shift it here again it is one of the point group operation plus a translation ok that is how the symmetry elements are coming.

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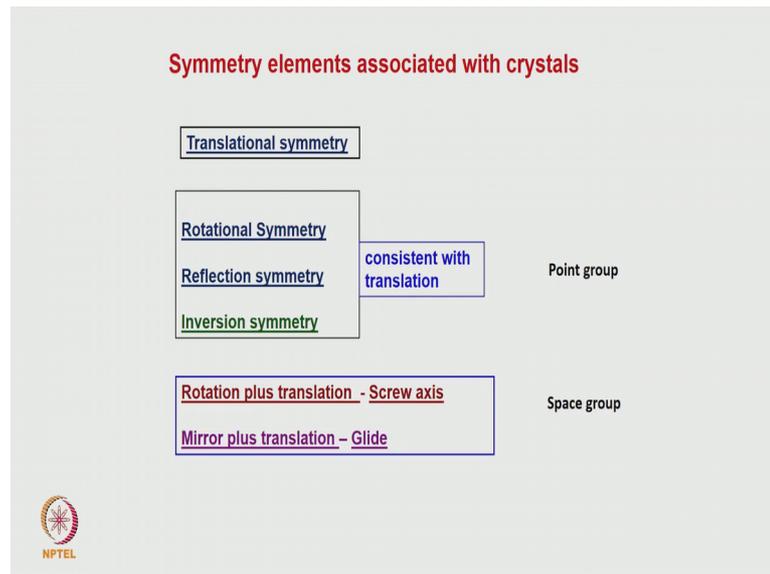
So, space group is essentially as I had mentioned and all this symmetry operations are there, but along with that there is a translation then only a lattice will be generated right.

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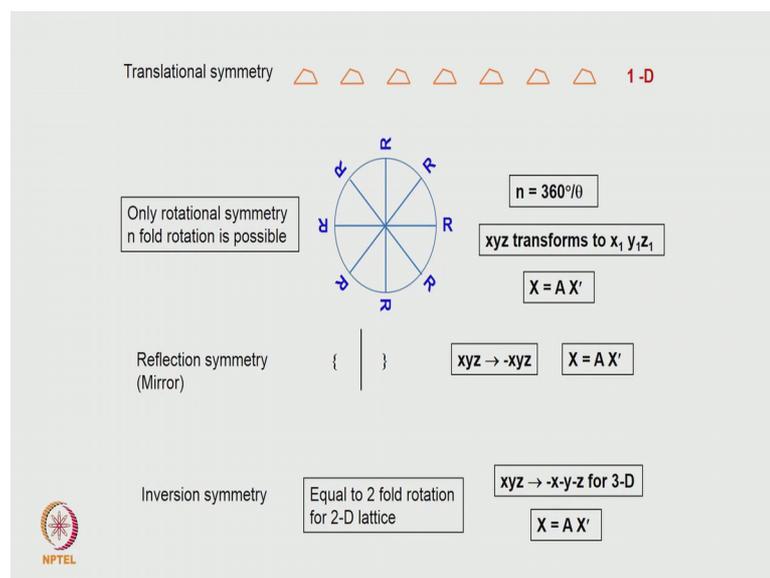
So, I had mentioned that only translation symmetry that is one, rotational symmetry what we can consider it is that. Around any point like what is being shown here, if we take a motive rotate it by some angle that we can divide it 360 by angle it gives a number n ok.

Then it is just a rotation is possible, but this rotation is not going to be consistent. Like here if some particular angle by which suppose I rotate it by 90 degree, this will this point will here this is not the lattice point. So, that is why these set of translations are

permitted. So, that specifies for each type of a lattice which we consider only some particular types of rotation is possible. So, that is one type of a symmetry mirror I had mentioned inversion and this can be represented in various ways one is with respect to a coordinates of this position. So, from one coordinate to another coordinate if the coordinate changes by this transformation, then what is the matrix which we have to use that is also way in which we can represent it. This can be represented in stereogram, there are so many ways in which it could be (Refer Time: 21:56) the all these aspects have been covered in the class.

Then another important thing which we should remember is that the rotation is one which brings if when an object is right handed like for example, here this R when it is written, this is always brought to R which is a right handed one. If an operation of mirror is involved a right hand object is made into a left hand object that will always be there in the history. Why I am mentioning it is that these (Refer Time: 22:36) types of transformations that is if you have got only a rotation is involved, then we can have a crystal where one particular type of a molecule it only has a right hand type, and another which has left hand type which moves. So, these are called as a optically active materials

One will give right hand cash if another will give a left hand (Refer Time: 22:56). So, understanding this sort of symmetry when we understand, we can talk about what sort of properties which the material we will exhibit or if we know about what type of properties which a material exhibit, we can tell what is the sort of symmetry elements which the material will have.
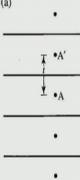
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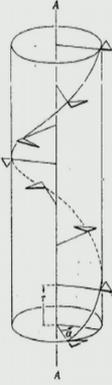

That makes life simpler in getting information about the crystal structures ok.

These aspects have all been covered and just for the sake of continuity I had included slight, but you can go through this get all the information this is for the inversion symmetry.

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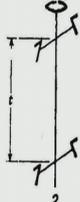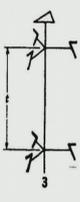
So, essentially the xyz goes into minus x minus y minus z. Similarly the screw axis as I had mentioned here you can make out that this is like a staircase round up point from here you give a translation and then give a rotation, then again a translation and rotation by doing this, this point you find that after 6 volt operation it comes here, this is what essentially a screw axis is.

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Similarly, glide I had explained, but there are different symbols which are used to explain different types of glides along different directions in the lattice all these details have been covered in the class. So, essentially if you look at what are the types of symmetry operations we can have in different dimensions. Having just briefly mentioned about the

different types of symmetry elements, if we take an one dimensional lattice the symmetry elements which we can have is one fold.

That is if I take this particular one lattice one dimensional lattice, I give an one fold to rotation around any point it will come back to it is original position or around this point if I give a twofold rotation it will come back, or if I put a mirror here I can have. So, these are all the only symmetry operations which are possible around a point. So, the point looks symmetry operations are only this ok.

In two dimensional lattice if you consider, we can have one fold, two fold, three fold, fourfold, six fold and a mirror. What all symmetry operations which we can have as far as three dimensional lattice is concerned? Here we can have 1, 2, 3, 4, 6 mirror inversion and then one bar, two bar, three bar, four bar, six bar these operations as I had explained in the class is essentially nothing, but a rotation and an inversion which is all that completes one operation and their combination of these operations are possible.

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If we consider this sort of a combination, how many types of point groups which are possible in one dimension that can be 5, in two dimensions we can have 10 point groups are possible, in three dimensions if we consider we can have 32 distinct point group are possible, but if you take the combinations of this the combinations will be quite a lot. Here for the three dimensions it can be used more than 1000, but finally, from the symmetry when we consider only 32 distinct point groups are possible ok.

Let us take the space group. So, here also I had mentioned like point group it is essentially as I mentioned consistent with translation, but it is not translation is added, but in space group it is a point group plus a translation has to be there. Both are there together in this if we consider a one dimensional lattice, point group then one more all the point group which are considered plus 1 will come which is called as a glide. Then the total number of space groups which we can have is 7.

Similarly in two dimensional lattice if we consider point group which are ten plus that glide also will come then the total number of distinct space groups which we can have is 17, three dimensional lattice if we consider then we can have that 32 point groups plus in addition to it is screw and glide also will come. If all the symmetry operations if there are operating on a lattice, then we can have 230 distinct space groups are possible. These are all the structures to which periodic crystals can form or crystallize into ok.

That if we consider an example in one dimensional crystal, I had just shown this illustration in this slide ok.

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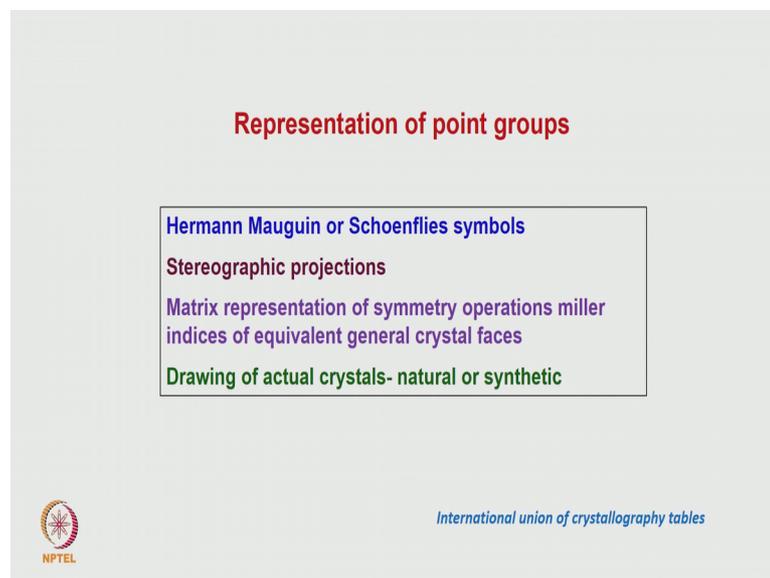
These five are the ones, where you can just put one or this is with the rotation and this is with the mirror this is a mirror, which is perpendicular here it is a rotation and a mirror.

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Examples of symmetry in 1-D crystal
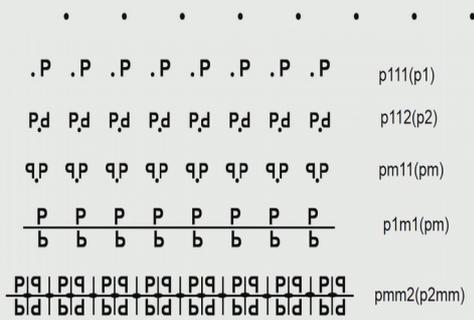
so essentially around a point if you see there are five are there point groups, and these are all the five types of crystal structures just taking only point groups into consideration.

If we add glide to it, there are two more will come. So, now, total 7 space groups are possible in one dimensional lattice correct. There are various ways in which these representation of point groups can be done in the table if you look at (Refer Time: 28:58) table one is Hermann Mauguin I had explained in detail or Schoenflies symbols. Schoenflies symbols I had not talked about it that is space spectroscopy people, but cryptography we are more of we use we use more often Hermann Mauguin Sysmbol that I had explained in detail anyway I will explain it briefly again here today ok.

Then in stereographic projection formalism also it could be represented, then a matrix formalism which we could represent, which I had mentioned then our drawing of that actual crystals are showing the for this itself could be there are drawings which is synthetic or a natural crystal these are all the various ways in which it could be represented ok.

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Examples of 2-D Point group representation using stereogram

Stereographic representation, general positions as well as symmetry elements are given.
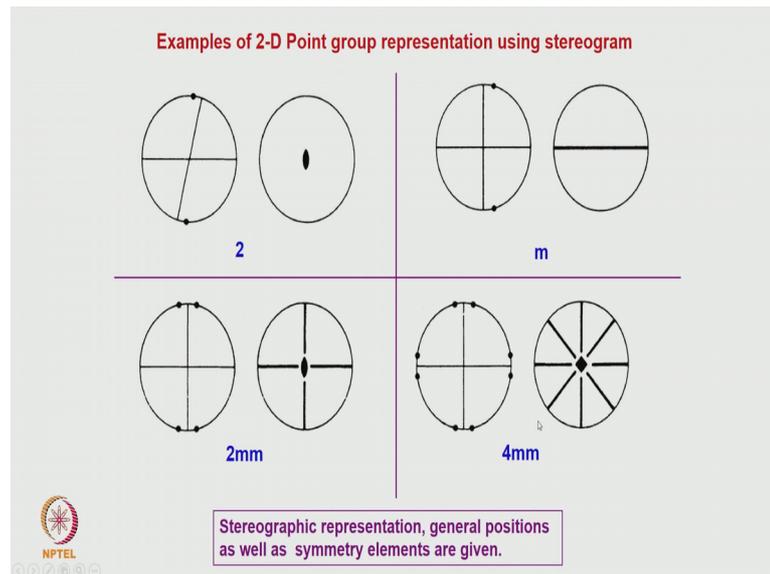
These aspects of rotational symmetry in the matrix formulation this is how we could do these are. In the when you wanted to represent it in a stereogram, essentially what we do it is that we take the primitive circle, on which these are all the coordinates and then if you take one point on that circle because this for a two dimensional points, these gets since for a monoclinic structure. So, two fold rotations this will come here again one more rotation it will come here.

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Symmetry Elements in 2-D lattice / crystal

Periodic arrangement in 1, 2or 3 dimensional space can be described in terms of symmetry elements. Symmetry arises because of groups of atoms or lattice point repeats in regular way to form a pattern

Symmetry operation in 2-d lattice:

Translational symmetry   Rotational Symmetry

Reflection symmetry   Inversion (nothing but 2-fold rotation in 2-D)

Glide

17

One way this is one way we can represent or other is the two fold rotation is represented by this sort of a symbol. So, these are all the two options like mirror this is one here if you put a mirror this will gets reflected here. So, this is here only the symmetry is

represented, here essentially one particular point, how it transforms or moves from one to another position by the operation of the symmetry. This is for 2 mm this is for 4 mm these are all the ways in which it is done the all the details which I had shown earlier and that is available in all standard books which you can see ok.

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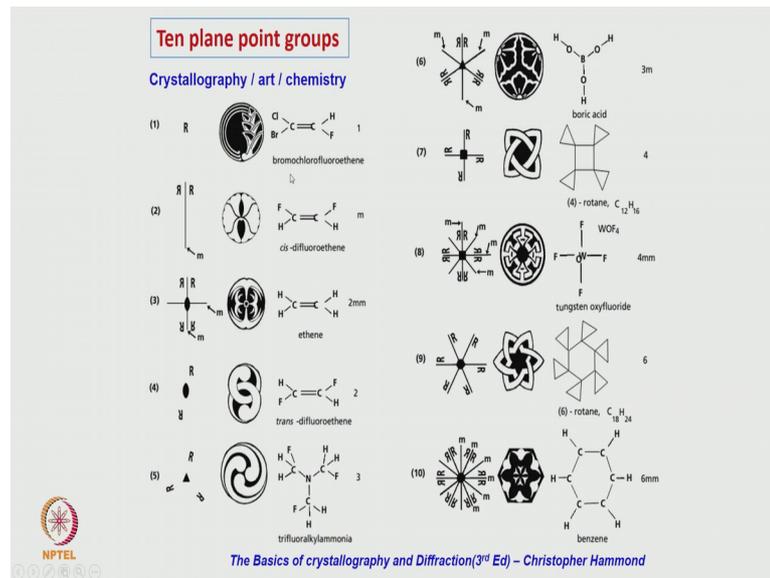
So, this is what we have considered so, far is essentially what all the various ways in which the two dimensional point groups can be represented in stereographic projection. The same point group can be represented in another way just taking a like a crystal that is as symmetric motif and you show what is that operation of it. What is the type of patterns if you see, which exhibits we can argue it is taken from a naught which exhibit the whether one fold or two fold or a mirror symmetry all these plus some crystals which exhibit or molecules which exhibit this sort of symmetry operations that is shown in this.

If you look at it here it is one fold mirror, 2, 3, 4, 5, 6 and then combinations of this rotation and. So, this brings out only 10 distinct points which I had already mentioned ok.

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Planar lattice + (combination of rotation, mirror and glide) = Planar group
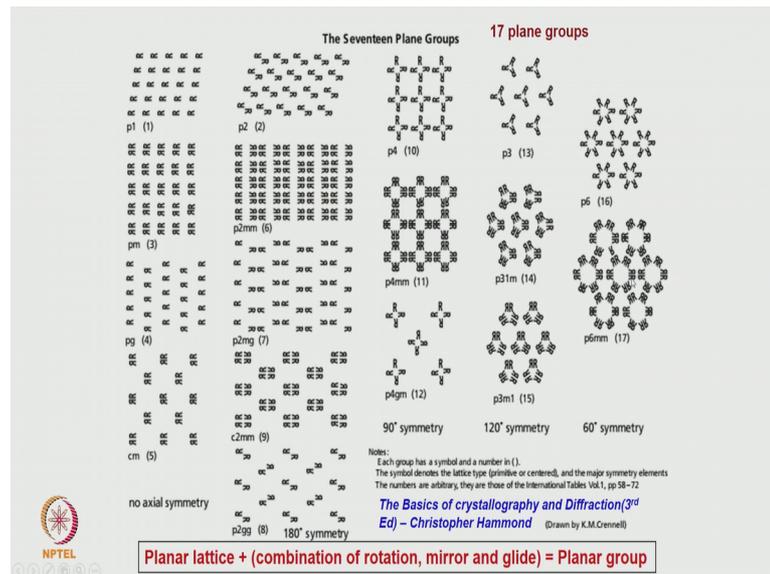
Then I mentioned that if you add glide, we will have a 17 will come into the picture this is for an isometric motif all the seventeen types of crystal which can form ok.

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Two dimensional lattices, point group and space group

System and lattice symbol	Point group	Space group symbols		Space group number
		Full	Short	
Parallelogram	1	p1	p1	1
p (primitive)	2	p211	p2	2
Rectangular	m	p1m1	pm	3
p and c (centred)		p1g1	pg	4
		c1m1	cm	5
	2mm	p2mm	pmm	6
		p2mg	pmg	7
		p2gg	pgg	8
		c2mm	cmm	9
Square p	4	p4	p4	10
	4mm	p4mm	p4m	11
		p4gm	p4g	12
Triequiangular	3	p3	p3	13
(hexagonal) p	3m	p3m1	p3m1	14
		p31m	p31m	15
	6	p6	p6	16
	6mm	p6mm	p6m	17

A. Kelly and K. M. Knowles, Crystallography and Crystal Defects, 2nd Ed., John Wiley & Sons, 2012

This space group which can come that is shown here. And these are given in international you know crystallography it is given as the each space group is given a particular number, one such number is know you open that page.

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3-D point groups

Pure rotation is called operation of *first kind*. (It cannot bring a right handed object in coincidence with left handed object)
Inversion and mirror are called operation of *second kind* (they bring right handed object in coincidence with left handed object)

Various combinations of 1, 2, 3, 4, 6 and -1, -2, -3, -4, and -6 generate 32 point groups or crystal classes.

Operation of proper rotation and their combination constitute 11 classes. (first kind)

Roto inversion another 5.

Combination of proper and improper rotation axes another 16.

Point group - Representation of symmetry of a motif around a point

In that book with that number then they give the full symbol as well as the short symbol what is the point group corresponding to it, all these informations are given in the table and the details which has been explained in the class. Similarly three dimensional point group also we can represent it in that same way and here.

(Refer Slide Time: 33:03)

32 point groups

Taken from crystallography and crystal defects book by Kelly and Knowles

Most of the times you find that these are represented in a stereographic form, in this stereographic projection if you look at it for a fourfold rotation you show the axis ok.

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(Refer Slide Time: 33:39)

On a stereograph and then take a motivate a general point and how it gets repeated itself (Refer Time: 33:24) or as I has mentioned you can show by the cemetery ok.

So, here all the symmetry elements that 32 point groups are shown in these two slides, which has been explained earlier. This can be given in many books you will find that these are given in a table form also, in this table form if you see it the one which is shown with these colour. These essentially corresponds to what is the maximum symmetry which the crystal will exhibit this is what the symmetry which the lattice exhibits, lattice exhibits the full symmetry and this one if you see it are the ones which show what is the minimum symmetry which should be there ok.

This is the minimum symmetry with which all these classification which has been pulled. All these details you are going to and in these table if you look at it when we say that 432 what does this order 432 mean ok.

(Refer Slide Time: 34:33)

Order of axes of symmetry elements in point group for crystal systems

Crystal System	Symmetry Direction		
	Primary	Secondary	Tertiary
Triclinic	None		
Monoclinic	[010]		
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	[100]/[010]	[110]
Hexagonal/ Trigonal	[001]	[100]/[010]	[120]/[1 1 0]
Cubic	[100]/[010]/ [001]	[111]	[110]

Example: 422 – 4 fold along [001] direction, 2 fold along [100]/[010] direction and another 2 fold along [110] direction

So, this is explained in this sort of a table for the primary number mean, for each of the crystal system here it is a 0 1 so on axis along, which that two when we open that two fold rotation comes and here if you look at it around 1001 is along that c axis it comes. So, what all types of symmetries which will be coming along with particular direction crystal structures that is how they are represented in this table, in the Hermann Mauguin symbol ok.

And this basis I had just shown the various crystal structures ok.

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Bravais Lattices
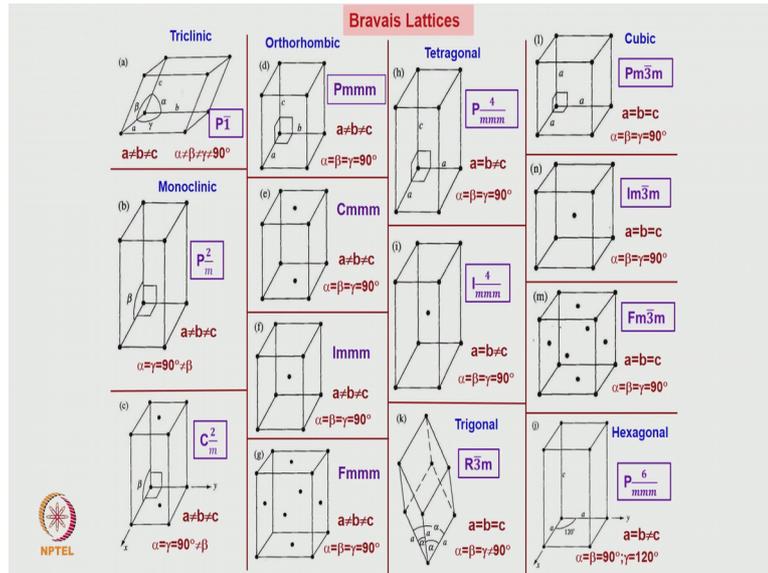
And their maximum symmetry elements which are there, this I had already explained. Now I mentioned that the space group is essentially nothing, but a combination of point groups plus translation symmetry associated with it all the point groups. And on this basis if the point group itself if you look at it, we can say whether it is a polar or it has got a centre symmetry, on this basis we can tell polar will not have a centre symmetry and then an endomorphic or non endomorphic that will show optical activity ok.

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Space groups

Space-group symmetry is a combination of symmetry elements such as rotation, mirror, inversion, screw axes or glide planes.

The determination of space-group symmetry of material is an essential step in structure analysis since it minimises the amount of information needed for the complete description of the contents of the unit cell.

The number of permutations of Bravais lattices with rotation and screw axes, mirror and glide planes, plus points of inversion is finite: there are only 230 unique combinations for three-dimensional symmetry, and these combinations are known as the 230 space groups.

Polar, non-polar, enantiomorphic / non- enantiomorphic

So, ferroelectric material and piezoelectric material, various properties with a elastic properties all these properties could be defined looking into which sort of crystallography. If you know the property how it changes in different directions if it is

measured, we can tell that this is a particular type of a crystal class in which the sample should fall into. These are all the various symbols which are used to represent all the symmetry operations this I had explained in detail.

(Refer Slide Time: 36:20)

Now the space group also can be represented, what all the ways in which the space group could be represented one is the Hermann Mauguin symbol could be used to the represent this space group. So, essentially what is being done in this is that, what is the type of us the classification which I had mentioned for depending upon the different directions for different crystals, how it is to be; how the first number second number and the third number will come then P that is primitive is represented as P, I for body centered F for face centered A, B, C and then R for trigonal. These sort of symbols will be put in front of it that is how the full space group is represented in Hermann Mauguin symbol then just mentioning all the symmetry operations also that can be represented in the international (Refer Time: 37:34) of cryptography table all these representation in which the space group represented.

Another is the we can show a symmetry diagram; what is essentially done is along any one of the axis any along one of the principle axis which we use, around that along that axis show the unit cell the show all the symmetry element which are associated that is one way or another way which is done is that, like suppose it is going to be a rectangle this is going for a simple orthorhombic structure, then we can either show all the

symmetry elements or you take a general point that general point means that one which does not have any symmetry associated with it. So, you have to apply all the symmetry operation it will generate all other points around that lattice point you show that.

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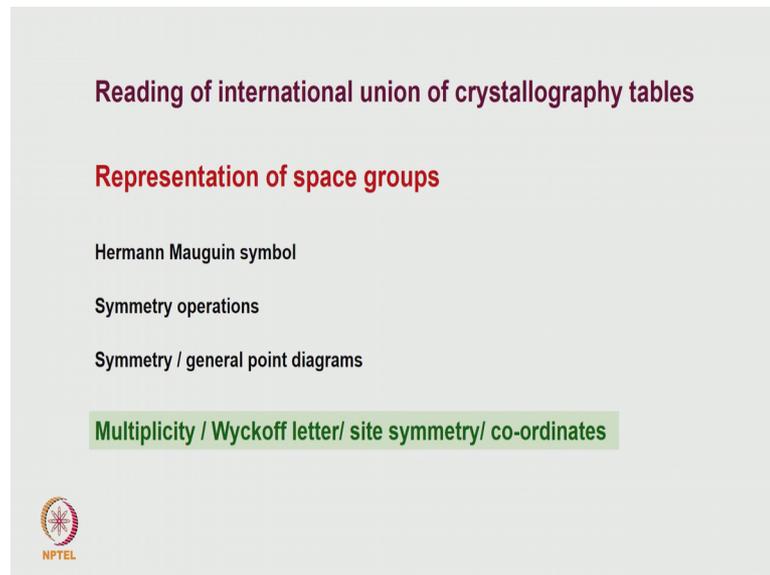
These are all the two ways in which it is represented. The third is the fourth way in which it is represented is multiplicity which is associated with the different points, then Wyckoff letter site symmetry and coordinates. Because what happens is that when you represent with symmetry elements, these point may have some symmetry associated with it maybe this centre has got some symmetry, there are many points which does not have a symmetry associated with it.

So, there are some points which have some specific symmetry associated with that point in that unit cell that decides how many atoms have to be placed in the unit cell is decided by that all those informations are given, and each of this special points or general points or general points are represented by the Wyckoff letter, and around each of this points adjacent neighbours if you consider what sort of a side symmetry which it will have that is also given, and then once that is decided how many points are there what all the coordinates of that points that is all mentioned that sort of a table.

This is a table which can be used to construct crystal structures. So, what is the way to understand this? This is aspect which I will explain it a little bit in detail; here what I had considered is P4 mm ok.

Graphical representation of General and Special positions for P 4mm

Which type of Wyckoff position, motif or atom will occupy will be determined by energetic consideration.
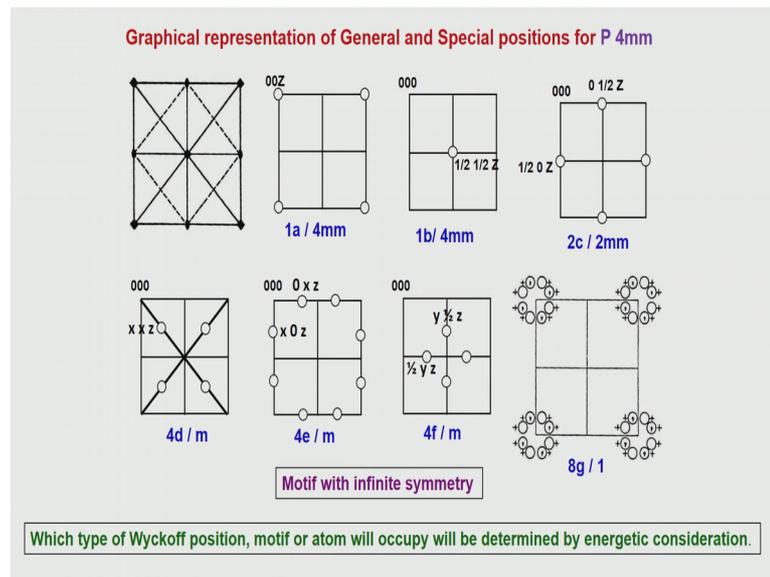
That means that point group symmetry is 4 mm it is a tetragonal structure because that four is coming as a first letter then two mirrors are coming, then 99 minutes that that sequence in which it is been mentioned, the 99 is the number corresponding to this for P4 mm.

For each 230 that one to 230 they are numbered and then you look at this symmetry diagram this is along z axis is then be a and b axis then the unit cell is being shown then the unit cell is being shown, then around each of the lattice points you consider this is the four fold symmetry associated with it, and at the centre also it is a consequence of four fold symmetry comes which I had explain how this happen, then at this midpoint on each of these axis you have a twofold symmetry special points are coming, and then these are all the mirror reflections which are coming the mirror planes are shown.

Then this is a glide plane which comes. In this if you put a general 0.1 here by all the symmetry operations; this is where that all the symmetry operation by doing the symmetry operation we can generate all the other positions where they should come. So, this is these all the two information which is given and where is that origin (Refer Time: 41:25). All these special points if we consider we will have some coordinate associated with it, for each of the special points the coordinates are given in this table form. And what is the site symmetry corresponding it that is given in this column, and that Wyckoff

number is it starting from one having maximum symmetry is starting from the origin it is been given a b c d like this.

And for example, if we put at a general point for this particular one essentially another seven more points have to be generated, these are dictated by symmetry then only this complete this when the motifs are placed around it like this the unit cell, it will exhibit the forum symmetry correct. Now at this central point if you consider if you have placed, it the centre point also if you look at these points are there, the same symmetry it will exhibit. If I wanted to place an atom at the centre, if I keep it here or here or here we keep it this one point which has been put, a prior translation that is why I said the (Refer Time: 42:46) translation. So, this point gets repeated that is how the full lattice is generated ok.

Then only if you consider an atom like this ball, it has got an infinite symmetry. So, all the symmetry elements it will have we can keep it at this point only one is required. Whereas, if we keep at this one which has one fold symmetry then we require 8, like here if we look at it we have a twofold symmetry which is associated with it, then we require a two points then we can keep along this mirror symmetry, then what all points at which it has to be kept all those coordinates are given here where the atom should be there in the lattice ok.

This is what this table essentially illustrates. So, here what I have done is this and this that Wyckoff position the letter which is being used a b c corresponding to which type of a symmetry element in the unit cell this is what I had shown. But what is essentially important is that this same thing as I mentioned with respective to a one a position, if I keep an atom here or here it just satisfy. This way now it has got a forum of symmetry instead of it I can put this same atom at this particular position at half (Refer Time: 44:14) then also if the lattice put unit cells together this also satisfies the four mm symmetry.

Here if I put atoms at these points on the unit cell, like this then we join all unit cells together adjacent, to each other this also satisfies the four mm symmetry. If I put it on this particular one on this mirror symmetry plane, then these are all the positions and which it will be pulled and this also satisfies four mm. So, here if you look at it this is the way it has to be put, here this is a way and though symmetry if you put it this is a way it

will come; that means, that given an atom these are all the options which are available for this crystal structure, where that atom could be place.

If you place that atom like that at any of these positions, irrespective of whichever be the position we have kept it each of these unit cells satisfy the four mm symmetry this is the first. So, the option which atom has got these are all the possibilities that is what that we see it is the geometrical cryptography. The next one which happens is that if we keep it at these positions the number of atoms per lattice point it turns out to be one, if you keep it here also one, if you keep it here how many are required in the unit cell we have 2. If you keep it here in each unit cell we have 4, if you keep it here 4, here also 4 here also will be 8t ok.

Given an atom suppose it chooses some particular choice which is dictated by some energetic concentrations, which is beyond the scope to discuss in the class now. Then depending upon suppose it is taken 4; that means, that the density of the material will be changing depending upon the once a lattice parameter is fixed. So, you understand that. So, essentially this tells all the possibilities and if it takes it this way, then immediately if you know the unit cell parameter thee number of atoms which are density, then you can find out that this is a type of position which it can occupy we can infer some information about it correct ok.

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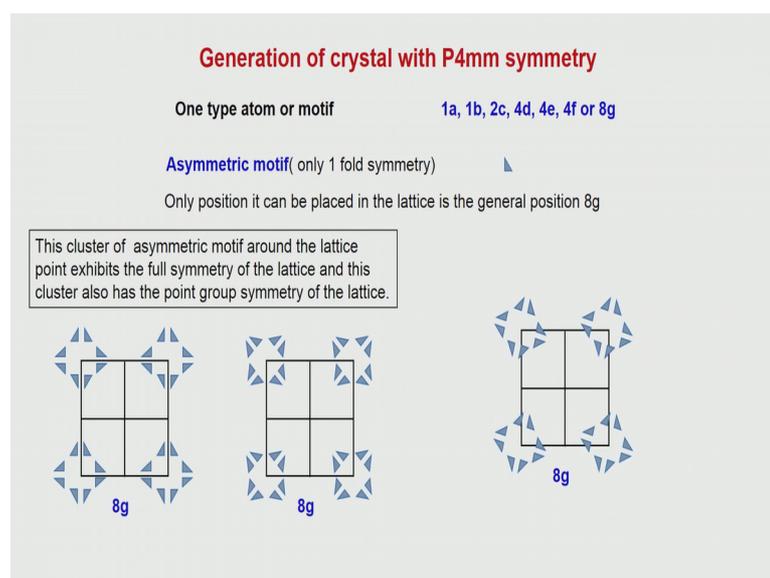
Then another one which is very important only this aspect I will cover is that suppose we consider a motif which is made up of an asymmetric motif, which has got the in this corresponding to this particular case four mm symmetry, how it can be placed around lattice point. Either we can keep it in this position then it is satisfies the four mm symmetry of the lattice or we can keep it rotated by 45 degree, then fold it satisfies. If I keep it at any other rotated by any other angle like in this particular case, this does not satisfy the 4mm symmetry.

Now, it will have only a fourfold symmetry; though this has got a four mm symmetry, the motif has got a four mm symmetry, the crystal also had lattice also has got a symmetry which is the same as that of here depending upon how we position it. So, essentially the symmetry which is shown by the crystal depends upon, if we keep a motif at a particular position what all the symmetry elements which are associated with that position consider it, what all the symmetry element which the motif has got, whichever symmetry elements are coinciding that is the symmetry element which the crystal will exhibit you understand that.

(Refer Slide Time: 48:25)

Suppose a motif has got one fold symmetry you put it around a square lattice which has fourfold symmetry, but motif has got one fold symmetry then the crystal final exhibits only a one fold symmetry, that is the example which we have shown in the first slide. So, this is one which is important, then these aspects. Then the another aspect is that suppose

if the same type of an atom the questions which comes is that, we said that these are the possibilities which are there can I keep that same atom at for example, in this position and in this position.

If I put the same type of an atom in these two position, then the space group (Refer Time: 49:11) will change it will no longer maintained (Refer Time: 49:12) symmetry. So, that is not possible suppose we have another type of an atom which is the there a type of an atom and a b type of an atom then a can be put here b can be put here.

(Refer Slide Time: 49:34)

So, that is possible. So, if we (Refer Time: 49:31) then if we put a here and b here then what will happen is that a b is the stoichiometry and the number of molecular formula is only one that is what it will be there, but the same molecule of a b stoichiometry I can put it by putting one here and another here.

So, there are many combinations are possible. So, this decides what is the type of stoichiometry with which we can generate our life when we have different type of species are given with which we are forming compounds. So, suppose it is AB A and B we can have AB composition AB 2 AB 4 these are all the ones which are possible directly looking at it we can tell the question which comes is that suppose this is not what I am telling is th suppose, but it has been observed that is a material with a b 3 or a b 5 is it possible to form.

If you look at these position in fact, if you ask me I will tell that yes it is possible how exactly it is that in this a item can be placed at this position 0 0 itself, what does it means that? It is an arbitration position which you can choose it a is put b can be put at 0 0 (Refer Time: 51:04) 1 then that satisfies also again that same cemetery, c can be put at and an another b atom can be put at another distance like this you can put it and form still having the same symmetry is being maintained it is possible ok.

In fact, these sorts of things have been seen. So, because which type of a crystal structure it forms it is dictated by the energetics, but if you look at this sort of a table simply looking at the ratios you find that it appears that it is not possible. The only way it is possible is that these what is essentially important is it suppose this turns out to be 0 0 0 putting one atom here if you not put an another atom in that procession ok, that is what the question which a (Refer Time: 51:58) crystal have a structure and stoichiometry other than what is dictated by this table yes it is possible.

(Refer Slide Time: 52:04)

This is one example which I had given one atom at the 0 0 Z, the other atom can be placed at 0 0 Z1, this also both of them exhibit that fourfold symmetry 4 mm symmetry will be there or a atom here b atom here or if you look here, this is 4 a atoms another atoms this also has got a AB stoichiometry, but it is A 4 view.

But what is going to happen is that depending upon the number of atoms, the density if the (Refer Time: 52:43) parameters maintains that thing the density change. This is the

same which is for a b stoichiometry these are all the possibilities which we are showing these are all various possibilities.

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Hierarchy of crystal systems
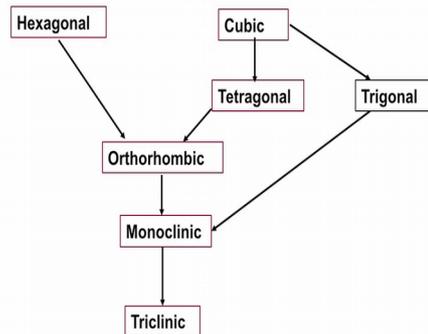
Diffusional /non-diffusional

So, from this what we can understand any type of a composition can be obtained for a any type of a composition a particular crystal structure it can form if energetic permit.

But the type of crystal structures which is possibly fixed to 230. So, if we consider between the various type of crystal classes from a hexagonal, suppose (Refer Time: 53:26) this is called as a hierarchy, that is a disorder status cut the maximum space group we can maximum symmetry operations which are possible; from this when a face transformation takes place it undergoes the transformation there will be lowering of the structures. So, if we take place by a replacive transformation, then what all the types of structures to which it forms.

Hexagonal when you transforms it can go to orthorhombic probably, hexagonal by a face transmission it cannot go to cubic. What I mean is that this is a square type of a lattice this is (Refer Time: 54:17) cubic. If we put an a atom at some particular position and b atom at some position, I can generate like if this is a cubic lattice which is a representation if I take it like this, a atom and b atom are here and the c is at this particular height it comes then it becomes a tetragonal structure, but it cannot be made into hexagonal.

But the replacement of atoms amend the sides when are when diffusional transformation occurs, where atoms which one atom goes and replaces to another site such transformation from cubic it will go to tetragonal or cubic to trigonal it can go or to monoclinic or triclinic hexagonal to orthorhombic to monoclinic to this one, these are all the way in which transform a this also tells that in a replacement transformation what all the types of structures which can be formed when a face transformation is occurring.

But these are all diffusional transformations, non diffusional transformations which are essentially called displacive type of transformation, there by deforming a crystal point homogeneously you can go from one particular structure to another structure it is possible that is what the martensitic transformation. Because in a martensitic transformation FCC can be made into HCP, that is cubic to this one without introducing and effect correct that transformation is occurring, but hexagonal to cubic if you have to go without introducing defect or a stacking fault, normally you can undergo this transformation whereas, by deforming structures from one structure to another city it is always possible to make.

Like BCC; BCC can be transforms into hexagonal, but cubic to this transformation generally here by this rule if you consider it is not possible, but martensitic it does occur essentially what we do we compress it like displace is like this all directions different directions to give different displacement, but you can change it to another structure. So, that is a non diffusional or that is called as displacive transmission.

So, everywhere crystallography plays a lot of role in understanding, then depending upon the which type of a structure which is their whether it is primitive that among the classes after structural (Refer Time: 56:55) all the crystals the 14 Bravais lattices could be represented in terms of primitive unit cell ok.

 (Refer Slide Time: 57:00)

Copper (A1, face-centered cubic, fcc)
Structure: cubic; $a = 0.3610$ nm; $Z = 4$; *Space group, $Fm\bar{3}m$* (No. 225);
Atom positions: Cu: 4a   0, 0, 0; $\frac{1}{2}, \frac{1}{2}, 0$;   0, $\frac{1}{2}, \frac{1}{2}$; $\frac{1}{2}, 0, \frac{1}{2}$

Tungsten (A2, body-centered cubic, bcc)
Structure: cubic; $a = 0.3160$ nm; $Z = 2$; *Space group, $Im\bar{3}m$* (No. 229);
Atom positions: W: 2a   0, 0, 0; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

Magnesium (A3)
Structure: hexagonal; $a = 0.3200$ nm, $c = 0.5200$ nm; $Z = 2$; *Space group, $P\,6_3/mmc$* (No. 194);
Atom positions: Mg: 2d $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$; $\frac{1}{3}, \frac{2}{3}, \frac{3}{4}$

Diamond (A4)
Structure: cubic; $a = 0.3567$ nm; $Z = 8$; *Space group, $Fd\bar{3}m$* (No. 227);
Atom positions: C: 8a   0, 0, 0; $\frac{1}{2}, \frac{1}{2}, 0$;   0, $\frac{1}{2}, \frac{1}{2}$; $\frac{1}{2}, 0, \frac{1}{2}$; $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$; $\frac{3}{4}, \frac{3}{4}, \frac{1}{4}$; $\frac{3}{4}, \frac{1}{4}, \frac{3}{4}$; $\frac{1}{4}, \frac{3}{4}, \frac{3}{4}$

But some of them are non primitive unit cells are used to represent, because these non primitive unit cells represent the full symmetry of the lattice that is the consideration which is used to represent that way.

(Refer Slide Time: 57:30)

Lattice point vectors in Bravais lattices

Crystal type	Symbol	Lattice point vectors
Primitive	P	000
Body centered	I	000; ½ ½ ½
Face centered	F	000 ; ½ ½ 0; ½ 0 ½ ; 0 ½ ½
A centered	A	000 ; 0 ½ ½
B centered	B	000 ; ½ 0 ½
C centered	C	000; ½ ½ 0
Trigonal	R	000 (rhombohedral axes)
Trigonal	R	000; $\frac{2}{3}\frac{1}{3}\frac{1}{3}$; $\frac{1}{3}\frac{2}{3}\frac{2}{3}$ (hexagonal-3 index)

So, when we do that that different lattice points which are there the unit cell, they have they will be represented in fractional coordinates. So, corresponding to each of them what is the sort of fractional coordinates which will be used that is given in this table. Generally in any of the crystal data book if you look at it, how do they represent the different materials all the cryptographic information. For example, if you take copper it is given copper a one is what it is called the structure baraic symbol, this is not a one

which is used in international (Refer Time: 57:56) of cryptography (Refer Time: 57:59) because international cryptography if we use it for copper we use DFM three bar and it is better to learn to start using that.

Then FCC is that I mentioned and then the structure is generally this it is a simple cubic structure in the cubic structure what is the lattice parameter and is; that means, that if it is a cubic structure if it is FCC you can say that around each lattice point there should be 4 (Refer Time: 58:25). So, the number of atoms just be there is four, this is a space group and the atoms positions at 4 a, because this is taken from the cryptography table these are all the position which the atoms will occupy there is if you have a particular atom and as we have seen in the case of P 4 mm.

If out of all the choices if only one particular element is there which one it will choose. Generally it will choose the one where that site exhibits maximum symmetry, then if it chooses that that is only at one position. So, the number of atoms per unit cell is going to be one that is one and generally whichever site has got maximum symmetry that always has got the energetically it has got from minimum and lower energy level. So, these two are related also structure and symmetry are quite related topics ok.

(Refer Slide Time: 59:41)

Similarly, tungsten which is body centered the same way we can say atom positions, but Z equals true similarly if you look at the graphite or sodium chloride for example, if we consider that is it is a sodium and chlorine is there, here if you see it sodium atom

occupies here the positions are 0 0 0 half of 0. That means, that this positions is a fixed special position, here only one atom can occupy one position we consider the case where 0 0 Z is there one atom and another atom can (Refer Time: 60:11) position with different value that is not possible here that is why here one position is occupied, next interspacial side, next other atom position comes like that it goes.

(Refer Slide Time: 61:08)

Crystal system	Bravais lattice symbol	Pearson symbol	Example of crystal structure
Triclinic (anorthic)	aP	aPn	
Monoclinic	mP	mPn	mP4-γBi
	mS (mA, mB, mC)	mSn	mS4-βBi
Orthorombic	oP	oPn	oP8-αNp
	oS (oA, oB, oC)	oSn	oS4-αU
	oI	oIn	
	oF	oFn	oF8-γPu
Tetragonal	tP	tPn	tP4-βNp
	tI	tIn	tI2-In
Trigonal (rhombohedral)	hR	hRn*	hR1-αHg
Hexagonal	hP	hPn	hP2-Mg
Cubic	cP	cPn	cP1-αPo
	cI	cIn	cI2-W
	cF	cFn	cF4-Cu

*In the Pearson symbol hRn, the number of atoms, n, refers to the primitive rhombohedral unit cell.

But when you go to higher intersections where this position which are given by mirror symmetry where the value x comes then there are many atoms can occupy along those lines that I will similarly for zinc blende and here if you see that the z is given by 4 because 4 NaCl that is 4 of sodium and 4 of chlorine. So, NaCl has (Refer Time: 61:54) if you consider only 4 is going to be there this is how similarly for zinc thing blende it going to be Z equals 4 this way we can understand this is one way of representation.

(Refer Slide Time: 61:02)

Table 1.7. Some Strukturbericht, Schoenflies, and Hermann-Mauguin Symbols

Strukturbericht	Schoenflies	Unit Cell	Hermann-Mauguin	Example
A1	O_h^5	FCC	$Fm\bar{3}m$	Copper
A2	O_h^9	BCC	$Im\bar{3}m$	Tungsten
A3	D_{6h}^4	HCP	$P6_3/mmc$	Magnesium
A4	O_h^7	FCC	$Fd3m$	Diamond
A5	D_{4h}^{19}	BCT	$I4_1/amd$	β-tin
B1	O_h^5	FCC	$Fm\bar{3}m$	NaCl
B2	O_h^1	PC	$Pm\bar{3}m$	CsCl
B3	T_d^2	FCC	$F\bar{4}3m$	ZnS (sphalerite)
B4	C_{6v}^4	PH	$P6_3mc$	ZnS (wurtzite)
C1	O_h^5	FCC	$Fm\bar{3}m$	CaF_2
C2	T_h^6	PC	$Pa\bar{3}$	FeS_2
C3	O_h^4	PC	$Pn\bar{3}m$	Cu_2o
DO_3	O_h^5	FCC	$Fm\bar{3}m$	BiF_3
DO_{11}	D_{2h}^{16}	PO	Pnma	Fe_3C
$E2_1$	O_h^1	PC	$Pm3m$	$CaTiO_3$
$H1_1$	O_h^7	FCC	$Fd3m$	Al_2Mgo_4
$L1_0$	D_{4h}^1	PT	$P4/mmm$	AuCuI

Different type of symbols used in literature to represent crystal structures

Another way in which it is (Refer Time: 00:00) it is called the Pearson symbol which is being used. In that triclinic is represented by anorthic. So, it is represented at a, monoclinic is a m orthorhombic is o, tetragonal t, trigonal h, hexagonal h and cubic is c and then whether it is a primitive or body centered. So, those symbols are used then n represents what is going to be the total number of atoms which are present in the unit z this is an another way of representation. So, for copper if you have to represent it we will put c F4 it will come ok.

Suppose we have to represent diamond it will be c F8 it will be come. Then if we see the books there are various types of symbols types of symbols which has been used. So, this is the symbol which is used by international (Refer Time: 62:05) of cryptography then we use another BCC BCT all these used to represent crystal structures, then the Schoenflies symbols are used because the Schoenflies symbols and the point group symbols have got one to one correspondence ok.

But as far as the space group is concerned the Schoenflies when he formulated this independently be found out, what he did was that depending upon which crystal which he determined he gave the number after giving this he gave number one two three like that, which was arbitrary that is why it is better to use crystallographers prefer this one and chemist especially people who work on spectroscopy prefer this because this directly tells because they look at what is the molecule, what is the vibrational spectrum, what is the rotational spectrum for which it is essentially a point group, which is more important rather than the space groups. So, they use this ok.

Then another symbol which is strukturbericht which was the (Refer Time: 63:13) this is what all the more confusing A1, A2, A3, A4 these are all there, but I think logically explaining how it is has come is going to be very difficult here there is some logic is there. So, it is better one starts using this sort of symbols to represent crystal structures because if you represent it this way then immediately you can go to international union cryptography table, look at that specific number all the information atom positions everything is available ok.

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So, here it is for a primitive cubic like up to this position if you see if an item is put at this position only one item can be put, the next atom has to if comes next type of an species it has to be put here or here or here, but if I like here I can put one atom at these position xx this one, this x is a variable number, one more atom can be put with a value of x which is different. So, that is possible only for this that is suppose like here if you consider general position if I put 48 positions are there. What I can do it is that I can put a atom which occupies a general position, since in this unit cell this is one general point.

At this general point I can put a suppose a atom has been kept here b atom is kept here, then by symmetry elements I will be generating all other ones like this I can put it. In another position b atom can be again put in a general point, again be symmetry that is still it is space feeling nothing it touching each other, by symmetry operations we consider this page also atoms can be placed in the unit cell if energetic demands.

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That is what I wanted to tell here I am just showing the structures based done you take in a simple case of a sodium chloride, here if you see it that is sodium atom assume that it occupies this position because here it is fixed. So, only one atom can come, any other position if you considered as difference symmetry.

So, the next atom which it has to occupy either it has to go to this are this position because from the energetic consideration this is how it happens, but it is by a reflection which comes there are many options are available, that is why in those position though the crystallography table says the this is the value of x, we have to do x ray diffraction and do the intensity of the peak from that we can find out what is the value of x that is what all the crystallography is about, that is the whole x ray crystallography is to find out not only the crystal structures, but also what is the specific position which each atom is occupying that value x in the table is not defined. So, it is the job of the crystallographers to find out what the value is.

This will vary from element to element. In one element that value of x could be some particular value point some three another it could be some 0.35, another element when it forms the same crystal structure. So, that is how it changes.

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Structures based on filling up of interstices – FCC lattice

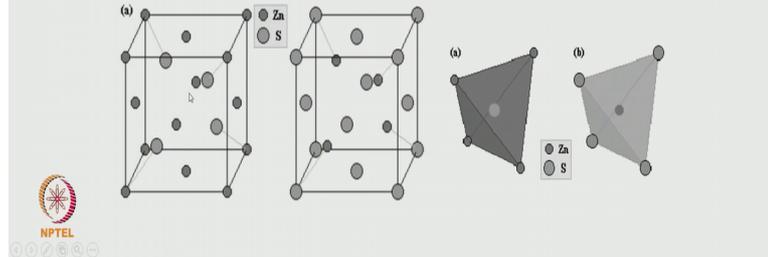FCC (tetrahedral sites) – half filled by different type of atom - ?????

Different type of atoms at tetrahedral sites - ZnS

Zinc Blende (sphalerite), cubic ZnS
Structure: cubic; $a = 0.5420$ nm; $Z = 4$; *Space group*, $F\bar{4}3m$ (No. 216);
Atom positions: Zn: $4a$ $\quad 0, 0, 0; \quad \frac{1}{2}, \frac{1}{2}, 0; \quad \frac{1}{2}, 0, \frac{1}{2}; \quad 0, \frac{1}{2}, \frac{1}{2};$
$\qquad\qquad$ S: $4c$ $\quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4}; \quad \frac{3}{4}, \frac{3}{4}, \frac{1}{4}; \quad \frac{3}{4}, \frac{1}{4}, \frac{3}{4}; \quad \frac{1}{4}, \frac{3}{4}, \frac{3}{4}$

So, similarly like zinc sulphide I have taken, here also you can see that this is the way that the zinc atoms they occupy some specific positions. So, the sulphur atoms we will occupies that 4 c position and when the number of atom increases. If you wanted to look at that unit cell it becomes quite difficult to understand it what is the best way in which can be done is take one atom; what are the nearest neighbors which are going to be there like this sort of a case and instead of showing the atom position now with these cases we can construct it, it becomes much simpler to under the crystal structure.

This is one way in which the crystals are represented, all these aspects I have been covered in that classes and then in addition to it what all the for a given a particular plane how the directions have to be represented, how the planes have to be represented, if two planes are they are what is that direction which is come on to it, if two directions are their what is the plane which is come on to it what is shown axis all this aspects have been covered. So, essentially what I have done it is some aspects of crystallography which has been covered over the course of 7 or 8 lectures, I had just tried to highlight these aspects of it.

Anyway, I hope I have given over all idea all various aspects which I considers important in electron diffraction and imaging. So, the examination is there shortly go through it and prepare wish you all success.

Thank you.