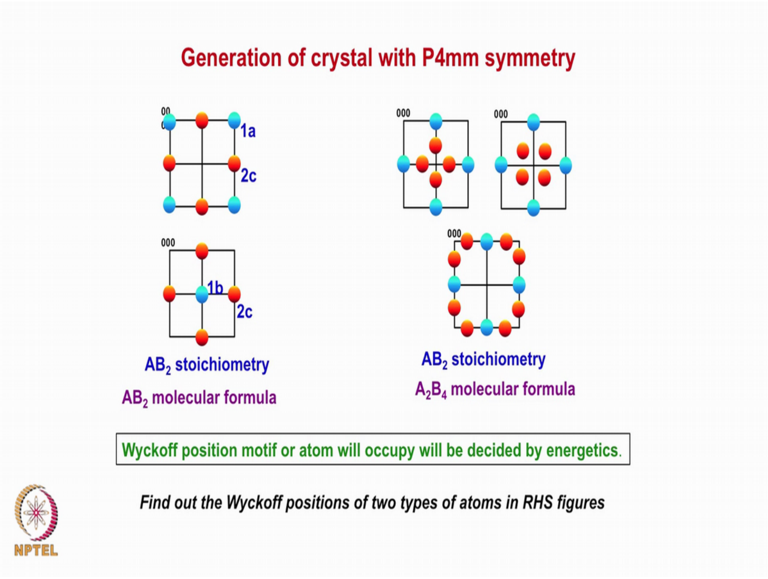
Electron Diffraction and Imaging
Prof. Sundararaman M
Department of Metallurgical and Materials Engineering
Indian Institute of Technology, Madras

Lecture – 08
Symmetry in 3-D Crystals

Welcome you all to this. In the last class what did we cover; that is given the Wyckoff table, how to use it to generate crystals having different stoichiometry all these things which we consider correct.

(Refer Slide Time: 00:45)



Generation of crystal with P4mm symmetry

AB_2 stoichiometry

AB_2 molecular formula

AB_2 stoichiometry

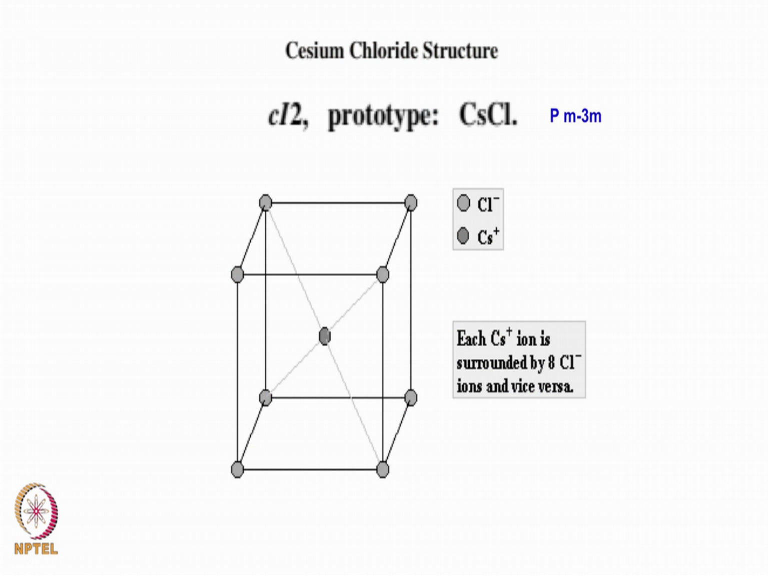
A_2B_4 molecular formula

Wyckoff position motif or atom will occupy will be decided by energetics.

Find out the Wyckoff positions of two types of atoms in RHS figures

So, essentially in that one the last slide which we use was to generate a crystal with P4mm symmetry and having stoichiometry AB 2 and with 2 different molecular formula one is having a AB 2, this one molecular formula another is A 2 B 4 correct. In this particular case if we consider this is a one type of an atom between 2 types of another atom.

(Refer Slide Time: 01:21)



Cesium Chloride Structure

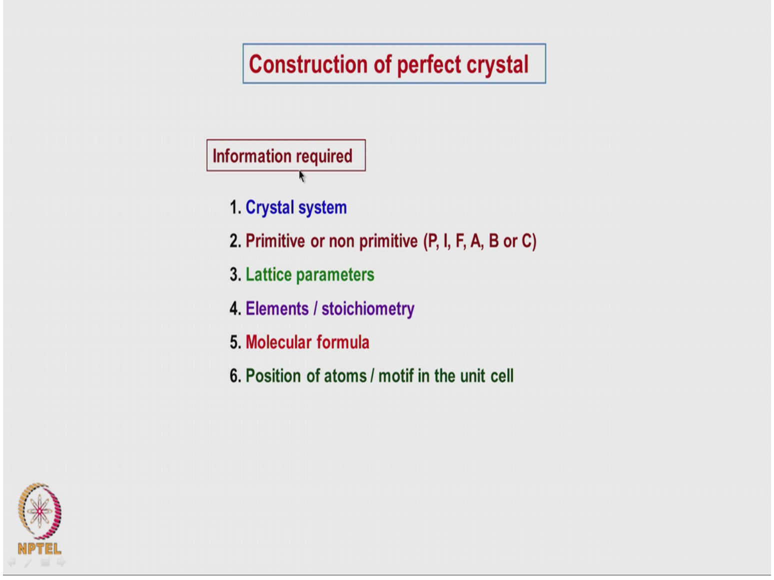
*cI*2, prototype: CsCl. P m-3m

Each Cs^+ ion is surrounded by 8 Cl^- ions and vice versa.

So, essentially this will be at a position which is exactly the middle of it because the force of attraction or repulsion whatever you look at it, it is going to be equal on either side. You look at these cases here what happens here these are like atoms which will have a repulsive force between them, these are unlike atoms which can attract each other, because of this depending upon the energetics and the type of interaction whether it is a covalent or ionic type of bonding these atom positions could move in these directions correct.

But even if it moves from here position to a closer position if you look at the symmetry remains that same that does not change right. Exact position atoms occupy in the crystal can change depending upon the type of atom which is involved where types of atom which are involved buts the symmetry remains the same that does not change.

(Refer Slide Time: 02:33)



Construction of perfect crystal

Information required

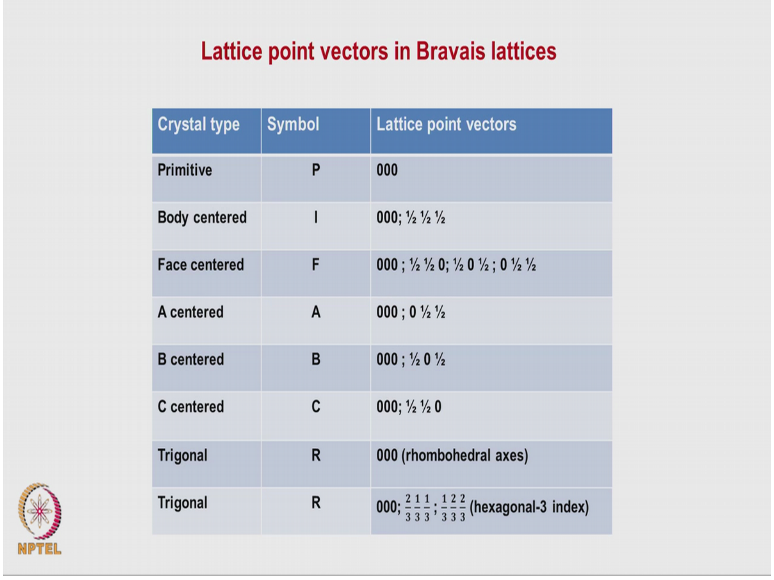
1. Crystal system
2. Primitive or non primitive (P, I, F, A, B or C)
3. Lattice parameters
4. Elements / stoichiometry
5. Molecular formula
6. Position of atoms / motif in the unit cell

So, far what we have considered is if we have to construct a perfect crystal what all information which we require the perfect crystal means that a crystal which does not contain any defects then one we should know what is the crystal system in which we want the crystal to be correct. So, this we are considering it that we are trying to construct a crystal then another is the other primitive or whether it is a non primitive lattice that information is necessary.

Then what all the lattice parameters which the crystal has, then what all the elements which constitute the crystal structure, and whether the elements occupy positions randomly in the lattice or they occupy some specific positions that is that information that is whether it is ordered or disordered. And then what is the molecular formula which compound should have in that unit cell that decides that also decides which position the atoms will occupy in the crystal.

If all these information is available, then we can construct a crystals looking at the Wyckoff position table which is given. The other one which is available in the international union of crystallography is the symmetry diagonal 2 dimensional representation of symmetry and also the position of a motive or an atom if you put at a general point how it is distributed, but this Wyckoff table is the one which is most important as far as construction of crystal structure is concerned.

(Refer Slide Time: 04:24)



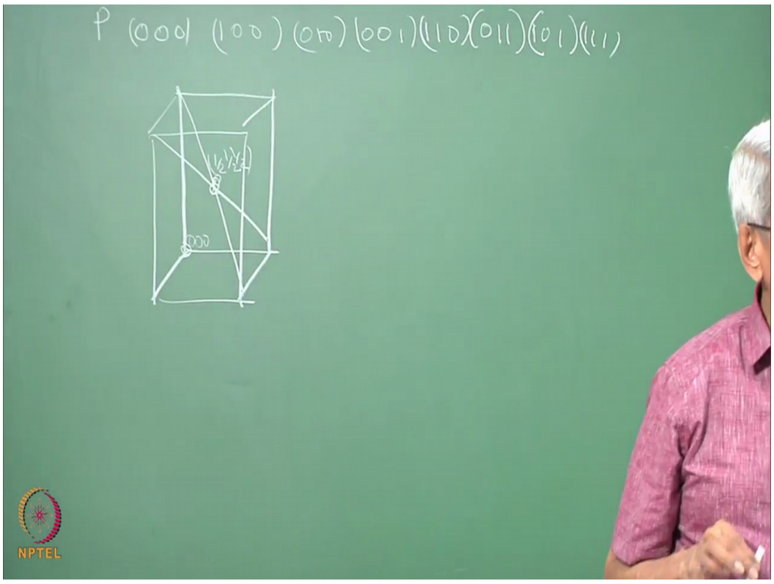
Lattice point vectors in Bravais lattices

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)

We will go into it in a little bit detail. The first thing is that all these crystals if we considered 3 dimensional crystals these are all based on 14 Bravais lattices correct. Essentially putting atoms at different positions in the lattice whether it is a general or special position, we generate different types of crystals with a different type of space groups correct. But how many types of lattices which we can have they are only 14.

So, the one is the lattice could be a primitive lattice correct. If a lattice is a primitive lattice then, we have to then one has to mention only that one position which is a lattice point at the origin if it is mentioned all other lattice points could be generated, because suppose we that for it is a primitive lattice all primitive lattices only one lattice point will be given.

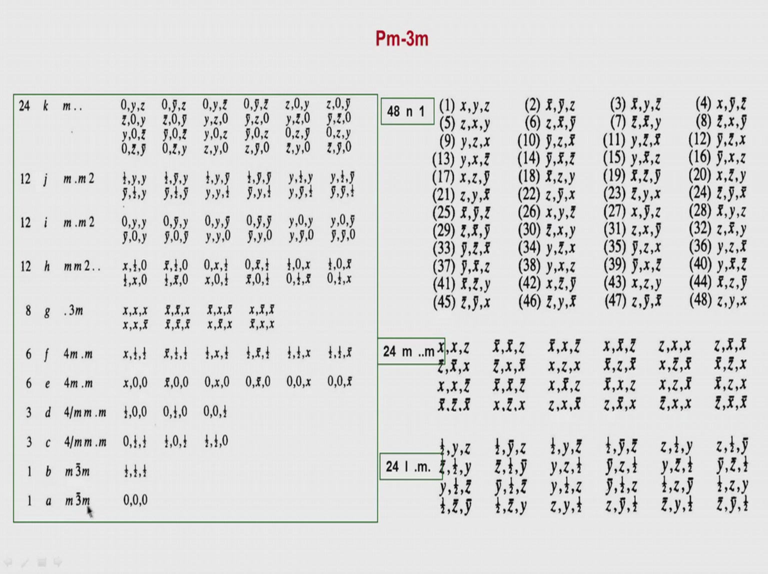
(Refer Slide Time: 05:30)



Once that lattice point is given then by applying the translations symmetry we can generate all of them this will become 100 then 010, 001, 110, 101, 111 like that we can go head and complete that full unit cell could be constructed, because this way using translational symmetry and knowing the position of the atom at the origin the lattice point we can construct the lattice correct.

If it is body centered lattice does not matter whether it is a cubic or whether it is tetragonal or whether it is orthorhombic. 2 lattice points are there in that unit cell. One lattice point is at the origin another lattice point is going to be at the middle. So, this will have coordinates 000, this will have coordinates half, half, half. This is distinctly different from the primitive lattice in the sense that from this lattice point to this lattice point by a lattice translation vector and the symmetry of that point is that side symmetry m 3 bar m. And it is designated in Wyckoff terminology as a and how many points are there the lattice that is only 1.

(Refer Slide Time: 07:21)



Pm-3m

24	k	m . .	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$z,0,y$	$z,0,\bar{y}$
			$\bar{z},0,y$	$\bar{z},0,\bar{y}$	$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$
			$y,0,\bar{z}$	$\bar{y},0,\bar{z}$	$y,0,z$	$\bar{y},0,z$	$0,z,\bar{y}$	$0,z,y$
			$0,\bar{z},\bar{y}$	$0,\bar{z},y$	$z,y,0$	$z,\bar{y},0$	$\bar{z},y,0$	$\bar{z},\bar{y},0$
12	j	m . m 2	$\frac{1}{2},y,y$	$\frac{1}{2},\bar{y},y$	$\frac{1}{2},y,\bar{y}$	$\frac{1}{2},\bar{y},\bar{y}$	$y,\frac{1}{2},y$	$y,\frac{1}{2},\bar{y}$
			$\bar{y},\frac{1}{2},y$	$\bar{y},\frac{1}{2},\bar{y}$	$y,y,\frac{1}{2}$	$\bar{y},y,\frac{1}{2}$	$y,\bar{y},\frac{1}{2}$	$\bar{y},\bar{y},\frac{1}{2}$
12	i	m . m 2	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$	$y,0,y$	$y,0,\bar{y}$
			$\bar{y},0,y$	$\bar{y},0,\bar{y}$	$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$
12	h	m m 2 . .	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$
			$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\frac{1}{2},\bar{x}$	$0,\frac{1}{2},x$
8	g	. 3 m	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$		
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$		
6	f	4m . m	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$
6	e	4m . m	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
3	d	4/m m . m	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$			
3	c	4/m m . m	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			
1	b	$m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
1	a	$m\bar{3}m$	$0,0,0$					

48 n 1

(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$
(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$
(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$
(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$
(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$
(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$
(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$
(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$
(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x

24 m ..m

x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$
$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$
$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$x,\bar{x},z$	$\bar{x},x,z$	$x,z,\bar{x}$	$\bar{x},z,x$
$\bar{x},\bar{z},\bar{x}$	$x,\bar{z},x$	$z,x,\bar{x}$	$z,\bar{x},x$	$\bar{z},x,x$	$\bar{z},\bar{x},\bar{x}$

24 l .m.

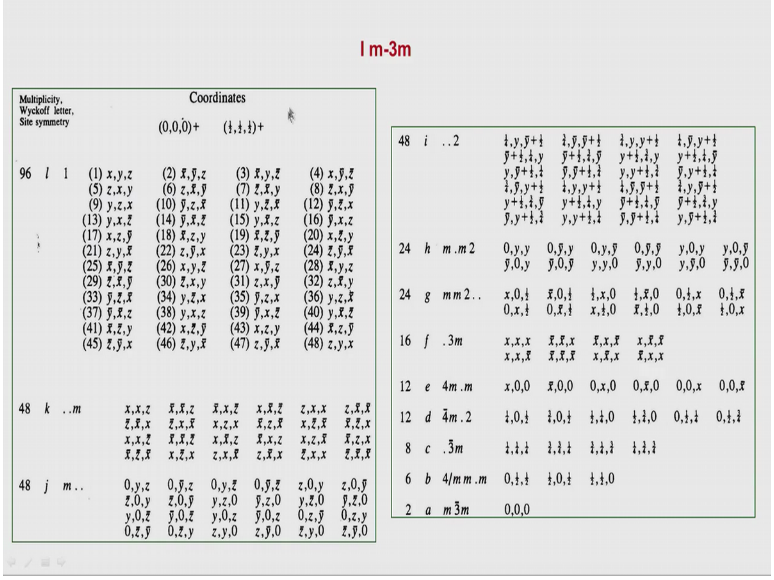
$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$	$\frac{1}{2},y,\bar{z}$	$\frac{1}{2},\bar{y},\bar{z}$	$z,\frac{1}{2},y$	$z,\frac{1}{2},\bar{y}$
$\bar{z},\frac{1}{2},y$	$\bar{z},\frac{1}{2},\bar{y}$	$y,z,\frac{1}{2}$	$\bar{y},z,\frac{1}{2}$	$y,\bar{z},\frac{1}{2}$	$\bar{y},\bar{z},\frac{1}{2}$
$y,\frac{1}{2},\bar{z}$	$\bar{y},\frac{1}{2},\bar{z}$	$y,\frac{1}{2},z$	$\bar{y},\frac{1}{2},z$	$\frac{1}{2},z,\bar{y}$	$\frac{1}{2},z,y$
$\frac{1}{2},\bar{z},\bar{y}$	$\frac{1}{2},\bar{z},y$	$z,y,\frac{1}{2}$	$z,\bar{y},\frac{1}{2}$	$\bar{z},y,\frac{1}{2}$	$\bar{z},\bar{y},\frac{1}{2}$

Then as I mentioned earlier if you are trying to construct a lattice or if you are trying to construct not lattice a crystal using only one element any one of this atom positions could only be fill correct. If we are keeping an atom in the simple cubic lattice at a general point, then another 48 points related by symmetry we have to keep the atoms to generate the simple cubic lattice you understand that is what this is being shown and there are others with when it is being kept on some other symmetry elements these are all the positions which are being given is it clear?

So, in a simple cubic lattice, if we do not keep atom at the lattice point put it as a general point, like a somewhere here if you try to keep an atom in this lattice in simple cubic then the number of positions in which the atom has to be there is 48 or a simple cubic lattice, then we place an atom at a random point within the unit cell there are another 48 positions are there which are related by symmetry at which the atoms are there.

Normally the lattices which we consider for when we try to fill up the different special positions the one which has the highest symmetry is what is filled that turns out to be this particular position. So, we get a simple cubic crystal structure with atom occupying the lattice point correct. Then the unit cell will have 48 atoms in it. That is a maximum which it can have. On this basis if we consider how many atoms are required to construct FCC lattice putting an atom at a random point that is one ninety 2 atoms will be there if we place an atom at a random point in an FCC unit cell. The crystal to exhibit that because 4 of 4 the FCC lattice contains 4 atoms per unit cell.

(Refer Slide Time: 10:26)



I m-3m

Multiplicity, Wyckoff letter, Site symmetry			Coordinates					
			(0,0,0)+	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+				
96	*l*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$		
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$		
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$		
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$		
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$		
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$		
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$		
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$		
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$		
			(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$		
			(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$		
			(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x		
48	*k*	..*m*	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$
			$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$x,\bar{x},z$	$\bar{x},x,z$	$x,z,\bar{x}$	$\bar{x},z,x$
			$\bar{x},\bar{z},\bar{x}$	$x,\bar{z},x$	$z,x,\bar{x}$	$z,\bar{x},x$	$\bar{z},x,x$	$\bar{z},\bar{x},\bar{x}$
48	*j*	*m*..	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$z,0,y$	$z,0,\bar{y}$
			$\bar{z},0,y$	$\bar{z},0,\bar{y}$	$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$
			$y,0,\bar{z}$	$\bar{y},0,\bar{z}$	$y,0,z$	$\bar{y},0,z$	$0,z,\bar{y}$	$0,z,y$
			$0,\bar{z},\bar{y}$	$0,\bar{z},y$	$z,y,0$	$z,\bar{y},0$	$\bar{z},y,0$	$\bar{z},\bar{y},0$

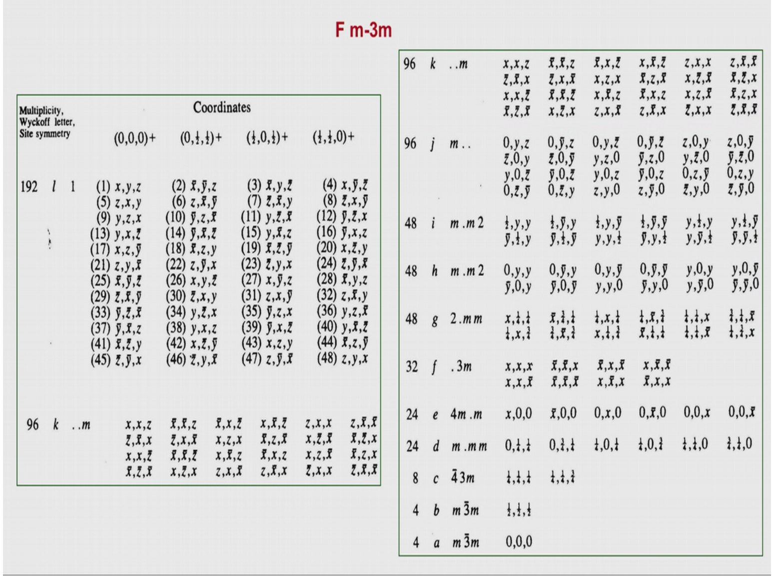
48	*i*	..2	$\frac{1}{4},y,\bar{y}+\frac{1}{2}$	$\frac{3}{4},\bar{y},\bar{y}+\frac{1}{2}$	$\frac{3}{4},y,y+\frac{1}{2}$	$\frac{1}{4},\bar{y},y+\frac{1}{2}$		
			$\bar{y}+\frac{1}{2},\frac{1}{4},y$	$\bar{y}+\frac{1}{2},\frac{3}{4},\bar{y}$	$y+\frac{1}{2},\frac{3}{4},y$	$y+\frac{1}{2},\frac{1}{4},\bar{y}$		
			$y,\bar{y}+\frac{1}{2},\frac{1}{4}$	$\bar{y},\bar{y}+\frac{1}{2},\frac{3}{4}$	$y,y+\frac{1}{2},\frac{3}{4}$	$\bar{y},y+\frac{1}{2},\frac{1}{4}$		
			$\frac{3}{4},\bar{y},y+\frac{1}{2}$	$\frac{1}{4},y,y+\frac{1}{2}$	$\frac{1}{4},\bar{y},\bar{y}+\frac{1}{2}$	$\frac{3}{4},y,\bar{y}+\frac{1}{2}$		
			$y+\frac{1}{2},\frac{3}{4},\bar{y}$	$y+\frac{1}{2},\frac{1}{4},y$	$\bar{y}+\frac{1}{2},\frac{1}{4},\bar{y}$	$\bar{y}+\frac{1}{2},\frac{3}{4},y$		
			$\bar{y},y+\frac{1}{2},\frac{3}{4}$	$y,y+\frac{1}{2},\frac{1}{4}$	$\bar{y},\bar{y}+\frac{1}{2},\frac{1}{4}$	$y,\bar{y}+\frac{1}{2},\frac{3}{4}$		
24	*h*	*m*.*m*2	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$	$y,0,y$	$y,0,\bar{y}$
			$\bar{y},0,y$	$\bar{y},0,\bar{y}$	$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$
24	*g*	*mm*2..	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$0,\frac{1}{2},x$	$0,\frac{1}{2},\bar{x}$
			$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$\frac{1}{2},0,\bar{x}$	$\frac{1}{2},0,x$
16	*f*	.3*m*	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$		
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$		
12	*e*	4*m*.*m*	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
12	*d*	$\bar{4}m.2$	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},0$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$
8	*c*	$.\bar{3}m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$		
6	*b*	4/*mm*.*m*	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			
2	*a*	$m\bar{3}m$	$0,0,0$					

Similarly, body centered if we consider cubic lattice, it will have 96. That is and another important factor which you see that here I am showing it for the body centered unit cell all the Wyckoff position tables which are available if you see here one thing which will be mentioned as the co ordinance 000 plus half, half plus this means that these are all the 2 lattice points in the Bravais lattice. And here the coordinates which are given is 1 with respect to only the origin. And if you see this is the symmetry of the point and then 000 it is Wyckoff position is a and it is mentioned the always that 2 atoms have to there. How do you generate the atom in the second position that is to these 2 lattice points you add this particular position where that atom should be there if you add it this will become 000 and half, half, half correct?

So, these are all the 2 positions the atoms will be therein if it is a single atom if you consider it. Suppose you are placing the atom not at the corner, but at the face center, then these are all the 3 general positions which are been trigonal indices, and with respect to origin where one of the lattice point, you take these 3 positions will be able to generate them. With respect to the other nonequivalent point in the crystal you will be able to generate another 3 more.

So, total 6 positions where the atom will be there. Is it clear? There is the atom is being put at this particular special point, if we try to keep it or it. So, happens that we assume that this crystal body centered units that is, but it contains 6 atoms then what is the position which it can acquire have then the atom have to occupy only this particular one. Is it clear? What we will do it is that some of these things as an assignment we will work it out on this Saturday. Then it will become very clear to you.

(Refer Slide Time: 13:09)



F m-3m

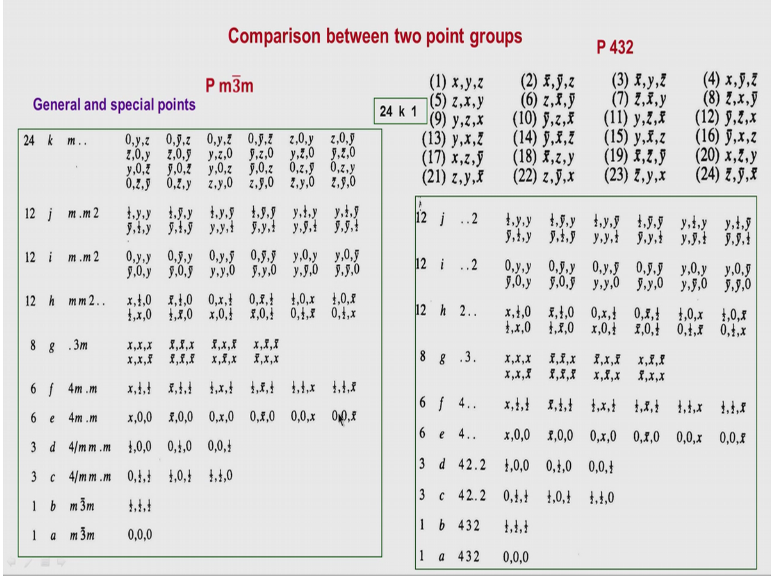
Multiplicity, Wyckoff letter, Site symmetry			Coordinates (0,0,0)+	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$
192	*l*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$
			(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$
			(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$
			(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x

96	*k*	..*m*	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$
			$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$x,\bar{x},z$	$\bar{x},x,z$	$x,z,\bar{x}$	$\bar{x},z,x$
			$\bar{x},\bar{z},\bar{x}$	$x,\bar{z},x$	$z,x,\bar{x}$	$z,\bar{x},x$	$\bar{z},x,x$	$\bar{z},\bar{x},\bar{x}$

96	*k*	..*m*	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$
			$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$x,\bar{x},z$	$\bar{x},x,z$	$x,z,\bar{x}$	$\bar{x},z,x$
			$\bar{x},\bar{z},\bar{x}$	$x,\bar{z},x$	$z,x,\bar{x}$	$z,\bar{x},x$	$\bar{z},x,x$	$\bar{z},\bar{x},\bar{x}$
96	*j*	*m*..	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$z,0,y$	$z,0,\bar{y}$
			$\bar{z},0,y$	$\bar{z},0,\bar{y}$	$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$
			$y,0,\bar{z}$	$\bar{y},0,\bar{z}$	$y,0,z$	$\bar{y},0,z$	$0,z,\bar{y}$	$0,z,y$
			$0,\bar{z},\bar{y}$	$0,\bar{z},y$	$z,y,0$	$z,\bar{y},0$	$\bar{z},y,0$	$\bar{z},\bar{y},0$
48	*i*	*m*.*m*2	$\frac{1}{2},y,y$	$\frac{1}{2},\bar{y},y$	$\frac{1}{2},y,\bar{y}$	$\frac{1}{2},\bar{y},\bar{y}$	$y,\frac{1}{2},y$	$y,\frac{1}{2},\bar{y}$
			$\bar{y},\frac{1}{2},y$	$\bar{y},\frac{1}{2},\bar{y}$	$y,y,\frac{1}{2}$	$\bar{y},y,\frac{1}{2}$	$y,\bar{y},\frac{1}{2}$	$\bar{y},\bar{y},\frac{1}{2}$
48	*h*	*m*.*m*2	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$	$y,0,y$	$y,0,\bar{y}$
			$\bar{y},0,y$	$\bar{y},0,\bar{y}$	$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$
48	*g*	2.*mm*	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}$
			$\frac{1}{4},x,\frac{3}{4}$	$\frac{3}{4},\bar{x},\frac{3}{4}$	$x,\frac{1}{4},\frac{3}{4}$	$\bar{x},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\bar{x}$	$\frac{1}{4},\frac{3}{4},x$
32	*f*	.3*m*	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$		
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$		
24	*e*	4*m*.*m*	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
24	*d*	*m*.*mm*	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$
8	*c*	$\bar{4}3m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$				
4	*b*	$m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
4	*a*	$m\bar{3}m$	$0,0,0$					

Similarly, in FCC if we consider what all the lattice points are there. Lattice points are 4 points are there correct. Within that lattice and with respect to these lattice points around each lattice point these are all the positions which we can have the atom. Then if we add with respect to each of this coordinates which are given we will generate 4 points. And that when they are occupied the simple cubic lattice like copper aluminum gold nickel all these elements we can generate, because there are only 4 atoms per unit cell. Is it not that is the way this going to fill up.

(Refer Slide Time: 14:01)



Comparison between two point groups

P $m\bar{3}m$

General and special points

24	k	$m..$	$0,y,z$ $\bar{z},0,y$ $y,0,\bar{z}$ $0,\bar{z},\bar{y}$	$0,\bar{y},z$ $\bar{z},0,\bar{y}$ $\bar{y},0,\bar{z}$ $0,\bar{z},y$	$0,y,\bar{z}$ $y,z,0$ $y,0,z$ $z,y,0$	$0,\bar{y},\bar{z}$ $\bar{y},z,0$ $\bar{y},0,z$ $z,\bar{y},0$	$z,0,y$ $y,\bar{z},0$ $0,z,\bar{y}$ $\bar{z},y,0$	$z,0,\bar{y}$ $\bar{y},\bar{z},0$ $0,z,y$ $\bar{z},\bar{y},0$
12	j	$m.m2$	$\frac{1}{2},y,y$ $\bar{y},\frac{1}{2},y$	$\frac{1}{2},\bar{y},y$ $\bar{y},\frac{1}{2},\bar{y}$	$\frac{1}{2},y,\bar{y}$ $y,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\bar{y}$ $\bar{y},y,\frac{1}{2}$	$y,\frac{1}{2},y$ $y,\bar{y},\frac{1}{2}$	$y,\frac{1}{2},\bar{y}$ $\bar{y},\bar{y},\frac{1}{2}$
12	i	$m.m2$	$0,y,y$ $\bar{y},0,y$	$0,\bar{y},y$ $\bar{y},0,\bar{y}$	$0,y,\bar{y}$ $y,y,0$	$0,\bar{y},\bar{y}$ $\bar{y},y,0$	$y,0,y$ $y,\bar{y},0$	$y,0,\bar{y}$ $\bar{y},\bar{y},0$
12	h	$mm2..$	$x,\frac{1}{2},0$ $\frac{1}{2},x,0$	$\bar{x},\frac{1}{2},0$ $\frac{1}{2},\bar{x},0$	$0,x,\frac{1}{2}$ $x,0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$	$\frac{1}{2},0,x$ $0,\frac{1}{2},\bar{x}$	$\frac{1}{2},0,\bar{x}$ $0,\frac{1}{2},x$
8	g	$.3m$	x,x,x $x,x,\bar{x}$	$\bar{x},\bar{x},x$ $\bar{x},\bar{x},\bar{x}$	$\bar{x},x,\bar{x}$ $x,\bar{x},x$	$x,\bar{x},\bar{x}$ $\bar{x},x,x$		
6	f	$4m.m$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$
6	e	$4m.m$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
3	d	$4/mm.m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$			
3	c	$4/mm.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			
1	b	$m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
1	a	$m\bar{3}m$	$0,0,0$					

P 432

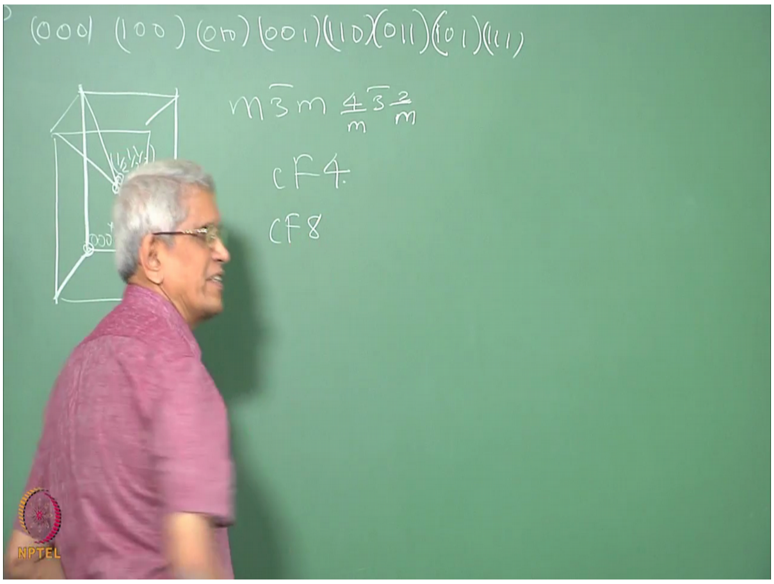
24 k 1

(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$
(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$
(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$
(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$
(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$
(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$

12	j	$..2$	$\frac{1}{2},y,y$ $\bar{y},\frac{1}{2},y$	$\frac{1}{2},\bar{y},y$ $\bar{y},\frac{1}{2},\bar{y}$	$\frac{1}{2},y,\bar{y}$ $y,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\bar{y}$ $\bar{y},y,\frac{1}{2}$	$y,\frac{1}{2},y$ $y,\bar{y},\frac{1}{2}$	$y,\frac{1}{2},\bar{y}$ $\bar{y},\bar{y},\frac{1}{2}$
12	i	$..2$	$0,y,y$ $\bar{y},0,y$	$0,\bar{y},y$ $\bar{y},0,\bar{y}$	$0,y,\bar{y}$ $y,y,0$	$0,\bar{y},\bar{y}$ $\bar{y},y,0$	$y,0,y$ $y,\bar{y},0$	$y,0,\bar{y}$ $\bar{y},\bar{y},0$
12	h	$2..$	$x,\frac{1}{2},0$ $\frac{1}{2},x,0$	$\bar{x},\frac{1}{2},0$ $\frac{1}{2},\bar{x},0$	$0,x,\frac{1}{2}$ $x,0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$	$\frac{1}{2},0,x$ $0,\frac{1}{2},\bar{x}$	$\frac{1}{2},0,\bar{x}$ $0,\frac{1}{2},x$
8	g	$.3.$	x,x,x $x,x,\bar{x}$	$\bar{x},\bar{x},x$ $\bar{x},\bar{x},\bar{x}$	$\bar{x},x,\bar{x}$ $x,\bar{x},x$	$x,\bar{x},\bar{x}$ $\bar{x},x,x$		
6	f	$4..$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$
6	e	$4..$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
3	d	42.2	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$			
3	c	42.2	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			
1	b	432	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
1	a	432	$0,0,0$					

Here what I have shown is comparing between 2 primitive lattices of the cubic unit. This is p m 3 bar m. I had just shown the few not the complete coordinates for all the Wyckoff positions I have not shown. Here it is for p 4 3 2. This is also primitive lattice cubic, but the space group symmetry these 2 are different. What is this m 3 bar m means actual symmetry elements?

(Refer Slide Time: 14:44)



4 by m 3 bar 2 by m, this is the full symmetry element which is associated you should, remember all these also because what is given is a convention is a short hand notation is this clear.

Here if you look at it this is also a simple cubic lattice. This symmetry this also 4 3 2, if I take an atom has got an infinite symmetry right assuming to be a sphere, then if I place it at the simple cube at 0 0 position. Then what is the symmetry which it will exhibit. What is the symmetry the crystal will have, 4 3 2 or p m 3 bar m?

Student: Sir, both of the symmetry elements will be there.

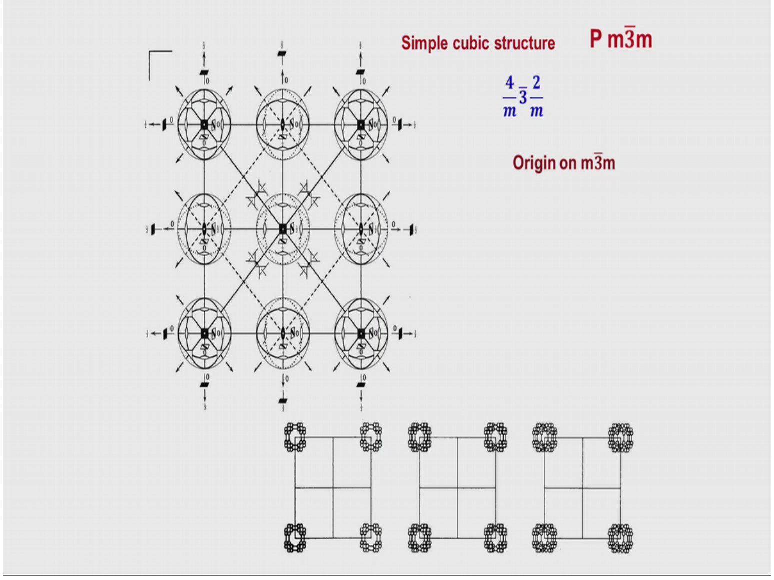
Both of the symmetry elements, but which has got the maximum symmetry element.

Student: M 3 bar m.

M 3 bar m. So, that symmetry element it will exhibit. So, if you see here all these Wyckoff positions up to a certain point here these Wyckoff positions remains that same identical, which because it is a simple cubic unit cell on which if you try to fill up these positions there all identical positions. So, then the symmetry which will exhibits the one which is maximum which it can have, but only here when you come to this Wyckoff position and here this Wyckoff position you find that suddenly there are differences in the atom position only when we place atoms corresponding to these positions, then only the difference between these 2 structures will come. Is it clear? What does this suggest that only when we have a large number of atoms are there to be placed within the unit cell then only the subtle difference between these 2 primitive lattices with 2 different types of symmetries which we see the difference otherwise if it is only a one type of an atom and we are placing it as a lattice point it is like it will exhibit the symmetry of the lattice what is the symmetry of the lattice for a simple cubic lattice it is p m 3 bar m. So, that is a maximum symmetry.

The subtle differences in symmetry come only atom is kept at positions, where the number of atoms which has to be kept at for some Wyckoff positions we see the difference only. When those Wyckoff positions that is the number of atoms per unit cell suppose for a simple cubic lattice turns out to be 24. Then the options are whether it can be filled in this way or it can be filled in this way if the atom positions are kept at these particular positions. Then it will turn out to be p m 3 bar m. If the atoms are kept at these positions it will give a symmetry which is p 4 3 2 is that clear?

(Refer Slide Time: 18:28)



Simple cubic structure

P m$\bar{3}$m

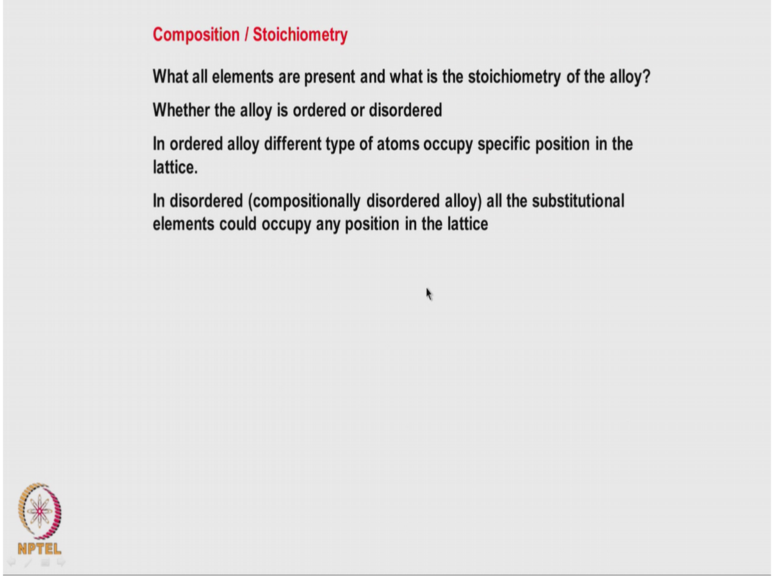
$\frac{4}{m}\bar{3}\frac{2}{m}$

Origin on m$\bar{3}$m

So far whatever the symmetry diagram and the positions of general point in the unit cell which has been shown in the international union of cryptography whatever I have considered or with respect to structures which have less number of smaller symmetry the when the symmetry becomes large this is p m 3 bar m I have taken you can see the type of symmetry elements which are involved is much more complicated.

When we look for a FCC structure it becomes still more complicated, when we look for a diamond cubic where a glide also is there screw comes into the picture, then these becomes very complicated structures that is so you do not have to really bother about it to construct a crystal structure, what we require is the Wyckoff positions and the coordinates which is given in the international union of crystallography that itself is good enough to construct a crystal structure here. You can see that how the atoms are distributed around the lattice point when it is being placed at a general position.

(Refer Slide Time: 19:47)



Composition / Stoichiometry

What all elements are present and what is the stoichiometry of the alloy?

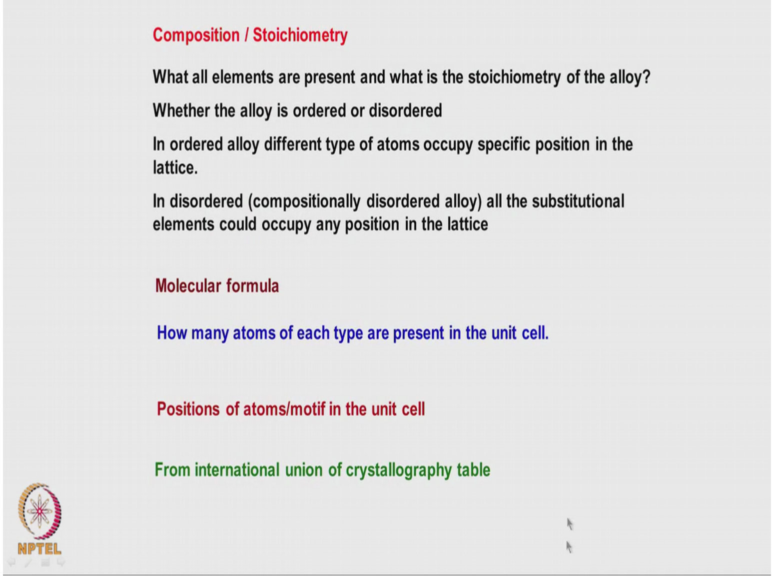
Whether the alloy is ordered or disordered

In ordered alloy different type of atoms occupy specific position in the lattice.

In disordered (compositionally disordered alloy) all the substitutional elements could occupy any position in the lattice

So, as I mention that composition is a necessary, if more than one element is there if it is disordered then atoms can be randomly placed at any position lattice point. If it is ordered, then we should know which particular type of Wyckoff position this atom is going to occupy that also will be decided by the molecular formula of the crystal structure.

(Refer Slide Time: 20:15)



Composition / Stoichiometry

What all elements are present and what is the stoichiometry of the alloy?

Whether the alloy is ordered or disordered

In ordered alloy different type of atoms occupy specific position in the lattice.

In disordered (compositionally disordered alloy) all the substitutional elements could occupy any position in the lattice

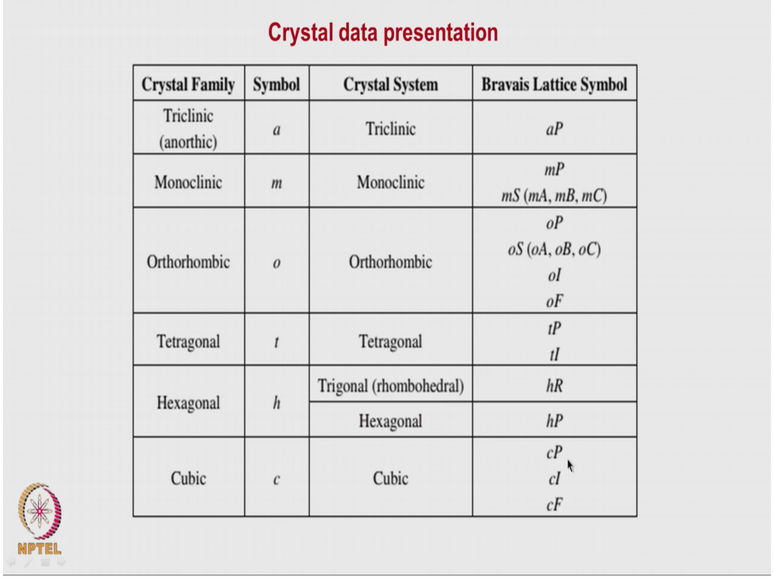
Molecular formula

How many atoms of each type are present in the unit cell.

Positions of atoms/motif in the unit cell

From international union of crystallography table

(Refer Slide Time: 20:17)



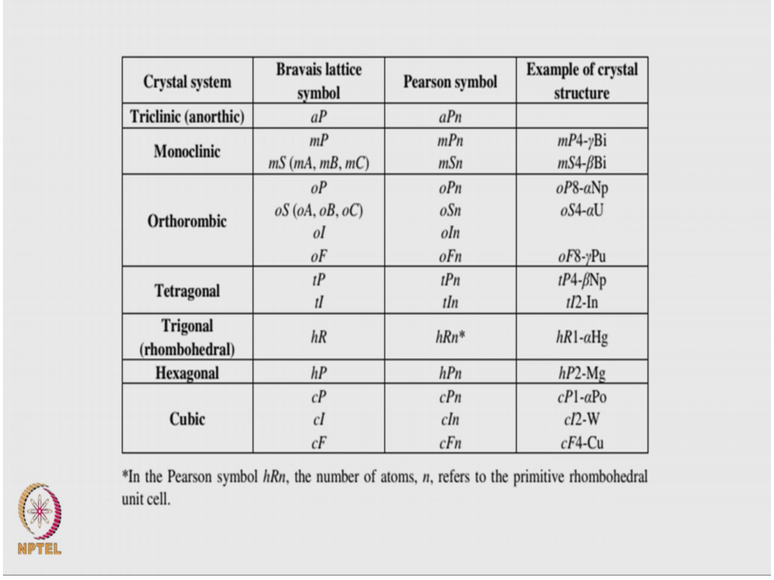
Crystal data presentation

Crystal Family	Symbol	Crystal System	Bravais Lattice Symbol
Triclinic (anorthic)	*a*	Triclinic	*aP*
Monoclinic	*m*	Monoclinic	*mP* *mS* (*mA*, *mB*, *mC*)
Orthorhombic	*o*	Orthorhombic	*oP* *oS* (*oA*, *oB*, *oC*) *oI* *oF*
Tetragonal	*t*	Tetragonal	*tP* *tI*
Hexagonal	*h*	Trigonal (rhombohedral)	*hR*
		Hexagonal	*hP*
Cubic	*c*	Cubic	*cP* *cI* *cF*

So, all this information we can get it from international union of crystallography. If you look at many of the crystal data presentation in many of the books, which are given there are many symbols Pearson’s hand book also. If you look at it, they follow a particular system that is a quite of10 for most of them elements where the crystal structure has been identified elements are many compounds where the crystal structure has been identified. It is tabulated in some form it is available in a some crystal data set. In that they follow a particular symbol to explain this. One triclinic is essentially symbol which is used is a and if it primitive is with respect to p if it is monoclinic it is m and m p and that m s is used where it could be m ABC.

Similarly, orthorhombic if we use o p if is a o is for orthorhombic p is for primitive, o I is for orthorhombic for body centered, o f is orthorhombic face centered like that we have these symbols.

(Refer Slide Time: 21:47)



Crystal system	Bravais lattice symbol	Pearson symbol	Example of crystal structure
Triclinic (anorthic)	*aP*	*aPn*	
Monoclinic	*mP*	*mPn*	*mP*4-γBi
	mS (*mA*, *mB*, *mC*)	*mSn*	*mS*4-βBi
Orthorombic	*oP*	*oPn*	*oP*8-αNp
	oS (*oA*, *oB*, *oC*)	*oSn*	*oS*4-αU
	oI	*oIn*	
	oF	*oFn*	*oF*8-γPu
Tetragonal	*tP*	*tPn*	*tP*4-βNp
	tI	*tIn*	*tI*2-In
Trigonal (rhombohedral)	*hR*	*hRn**	*hR*1-αHg
Hexagonal	*hP*	*hPn*	*hP*2-Mg
Cubic	*cP*	*cPn*	*cP*1-αPo
	cI	*cIn*	*cI*2-W
	cF	*cFn*	*cF*4-Cu

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

These Bravais lattice symbol just tell what is the crystal system to which it belong, and whether it is primitive or a non primitive lattice right. To give the complete information; one more information which is required is how many atoms are there in that unit cell right. Like triclinic if we say a p the last number n this number could be have this number can have different values. Like for example, suppose it is copper how will we represent what is the symbol in these notations.

Student: C.

C f 4 this what it will turn out to be suppose it is diamond.

Student: C f 8.

It will be c f 8 there are going to be 8 positions motive is motive or an atom or a molecule is going to be kept. This is how this representation is, is this clear? This the way it is represented in many books. That is what essentially given in this table also.

(Refer Slide Time: 23:00)

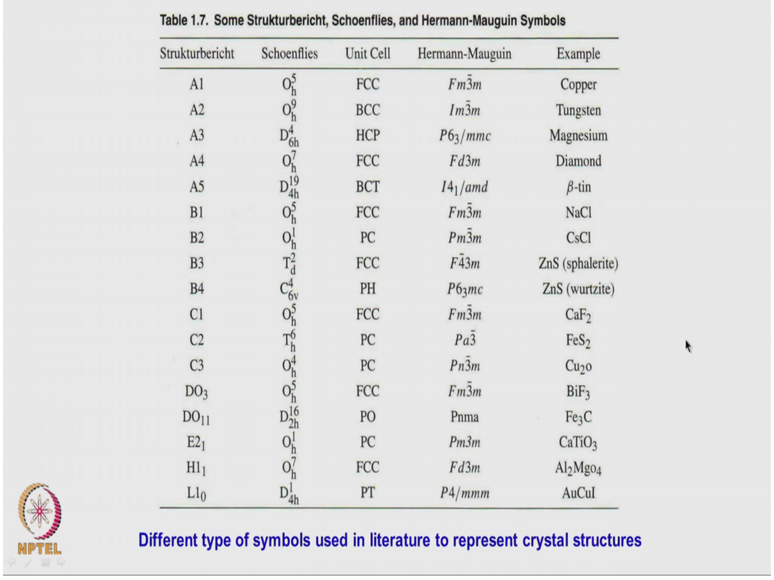


Table 1.7. Some Strukturbericht, Schoenflies, and Hermann-Mauguin Symbols

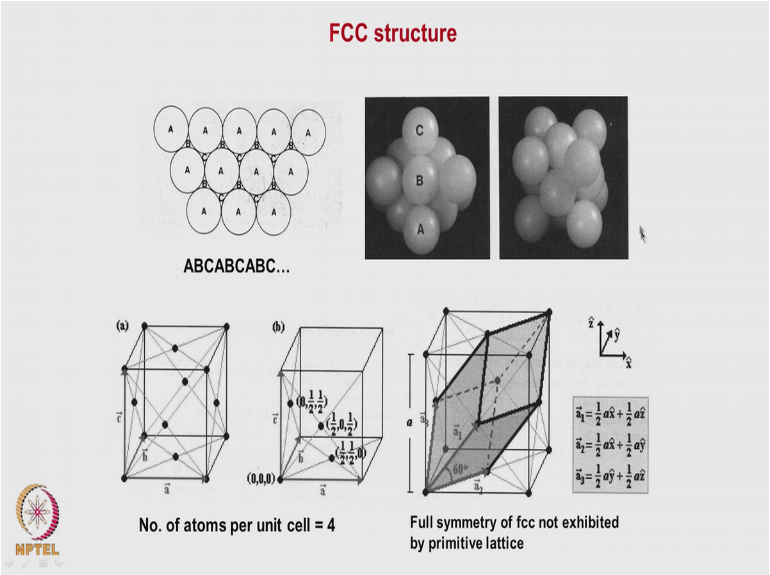
Strukturbericht	Schoenflies	Unit Cell	Hermann-Mauguin	Example
A1	O_h^5	FCC	$Fm\bar{3}m$	Copper
A2	O_h^9	BCC	$Im\bar{3}m$	Tungsten
A3	D_{6h}^4	HCP	$P6_3/mmc$	Magnesium
A4	O_h^7	FCC	$Fd3m$	Diamond
A5	D_{4h}^{19}	BCT	$I4_1/amd$	β-tin
B1	O_h^5	FCC	$Fm\bar{3}m$	NaCl
B2	O_h^1	PC	$Pm\bar{3}m$	CsCl
B3	T_d^2	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

Then when you go through papers you will find that to describe this crystal structure there are many types of symbols which are being used right. In most of the metallurgical journals if you see, that a 1 a 2 a 3 a 4 a 5 then b one b 2 then c 1 c 2 c 3 d o 3 d o to and d 2 l 1 2 l 1 0 this sort of symbols you will notice correct. That is one that is called strukturberichit, because of the oldest one. Then the Schoenflies symbol is the one which what the chemist use it which just represents what is the type of symmetry elements which are rotational and inversion mirror or these things are associated with.

Then the other way is that we can use that just a unit cell FCC BCC this also we see this type of nomenclature used then Hermann-Mauguin is the space group symbol which we will be noticing it and nowadays. This is a one which is used as a standard symbol this as well as this symbol is the Schoenflies symbol these are all the 2 because mostly the solicit chemistry people who work on crystallography they use this symbol. Material scientist uses these symbols. And then typical what is the element which is a element or a compound which is having the crystal structure that also that information is always given.

(Refer Slide Time: 24:31)



FCC structure

ABCABCABC...

No. of atoms per unit cell = 4

Full symmetry of fcc not exhibited by primitive lattice

$\vec{a}_1 = \frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{z}$

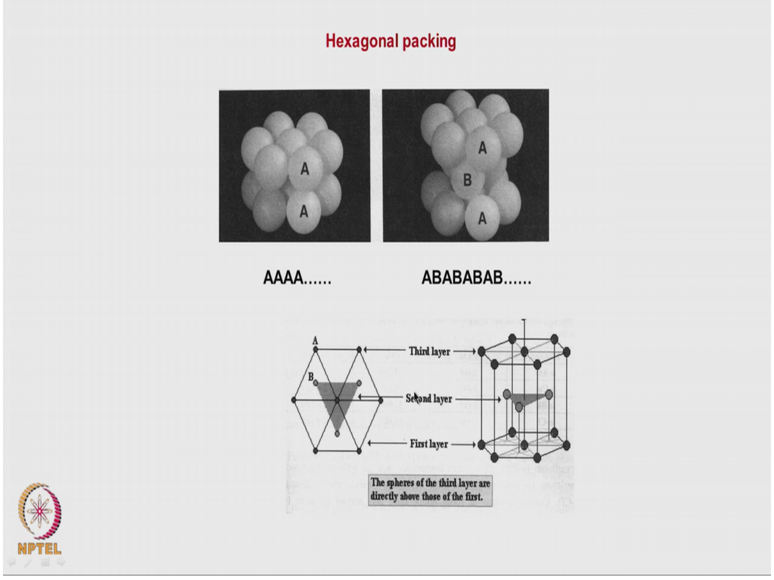
$\vec{a}_2 = \frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y}$

$\vec{a}_3 = \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z}$

What all the ways in which we can represent this structures. One is construction of a unit cell which we have looked at it how to construct a unit cell. Another is arrangement of 2 dimensional layers one on top of each other right. Like for FCC if we take A B C stacking sequence a layer B layer C layer. That is on top of hexagonal lattice, one on kept on top of the other at some different positions we can generate this lattice, that is what essentially is being shown and in the unit cell form also we can represent them. Other way it will be represented is that not only just you do not have to show all the atom positions, we just show the points non points where the atoms are going to be the by 000 the coordinates are given here.

Then this one exhibit this figure tells us about what is the primitive lattice of FCC. Here it is essential a rhombohedral lattice or trigonal. This is one coordinate. So, it is essentially all these 3 together. Half, half 0 half 0 half and 0 half, half, they are the once which derive once the 3 lattice parameters corresponding to this trigonal lattice. This way we can construct it. And this has only one atom per unit cell. So, it is a primitive unit cell. And this is the way we will be representing this coordinates of this lattice in terms of the FCC coordinate correct.

(Refer Slide Time: 26:43)



Hexagonal packing

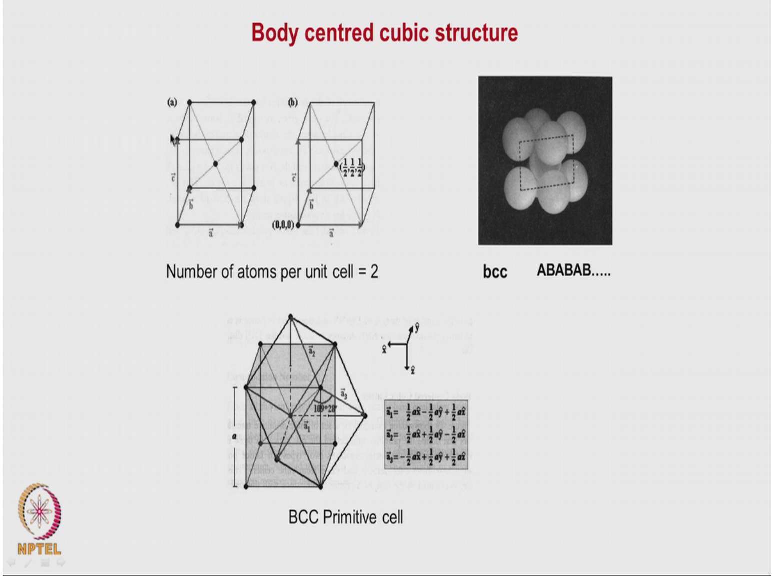
AAAA......

ABABABAB......

The spheres of the third layer are directly above those of the first.

Similarly, we can have hexagonal lattice also we can represent it in this form. It is an A, A, A and HCP as I mentioned is not a Bravais lattice. So, it will have 2 positions the AB, AB. So, essentially if we consider 2 lattice points together that determine the Bravais lattice of hexagonal prospect. And this is another way in which we can represent the projection also right and then at what position these atoms come that also we can mark it to explain.

(Refer Slide Time: 27:24)



Body centred cubic structure

Number of atoms per unit cell = 2

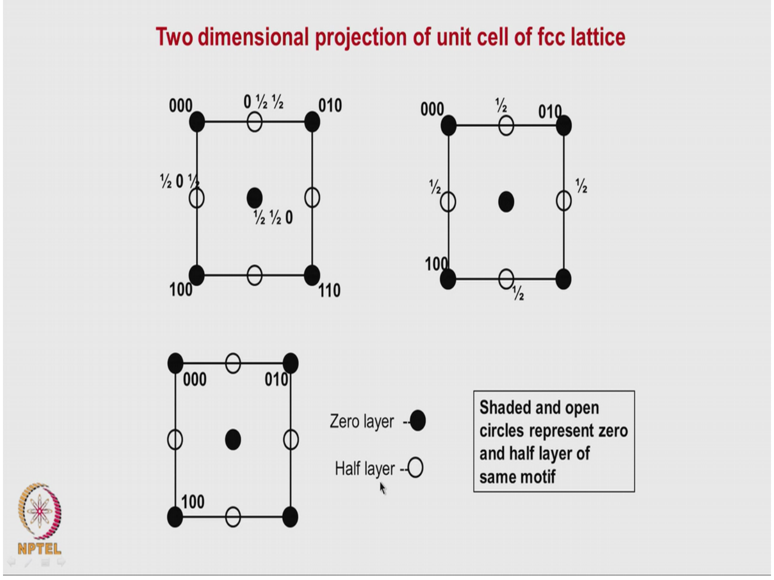
bcc ABABAB.....

$$\vec{a}_1 = \frac{1}{2}a\hat{x} - \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z}$$
$$\vec{a}_2 = \frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} - \frac{1}{2}a\hat{z}$$
$$\vec{a}_3 = -\frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z}$$

BCC Primitive cell

The same way we can represent body centered cubic lattice also, the various representations are possible. And here this one is essentially the rhombohedral lattice unit cell and this is nothing but a primitive lattice, but what is the difference between this primitive lattice and the FCC lattice, FCC are the BCC lattice is that the BCC lattice exhibits to the complete symmetry of the lattice. Whereas, the primitive lattice which we choose that does not exhibit the complete symmetry. And these are all the various ways we can project it also the lattices this is for an FCC lattice.

(Refer Slide Time: 28:17)


Two dimensional projection of unit cell of fcc lattice

Shaded and open circles represent zero and half layer of same motif

Student: In BCC we should represent the primitive lattice. So, why do we represent why do not we represent BCC as the primitive lattice.

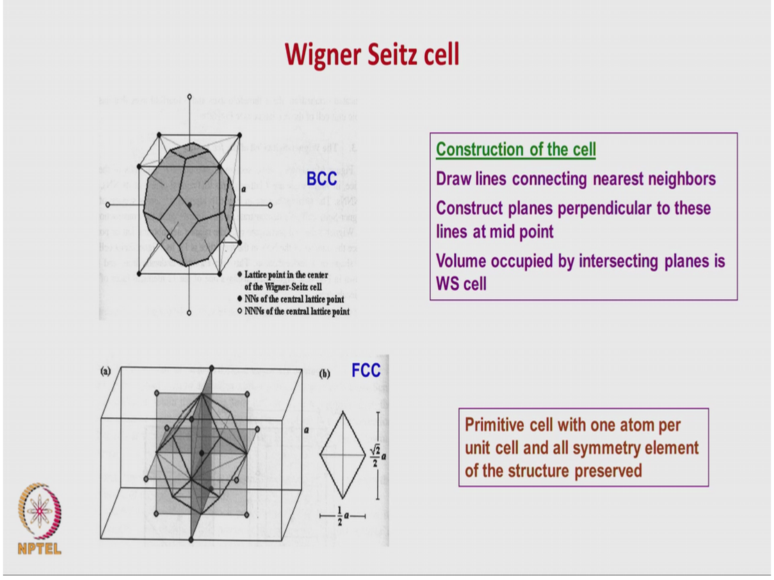
No we can represent it is a primitive lattice, but the problem which happens is that when you represent it as a primitive lattice the symmetry complete symmetry you do not see it in that unit cell.

Student: But, you said in BCC you can.

No, BCC you have the full symmetry is there. The symmetry of the BCC lattice can be seen in the BCC unit cell, but not in the primitive because BCC unit cell is a non primitive. Rhombohedral is the non primitive unit cell. That does not exhibit that symmetry. So, what is the other way in which this could be represented, the projection we can take it along any particular direction, and then show these are the atoms which are there in the projected layer, which is a 001 and then atoms at other positions they can be represented with different symbol and we give the coordinates.

Or we can just give with this positions which essentially tells that it is half layer up. That is another way in which we can represent them also, we just use 2 symbols, but you just right it down zeroth layer and half layer. This sort of notation when you go through many of the publish papers you will find all types of notations are used to represent unit cells.

(Refer Slide Time: 29:58)



Wigner Seitz cell

Construction of the cell

Draw lines connecting nearest neighbors

Construct planes perpendicular to these lines at mid point

Volume occupied by intersecting planes is WS cell

Primitive cell with one atom per unit cell and all symmetry element of the structure preserved

If this is called as a Wigner Seitz: Wigner Seitz cell what do you understand from this.

Student: It is primitive.

Primitive what else.

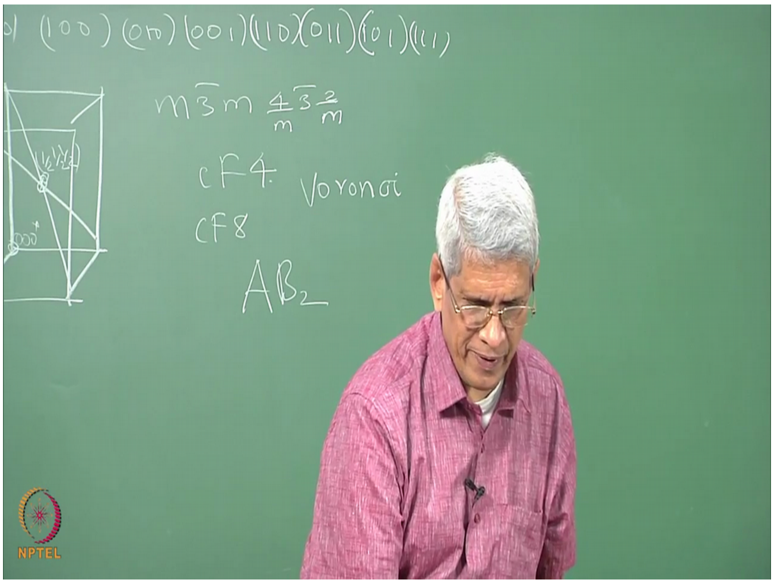
Student: Exhibits full symmetry.

This lattice exhibits this is a primitive lattice which is constructed which exhibits the full symmetry of the crystal structure. How is it constructed from the origin find out all the nearest neighbor points, draw lines to them find out the midpoint draw a plane normal to it? When you draw a plane normal to it all these planes will intersect and it will enclose a volume correct. This volume within that only one atom is there and this has a specific shape which is associated with it. And if you look at the faces which it has it exhibits the full point group symmetry of the crystal it exhibits. Here what we have is that a hexagon and a square with the one with which the surface are formed for BCC. This is called as a Wigner Seitz cell. A similar correspondence to this in another cell is there in reciprocal lattice. You know what it is.

Student: Is the Wigner Seitz cell of reciprocal lattice.

Wigner Seitz cell in reciprocal lattice; here it can be any structure because Wigner Seitz cell is for all the structures you have. It need not be for FCC or BCC it is for every non primitive cell we can construct one, you heard of Brillouin zone; Brillouin zone is nothing but in reciprocal space Wigner Seitz cell corresponding to Brillouin zone in real space what you draw is Wigner Seitz cell. What is the importance of this is that whenever some computation you wanted to do, you have only it is a non primitive lattice at one lattice point if you take the electronic structure whatever is the property corresponding to this cell and it can be by periodic when it can repeated in the full space and you can do it for computation becomes much easier.

(Refer Slide Time: 32:57)

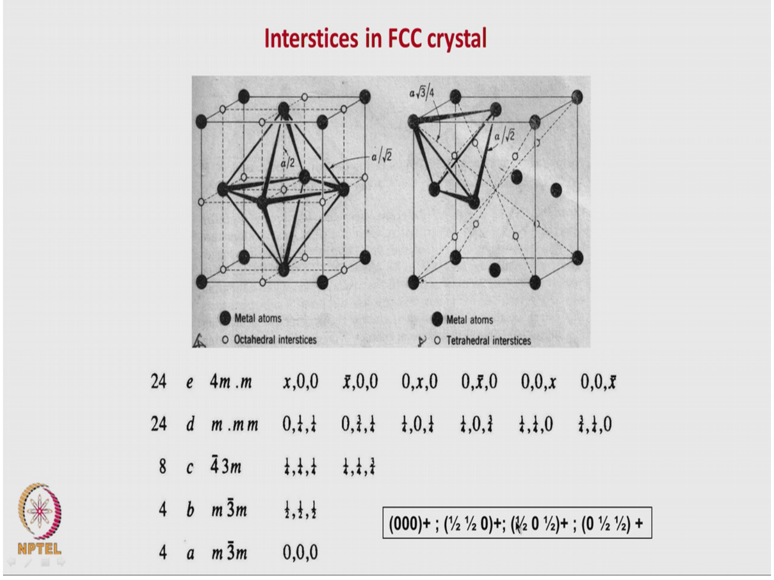


So, most of the time you will find that these sort of cells are used another name also which is used at Voronoi Polyhedra. That is also another name which you will see it in this name you will see in many books using this name also this is all nothing but the

Wigner Seitz cell. This is a primitive cell which exhibits the full symmetry of the lattice and the construction is explained how to construct this cell. Is it clear? If you have any doubt, please do clarify.

Similarly, for FCC if you try to consider this will be essentially like rhombuses. That is assently 110 type of surface with which that polyhedra will be made up of. So, once we have got a specific crystal structure with a lattice parameter which we know this is considered for a cubic structure, we can do it for a tetragonal structure also there we should know the lattice parameters right then you will find the depending upon the lattice parameter ratios there will be some small changes which once you draw you will it will become very clear to you.

(Refer Slide Time: 34:22)



Interstices in FCC crystal

24	*e*	$4m.m$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
24	*d*	$m.mm$	$0,\frac{1}{4},\frac{1}{4}$	$0,\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},0,\frac{1}{4}$	$\frac{1}{4},0,\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},0$	$\frac{3}{4},\frac{1}{4},0$
8	*c*	$\bar{4}3m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$				
4	*b*	$m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
4	*a*	$m\bar{3}m$	$0,0,0$					

(000)+ ; (½ ½ 0)+; (½ 0 ½)+ ; (0 ½ ½) +

This sort of cell can be constructed. This is a very important aspect of geometry crystallography which one should always remember. Now I you have studied that in crystals like if we take a simple FCC lattice if atoms occupy all the corners at the face centers there are tetrahedral and octahedral positions correct. These are all the positions they are normally we say that there interstitial atoms can come and occupy position, it need not be interstitial the second element can come if that first element has occupied this position the second element can come and occupy these particular position. What all these positions correspond to? These are all special points in the crystal which if you see here. Here I had just taken a few Wyckoff positions starting from the one having the lowest highest symmetry and going up with lower symmetry I had given.

If you look at it these are all the positions 000 represents the position which corresponds to a lattice point and when we add to the other 4 equivalent lattice points is we can generate all the points then we have to apply that translation symmetry root then we will be able to find out what all points in the unit cell atom should be kept and then we can complete the structure. Which is the next position which it can be fill is m 3 bar m the same side symmetry as the origin is there at the center. That position 4 positions are possible equivalent positions are possible. This is half, half, half. If we add this to this equivalent positions in the a lattice then we will be able to generate all the positions and generate these are all the positions where atoms can be kept.

This could be interstitial or this could be another. This is how most of the lattices ordered lattices are generated. And then this position if we try to fill up, this Wyckoff position c then this will all correspond to tetrahedral sites. This we call it as generally as octahedral sites. All these sites are as per the Wyckoff tables special positions in the unit cell understand that. So, if we try to fill these positions then what is the type of a structure which we will generate, what will be the stoichiometry there is a atom is placed here and b atom is placed here.

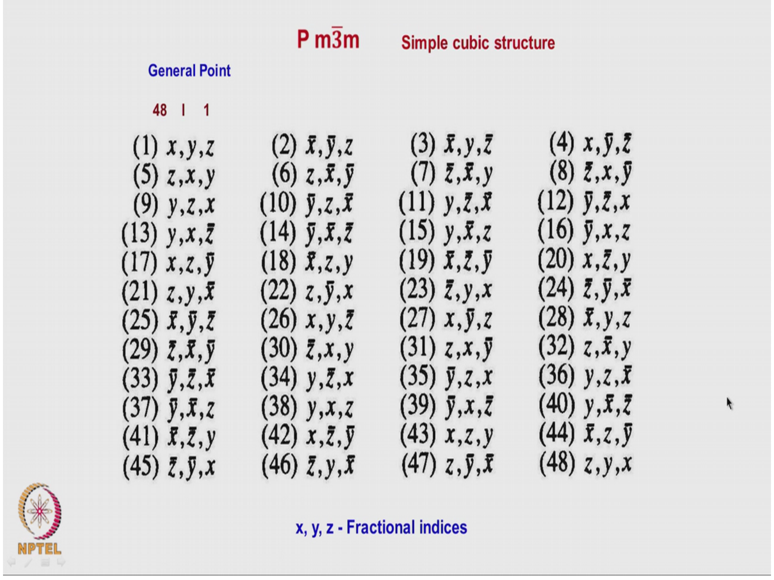
Student: A b.

A b type of has stoichiometry, which is a crystal which has this stoichiometry which it form.

Student: NaCl.

Nacl titanium nitrate there are many compounds are there which form with these crystal structures. This is how it happens. Suppose in a titanium nitrate or sodium chloride these positions are occupied now which is the next position interstitial position which will be there, then only the tetrahedral positions are available to which the third atom if we wanted to put they can go and occupy. This is how the crystal structures are constructed. And then the compound will have AB and if it is even A B C 2 will be the stoichiometry of this particular compound right, is this clear.

(Refer Slide Time: 38:21)



P m$\bar{3}$m   Simple cubic structure

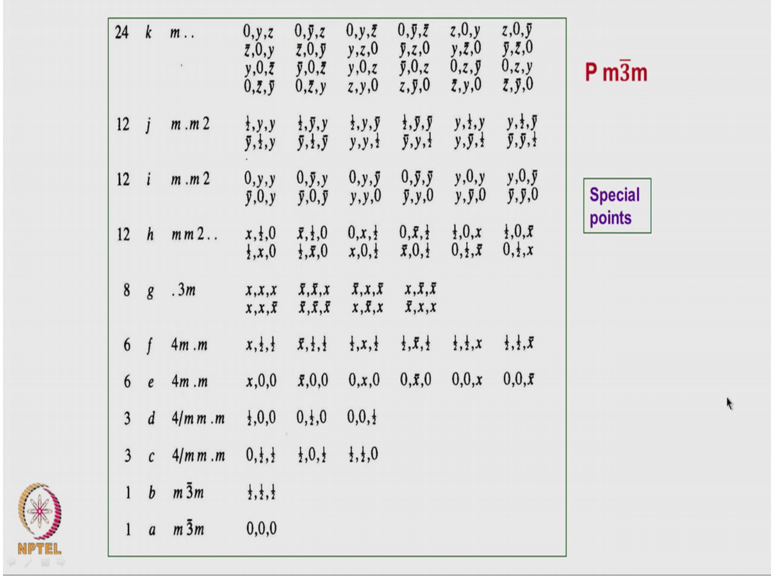
General Point

48 l 1

(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{x},y,\bar{z}$ (4) $x,\bar{y},\bar{z}$
(5) z,x,y (6) $z,\bar{x},\bar{y}$ (7) $\bar{z},\bar{x},y$ (8) $\bar{z},x,\bar{y}$
(9) y,z,x (10) $\bar{y},z,\bar{x}$ (11) $y,\bar{z},\bar{x}$ (12) $\bar{y},\bar{z},x$
(13) $y,x,\bar{z}$ (14) $\bar{y},\bar{x},\bar{z}$ (15) $y,\bar{x},z$ (16) $\bar{y},x,z$
(17) $x,z,\bar{y}$ (18) $\bar{x},z,y$ (19) $\bar{x},\bar{z},\bar{y}$ (20) $x,\bar{z},y$
(21) $z,y,\bar{x}$ (22) $z,\bar{y},x$ (23) $\bar{z},y,x$ (24) $\bar{z},\bar{y},\bar{x}$
(25) $\bar{x},\bar{y},\bar{z}$ (26) $x,y,\bar{z}$ (27) $x,\bar{y},z$ (28) $\bar{x},y,z$
(29) $\bar{z},\bar{x},\bar{y}$ (30) $\bar{z},x,y$ (31) $z,x,\bar{y}$ (32) $z,\bar{x},y$
(33) $\bar{y},\bar{z},\bar{x}$ (34) $y,\bar{z},x$ (35) $\bar{y},z,x$ (36) $y,z,\bar{x}$
(37) $\bar{y},\bar{x},z$ (38) y,x,z (39) $\bar{y},x,\bar{z}$ (40) $y,\bar{x},\bar{z}$
(41) $\bar{x},\bar{z},y$ (42) $x,\bar{z},\bar{y}$ (43) x,z,y (44) $\bar{x},z,\bar{y}$
(45) $\bar{z},\bar{y},x$ (46) $\bar{z},y,\bar{x}$ (47) $z,\bar{y},\bar{x}$ (48) z,y,x

x, y, z - Fractional indices

(Refer Slide Time: 38:24)

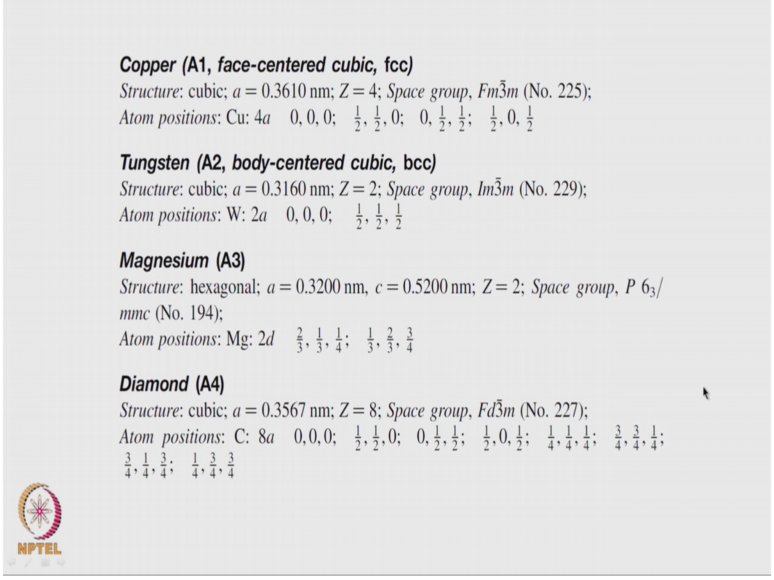


24	k	m . .	$0,y,z$ $\bar{z},0,y$ $y,0,\bar{z}$ $0,\bar{z},\bar{y}$	$0,\bar{y},z$ $\bar{z},0,\bar{y}$ $\bar{y},0,\bar{z}$ $0,\bar{z},y$	$0,y,\bar{z}$ $y,z,0$ $y,0,z$ $z,y,0$	$0,\bar{y},\bar{z}$ $\bar{y},z,0$ $\bar{y},0,z$ $z,\bar{y},0$	$z,0,y$ $y,\bar{z},0$ $0,z,\bar{y}$ $\bar{z},y,0$	$z,0,\bar{y}$ $\bar{y},\bar{z},0$ $0,z,y$ $\bar{z},\bar{y},0$
12	j	m . m 2	$\frac{1}{2},y,y$ $\bar{y},\frac{1}{2},y$	$\frac{1}{2},\bar{y},y$ $\bar{y},\frac{1}{2},\bar{y}$	$\frac{1}{2},y,\bar{y}$ $y,y,\frac{1}{2}$	$\frac{1}{2},\bar{y},\bar{y}$ $\bar{y},y,\frac{1}{2}$	$y,\frac{1}{2},y$ $y,\bar{y},\frac{1}{2}$	$y,\frac{1}{2},\bar{y}$ $\bar{y},\bar{y},\frac{1}{2}$
12	i	m . m 2	$0,y,y$ $\bar{y},0,y$	$0,\bar{y},y$ $\bar{y},0,\bar{y}$	$0,y,\bar{y}$ $y,y,0$	$0,\bar{y},\bar{y}$ $\bar{y},y,0$	$y,0,y$ $y,\bar{y},0$	$y,0,\bar{y}$ $\bar{y},\bar{y},0$
12	h	m m 2 . .	$x,\frac{1}{2},0$ $\frac{1}{2},x,0$	$\bar{x},\frac{1}{2},0$ $\frac{1}{2},\bar{x},0$	$0,x,\frac{1}{2}$ $x,0,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$ $\bar{x},0,\frac{1}{2}$	$\frac{1}{2},0,x$ $0,\frac{1}{2},\bar{x}$	$\frac{1}{2},0,\bar{x}$ $0,\frac{1}{2},x$
8	g	. 3m	x,x,x $x,x,\bar{x}$	$\bar{x},\bar{x},x$ $\bar{x},\bar{x},\bar{x}$	$\bar{x},x,\bar{x}$ $x,\bar{x},x$	$x,\bar{x},\bar{x}$ $\bar{x},x,x$		
6	f	4m . m	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$
6	e	4m . m	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
3	d	4/m m . m	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$			
3	c	4/m m . m	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			
1	b	m $\bar{3}$m	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
1	a	m $\bar{3}$m	$0,0,0$					

P m$\bar{3}$m

Special points

(Refer Slide Time: 38:26)



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: 4*a* $0, 0, 0$; $\frac{1}{2}, \frac{1}{2}, 0$; $0, \frac{1}{2}, \frac{1}{2}$; $\frac{1}{2}, 0, \frac{1}{2}$

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: 2*a* $0, 0, 0$; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

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: 2*d* $\frac{2}{3}, \frac{1}{3}, \frac{1}{4}$; $\frac{1}{3}, \frac{2}{3}, \frac{3}{4}$

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

I will just leave this; this I had already explained in the last class how in that Pearson’s data book they give all this information correct. The last class I mentioned, like cubic structure the lattice- yes.

Student: Sir, if the FCC lattice even the body centered

Yes, the symmetry the site symmetry of this position and this position remains identical.

Student: Why is it that not that any atom is occupying that place in the first place why is it.

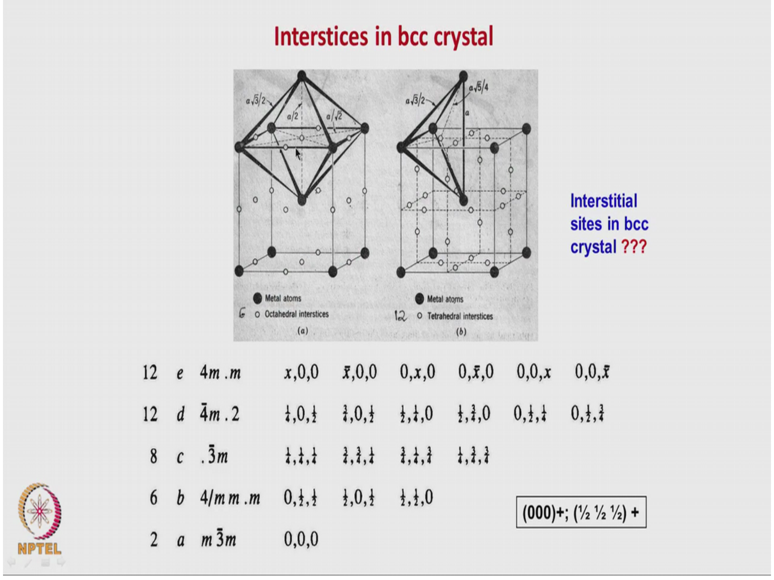
If you put an atom at these corners, and if you put at that position it becomes a BCC.

Student: Like all the corners face structures and the bodies.

No. The first rule is that only one special position can be filled with a one particular type of an atom. If you put the same type of atom on 2 Wyckoff positions then the symmetry of the lattice changes, symmetry will not be the same. How do you identify a symmetry is the environment remains identical correct. That is if you put a position at that position that environment the same position if you atom you put it the environment changes. If you put a different type of an atom then the environment around it does not change. That is the main governing rule in constructing these lattices using this Wyckoff table.

Like diamond: if we take it the lattice parameters and z equals 8 means that the molecular formula. That is a total 8 atoms are going to be there in this space group is f d 3 bar m. This is the number also which is given. This is the space group number which is given in the international union of crystallography. So, we can go to that page and get all other detailed information and atomic positions are only a position are occupied, but 8 atoms will be occupying these position within the unit cell. Once this information is there we can construct the crystal structure. Essentially this information has been obtained from x ray diffraction or electron diffraction various (Refer Time: 41:03) when they complete data analysis has been done. And the complete crystal structure information is given it is published in these books.

(Refer Slide Time: 41:19)



Interstices in bcc crystal

Interstitial sites in bcc crystal ???

12	e	4m.m	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
12	d	$\bar{4}$m.2	$\frac{1}{4},0,\frac{1}{2}$	$\frac{3}{4},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{4},0$	$\frac{1}{2},\frac{3}{4},0$	$0,\frac{1}{2},\frac{1}{4}$	$0,\frac{1}{2},\frac{3}{4}$
8	c	.$\bar{3}$m	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},\frac{3}{4}$		
6	b	4/mm.m	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			
2	a	m$\bar{3}$m	$0,0,0$					

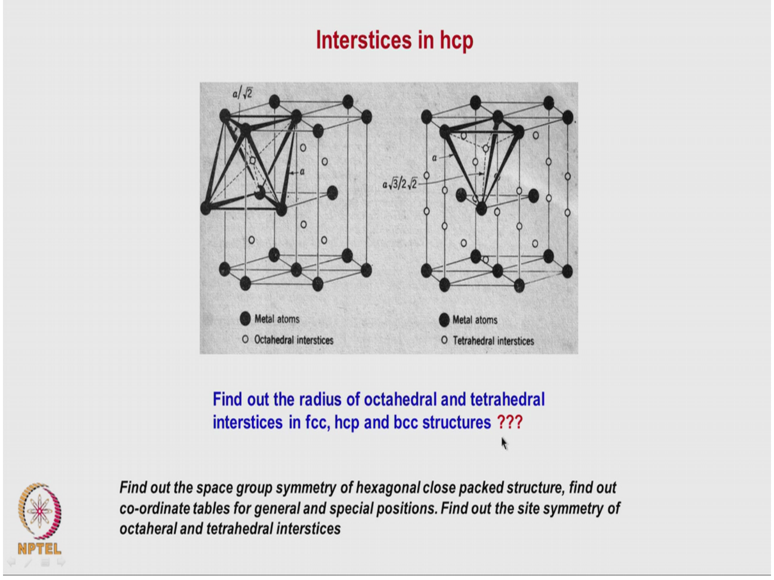
(000)+; (½ ½ ½) +

Similarly, we can consider it for BCC. Here if you see it the atoms occupy the lattice points which correspond to this a position Wyckoff position. The other Wyckoff position the next atom can occupy is that 4 by mmm. If you look at this Wyckoff position, what is the symmetry of that position that site, that as a tetragonals symmetry right. There is m 3 bar m, there is if it has to have a cubic symmetry that is the atom can the crystal can have as a whole a cubic symmetry, but each lattice position can have a symmetry which need not be cubic. How is it determined is that if you look at this special position, what all the positions at which the nearest neighbors are there whether they exhibit a cubic symmetry or not this case you look at it that tells you what if you look here from this position this 1 2 3 4 these are at a by root 2 distance from here to here and these is set a by 2 correct.

So, 2 are and their 90 degree perpendicular to each other these 2 the third which is perpendicular axis is at a distance which is not the same. So, the symmetry which at exhibits is a tetragonal symmetry; that is what essentially that is what is being represented here this site symmetry. So, this is what we this is an octahedral cage correct. There an atom can come. The other is that if you see the next one it is the with respect to a lattice it is tetrahedral position, but if you look what is the symmetry which it has in cubic in l body centered it is 3 bar m, it is a rhombohedral symmetry, but if you look here this particular position, it is assently 4 bar m 2 this also exhibits a tetragonal symmetry this site.

So, either this gets filled or the next site which you always find is that these are all the positions which the atoms because that is having a lower symmetry compared to the other one. Is it clear? So, this is how finally, the symmetry determines. First we take an atom and we know that these are all the positions which are available in the unit cell where we can place it then it will occupy those points which has got the highest symmetry. Once that is completed the next atom will go to position of the available special position which are available which has got the lowest symmetry, it will go to that position that is how the lattice is generated, that is how the crystals are generated by placing atoms at different positions.

(Refer Slide Time: 44:35)

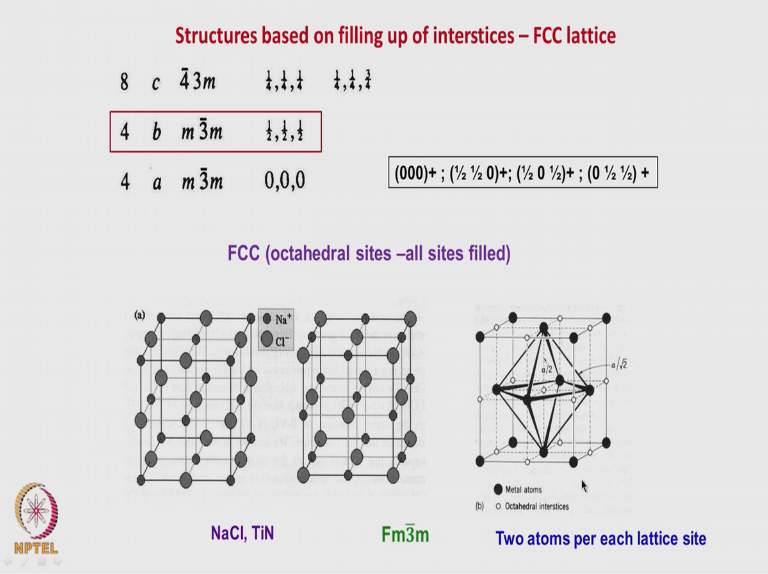

Interstices in hcp

Find out the radius of octahedral and tetrahedral interstices in fcc, hcp and bcc structures ???

Find out the space group symmetry of hexagonal close packed structure, find out co-ordinate tables for general and special positions. Find out the site symmetry of octaheral and tetrahedral interstices

This is I had just shown it for HCP lattice which one can fill it up similar way this you can work it out.

(Refer Slide Time: 44:44)


Structures based on filling up of interstices – FCC lattice

8	c	$\bar{4}3m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$
4	b	$m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	
4	a	$m\bar{3}m$	0,0,0	

(000)+ ; (½ ½ 0)+; (½ 0 ½)+ ; (0 ½ ½) +

FCC (octahedral sites –all sites filled)

NaCl, TiN

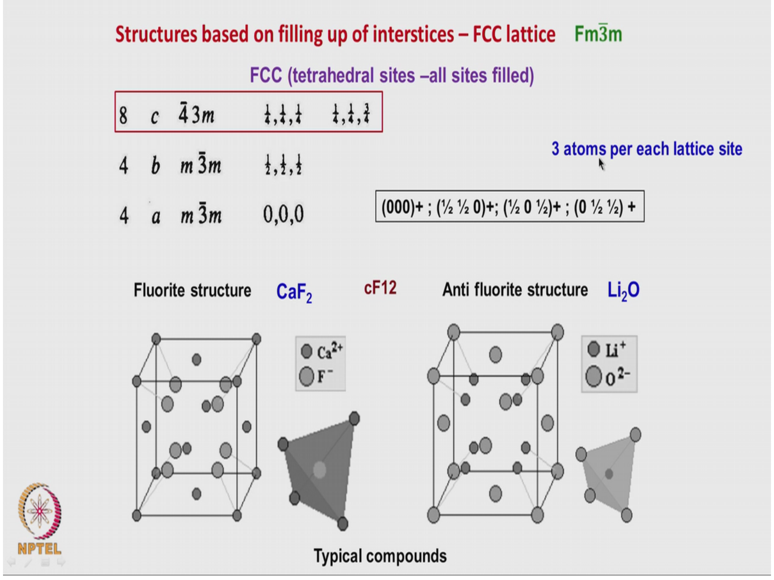
$Fm\bar{3}m$

Two atoms per each lattice site

Here again structure based on filing up of interstices. FCC lattice which we are familiar with, these a sodium chloride structure, a titanium nitride also have the same structure. The anions occupy the corners, the cations occupy the face centers and the edges edge center, this is how the structure is generated correct. And in these with respect to the

Bravais lattice each lattice point has got 2 atoms per lattice point correct. Is it clear? Because around each lattice point, one position and one more position which will be there, that is 2 atoms are going to be there, because there how many atoms are totally there in this cell 8 1 n a and one c l occupies each of the lattice points that is the way it is

(Refer Slide Time: 45:53)



Structures based on filling up of interstices – FCC lattice $Fm\bar{3}m$

FCC (tetrahedral sites –all sites filled)

8	c	$\bar{4}3m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	$\frac{1}{4},\frac{1}{4},\frac{3}{4}$
4	b	$m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	
4	a	$m\bar{3}m$	0,0,0	

3 atoms per each lattice site

(000)+ ; (½ ½ 0)+; (½ 0 ½)+ ; (0 ½ ½) +

Fluorite structure CaF_2 cF12 Anti fluorite structure Li_2O

Typical compounds

Similarly, suppose we try to fill the tetrahedral lattices, then what is the stoichiometry which this material will have? The tetrahedral positions are c right, and this is a 4 and 8. So, it has to be essentially AB 2 type of a stoichiometry which it should have. A typical example is calcium fluoride if we see that has a (Refer Time: 46:31) the calcium atoms occupy all the corners the fluorine atoms occupy the centers of the tetrahedral sites. And this also can be represented as, like around each cation there are anions which are situated this cage is essentially a tetrahedral cage, because so far here we have considered only how many atoms are there total number of atoms which are going to be there.

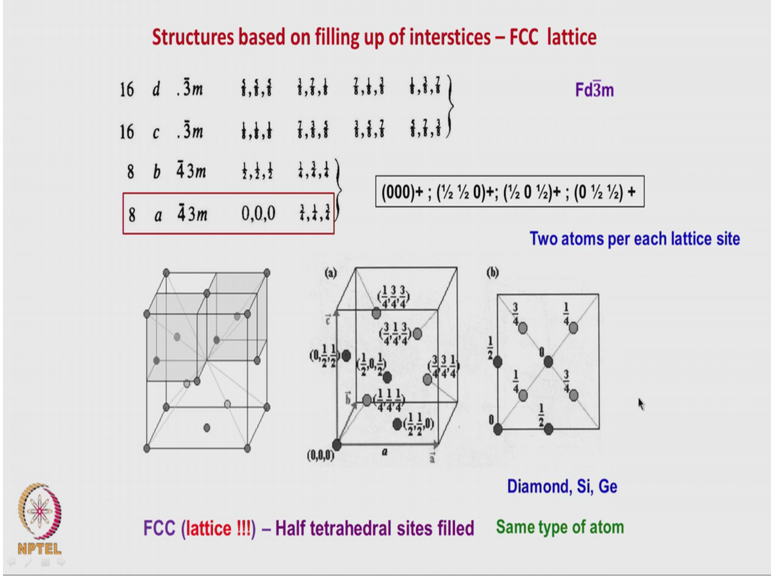
Student: 12.

12 is going to be there correct. And like the earlier class we considered that we can have like for m 23 c 6 116 atoms could be there. So, if you have to place all the 116 atoms in the unit cell, it is going to be a very big mess to visualize it right in the unit cell one way

in which we can represent it is this sort of cages, if we consider around cation or an anion and we can construct the crystal structure that way as one we will come to it.

Similarly, another structure is called as anti fluorite structure where the lithium atoms these are oxygen and lithium. The lithium ions are kept at this one oxygen atoms come at these positions this way also we can. Here also we have 3 atoms per each lattice point we will have that is with respect to a Bravais lattice.

(Refer Slide Time: 48:27)



Structures based on filling up of interstices – FCC lattice

16	*d*	$.\bar{3}m$	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{3}{8},\frac{7}{8},\frac{1}{8}$	$\frac{7}{8},\frac{1}{8},\frac{3}{8}$	$\frac{1}{8},\frac{3}{8},\frac{7}{8}$
16	*c*	$.\bar{3}m$	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{7}{8}$	$\frac{5}{8},\frac{7}{8},\frac{3}{8}$
8	*b*	$\bar{4}3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$		
8	*a*	$\bar{4}3m$	0,0,0	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$		

Fd$\bar{3}$m

(000)+ ; (½ ½ 0)+; (½ 0 ½)+ ; (0 ½ ½) +

Two atoms per each lattice site

Diamond, Si, Ge

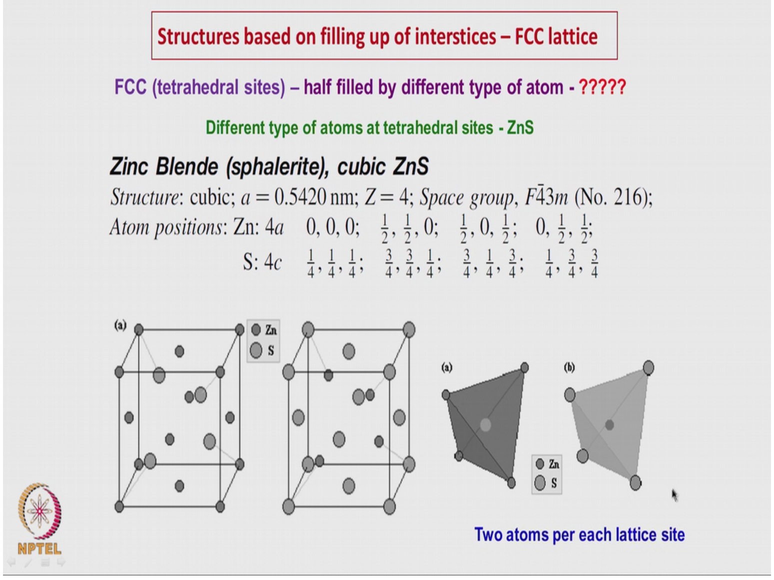
FCC (lattice !!!) – Half tetrahedral sites filled

Same type of atom

Then here is this diamond is also a lattice which is based on a it is a crystal which is based on FCC lattice correct. The number of atoms per lattice point will be 2 in this particular case.

Earlier we have discussed how what all the various ways in which it can be represented. Here what is going to happen is that if we divide this lattice into 8 smaller cubes, at the center of these 2 cubes if we place another carbon atom with respect to a bottom the center of this one and the one with respect to center of the bottom half if we keep then we will be generating the diamond structure. Essentially with respect to if we look at the bonding with respect to every carbon atom it is a tetrahedral 1 4 carbon atoms are there bonded to each.

(Refer Slide Time: 49:41)



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);

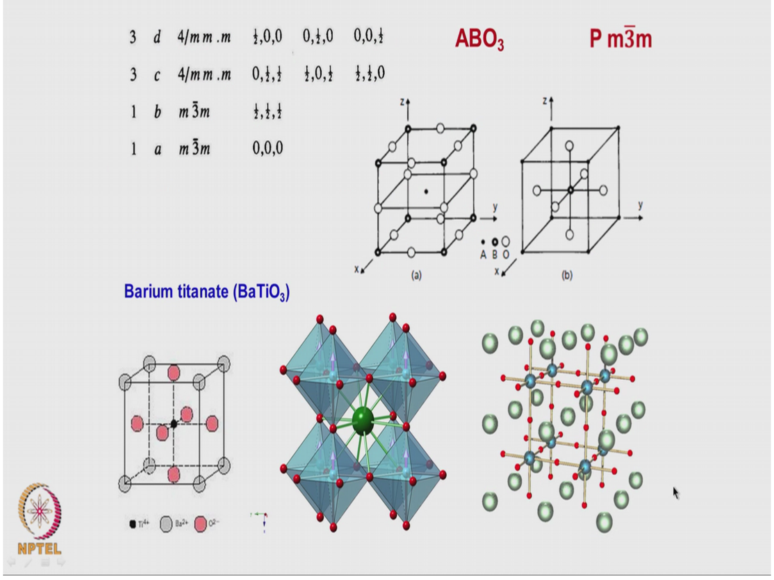
Atom positions: Zn: $4a$ $\quad 0, 0, 0; \quad \frac{1}{2}, \frac{1}{2}, 0; \quad \frac{1}{2}, 0, \frac{1}{2}; \quad 0, \frac{1}{2}, \frac{1}{2};$

S: $4c$ $\quad \frac{1}{4}, \frac{1}{4}, \frac{1}{4}; \quad \frac{3}{4}, \frac{3}{4}, \frac{1}{4}; \quad \frac{3}{4}, \frac{1}{4}, \frac{3}{4}; \quad \frac{1}{4}, \frac{3}{4}, \frac{3}{4}$

Two atoms per each lattice site

Another type of a lattice which we can consider it is because I am just taking FCC as an example FCC lattices an example. Similarly, we can take with respect to all the Bravais lattices we can fill it up this way and construct various types of crystals can be constructed. These we will forgive it as some assignment to you people to work it out here on a Zinc Blende that is cubic zinc sphalerite, there are 2 forms are there hexagonal as well as the cubic right is Zinc Blende another is the Wurtzite site. Here if you if we consider it similar to diamond structure only all the corners at face centers are occupied by zinc and the sulphur occupies 4 positions inside at 4 tetrahedral positions out of the 8 which are possible right: so here also this sort of representation which we can use to fill up the lattice.

(Refer Slide Time: 50:53)



3	d	4/mm.m	½,0,0	0,½,0	0,0,½
3	c	4/mm.m	0,½,½	½,0,½	½,½,0
1	b	$m\bar{3}m$	½,½,½		
1	a	$m\bar{3}m$	0,0,0		

ABO_3

P $m\bar{3}m$

Barium titanate ($BaTiO_3$)

Here I have just considered Perovskite structure barium titanate is one example. And these are all the atom positions which are there this is a primitive lattice yes.

Student: Sir, sometimes it can occupy half the total number of positions as well right like in z n s sulphur occupies half the 8 position half the 8 position.

Suppose the Sulphur occupies the other half also.

Student: Same.

The stoichiometry will become z n s 2, but electrostatic charge balance has to be maintained that decides what is going to be the stoichiometry which is the material can have that depends upon the valence

Student: So.

The elements which are involved.

Student: Half the total number of positions can be felt or is it like water.

Like carbon if you say the diamond. Diamond is also of out of the tetrahedral positions 8 which are possible only half the positions are occupied it is possible.

Student: Positions are similar positions right earlier when we (Refer Time: 52:07)

No.

Student: While putting a atom at one point we have to like to maintain the symmetry we put it in all the similar point.

Exactly!

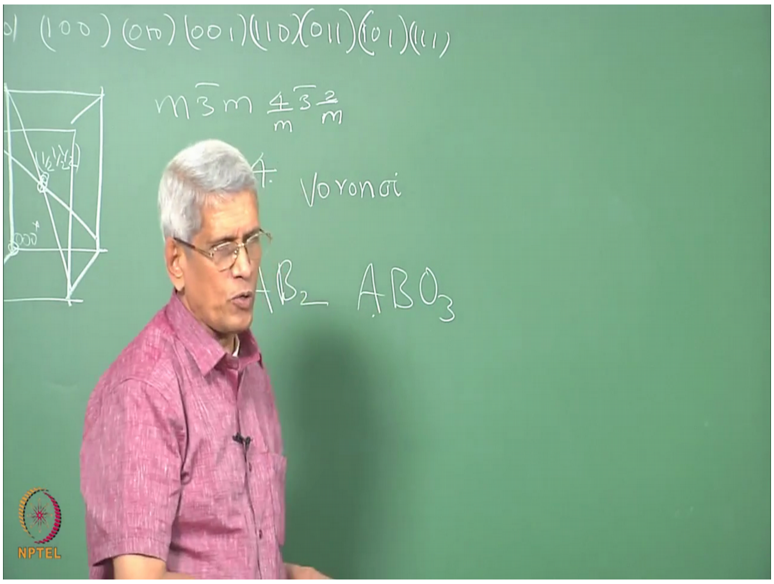
Student: So, how do we explain this in this?

What you have to consider it is what all the lattice points where we can have the atoms, correct. If you look at the Wyckoff table which is given here, with respect to diamond cubic it is a face centered, but d 3 bar m. So, since it is a face centered lattice these are all the 4 equivalent positions are there. Around each lattice point these are all the positions where the atoms are going to be there. It is not the same as in FCC. The lattice is FCC, but around each lattice point the atom is occupying some special positions.

You understand that when we filled up in this particular structure, here it is essentially the Wyckoff position table which we give it is for a structure which is essentially an FCC structure. You understand that. Here the symmetry is not the same. So, essentially these 2 are slightly different, but the lattice essentially is an FCC lattice, you understand that. That is the subtle difference between them it is not filing up of some of the positions in that FCC lattice. Is it clear? These are decided by the type of bonding which we have.

So, here if you consider barium titanate, the number of atoms in the unit cell if you see this is what essentially it is going to be the total number of atoms around 8 unit cell to have this molecular formula. Then you can make out that showing the positions is going to be quite tricky right, hence very difficult to visualize it. The one way in which it is being done is that if you show with respect to a cage this an octahedral cage in which the red atom is kept here and these are all the oxygen atoms now it becomes much easier to understand this.

(Refer Slide Time: 55:16)



There is these are all the positions one type of an atom occupy these are all and then this is the another position that is this is one which has an ABO 3 right. An atom occupies one particular position all the, b atom occupies another position in the primitive lattice and the c atoms are the oxygen atoms which occupy these positions.

So, this way also we can represent it you will find in many books this sort of a representation is being given to describe this structures you know what is the property of barium titanate.

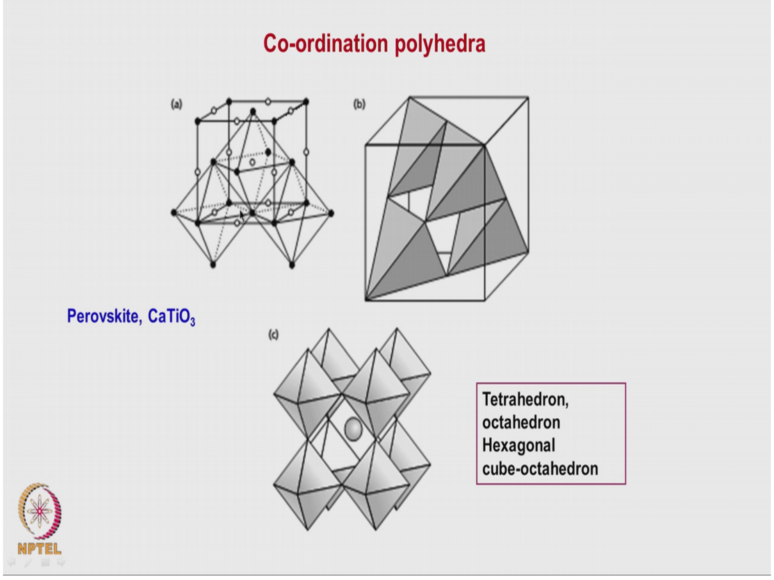
Student: Piezo.

It is a piezoelectric; so piezoelectric means that what it should have.

Student: It is applying a.

It should be a polar molecule right by application of stress you should be able to, but looking at it do we see any of this from the structure it looks like a cubic structure. When it undergoes the transformation that is a slight distortion is there.

(Refer Slide Time: 56:14)



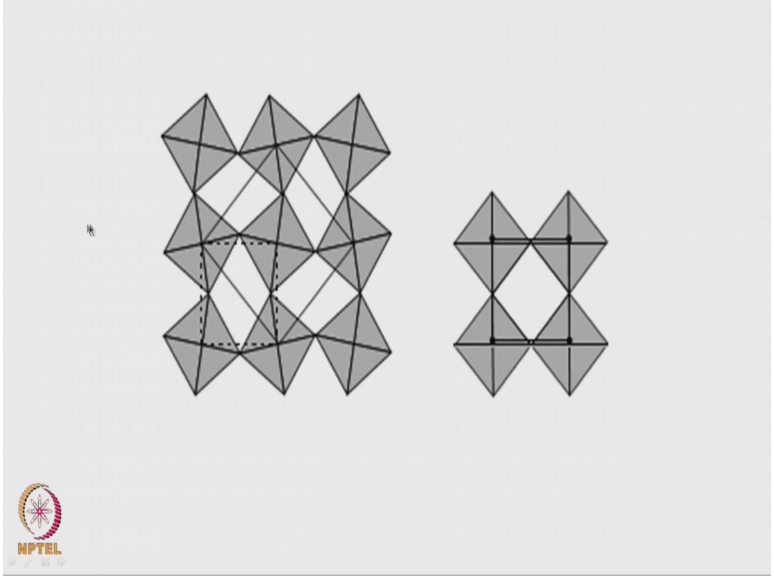
Co-ordination polyhedra

Perovskite, CaTiO$_3$

Tetrahedron,
octahedron
Hexagonal
cube-octahedron

I will just come back to this that is these cages are essentially a to maintain the charge balance, that is the slight distortion. That distortion is when you see that it is tilted in another is tilted in a slightly different way.

(Refer Slide Time: 56:18)



Because, this is the same type of a octahedron position when it comes with respect to a charge if we consider it all the positive charges and the another negative charge which comes at the center they are going to be slightly displaced.

So, it is essentially only a tetragonal structure can exhibit that, cubic structure by symmetry they have to coincide. So, it cannot exhibit all polar molecules cannot have a cubic symmetry understand that.

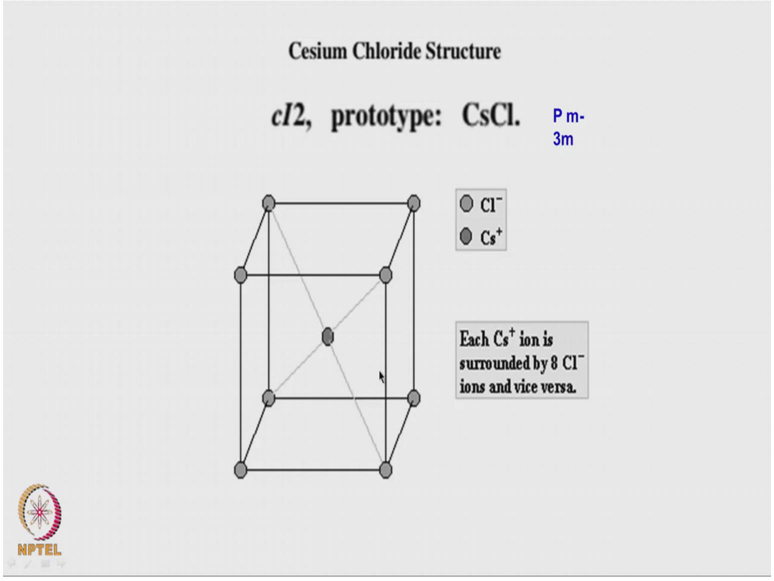
Student: Sir, then what to do along only along this axis.

Along this axis.

Student: Other axis.

Like that in another unit cell it can be along the all the 3 are equally possible. That is why we say that this can exist in 3 variance, or this 3 variance are called as orientation variance the 3 orientations, it can choose and this is an another form in which it is exhibited where this is where the atoms are slightly shifted the central atom, because of which it will exhibit this piezoelectricity or fellow electricity. All these will have this sort of crystal structures. That is just looking at from the crystallography itself if we find this is the property which exhibits we can expect what is the positions which atom should occupy that some guidelines we can get it.

(Refer Slide Time: 58:06)



Cesium Chloride Structure

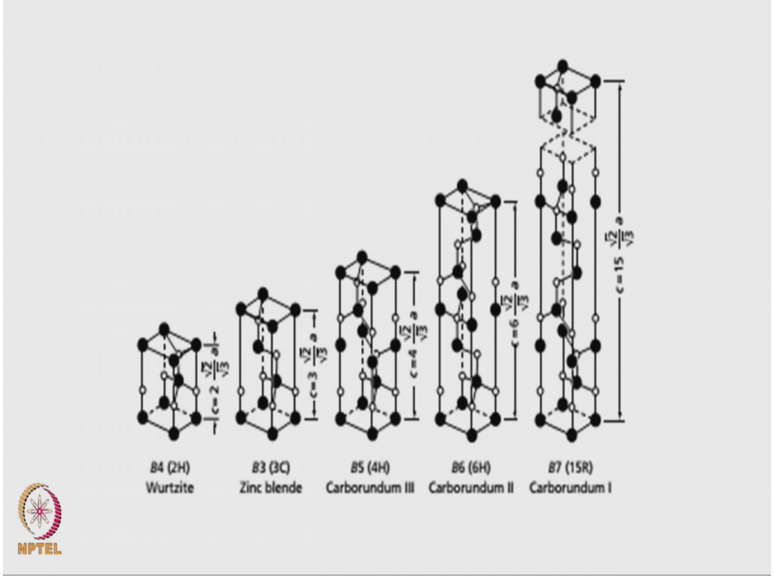
*cI*2, prototype: CsCl. P m-3m

● Cl^-
● Cs^+

Each Cs^+ ion is surrounded by 8 Cl^- ions and vice versa.

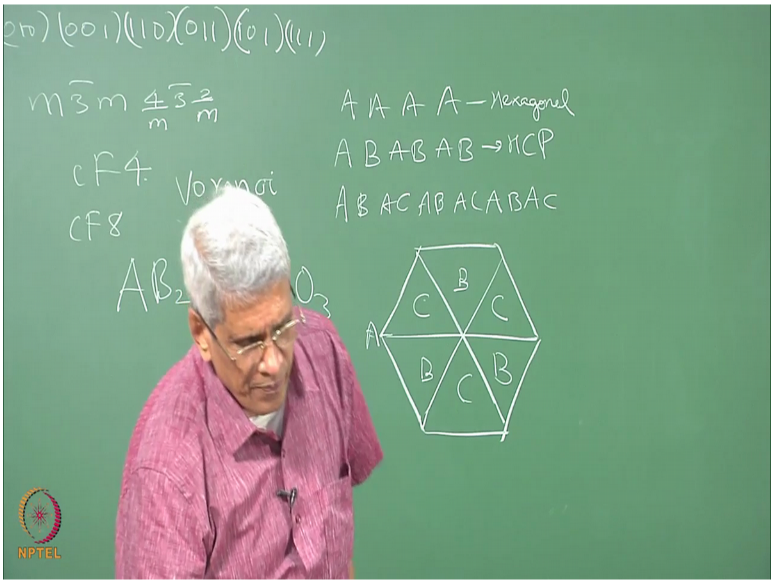
Similarly, we can take a Cesium chloride structure. This is a also a simple cubic lattice right 2 interpenetrating if the atoms turns out to be the same type of an atom, it will be a body centered. That is a disordered lattice will be body centered. The ordered lattice is essentially a primitive lattice, primitive simple that is a simple cubic lattice. Here also in these sorts of lattices we can fill atom positions and various types of crystal structures could be constructed.

(Refer Slide Time: 58:47)



This is essentially with a tetrahedral that is here also, Wurtzite Zinc Blende carborundum there are many forms which are possible with various types of stacking sequences are possible. Like tetragonal lattice what we considered is essentially A, A is one type of a hexagonal lattice.

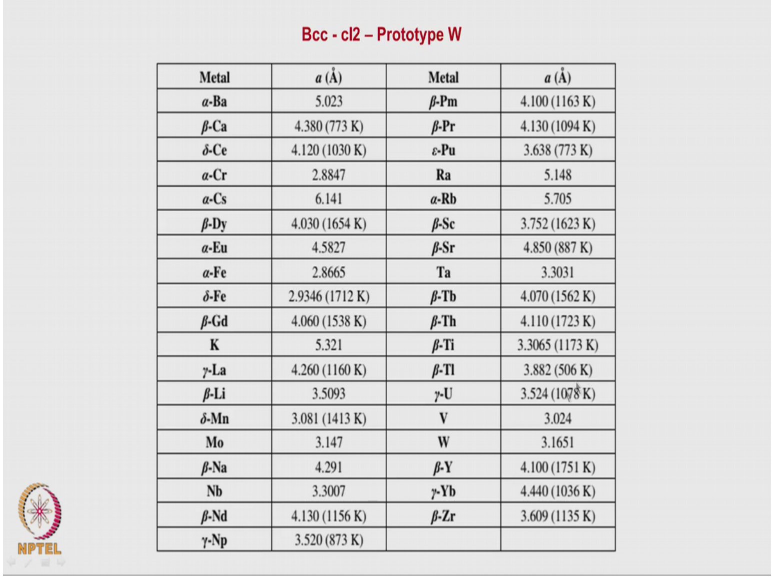
(Refer Slide Time: 59:13)



Another is this is hexagonal, this is hexagonal close pack. Another type which we can have is this type of a lattice also is possible this also will be a hexagonal lattice there are various types of stacking sequences which are possible.

This I will just show you just a minute, now before that so far we have considered.

(Refer Slide Time: 60:01)



Bcc - cI2 – Prototype W

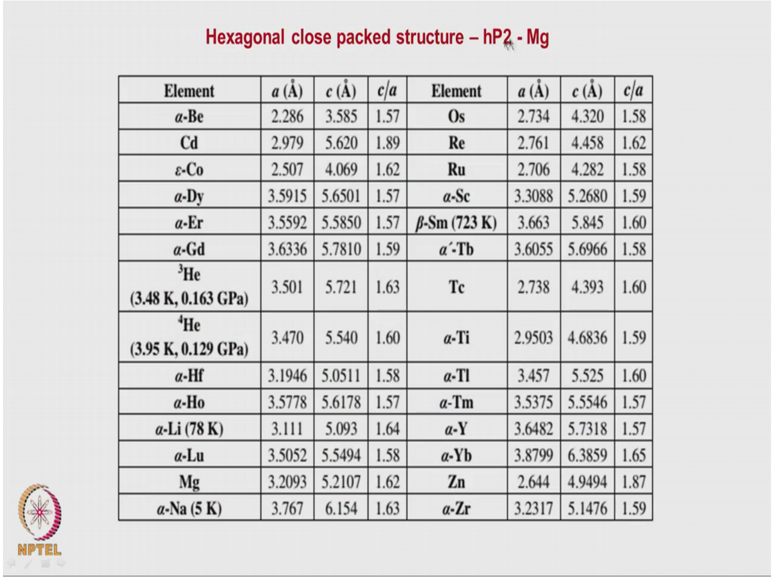
Metal	a (Å)	Metal	a (Å)
α-Ba	5.023	β-Pm	4.100 (1163 K)
β-Ca	4.380 (773 K)	β-Pr	4.130 (1094 K)
δ-Ce	4.120 (1030 K)	ε-Pu	3.638 (773 K)
α-Cr	2.8847	Ra	5.148
α-Cs	6.141	α-Rb	5.705
β-Dy	4.030 (1654 K)	β-Sc	3.752 (1623 K)
α-Eu	4.5827	β-Sr	4.850 (887 K)
α-Fe	2.8665	Ta	3.3031
δ-Fe	2.9346 (1712 K)	β-Tb	4.070 (1562 K)
β-Gd	4.060 (1538 K)	β-Th	4.110 (1723 K)
K	5.321	β-Ti	3.3065 (1173 K)
γ-La	4.260 (1160 K)	β-Tl	3.882 (506 K)
β-Li	3.5093	γ-U	3.524 (1078 K)
δ-Mn	3.081 (1413 K)	V	3.024
Mo	3.147	W	3.1651
β-Na	4.291	β-Y	4.100 (1751 K)
Nb	3.3007	γ-Yb	4.440 (1036 K)
β-Nd	4.130 (1156 K)	β-Zr	3.609 (1135 K)
γ-Np	3.520 (873 K)		

How to construct the lattices and some basis of filling up interstitial and there is tetrahedral or octahedral voids? We can construct different types of lattices whether it could be an ionic type of a compound or it could be a alloys or intermetallic alloys or it could be covalent type of bond. Most of the metals if we look at it in the periodic table most of them form either FCC BCC or HCP very few go into tetragonal structure. The simple cubic structure only one element goes which one.

Student: Polonium.

Polonium that is the only element which takes a simple cubic, that is the rarest one as far as the elements are concerned.

(Refer Slide Time: 61:09)

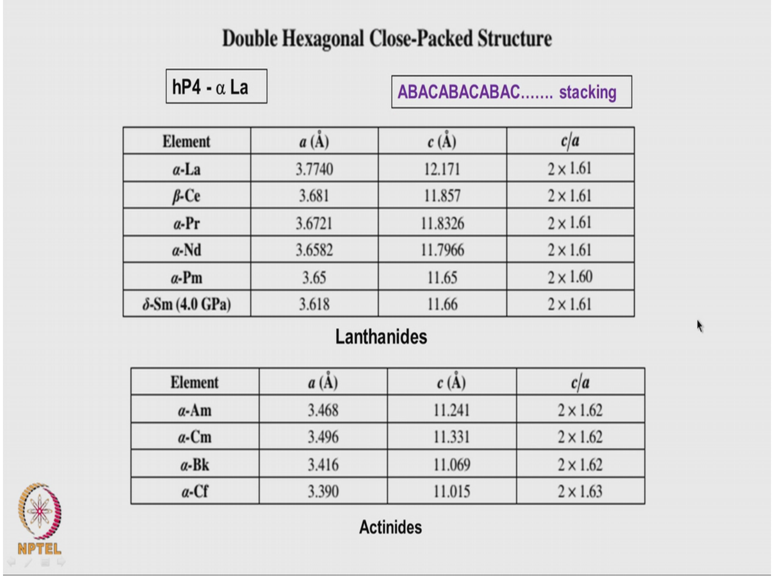


Hexagonal close packed structure – hP2 - Mg

Element	a (Å)	c (Å)	c/a	Element	a (Å)	c (Å)	c/a
α-Be	2.286	3.585	1.57	Os	2.734	4.320	1.58
Cd	2.979	5.620	1.89	Re	2.761	4.458	1.62
ε-Co	2.507	4.069	1.62	Ru	2.706	4.282	1.58
α-Dy	3.5915	5.6501	1.57	α-Sc	3.3088	5.2680	1.59
α-Er	3.5592	5.5850	1.57	β-Sm (723 K)	3.663	5.845	1.60
α-Gd	3.6336	5.7810	1.59	α′-Tb	3.6055	5.6966	1.58
^{3}He (3.48 K, 0.163 GPa)	3.501	5.721	1.63	Tc	2.738	4.393	1.60
^{4}He (3.95 K, 0.129 GPa)	3.470	5.540	1.60	α-Ti	2.9503	4.6836	1.59
α-Hf	3.1946	5.0511	1.58	α-Tl	3.457	5.525	1.60
α-Ho	3.5778	5.6178	1.57	α-Tm	3.5375	5.5546	1.57
α-Li (78 K)	3.111	5.093	1.64	α-Y	3.6482	5.7318	1.57
α-Lu	3.5052	5.5494	1.58	α-Yb	3.8799	6.3859	1.65
Mg	3.2093	5.2107	1.62	Zn	2.644	4.9494	1.87
α-Na (5 K)	3.767	6.154	1.63	α-Zr	3.2317	5.1476	1.59

There are the like magnesium here this hexagonal structure. This is the symbol which we use it, if we look at the book h is hexagonal p is primitive 2 is 2 atoms per unit cell. So, it is a hexagonal close packed lattice.

(Refer Slide Time: 61:25)



Double Hexagonal Close-Packed Structure

hP4 - α La

ABACABACABAC....... stacking

Element	*a* (Å)	*c* (Å)	*c*/*a*
α-La	3.7740	12.171	2 × 1.61
β-Ce	3.681	11.857	2 × 1.61
α-Pr	3.6721	11.8326	2 × 1.61
α-Nd	3.6582	11.7966	2 × 1.61
α-Pm	3.65	11.65	2 × 1.60
δ-Sm (4.0 GPa)	3.618	11.66	2 × 1.61

Lanthanides

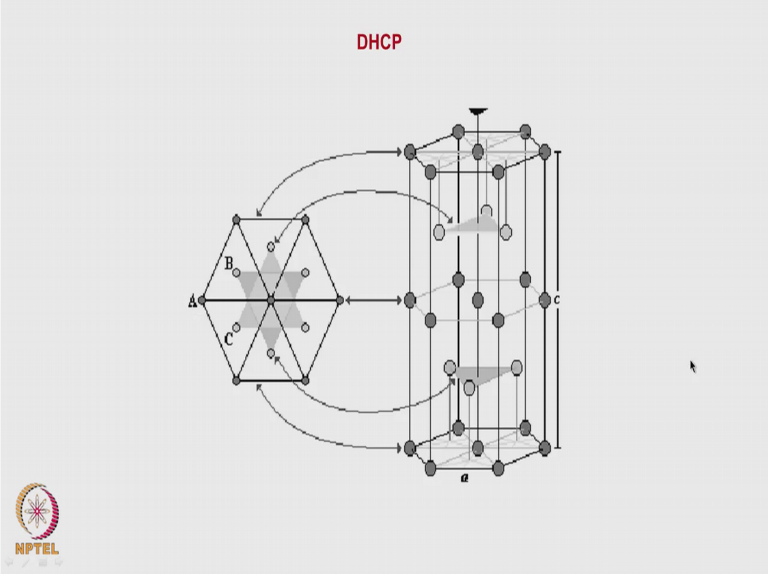
Element	*a* (Å)	*c* (Å)	*c*/*a*
α-Am	3.468	11.241	2 × 1.62
α-Cm	3.496	11.331	2 × 1.62
α-Bk	3.416	11.069	2 × 1.62
α-Cf	3.390	11.015	2 × 1.63

Actinides

Similarly, this is called as a double hexagonal lattice which is that ABAC, ABAC, ABAC type of a stacking sequence because we know that when we take a 2 dimensional hexagonal lattice in that lattice like this hexagonal lattice, these are all the positions in which another hexagonal lattice could be kept or these are all the other positions which the hexagonal lattice could be kept on top of it correct. These are the only 2 positions which are possible.

If we keep this a position and the next layer in this position hexagonal lattice next layer on top of a if we continue it turns out to be a HCP lattice. Instead if AB is kept here A on top then the next layer turns out to be a C layer then the next layer is again an A layer if that sequence this is called as in these many of the lanthanides they going to that is particular type of a structure.

(Refer Slide Time: 62:58)

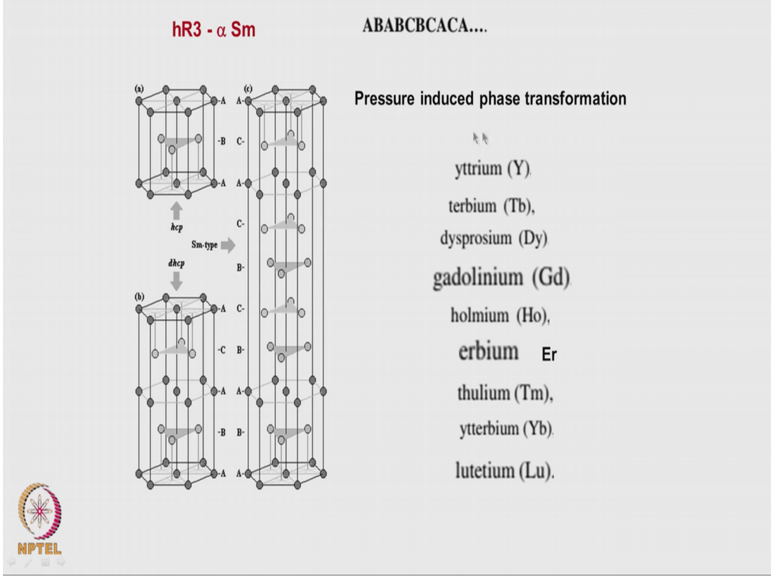


DHCP

Here you see this is the unit cell. This is a hexagonal lattice the other part of it only the atoms which are there within the unit cell is being shown. These are all the positions which they occupy then this is again a position this one if you see it if in this prism type of a structure an atom was there here next it comes on the other one correct.

These are all the 3 positions essentially this position if you rotate it by 60 degree, then we will be getting the other position that is every alternate position in an HCP lattice where the b position is there every next position you just rotate it by 60 degree and place it because that position is also from symmetry consideration equally possible. There are many crystal structures which are formed like I think Na3Ti goes into this particular type of a structure, you can verify that, then this is another type of structures yttrium gallonium these transformations occur under pressure.

(Refer Slide Time: 64:19)



hR3 - α Sm

ABABCBCACA....

Pressure induced phase transformation

yttrium (Y)

terbium (Tb),

dysprosium (Dy)

gadolinium (Gd)

holmium (Ho),

erbium Er

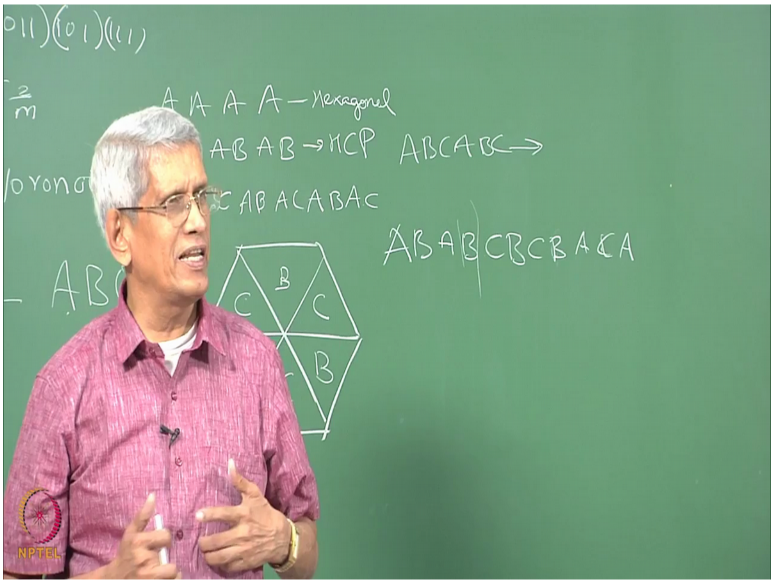
thulium (Tm),

ytterbium (Yb)

lutetium (Lu).

Pressure induced transformation many crystal structures can occur, here what is the stack sequence AB AB CB AB AB CB C then AC AC A and then this will repeat itself. There are many combinations of this type of sequences that is we have AB css sequence is there correct.

(Refer Slide Time: 64:56)



If we take ABC, ABC in this particular form, it will turn out to be a cubic structure right. If we take the combination as A, A, A it is hexagonal. If we take it AB AB AB it is HCP.

We can have this sort of a sequence which is possible, but if you look at all other sequences, nowhere you find that ABC will be come. If anywhere an ABC comes means that it is an FCC type of a structure. In this structure also if you see it is AB AB CB, I think CBA this is the sort of a structure no C; CB A like this the structure comes CB ACA, ACA this is also a combination of these three, but nowhere the sequence ABC comes correct. Is there any ABC is there?

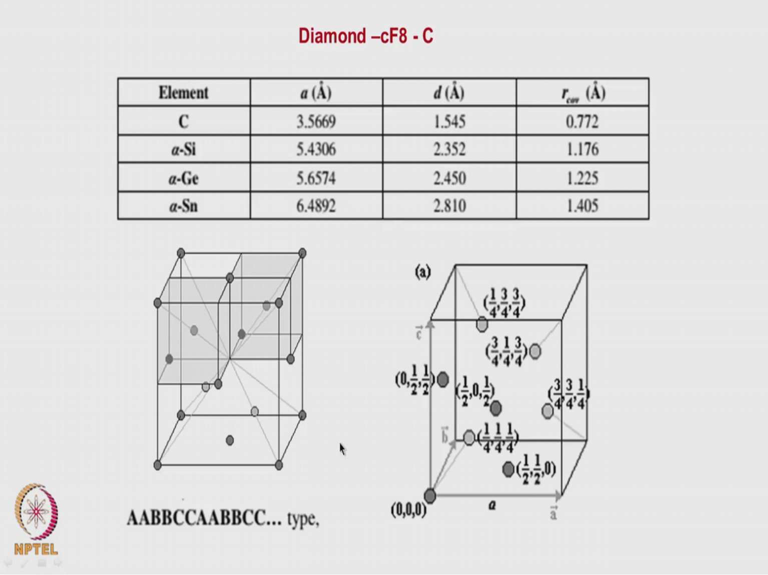
Student: Yes, sir AB.

AB, AB.

Student: AB AB is there.

Yes, ABC is there here it is there correct. This particular one will be like fault. This is essentially if you introduce fault in a particular layer, you can have this sort of a structures, but if you look at the unit cell this is still a hexagonal one. The symmetry which it exhibits is only the hexagonal symmetry.

(Refer Slide Time: 66:54)

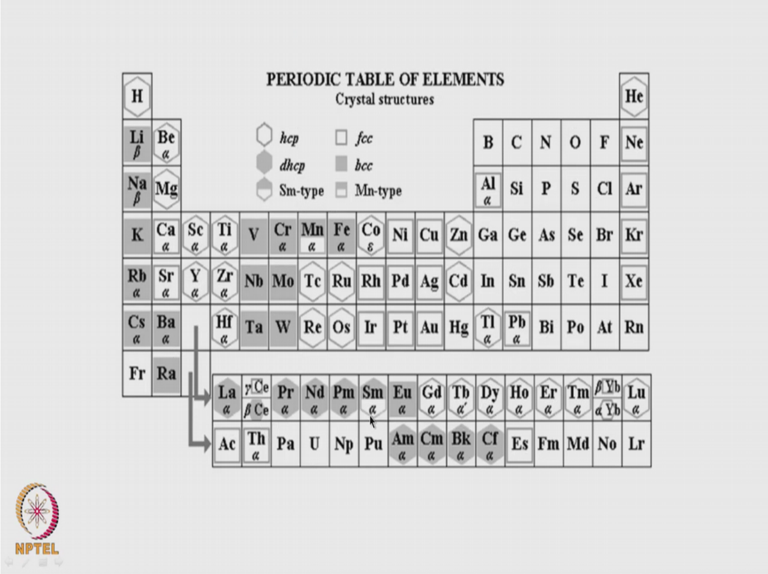


Diamond –cF8 - C

Element	a (Å)	d (Å)	r_{cov} (Å)
C	3.5669	1.545	0.772
α-Si	5.4306	2.352	1.176
α-Ge	5.6574	2.450	1.225
α-Sn	6.4892	2.810	1.405

AABBCCAABBCC... type,

(Refer Slide Time: 66:58)

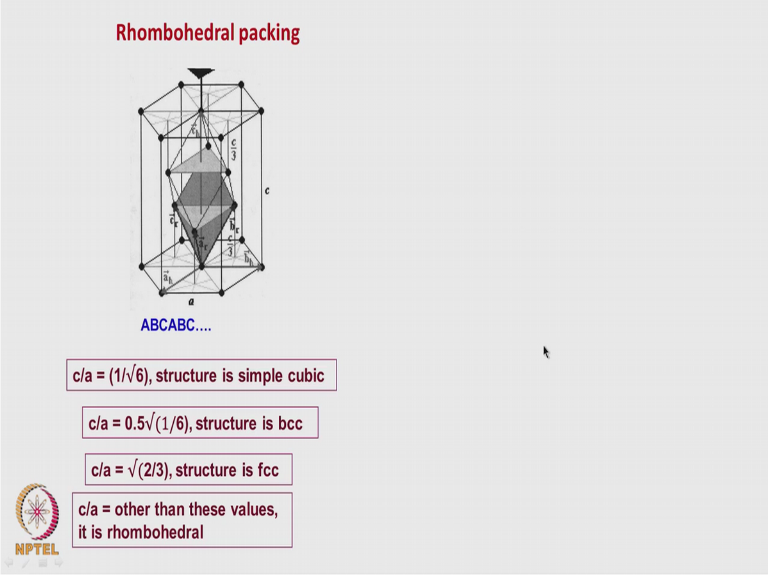


PERIODIC TABLE OF ELEMENTS
Crystal structures

- ⬡ hcp
- ⬢ dhcp
- ⬡ Sm-type
- ☐ fcc
- ■ bcc
- ▨ Mn-type

Then there are various structures which we have considered. This is just giving a periodic table where one can what all the types of crystal structures which it can hold either HCP.

(Refer Slide Time: 67:33)



Rhombohedral packing

ABCABC....

c/a = (1/√6), structure is simple cubic

c/a = 0.5√(1/6), structure is bcc

c/a = √(2/3), structure is fcc

c/a = other than these values, it is rhombohedral

Double hexagonal that manganese type BCC, FCC these are all the structures to which most of the elements in the periodic table follow into. Majority go into FCC BCC or HCP structures here. What I will do is I will stop it here.