Condensed Matter Physics
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Lecture - 03
Symmetry in Perfect Solids Worked Examples

Stated without prove to be in the lecture. They are asked to prove that fivefold rotational symmetry is not consistent translation symmetry in a perfectly periodic crystal.

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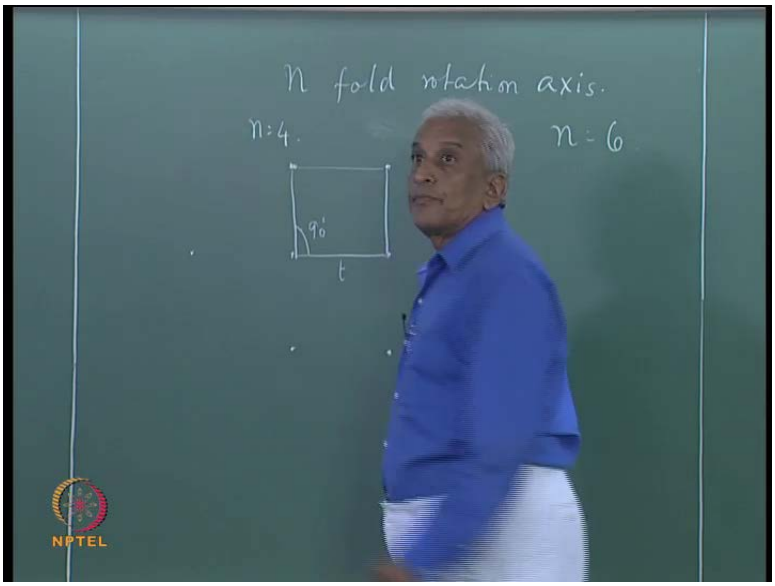

In order to prove this, suppose we consider an n fold rotation axis perpendicular to a plane of the board. Let us for example, consider a fourfold n equal to 4.

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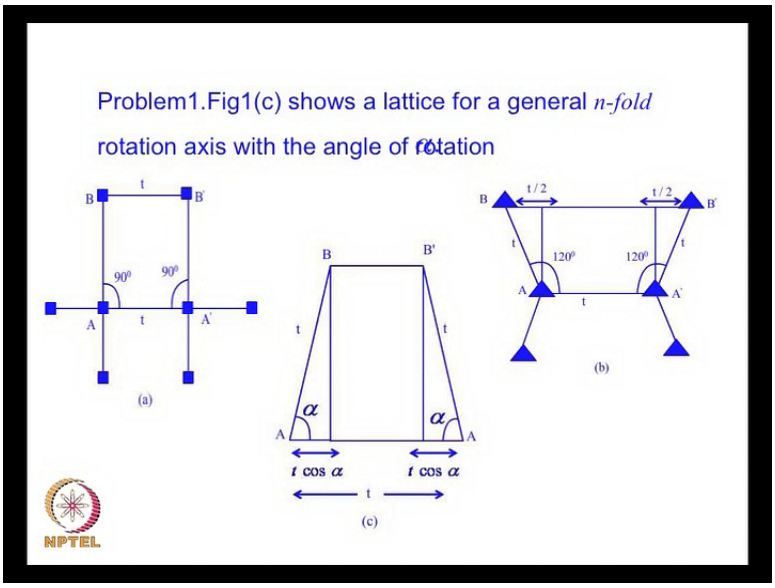

Figure 1 a shows such a 4 fold rotation. A 4 fold symmetry axis in a translational invariant crystal lattice. So, one has atoms in this various lattice positions and this angle here, the angle is 90 degrees for n equal to 4. So, this is the also the case here and this is the lattice translation vector.

So, this rotation axis takes to this position and their 4 fold rotation axis takes to this position and now the final position of these two atoms should also be consistent with the translational symmetry of the lattice. Similarly, the next figure 1 b also shows the same thing for n equal to 6 for 120 degree rotation. Now, in general, we can show this in one to see the general situation is shown.

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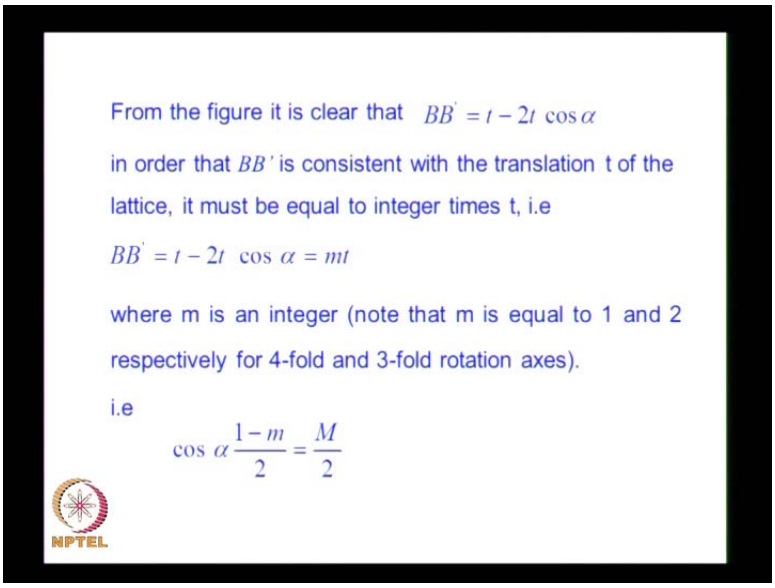

From which it is clear that we have the condition t minus 2 t plus alpha should be some integer times the translation vector, t is the translation in the translational periodic city of the lattice and alpha is the angle threw the rotation axis.

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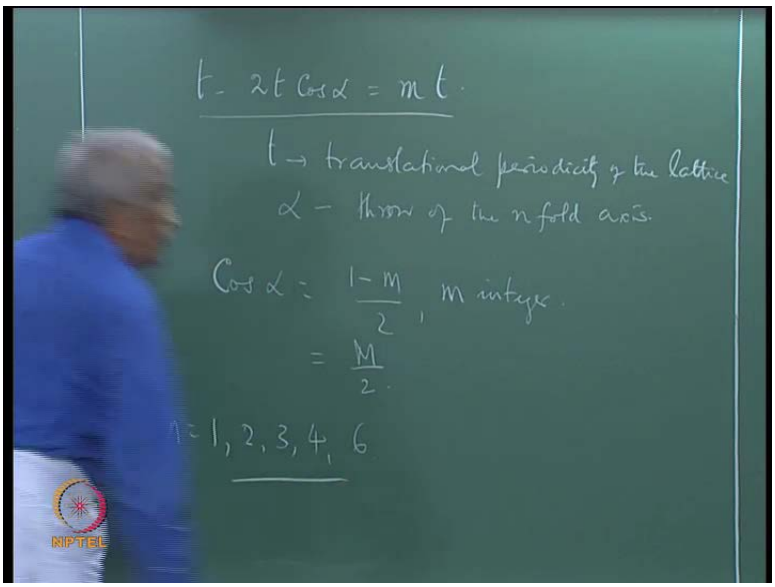

So, that would be the condition that has to be satisfied, which becomes therefore, which gives cos alpha equals 1 minus m by 2, where m is an integer. This it is an integer we can also write it as some other integer by 2.

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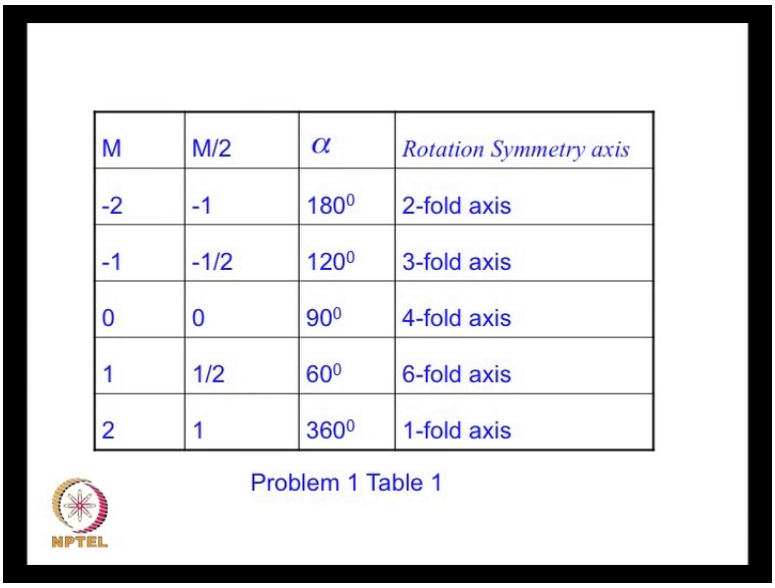

And so, the table shows the various values since case alpha cannot exceed minus 1 or plus 1. So, that imposes a restriction on the allowed values of M and hence the small n therefore, that the rotational the alpha values which corresponds to an integer M in this condition are given in table tabular form. So, from that it is clear that n equal to either 1 or 2, 3 or 4 or 6 and a 5 fold rotation therefore, not consistent with the translation periods.

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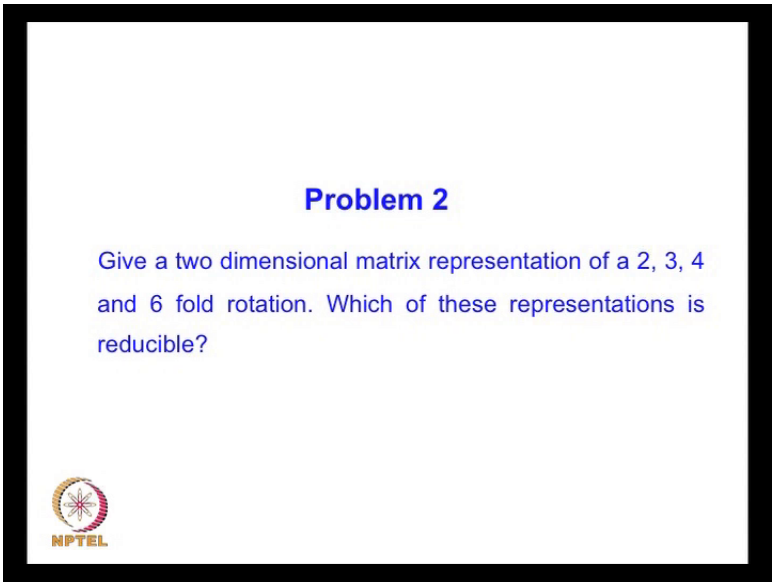

The next problem talks about a two dimensional matrix representation of 2 fold, 3 fold, 4 fold and 6-fold axis of rotation in the groups C 2, C 3, C 4,and C 6.

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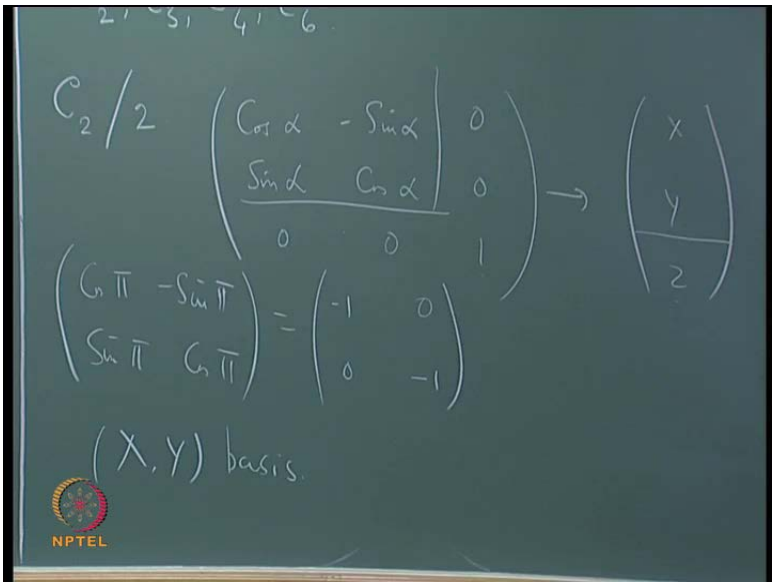

So, if you have a rotation corresponding to this axis. How do you represent them matrix in matrix form? This is important for a group theoretical understanding of the characters and represents basis of these fine groups. Suppose we consider C 2 is shown like symbol is C 2 and the international symbol is 2. And the matrix element since the angle of the rotation is high. So, we have general cos alpha, minus sin alpha, sin alpha, cos alpha in three dimensional.

This is the matrix rotate representation of rotational axis is about, which coincides along the z axis. Now, the basis for this is the coordinates x y z in three dimensional space. Now, we are all is to provide two dimensional representations. So, that will be for the 2 fold axis it will be cos pi, minus sin pi, sin pi, cos pi, which is cos pi is minus 1, this is zero, this is zero, this also minus 1. Provided we deal with this, which means these is the basis; the basis is for this x y that is one, two dimensional representation. Of course, one can choose y z or x z as the basis.

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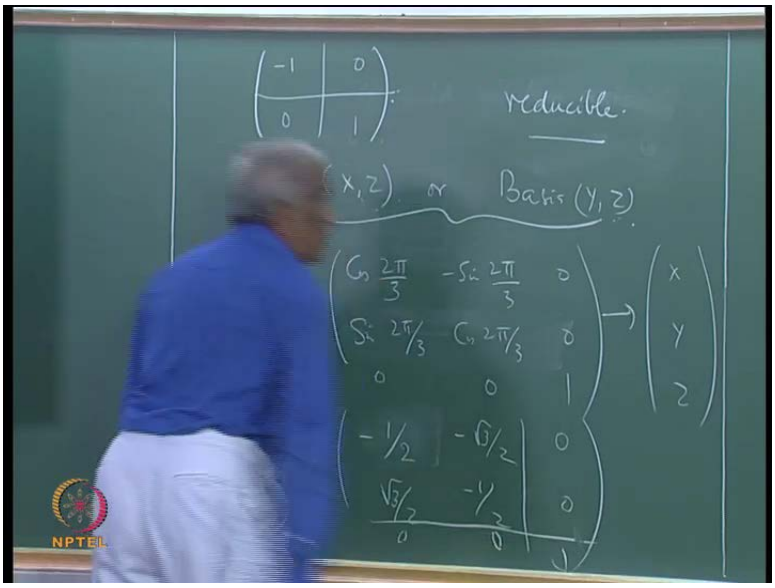

Suppose I choose x z as the basis, basis x z then the corresponding matrix elements are cos alpha 1 0 0 for alpha equal to pi. So the matrix representation is minus 1 0 0 1 this also an equally valid representational of the two axis for if we basis adopted is x z. alternatively we can also have basis y z is, that is the case then we have cos alpha 0 0 1. So, that is again same matrix for both these.

So, we have the possibility of two different representations depending on whether we choose x y as the basis or x z or y z or the basis. Depending on that these provide the two different representations for the C 2 rotation. Now, since it is of this farm we can of course, factor it further partition the matrix further and the corresponding basis can be one dimensional so, x or y.

So, this is a completely reducible basis, the reducible representation can be the two dimensional representation can be reduced into two, one dimensional representation. Similarly these also can be reduced. Now, we proceed to a C 3 axis. For the C 3 axis cosine alpha, alpha is 2 pi by 3. So I have cos 2 pi by 3, minus sin by 2 pi by 3, 0, sin 2 pi by 3, cos 2 pi by 3, 0, 0, 0, 1 is the three dimensional, full three dimensional representation is the bases x y z. So, this can be written as minus half, minus half, minus root 3 by 2 and root 3 by 2, 0 0 1,0 0.

So, we have the possibility depending on which representations we choose, we can partition this matrix like this. So, this can be a one two dimensional representation for C

3 rotational z axis. So, it can be minus half, minus root 3 by 2, root 3 by 2, minus half that would be a two dimensional representation for the basis x y or if we choose x z as the basis then that would be minus half, 0, 0, 1 that would be for the basis x z or it can be y z can be the basis.

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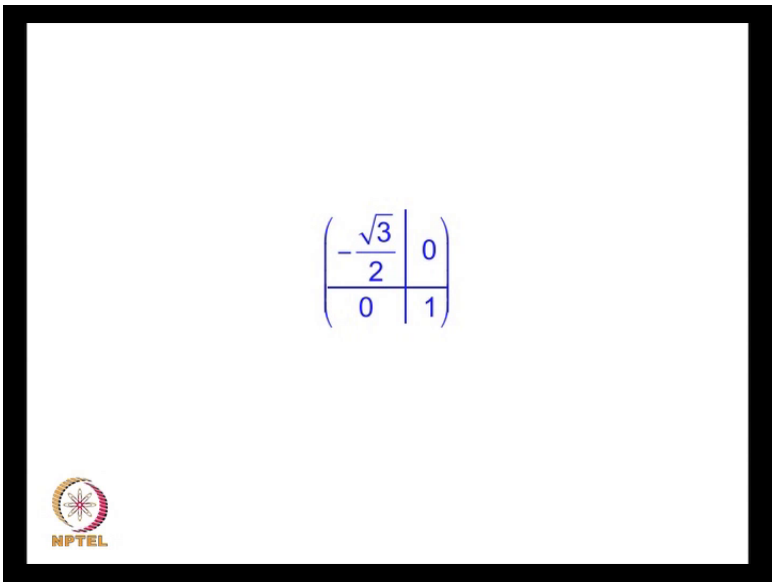

So, these are the three two dimensional representations and we can see that these is reducible this is also reducible since, the half diagonal matrix elements or all zeros. So, this both these are reducible.

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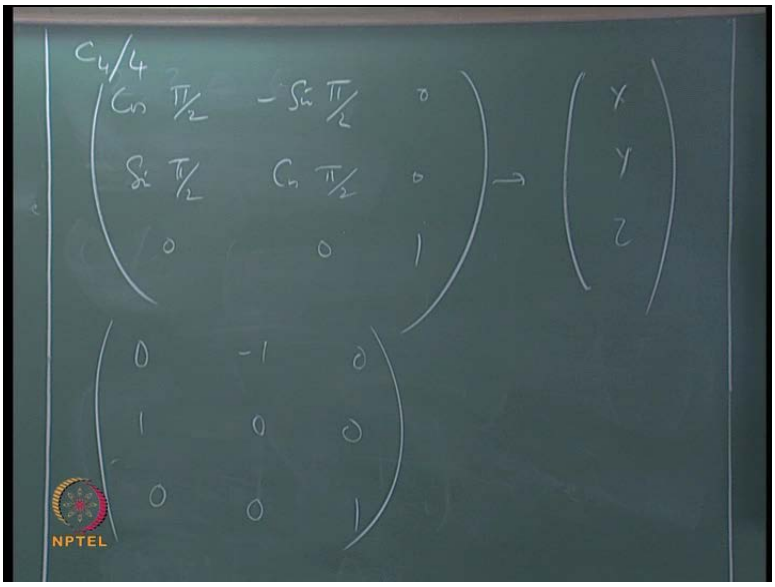

Whereas, going on to the case of the C 4 axis. A 4 fold rotation by the z axis so, it has cos pi by 2, minus sin pi by 2, sin pi by 2, cos pi by 2, 0 0 1, that is the three dimensional representation with x y and z. And that would correspond to cos pi by 2 is 0, minus 1, 1, 0, 0, 0, 0, 1.

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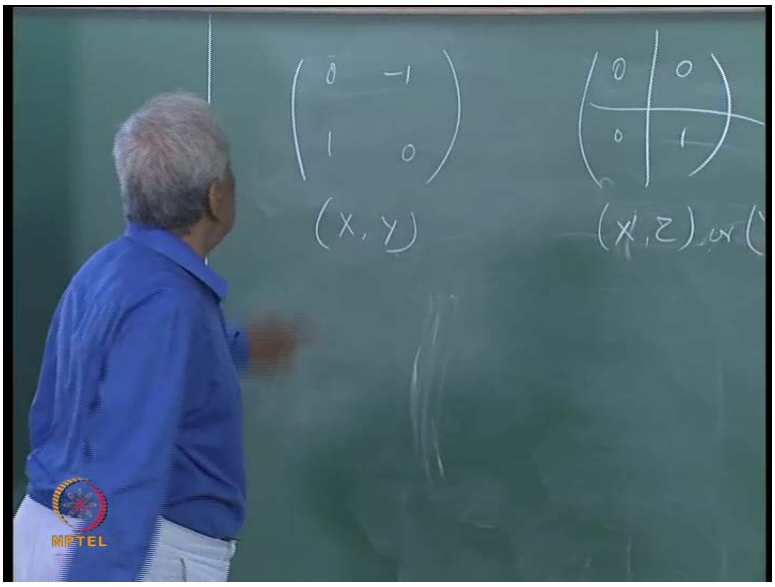

So, the corresponding two dimensional representations for the C4 axis will be 0, minus1, 1, 0, if we choose x y as the basis.

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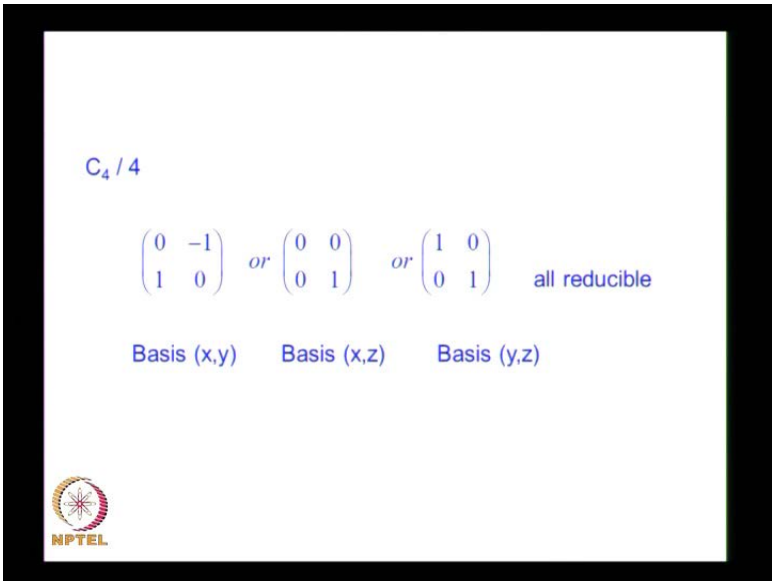

Whereas, it will be 0,0,0,1 if it is x z, y z will be also; obviously, is a reducible representation while this is not. Coming to the C 6 axis by the same reasoning one can arrive at the answers. So, we have cos 0, 0, 1 for the y z basis also. So, that answers the question we now pass on to problem 3 and 4.

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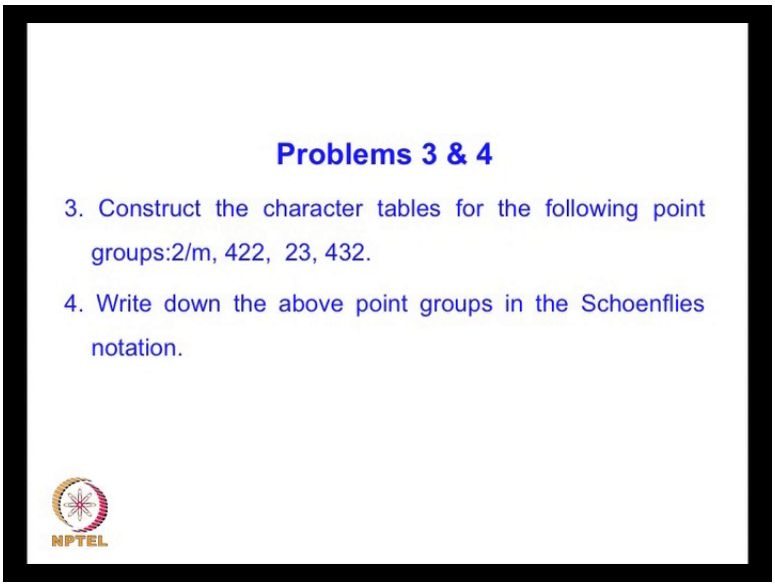

Which are taken together, we are required to construct the character table for the following point groups.

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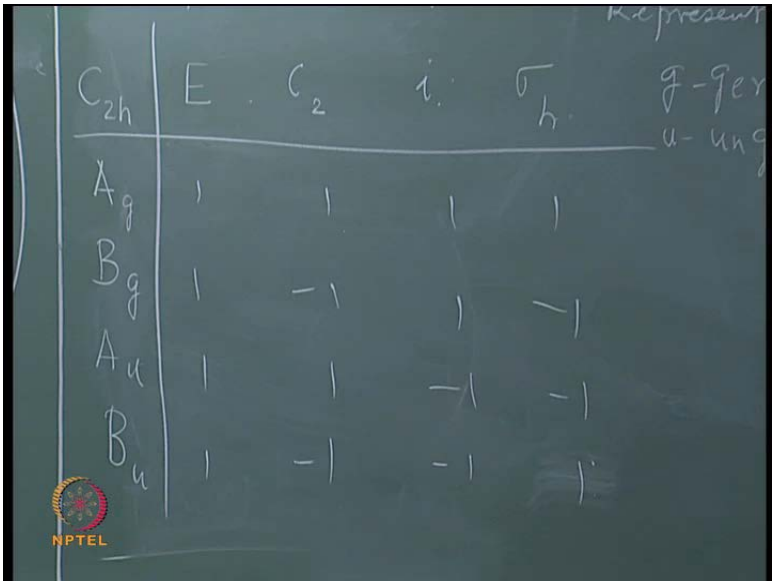

The first point group to be considered is 2 by m, which is a mirror perpendicular to a 2 fold axis. So, it goes by the nomenclature C 2 h in shown flies notation. So, C 2 h as the elements; these are the elements. C 2 square is high and because there is a mirror sigma h and that produces inversion symmetry. So, there are four elements in this group and therefore, there are four irreducible representations. The number of irreducible representation is equal to number of classes really. There are four different classes 1,2,3,4.

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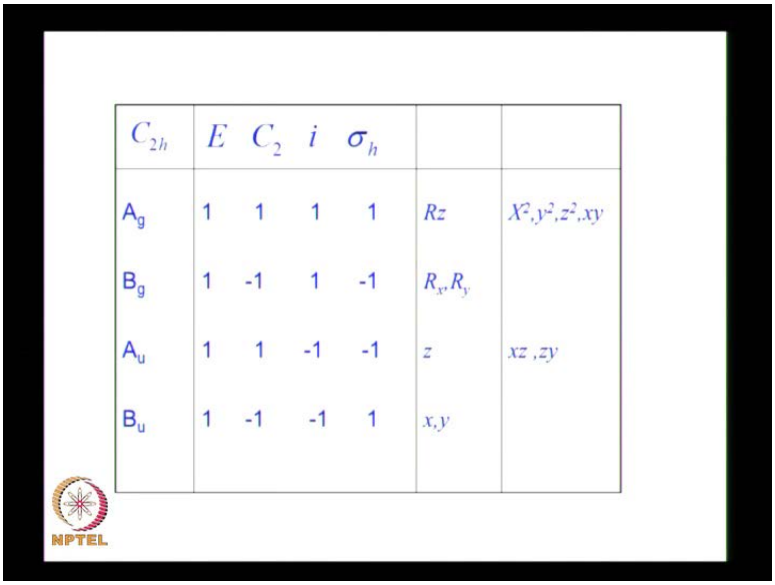

So, since there are four elements. So, one is the totally symmetric representation and then you can have and that is called g because, of the inversion symmetry g is gerade. So, it is symmetric with respect to the inversion. And there is also another one dimensional representation B g and then you have and ungerade, which is hard with respect to inversion and B u. So this will have 1, 1, 1, 1 and this will have 1, 1, minus 1, minus 1 and this will have 1, 1, minus 1 and minus 1. So, that would be the character table for the group 2 by m or C 2 h.

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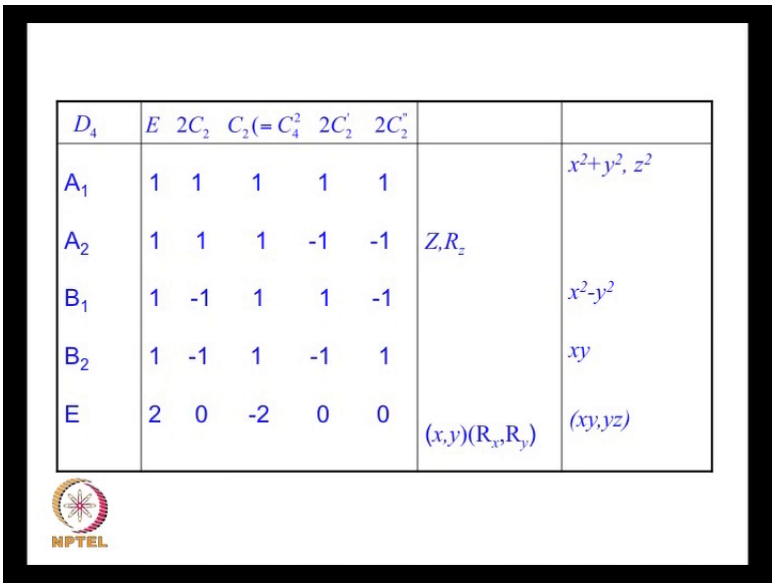

We now pass on to the next point group and proceed construct the character table. The next point group, which we take up is 4 2 2, which is D 4.

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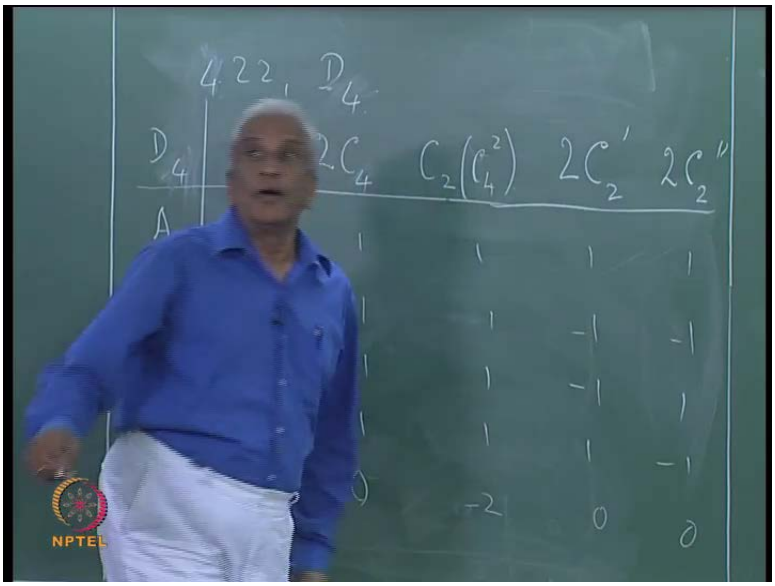

So, these are 2 C 4 and a C 2, which is C 4 square. And then you have the additional C 2 fold axis, 2 C 2, C 2 double dash. So, there are five classes. And therefore, five irreducible representations which are A 1, A 2, B 1, B 2 and then E, a two dimensional representations. So, the characters are which is totally symmetric of course. And then this will be anti symmetric is equal to this axis.

So you have B 1, which has anti symmetric with respect to this axis. And another one then you have two dimensional representations, which as the characters two for the identity it as the characters 0 as we saw already. This will be minus 2, 0, 0. So, that would be the character table for D 4. We next pass on to tetrahedral group, which is one of the cubic point groups O.

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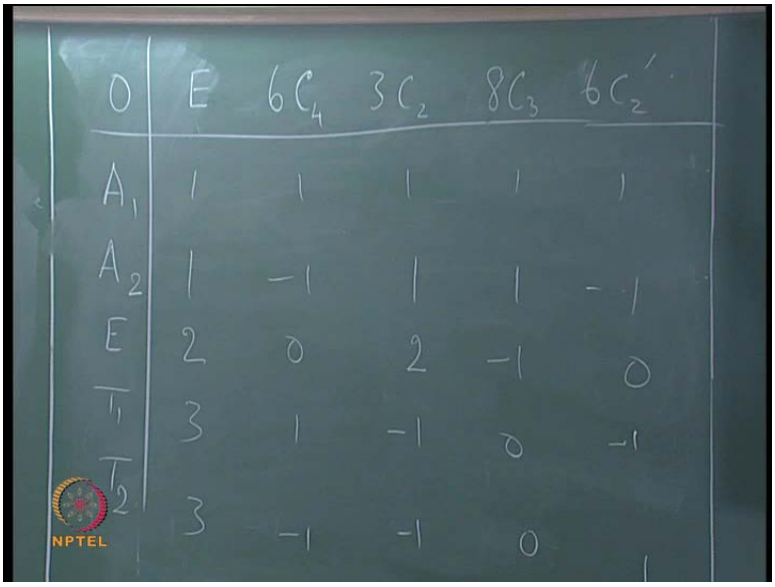

The group O, which is the octahedral group which is also a cubic point group. We considered the pure rotation axis the elements are identity and then has 6 C 4, 3 C 2 then 8 C 3, 2 3 C to dash.

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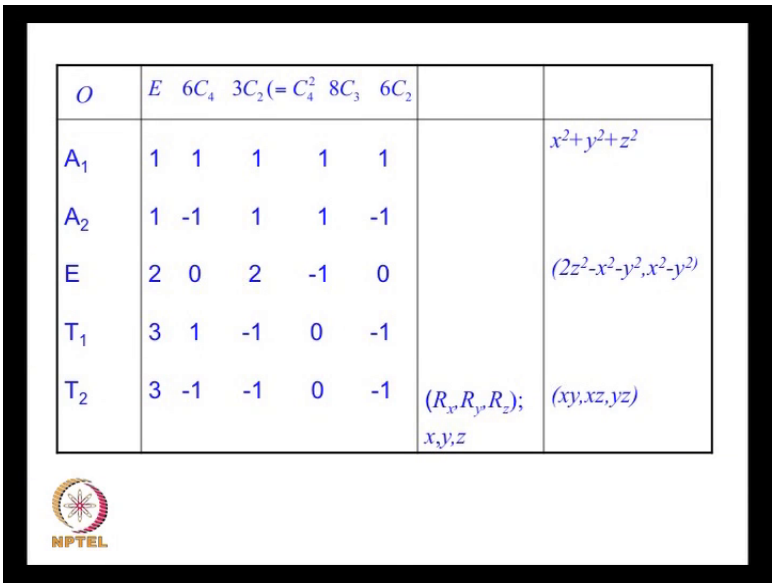

So, you have one plus six seven plus three ten 18 6 18 plus 624 because, of this you will have five irreducible representations. So, these will be A 1 one dimensional, A 2, E, T 1 two dimensional and three dimensional. So, this will have the character 1, 1, 1 then you will have 1, minus 1, 1, 1, minus 1 then you will have 2, 0, 2 to satisfy orthogonality. In the three dimensional rotation representations will have 3, 1, minus 1 and then 0, minus 1, in the other irreducible representation will have minus 1 here. So, these are the various irreducible representations of the and the next problem concern before the flies notation, which are also given here.

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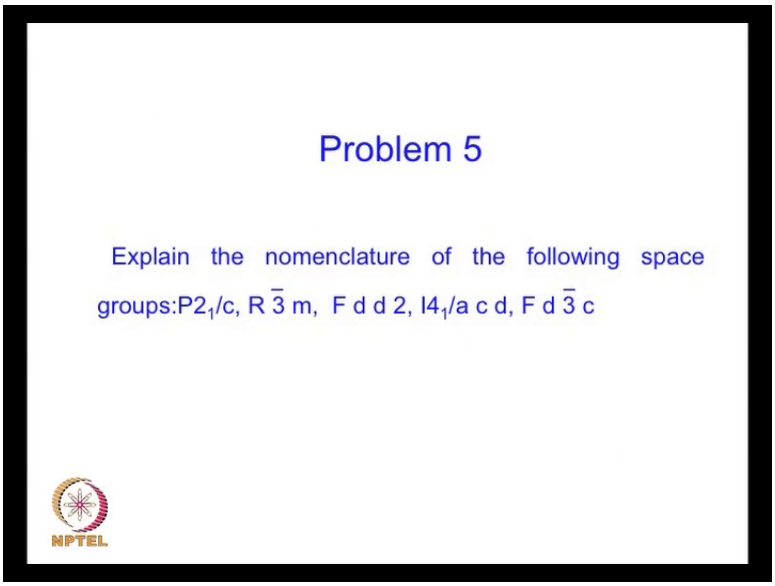

We now pass on to the next problem which concerns the space group notations.

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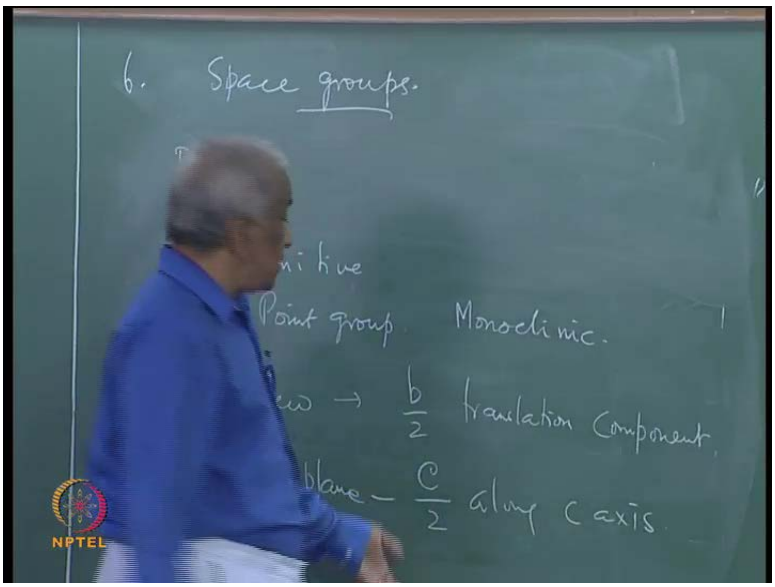

So, problem is on space groups. We are given the symbols for the difference space groups, you have P 2 1 by C. As we already explained during the lecture the P stands for a primitive crystal lattice, if one atom in the unit cell. And the ice organelle point group is 2 by m is the point group symmetry of the space group, which means that it is a monoclinic crystal lattice the brave lattice is a monoclinic primitive.

And you have two one screw instead of a pure two four axis, which means that there is a twofold axis followed by a translation component which is b by 2 of the translation along the b axis. And the symbols c means that, instead of the pure mirror symmetry we have a glide plane, in the plane perpendicular to this b axis. So, with a translation components c by 2 or along the c axis. So, you have a mirror plane which is a c plane and it is a mirror plane translation of the in front of c by 2 along the c axis so, that is the explanation.

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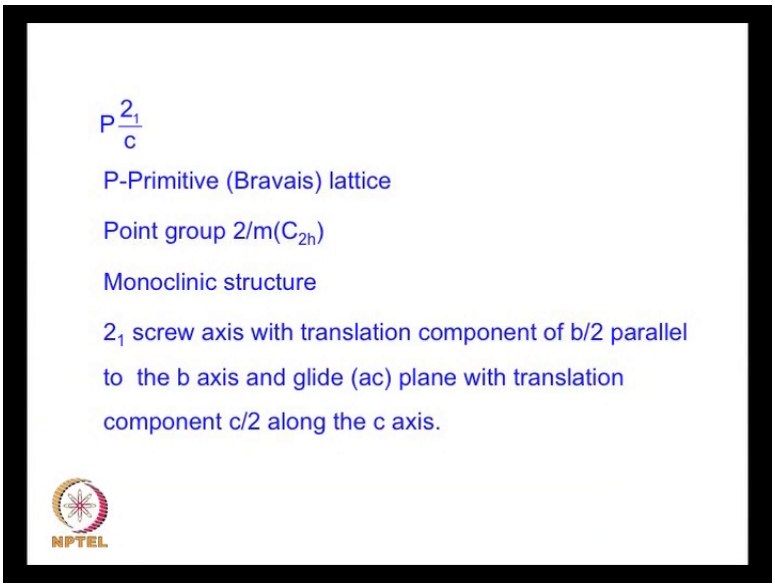

The next space to be considered is R 3 bar m.

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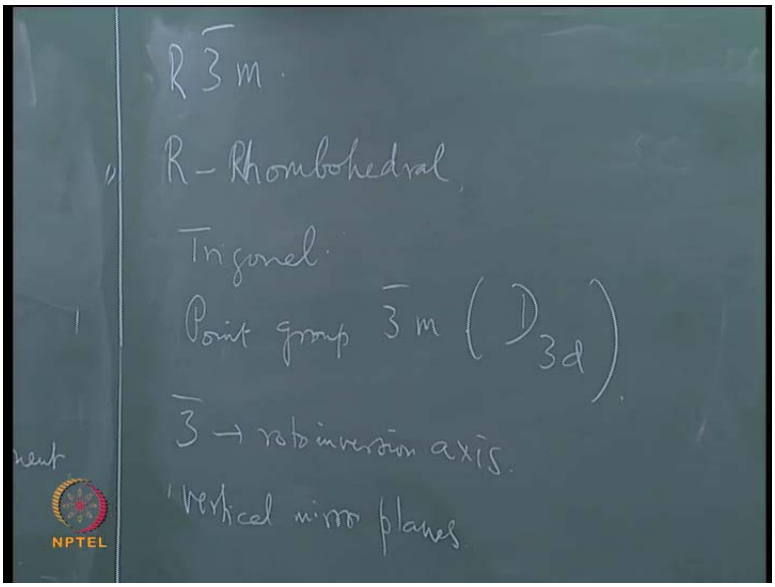

So, the symbol R stands for a rhombohedral crystal lattice, which belongs to a trignal point group. Trignal crystal system with a point group symmetry of 3 bar m. So, this is what is called D 3 d in shone flies notation. So, the 3 bar m means that, there is roto inversion axis, 3 bar is roto inversion along the z, along the c axis.

And then you have vertical mirror planes, pure mirror planes is no translation components coinciding is the roto inversion axis. So, that is the symmetry. The next space group to be considered is F d d 2.

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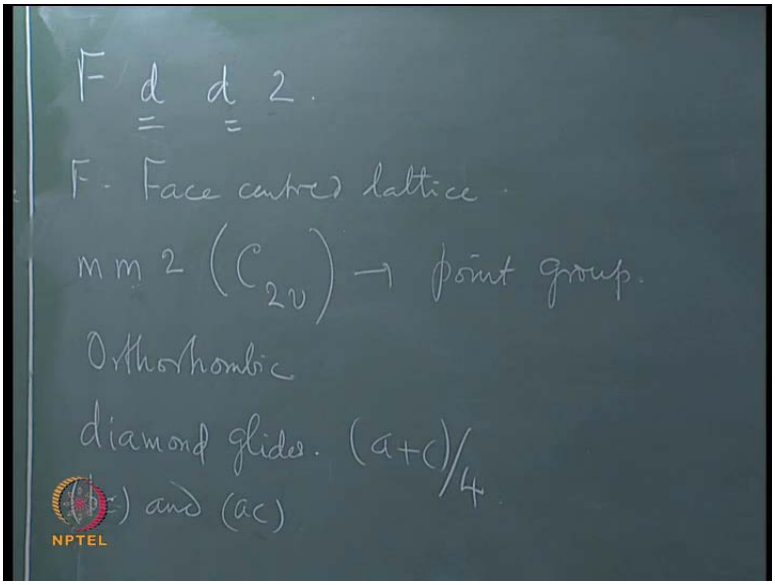

So, the symbol F means, it is face centered lattice, brave a lattice is a face centered lattice. Then since d d corresponds to mirror symmetry so, it is m m 2 is the point group, which is also known as the C 2 v this is the point group. So that means, this is an orthorhombic, since you have mirrors along the a and b so, planes perpendicular to the a and b axis under twofold axis in the along the z.

And the symbol d means, these are not pure mirror symmetries, but diamond glides with a translation component. So, this is first one is a perpendicular to the a axis. So, the b c plane and this one is perpendicular to the b axis through a c plane so, the conference of a plus c by 4. In this plane, in these two planes and you have a pure twofold axis.

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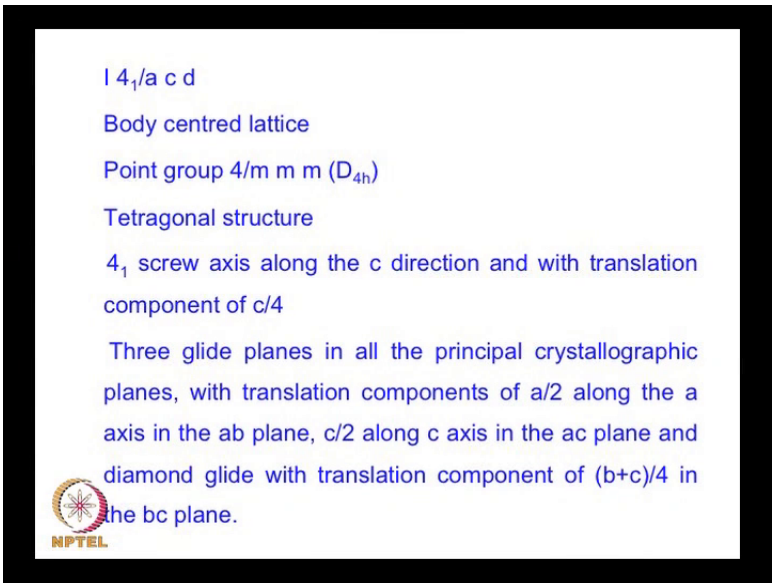

Next we move on to this space group symbol 4 1 for a c d with an I in front.

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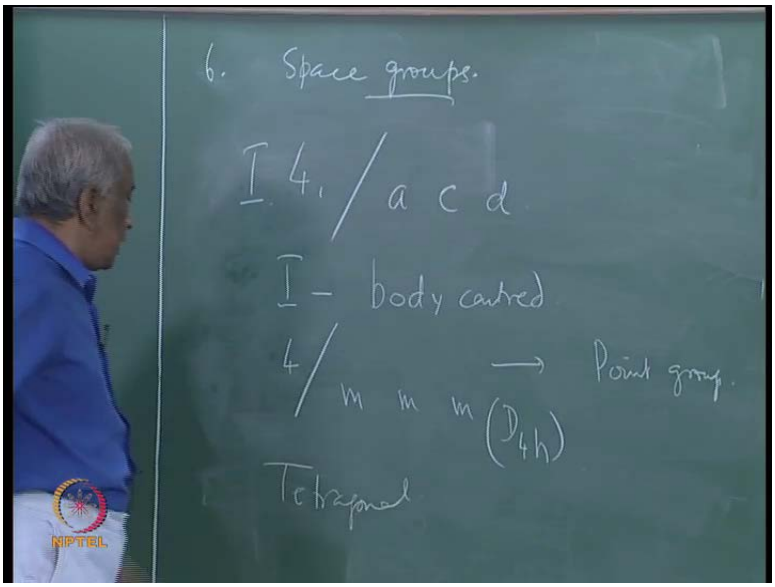

So, the symbol I stands for body centre lattice and the symbol 4 1 means the ice organelle point groups is 4 by there all mirrors. So, this is the point groups 4 by m m. The four fold axis with vertical. So, this is D 4 h. So, it is a tetragonal system because, you have a unique to fourfold axis. The interesting thing is that, we have not just a fourfold axis, but a 4 1 screw with a translation component of these along c axis.

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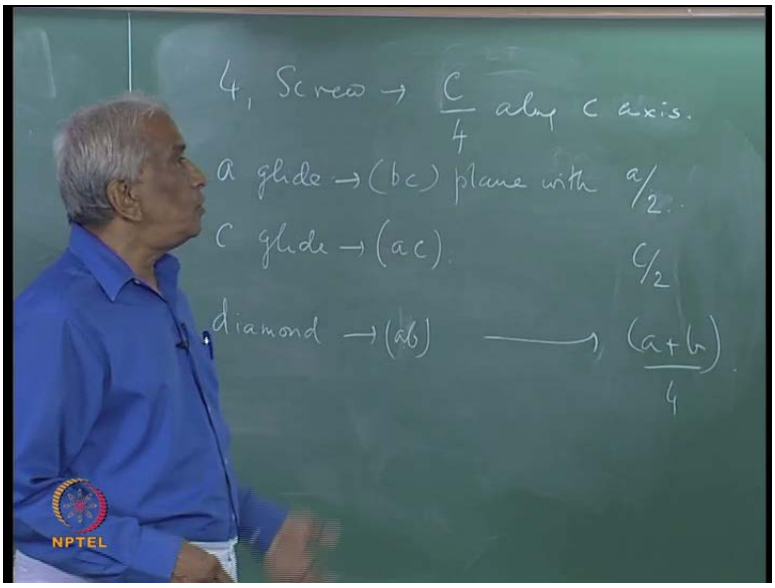

So, the translation component is c by 4 that is the translation component. And we have a glide and then c glide in the plane perpendicular to the b axis which is the a c plane. So, these again c by 2 and we have also a diamond glides in the b c. So, there are three glide planes in all the principal crystallographic plane. The translation components are a by 2, c by 2 and a plus b by 4 respectively.

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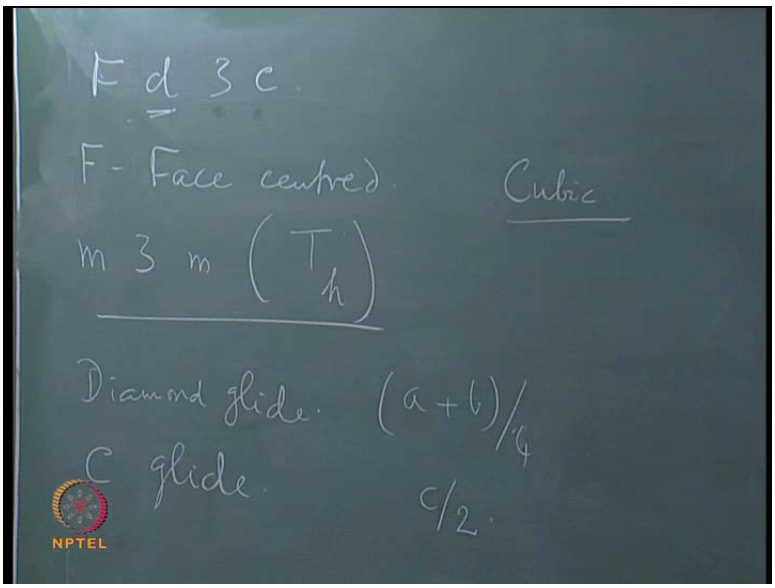

Lastly we take in the case F d 3 c, the symbol F; obviously, refers to a face centre lattice and d 3 c means it is m point group is m 3 m and that is nothing, but T h tetrahedral cubic

point group. So, it is a cubic crystal body centered cubic brave a lattice with an ice organelle point group m 3 m of p h in the behave a diamond glide.

So, instead of the pure mirror plane is the diamond glide is a pure threefold axis and a c glide corresponding to this. So, the diamond glide means it is a plus b by 4 and the c glide is the translation component the c by 2. And this is in the b c plane and this is the diamond glide in the a b plane. So, that explains the space groups symbols of, this space group F d 3 c is the cubic space group.

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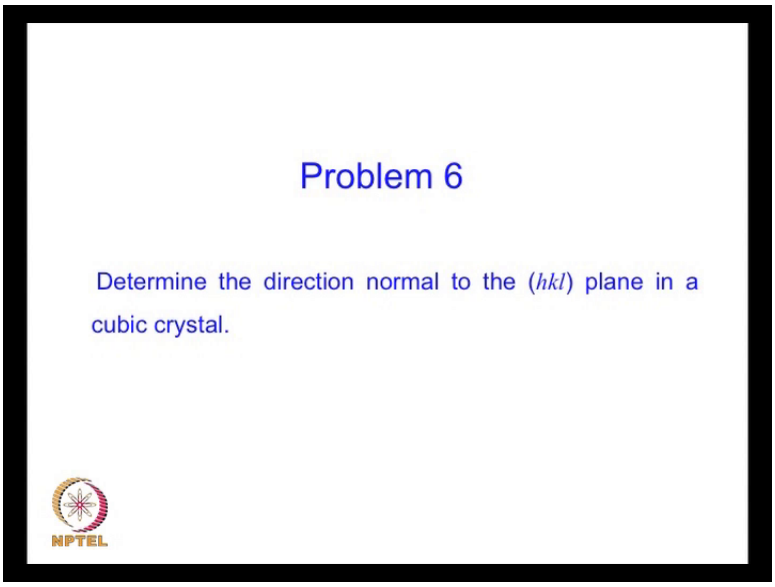

The next problem is to determine the direction normal to the h k l plane in a cubic crystal.

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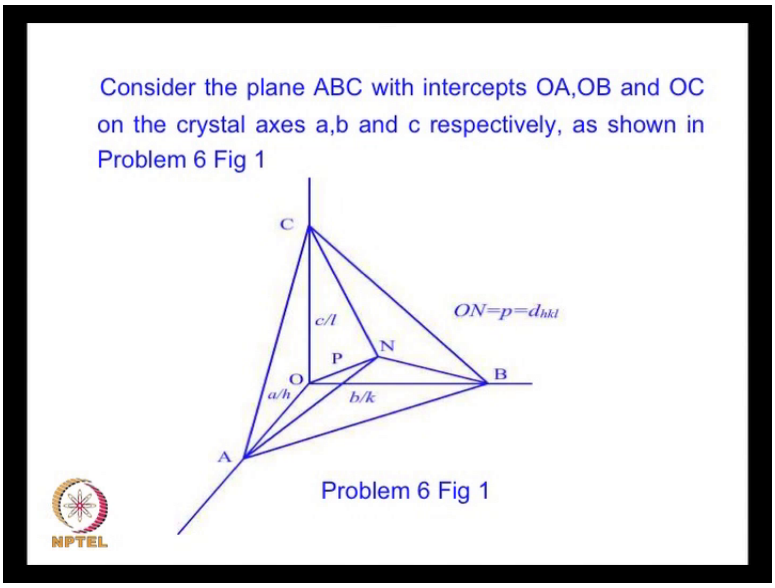

Figure 2 shows the plane A B C, which have the intercepts OA, OB and OC on the crystallographic axis, a axis, b axis, and c axis respectively. So, OA OB and OC are the intercepts the miller indices of this plane A B C or chosen to be h k l. So, that by the definition of the miller indices OA is a by h, OB is b by h, b by k well it is a cubic crystal.

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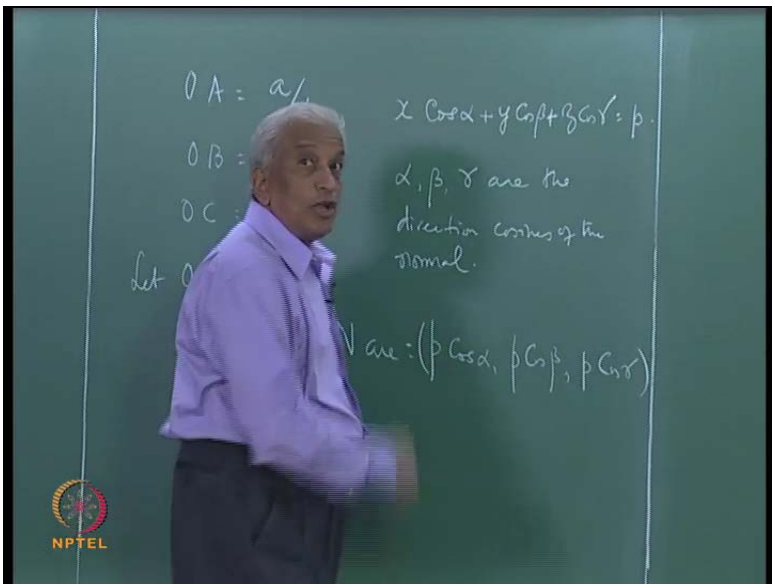

So, it is all a by k, OC is a by l. Now, in the figure let ON is the normal to the h k l plane.

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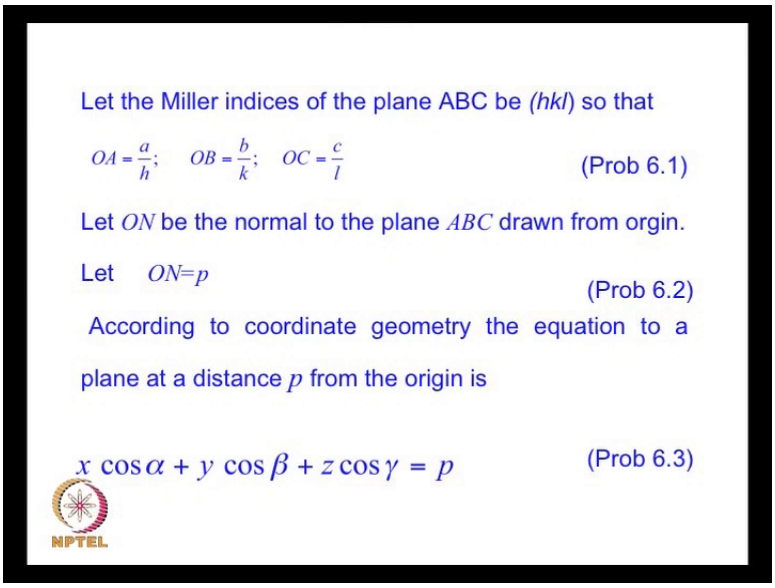

So, this length ON let it be chosen as p. If that is so, the normal form of the equation to a plane at a distance p from the origin is given by it is well known. That is given by x cosine alpha plus y cosine beta plus z cosine gamma equals p where, alpha beta gamma or the direction cosines of the normal. So, these the standard resulting coordinate geometry. So, we will use this. So, now, therefore, we can write the coordinates in the point N, what are the coordinates of point N?

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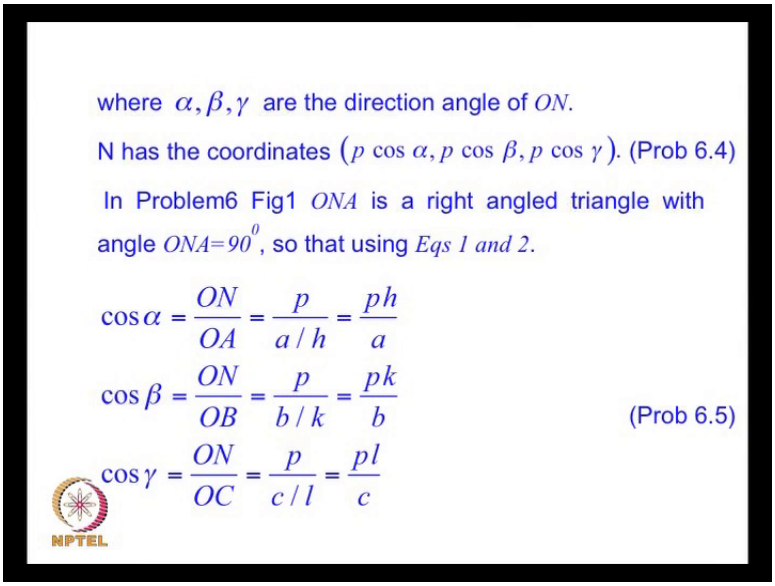

They are p cos alpha because, the length ON is p. So, it is p cos alpha, p cos beta and p cos gamma, these are the coordinates of the what? The point N so, now, going an referring to the figure they ONA the triangle. ONA is right angled triangle and with cos alpha which is ON by OA.

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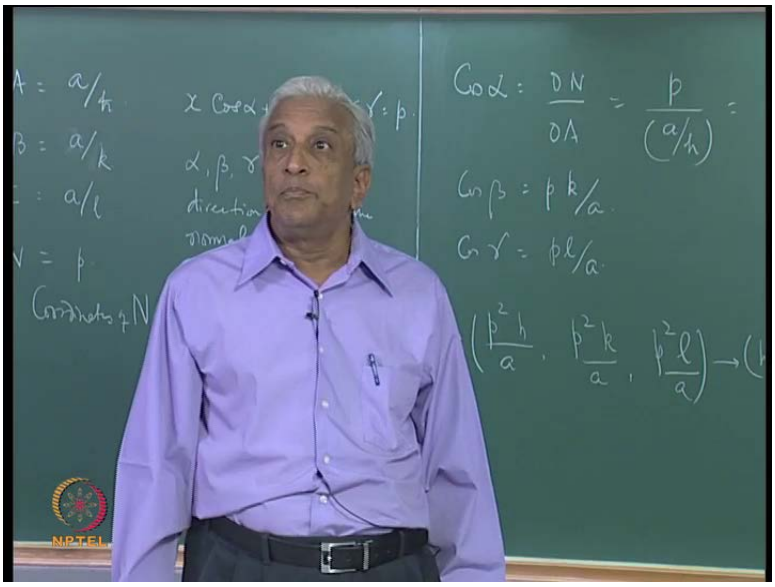

And ON is p and therefore, OA is a by h therefore, this is p h by a. Similarly, cos beta is p k by a, in cos gamma is p l by a. So, that the coordinates, these coordinates become fastening for cos alpha, cos beta and cos gamma, we get p square h by a, p square k by a, p square l by a. Therefore, reducing this to the smallest integers taking the common factors of away they arrive at h k l as direction normal to the plane, h k l plane. So, that is the direction h k l.

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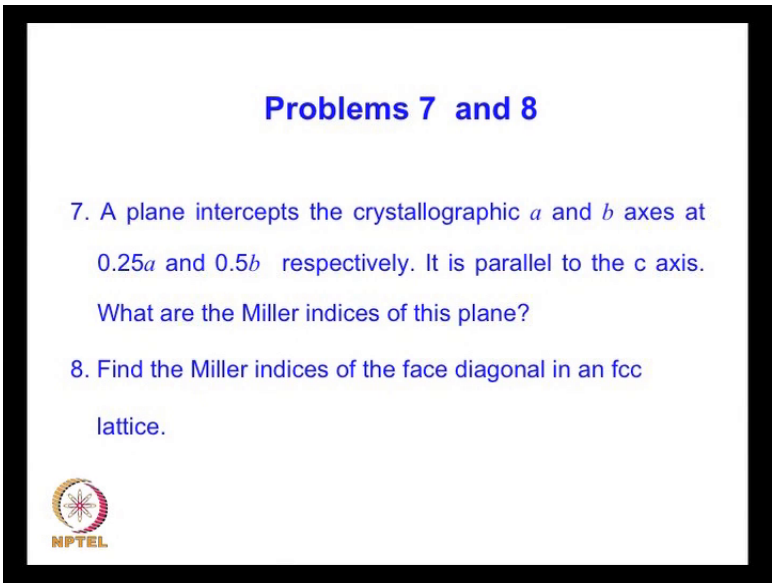

The next problem is to find the miller indices of a plane which intercepts the crystallographic a and b axis intercepts are 0.25 a and 0.5 b.

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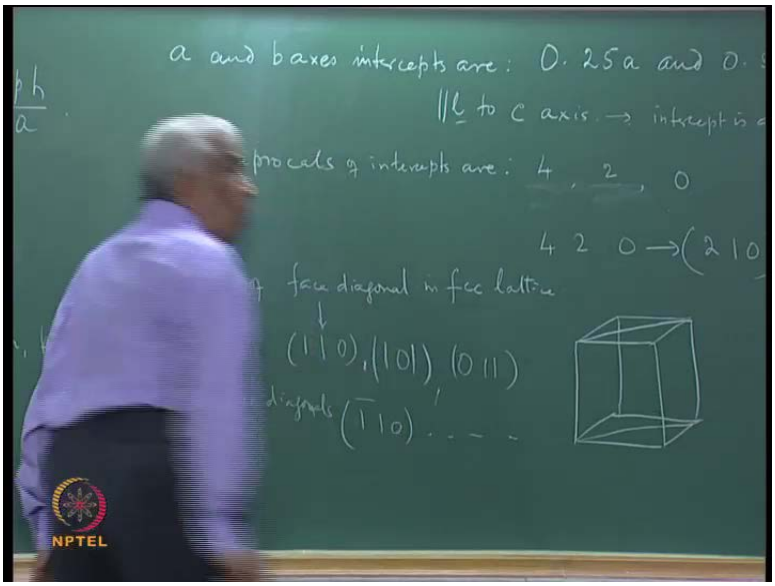

And it is also parallel to c axis. This is the plane therefore, there has to find the miller indices, for miller indices we go from the intercepts by taking the reciprocals to the intercepts. The reciprocals are this is 1 by 4. So, it is 4 of course, by a and 2 by b. Then since it is parallel to c axis the reciprocal is 0 because, this is parallel. So, the intercept is

infinity. Therefore, the reciprocal of infinities is 0 therefore, this becomes 4 2 0. And therefore, no we need not write a and b since they are measured in units of a and b.

So, this is 4, 2 and 0, which reduced to smallest integer is 2, 1, 0. Those are the miller indices of the plane. Proceedings of the same way, we are also as to find the miller indices of face diagonal in an f c c lattice. So, in an f c c lattice the face diagonal look like this. So, the face diagonal for example, is like this, one of the face diagonal.

So, the plane containing the face diagonal is makes intercepts it is miller indices are given by its makes intercepts one and one on these axis and it is parallel to z axis therefore, in miller indices is; obviously, 1, 1, 0. Now, not only 1, 1, 0, but also there are 12 face diagonal is and the different planes which contain this face diagonals are all the entire setup family of planes 1 1 0, 1 0 1, 0 1 1, also 1 bar 1 0 and so on. All of them they are twelve of them all of them belong to the same family of planes.

(Refer Slide Time: 40:07)

Structure	Ratio between a, b and c	Value of α, β and γ	No.of atoms per unit cell
SC			
	$a=b=c$		4
		$\alpha = \beta = \gamma = 90^0$	2
Body centred Tetragonal			
HCP	$a = b \neq c$		4

NPTEL

Problem 9 Table 1

The next problem is in the form of a table, in which we are given difference structures. And we are asked to fill in the blanks for a table, which gives the structure the ratio between a, b and c. The value of alpha, beta and gamma and the number of atoms for unit cell there are several blanks.

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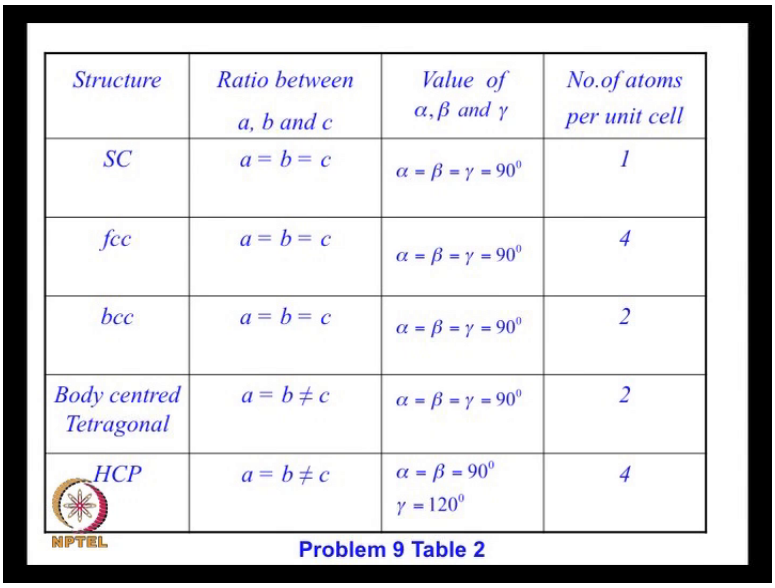

And the next table gives the answers with the missing entries, which are fill in the blanks, which are fill. So, the answers are obvious.

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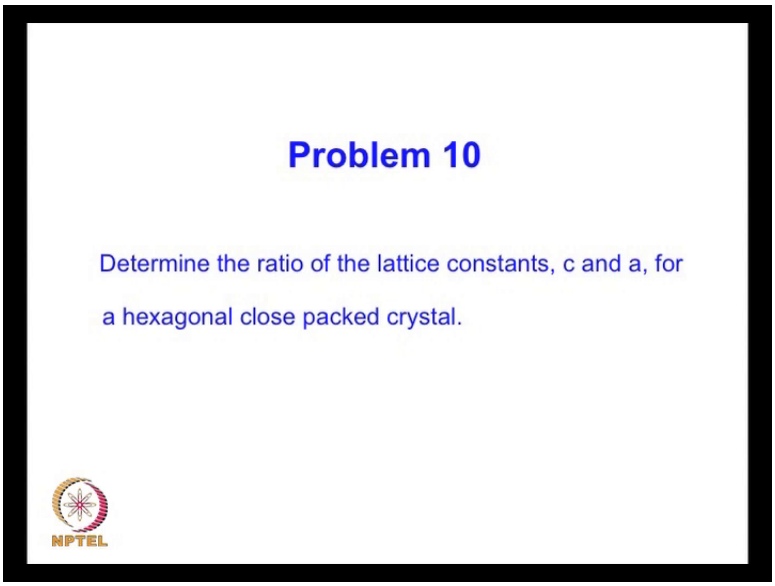

So, I do not provide any explanation for it, the table has self explanatory. The next problem we are asked to determine the ratio the lattice constants c and a.

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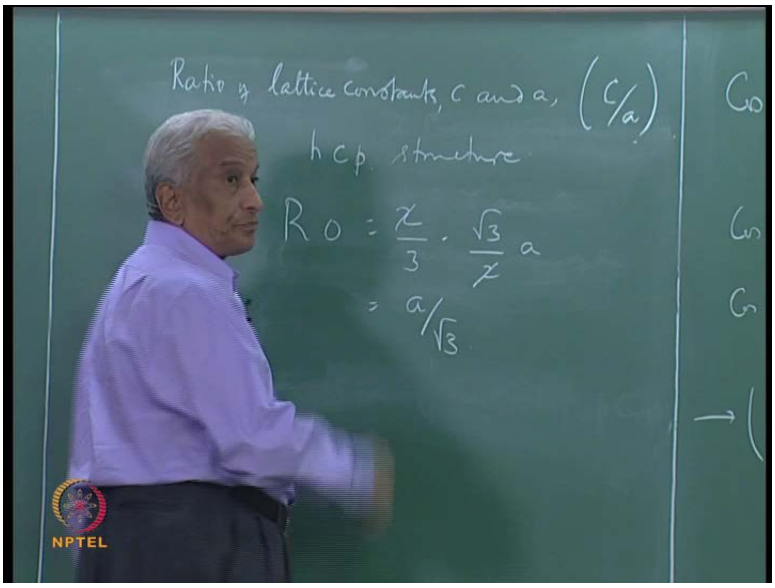

So, in other word, we are asked to determine c by a ratio for a H C P hexagonal close axis structure.

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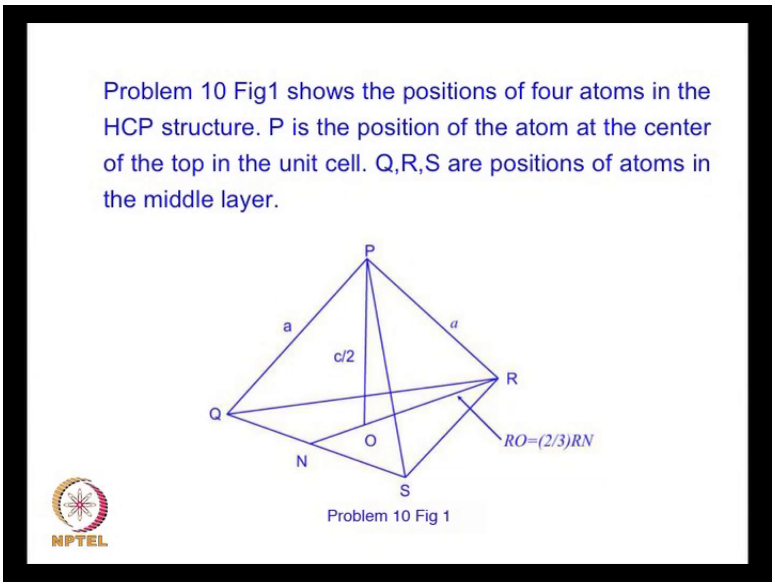

The next figure shows the positions of four atoms in the H C P structure. Now, you have p, which is the position of the atom at the center of the top in the unit cell, the topmost point in the unit cell. Which corresponds to one point in the unit cell and the next layer there are three corresponding positions of the atoms, in the middle layer they are written as Q R and S. Now, by geometry you can see that, the sides P R and R S are the sides of

the unit cell and that is given by a and therefore, since the angle is so, equilateral triangle in Q R S. Therefore, the side R N is root 3 by 2 a and the O R is two thirds of that because, O is the centroid of that, so, r n is divided in the ratio 1 is to 2.

(Refer Slide Time: 42:55)

$$PR = RS = a$$
$$c = 2PO$$
$$cla = (2PO)/a$$
$$RO = (2/3)RN$$
$$= (2/3)a\left(\frac{\sqrt{3}}{2}\right)$$
$$= \frac{a}{\sqrt{3}}$$

Therefore, we have R O in the figure as two thirds of root 3 by 2 a, which is a by root 3. So, that is the perpendicular distance R O from that is the distance R O. And we are required to find P O, the distance P O, which in the right angled triangle.

(Refer Slide Time: 43:33)

$$PO = \sqrt{(PR)^2 - (RO)^2}$$
$$= \sqrt{a^2 - \left(\frac{a}{3}\right)^2}$$
$$= \left(\sqrt{\frac{2}{3}}\right)a$$
$$\frac{c}{a} = \frac{2PO}{a} = \frac{2\left(\sqrt{\frac{2}{3}}\right)a}{a} = \sqrt{\frac{8}{3}} = 1.633$$

We are one side is a, another what we found just now as a by root 3. So, the distance P O is square root of a square minus a square 3, which is root 2 by 3 a.

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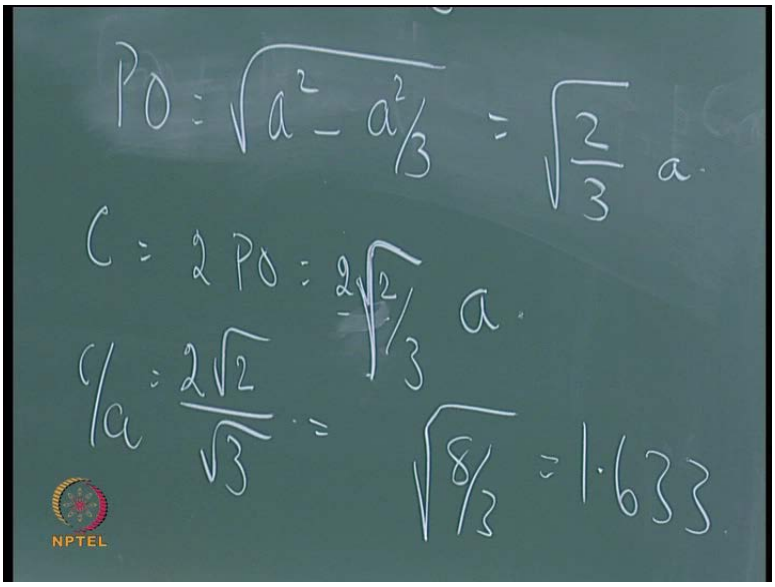

That is the distance from the top layer for atom P to the centroid in the next lower layer. So, the actual c axis ratio is twice c is two times P O and therefore, it is 2 root 2 by 3. And therefore, the c by a ratio is 2 root 2 by root 3 that is, it can also be written as root of 8 by 3. That works out to 1.633. So, that is the ratio of the c to the a axis, lattice para meters in the h c p structure.

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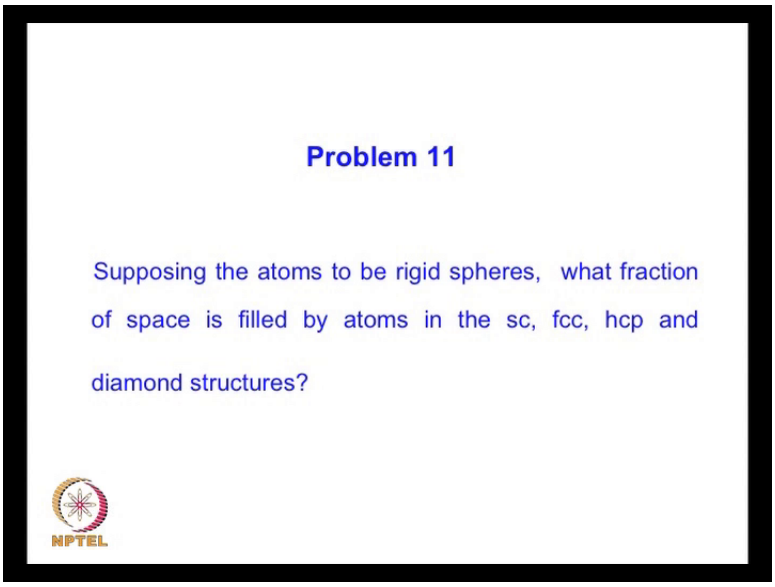

Next problem talks about atoms, which are treated a rigid sphere and then we are asked to calculate the fraction space field by atoms in different structures. The fraction is usually known as packing fraction, in short we can return as P F.

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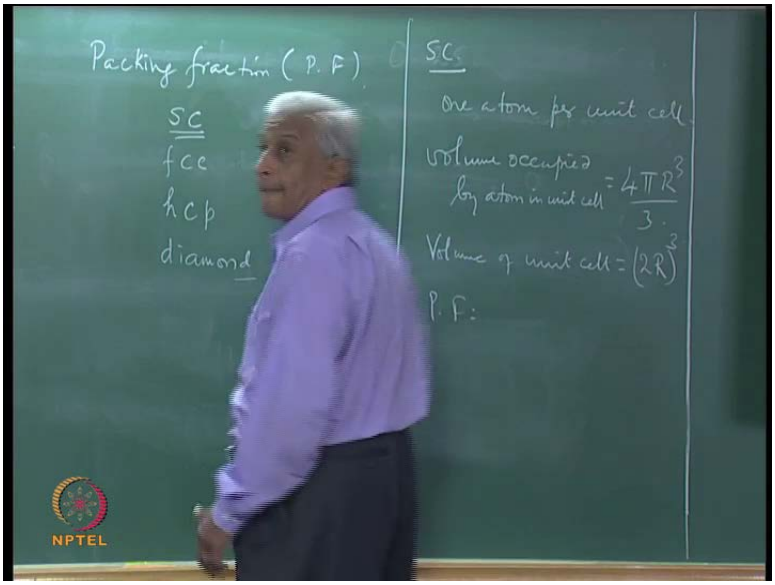

For this simply cubic structure, for the face centered cubic structure, for the hexagonal close packed structure and for the diamond structure, you proceed as follows let us, considered the a simply cubic. The simplest, in the simple cubic lattice we know there is one atom for unit cell. So, for R is the atomic radius, than the volume of occupied by the atoms in the unit cell is simply the atom volume 4 pi R cube by 3, since there is only one atom.

Whereas the volume of the unit cell itself depends on the side of the unit cell that will be the side of the cell has the distance 2 R, where R is the atomic radius. So, the volume will be 2 R cube, this cube of side 2 R. So, the packing fraction is the ratio of the two, so it will be on calculation this will be pi by 6.

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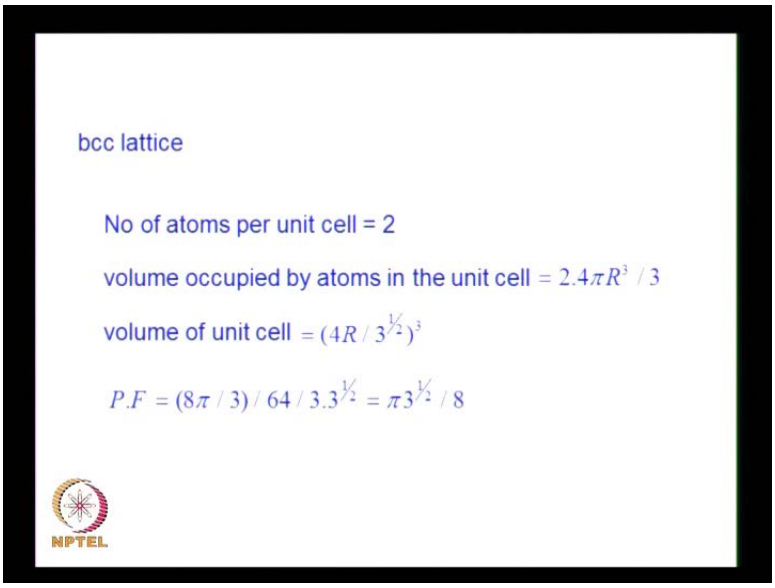

Next we consider b c c structure. For the b c c there are two atom, one at the body center and one at the corner, two atoms per unit cell.

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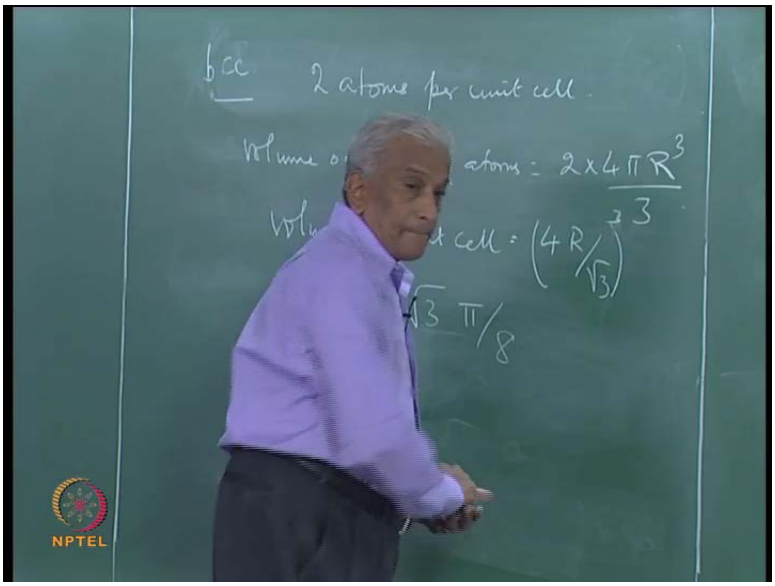

Therefore, the volume occupied by atoms equals 2 into 4 pi R cube by 3. Whereas, unit cell volume, we already saw the unit cell is 4 R by root 3. So, that is the side. So, the packing fraction which is the ratio of the two is just root 3 pi by 8.

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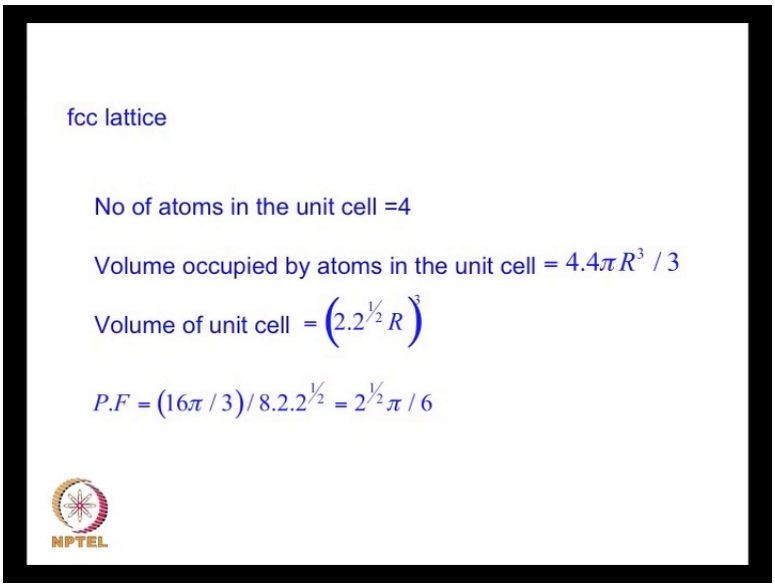

Next we consider the f c c structure, face centered cubic structure, where the number of atoms per unit cell is 4.

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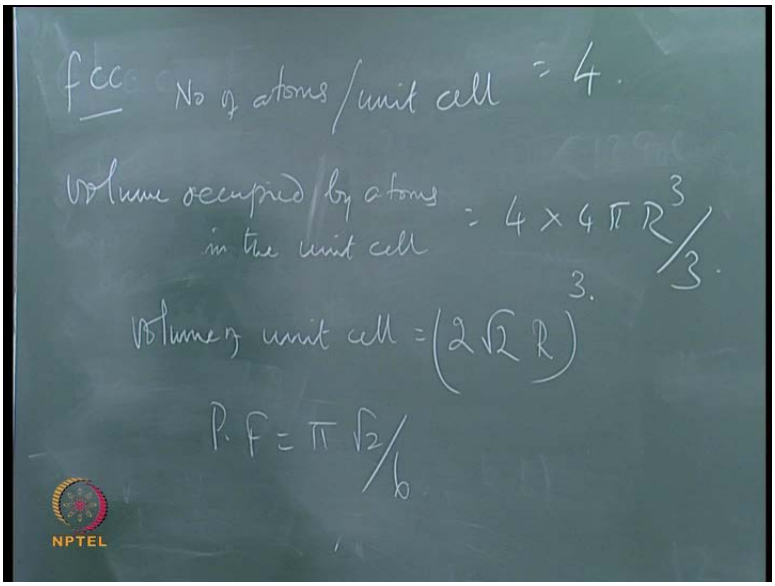

So, the volume occupied by atoms in the unit cell is 4 times 4 pi R cube by 3. In the volume of units cell is 2 root 2 R is the side cube of this. So, the packing fraction is pi into root 2 by 6.

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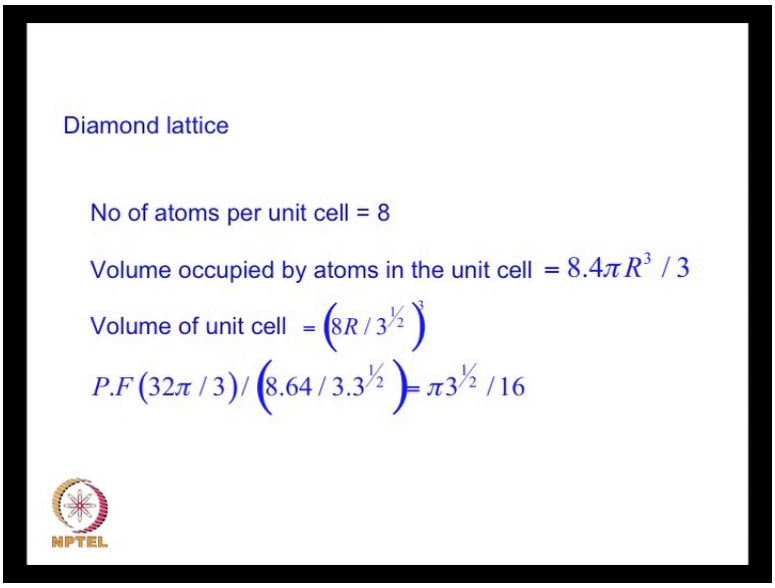

We will talk about the diamond lattice, which is a special lattice. The diamond cell as carbon atoms at the vertex and at the along the body diagonal at one quarter the one fourth, one fourth, one fourth of the coordinates of the carbon atoms and so on, all the equivalent of these.

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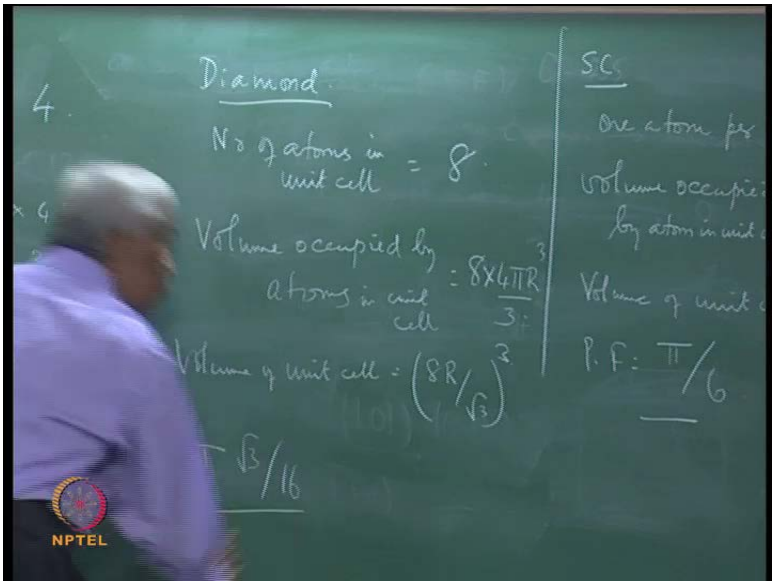

So, there are in total number of atoms in unit cell is 8 as one can readily verify. So, the volume occupied by atoms in unit cell is 8 times 4 pi R cube by 3. Whereas, the volume of the unit cell itself is 8 R by root 3 cube as one can readily see. So, the packing fraction

in this case works out to be pi root 3 by 16 is rather small number. So, this is not a very close packing fraction structure. The diamond is the rather open structure that is because, of the essential nature of the covalent bond between the carbon atoms.