Condensed Matter Physics
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Lecture - 3
Symmetry in Perfect Solids (Continued)

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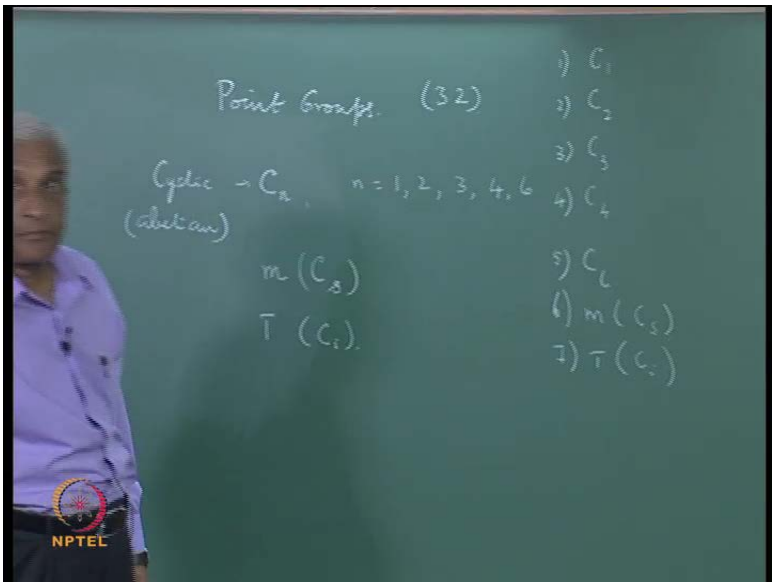

So, the last lecture, we introduced the concept of point groups which number 32, in three dimensions. So, we started in this lecture, we will enumerate these point groups in a rather systematic fashion; we saw that the first groups are the cyclic groups cyclic point groups given by the general symbol C n where n is 1, 2, 3, 4 and 6. So, we have C 1, C 2, C 3, C 4, and C 6. So, these are the cyclic point groups which are abelian these are the simplest in addition we have the m the mirror which is also given by the notation C s and i are one bar which is C i the inversion. So, i use the (( )) or the international symbols interchangeably

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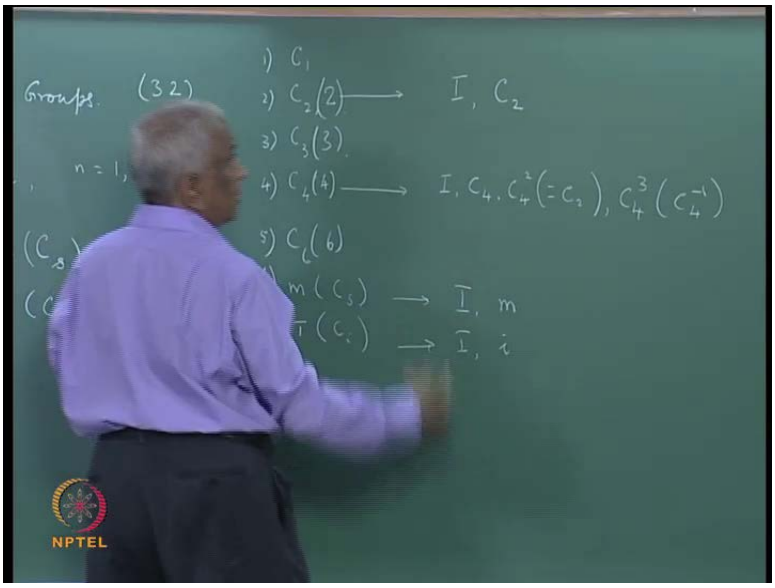

So, we have for example, if you take C 2, the point group C 2, the elements are the identity element and then the C 2 these are the elements. Whereas, for C 4, the elements are C 4, C 4 square, which is really C 2 and C 4 cube which is C 4 in the clockwise direction and so on. Similarly, for a mirror this is and for an inversion, the main elements are we then went on to add these mirrors to the various axis to get new point groups. And so we got the point groups two by m, this is also shown as two, this is shown as three, this is shown as four, shown as six, these are alternative rotations.

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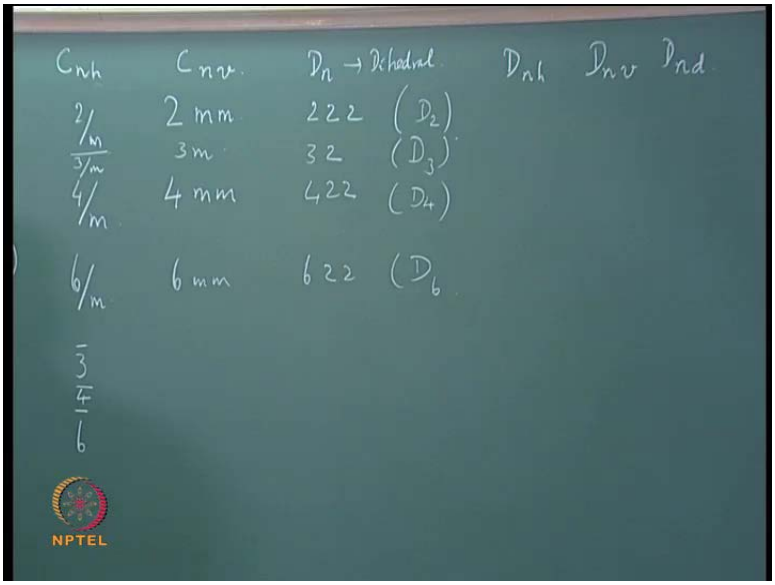

So, we get the point group two by m which is a direct product of C 2 and m and then we have similarly four by m and six by m. We can also get just like, we have one bar we can get other point groups like three bar six bar and four bar. We can also add mirrors parallel to the rotation axis and that would give lead to point groups, which are new such as six mm three m and so on. So, we get various point groups by the addition of mirrors either perpendicular to the rotation axis or parallel to the rotation axis. So, these are known as the C n h for a horizontal mirror plane and C n v for vertical mirror planes then we said that we have. So, called the dihedral D n the dihedral point groups which are got by combining rotation axis; this is also known as D 2 and you get 3 2, this is D 3 and a 4 2 2 6 2 2, this is D 4 this is D 6.

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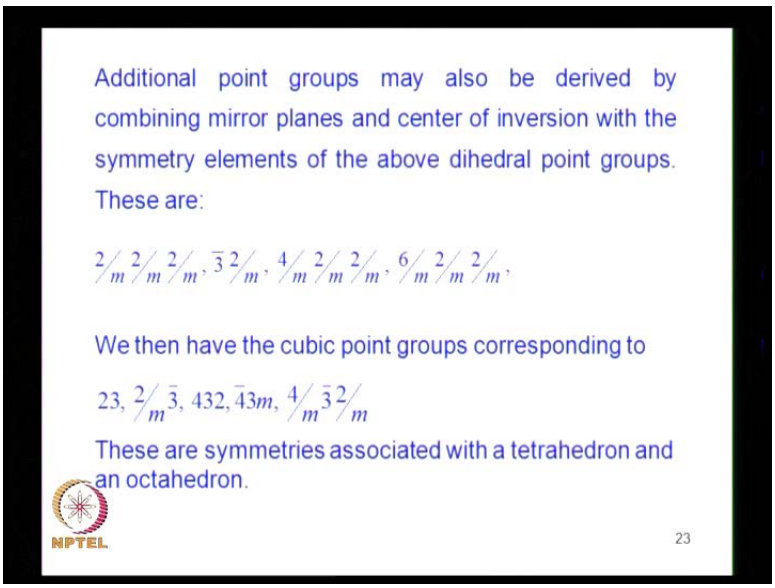

So, we can go on like this to get additional point groups. Now we can add mirrors to these to get things like 2 by m 2 by m 2 by m, 3 bar 2 by m, 4 by m 2 by m 2 by m, and 6 by m 2 by m 2 by m. So, these are known as the D n h where you add a horizontal mirror to the dihedral point groups. Similarly, you get also additional point groups by having D n v, we can also have diagonal mirror planes giving rise to D n d. All these are axial, they have a rotation axis, whereas we also have in addition to all this the cubic point groups.

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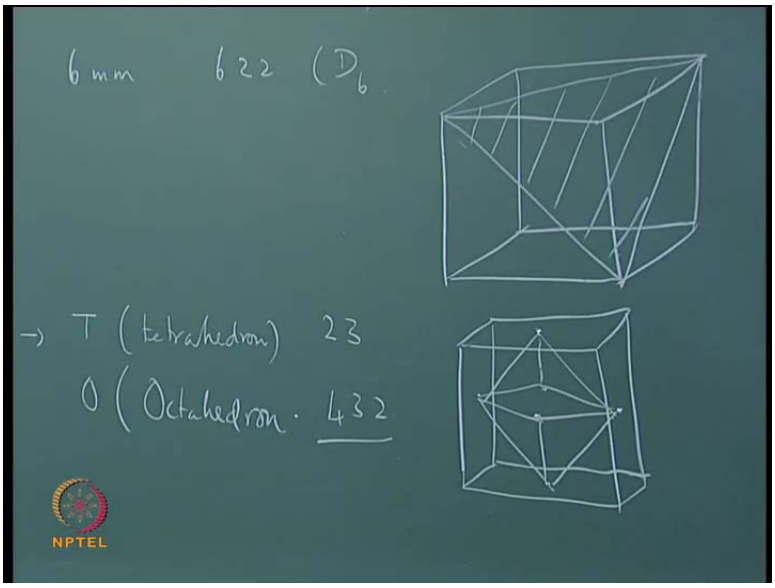

And a cube is a is an object of very high symmetry, which includes the symmetry of a tetrahedral and an octahedral. So, you have T and O which are also known as 2 3 and 4 3 2. Let us draw a cube and it can be readily seen that by joining these and the vertex opposite to this triangular plane you get a, so that is the one which has a obviously, a threefold axis and two fold axis of symmetry. Whereas, the same cube is also consistent with octahedral symmetry as can be seen by taking the mid points of these sides. So, one can see how a cube is has in implicit way octahedral symmetry and the octahedral symmetry is consistent with the four fold axis and a threefold axis and two fold axis.

So, it is to show that it is also known as 4 3 2, and then one can also have additional mirrors in a cube, for example, it is clear that there are mirrors present everywhere. So, addition of mirror symmetry gives rise to additional point groups like 2 by m 3 bar and then 4 by m 3 bar 2 by m and then 4 bar 4 m. So, this is the point group of highest symmetry among the 32, it is known as O h the octahedral with horizontal mirror planes. So, that would complete the enumeration the 32 point groups. Now these symmetry elements are all shown in the figure via.

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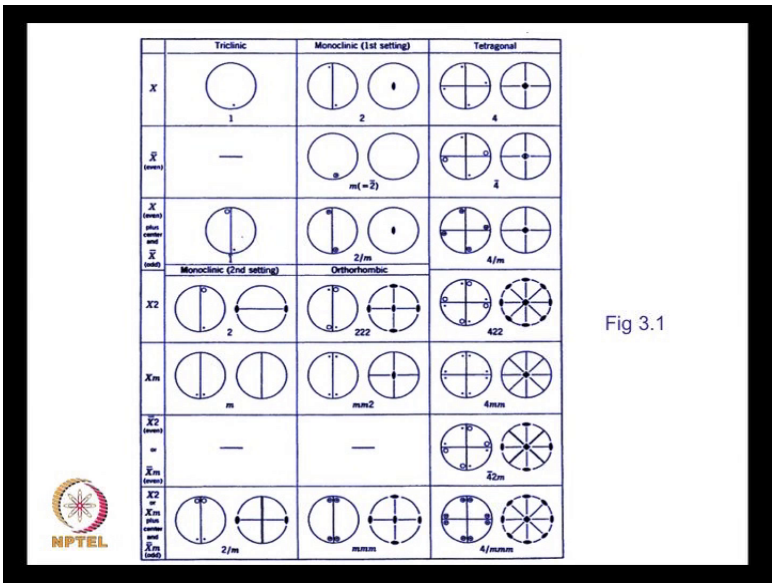

Fig 3.1

The technique of stereographic projection in this figure you also see a distribution of these various point group among the. So, called crystal classes what are these crystal classes these crystal classes are numbering seven their best understood by simply enumerating them.

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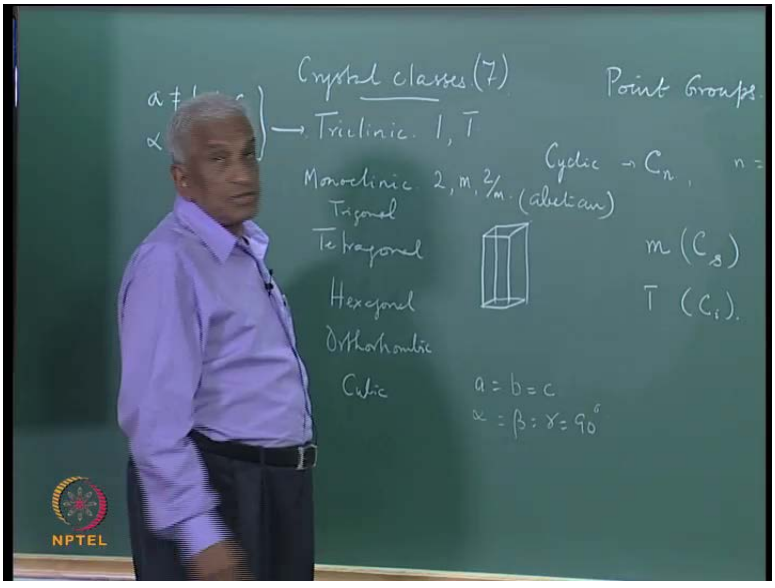

In order of ascending symmetry triclinic monoclinic tetragonal center well and then you have orthorhombic and cubic. So, these are the crystal classes, and you can see that the triclinic does not have any degree or symmetry and the point groups one and one bar.

This monoclinic is 2 m and 2 by m all these have a principal two fold axis, and then you have trigonal. Similarly, you can see the various this various symmetry elements associated with these are also shown by a what I explained as stereographic projection last time. So, the distribution of the 32 point group among the different crystal classes is shown.

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Crystal class	Description of unit cell	Point group
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90°$	$\bar{1}$ 1
Monoclinic	$a \neq b \neq c$ $\alpha = \beta = 90°, \gamma \neq 90°$	2/m m, 2
Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	2/m 2/m 2/m mm2, 222
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	4/m 2/m 2/m $\bar{4}$2m, 4mm, 422, 4/m, $\bar{4}$, 4
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90°$	4/m $\bar{3}$ 2/m $\bar{4}$3m, 432, 2/m$\bar{3}$, 23
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90°, \gamma = 120°$	$\bar{6}$/m 2/m 2/m $\bar{6}$m2, 6mm, 622, 6/m, $\bar{6}$, 6
Rhombohedral	$a = b = c$ $\alpha = \beta = \gamma \neq 90°$	$\bar{3}$ 2/m 3m, 32, $\bar{3}$, 3

In the next figure, now the crystal classe has the different characteristics with respect to the shape or the description of the unit cell of the crystal. And as you can see triclinic does not have any degree or symmetry in that is in the sense that three lattice periodicities in the three direction crystallographic directions need not necessarily be equal and this also true for the inter axial angels alpha beta and gamma. Whereas, in the case of monoclinic you have a not equal to b again, so this is triclinic and so on. So, a not equal to b not equal to c alpha equal to beta is not very clear gamma equal to 90 degrees then tetragonal has a equal to b not equal to c a tetragonal lattice is something like this. So, it is a square base and long the parallel like a rectangular parallel piped.

So, a equal to b not equal to c, but the inter axial angels are all ninety degrees then you have cubic which is the high symmetry and here all the three parameters lattice parameters (( )) equal. So, also the angels are also 90 degrees. So, that the axis are orthogonal to each other then you have the hexagonal which has a hexagonal symmetry and also the orthorhombic which I have already shown and then the trigonal or

rhombohedral. So, these are the various classes and the distribution of the various point groups is also shown.

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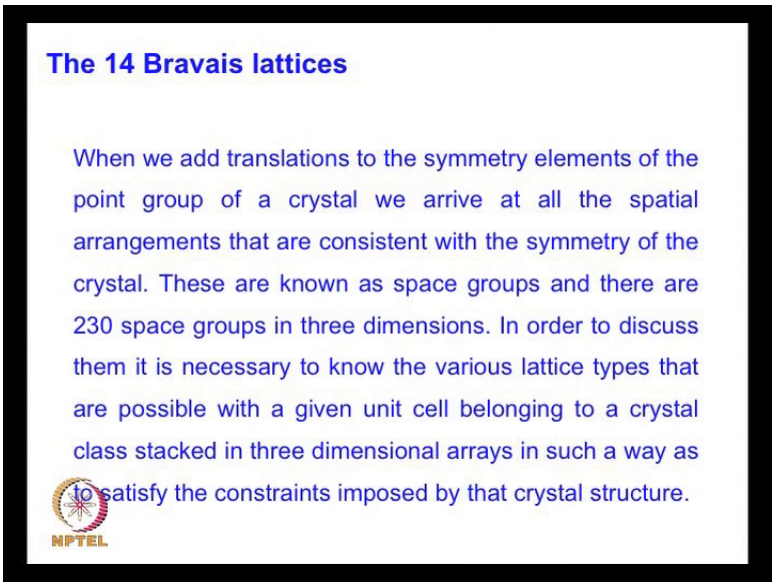

Now, we have discussed point group symmetries and the classification of the different crystals of different classes and the distribution of the various point groups into the these crystal classes. Next we have to consider the other symmetry which we already mentioned namely that of translational symmetry. So, we have to see what happens when we add translations to the symmetry elements of the point groups of a crystal then we arrive at all the special arrangements that are consistent with the symmetry of the crystal these are known as space groups. So, the space groups are derived from the point groups by adding translational symmetry elements in three dimensions in order to discuss space groups which are two hundred thirty in three dimensional space there are two thirty space groups in three dimensions. In order to discuss this, it is necessary to know the different types of lattices are a which are possible with a given unit cell belonging to a crystal class.

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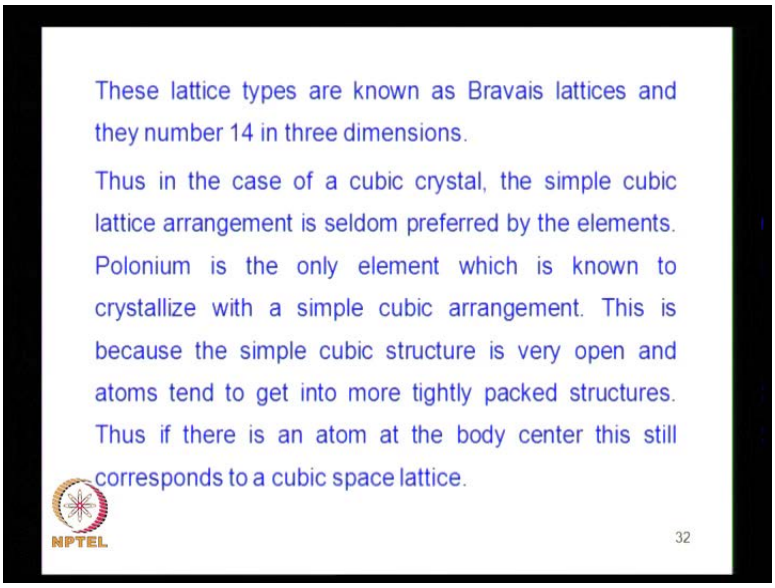

So, let us look let us look at this first, these lattice types are known as bravais lattices, they are fourteen in number, for example, in a cubic crystal

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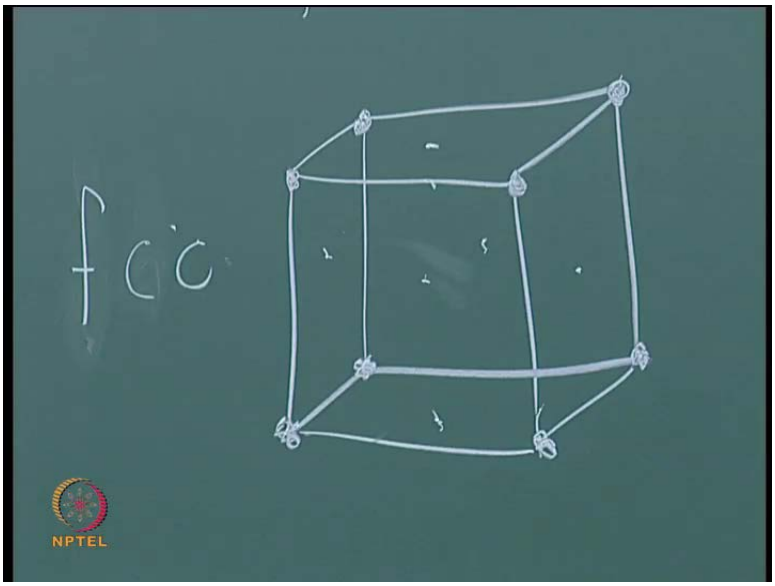

You have the simple cube like what I showed here a simple cube is just one in which there are atoms or molecules only at the vertices of a cube. So, it is a simple cubic lattice among the elements polonium is the only element which is known to crystallize with a simple cubic arrangement this is because the simple cubic structure is very open and the atoms tend to get into more tightly packed structures. So, these tightly packed structures

are got, for example, by adding an atom or molecule at the body center of the cube then the simple cube becomes a body centred lattice body centred cubic lattice bcc or we can also add atoms at the face centres. So, if you have atoms like this then this is a face centred cubic lattice fcc. So, these are much more tightly packed than a simple cubic space lattice.

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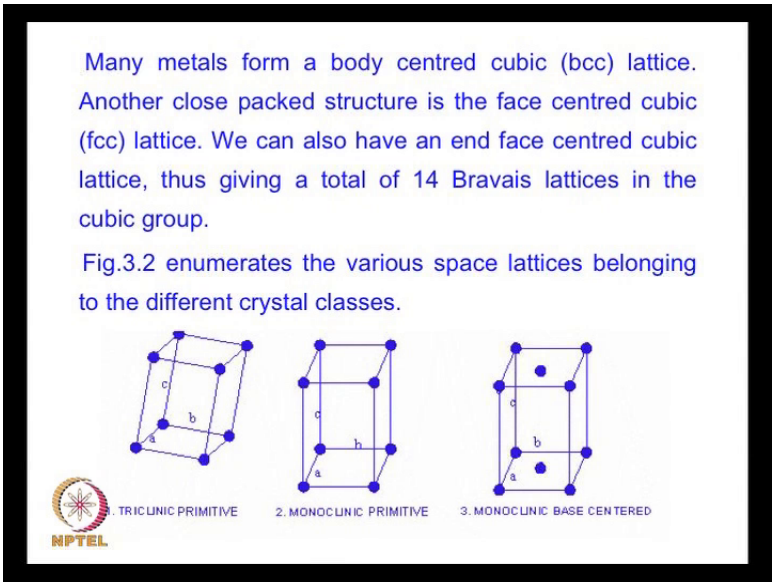

Many metals form body centred cubic lattice others have the face centred cubic lattice or sometimes the end face centred only one pair of end faces gets entered. So, these are the different Bravais lattices and figure shows the various space lattices belonging to the different crystal classes. For example, here we have the triclinic primitive lattice a primitive lattice is one in which there are atoms only at the corners then you have a monoclinic primitive and a monoclinic body centred.

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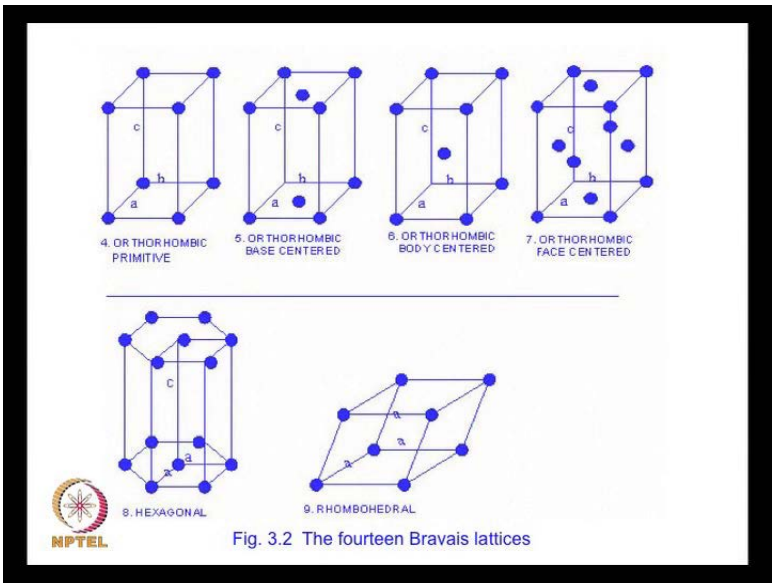

Then the orthorhombic as all possibilities orthorhombic primitive orthorhombic body centred orthorhombic face centred orthorhombic end face centred then you have a hexagonal and a rhombohedral lattice we then come to tetragonal primitive.

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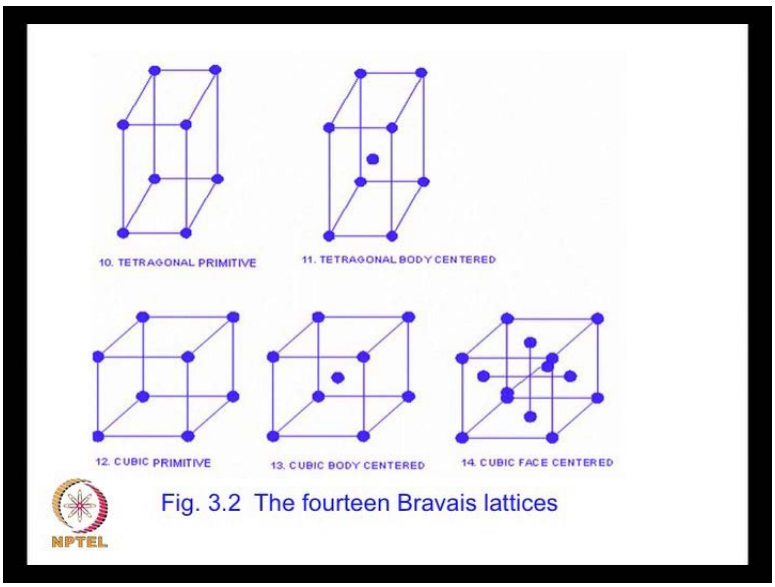

And tetragonal body centred as well as as I already said cubic primitive cubic body centred.

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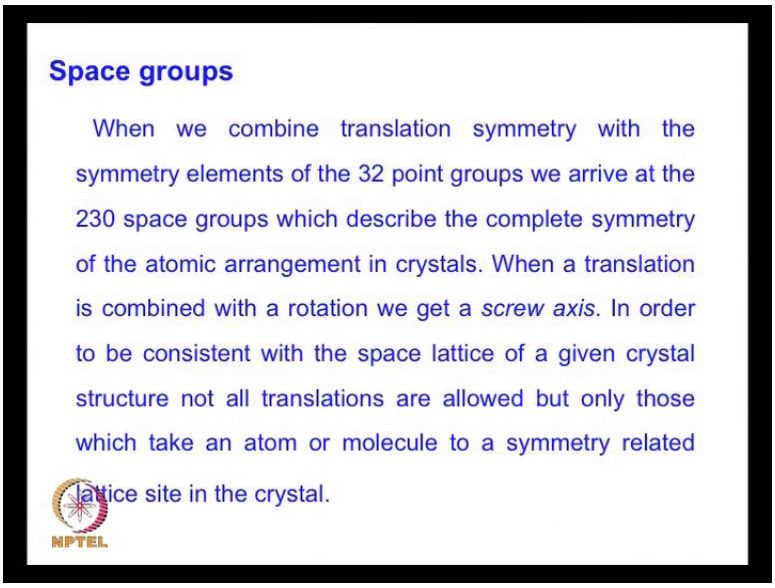

And cubic face centred. So, these are the fourteen lattice types now when we combine translational symmetry with symmetry elements of the 32 point groups we arrive at the two hundred and thirty space groups which describe the complete symmetry of the atomic arrangement in crystals.

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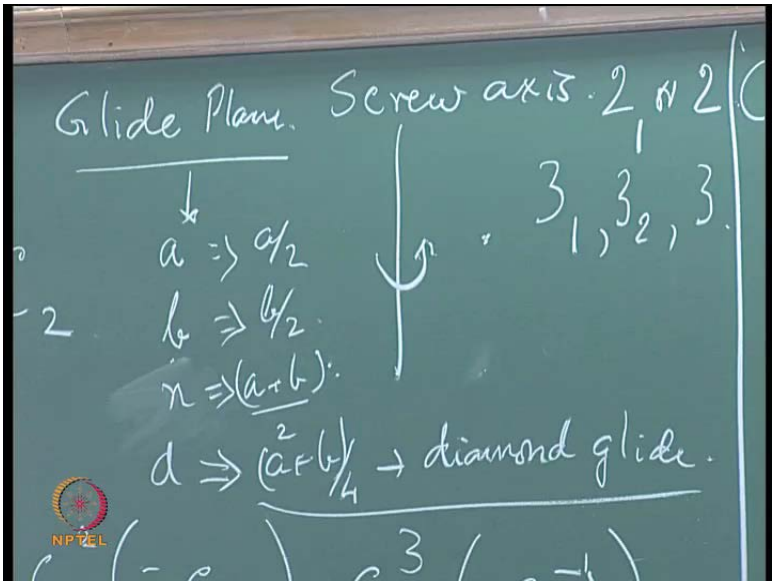

When a translation is combined with a rotation, so you have a rotation axis and then you perform the rotation bring it say here and then take this atom from here to a position by combining a translation the rotation is followed by a translation. This is amounts to what

is known as a screw axis when a translation is combined with a a mirror symmetry then we get what is known as a glide plane a mirror plane combined with translation is a glide plane. So, translation screw axis and glide planes form the elements of space groups

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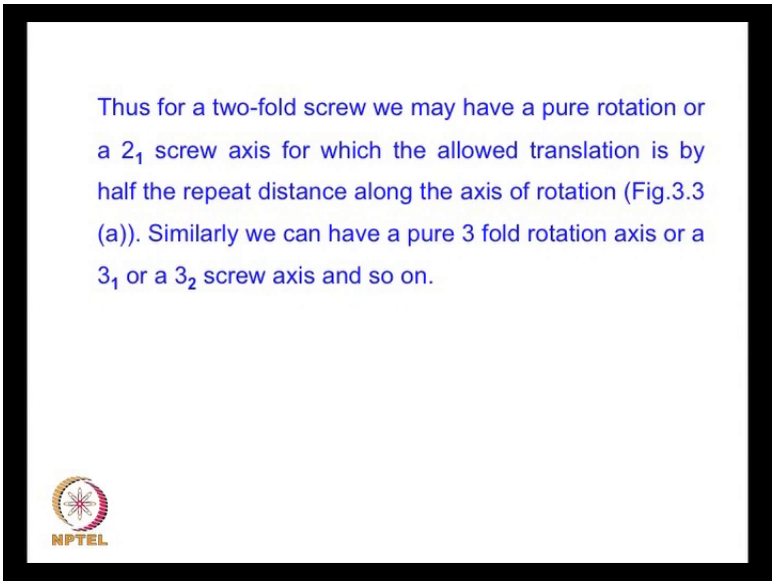

So, for example, for a twofold axis we can have a translation by half the repeat distance along the rotation axis as shown in the next figure.

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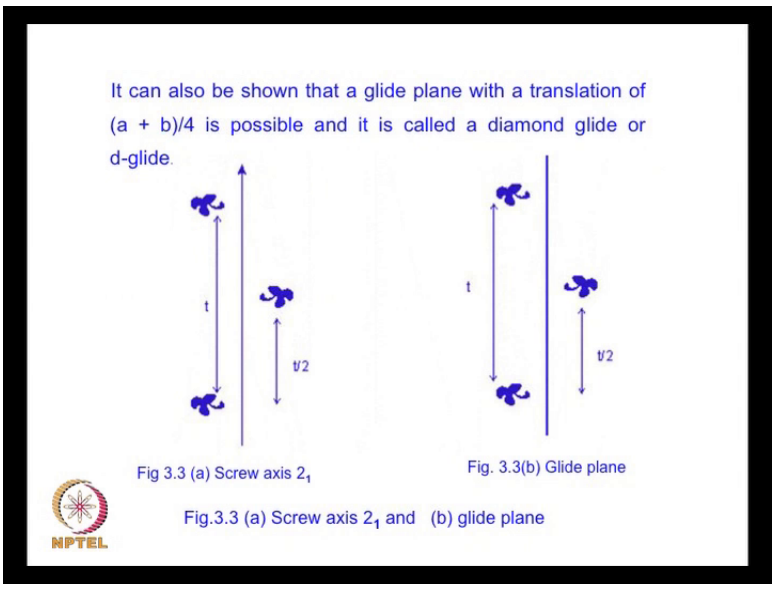

So, you have an atom which is brought into rotation and then translated along the rotation axis, so that is a screw axis similarly shows a glide plane where there is a mirror

symmetry and then a translation. The translation, in this case can be either in one of the sides of the mirror plane or the other side of the mirror plane or sometimes along the diagonal of the mirror plane. So, you have different types of glides and screws. So, in the case of a twofold axis, we can have a two one screw or a spur rotation axis two fold axis. Whereas, in the case of a threefold axis you can have three one or three two or three three one means a threefold axis of rotation followed by a translation parallel to the three fold axis by one-third lattice periodicity. Whereas, this one gives you a translation parallel to the axis by two thirds of the periodicity this is a pure rotation axis and so on.

So, you can have different screw axis like this and as I already said in the case of the glide planes you can have glide planes either along. For example, if a b plane is the mirror then it can be an a glide with translation component along the a axis or a b glide this is an end glide a diagonal glide with a translation component of a plus b by two. Whereas, this a by two this is b by two the translation component at d is a what is known as a diamond glide which can have a translation component of a plus b by four. So, these are the various possibilities of screw axis and diamond a glide planes.

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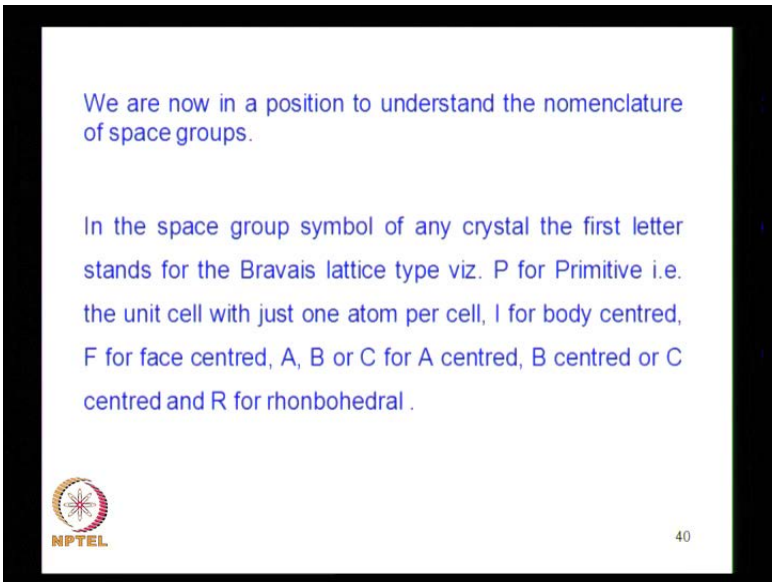

So, now we can talk about space groups and their nomenclature nomenclature the symbol for a given space group.

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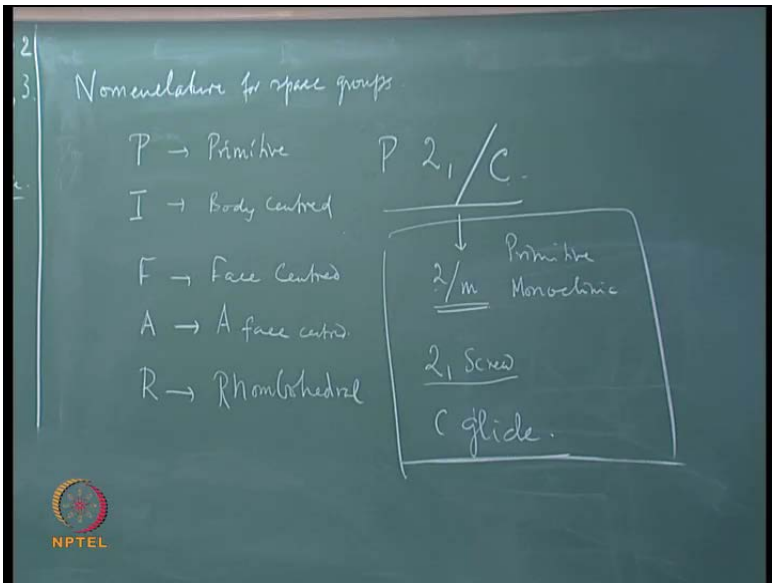

The first letter stands for a type of lattice for example, whether it is a primitive lattice or a body centred lattice face centred lattice or end face centred lattice, for example, A face centred and so on. So, you can have A or b or c face centred lattices and then you can also have rhombohedral lattice in case of a trigonal symmetry. So, the first letter in this space group symbol stands for the type of lattice.

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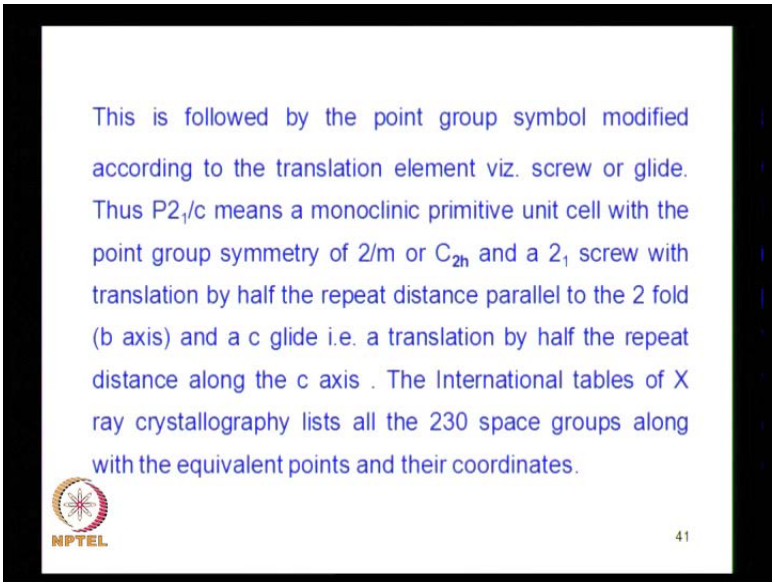

Then it is followed by the point group modified according to the translation element for example, whether it is a screw or a glide. For example, let us take an example and

illustrate this P 2 1 by C, this is the symbol for a a given monoclinic space group this means because the corresponding point group symmetry is just 2 by m, so that is a monoclinic point group. So, this is a monoclinic primitive lattice in which the two fold axis is replaced by a two one screw, a twofold axis followed by a translation component of b by 2 along the unique axis two fold axis. And then you have a glide plane perpendicular to the b axis the unique axis two fold axis and this has a translation component of C by two along the c a axis, so it is a C glide. So, these are the elements which go to make up the. So, it is a primitive monoclinic space group. So, this is how you understand the space group symbol for any given face group.

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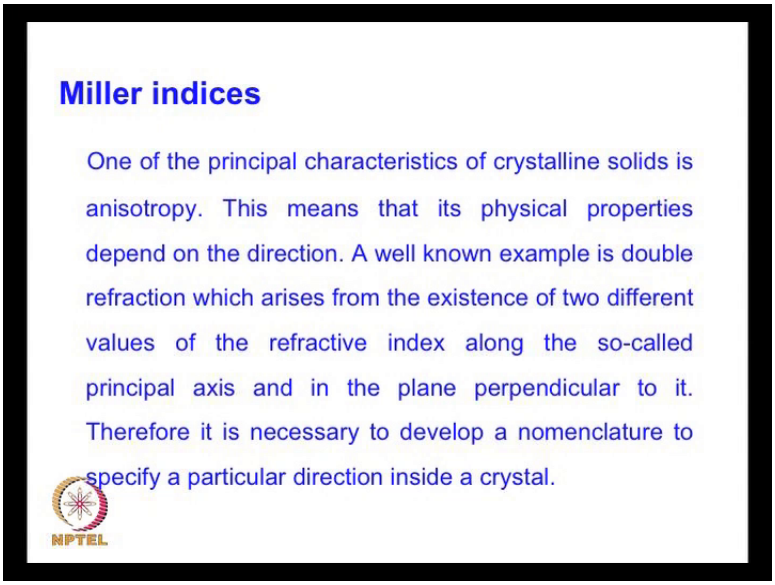

Next we come to the another important characteristic of crystalline solid which is anisotropy.

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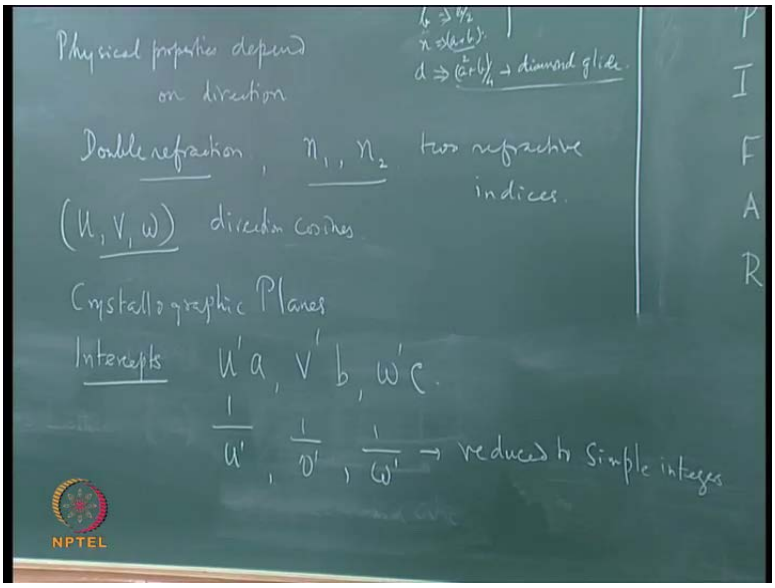

So, we talk about solids are in general anisotropic; isotropic means it is the same behavior in all directions; anisotropy means that the properties of the crystalline solids can be different along different directions. So, the physical properties depend on direction. So, it is very important to have a mechanism standard way of representing different directions in a crystalline solid. For example, we know double refraction, which means that the refractive index has two different values one along one direction and another along a plane in a plane perpendicular to that direction. So, you have n one and n two two refractive indices this is standard example of anisotropy.

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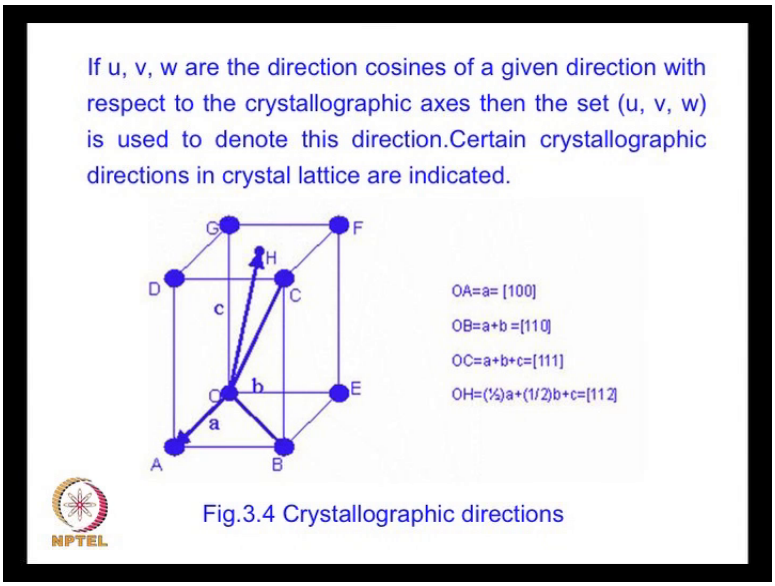

So, it is very important to specify the direction. How do we do it a given direction is always associated in three-dimensional space with u v and w, which are the direction cosines of this direction with respect to the crystallographic axis. So, the set u, v, w which are the direction cosines are used to denote the given direction, for example, in the figure, the different crystallographic directions 1 0 0, 1 1 0, 1 1 1, and 1 1 2 are shown. We also need to describe in a some standard way the different crystallographic planes how do we do that, for example, cleavage planes if you take a solid and try to cut it it gets broken more readily along certain specific directions. So, these are along the cleavage planes, because these planes are more densely packed with atoms.

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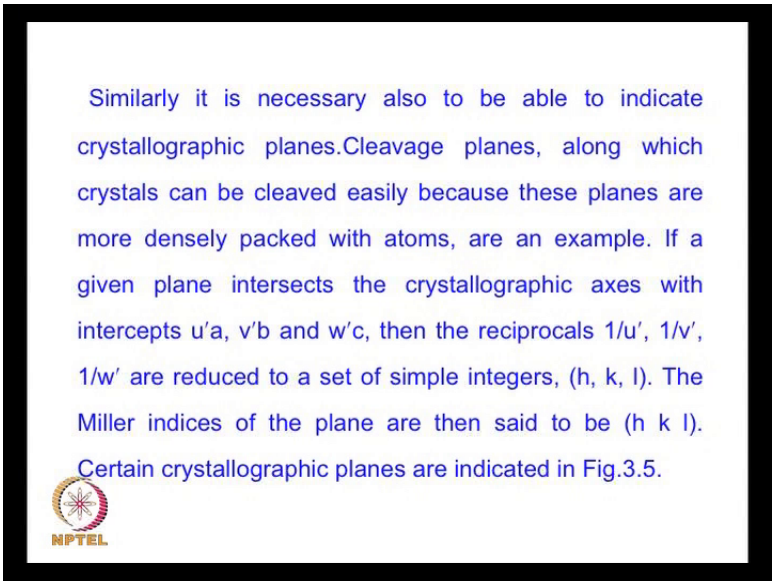

So, how do we talk about the different crystallographic planes we talk in terms of the intercepts that these crystallographic planes make with the crystallographic axis. So, we measure them in units of the lattice parameters. So, suppose we would say let us take u dash u dash a v dash b and w dash c are the intercepts then we take these. So, these are intercepts measured in units of a b and c the principal lattice parameters then we take the reciprocals 1 by u prime, 1 by v prime, 1 by w prime and these are reduced to a simple set of integers. So, the reciprocals or the intercepts measured units lattice parameters and reduced to simple integers that gives the set of number which are put together to refer to a given crystallographic plane and these integers are usually written as h, k and l and these are known as the miller indices. So, usual standard symbol for miller indices is h, k l.

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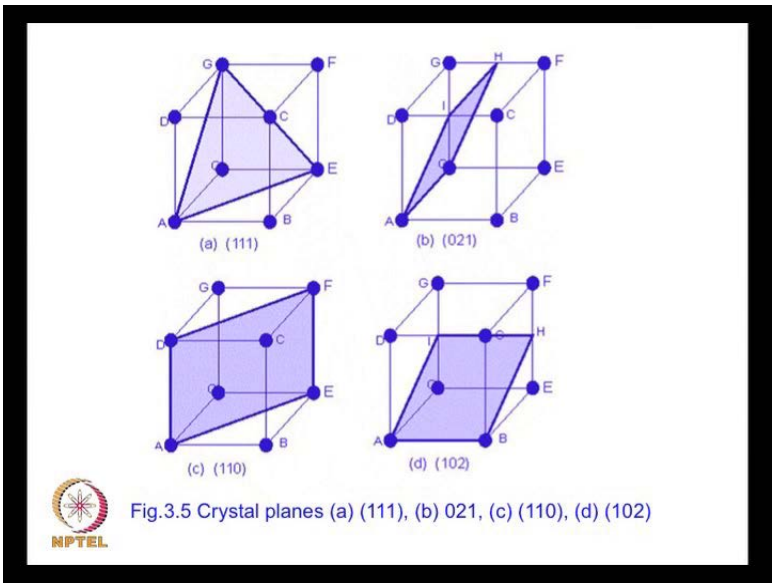

And the figure shows different crystal planes with different miller indices such as 1 1 1, 1 1 0, 0 2 1, and 1 0 2.

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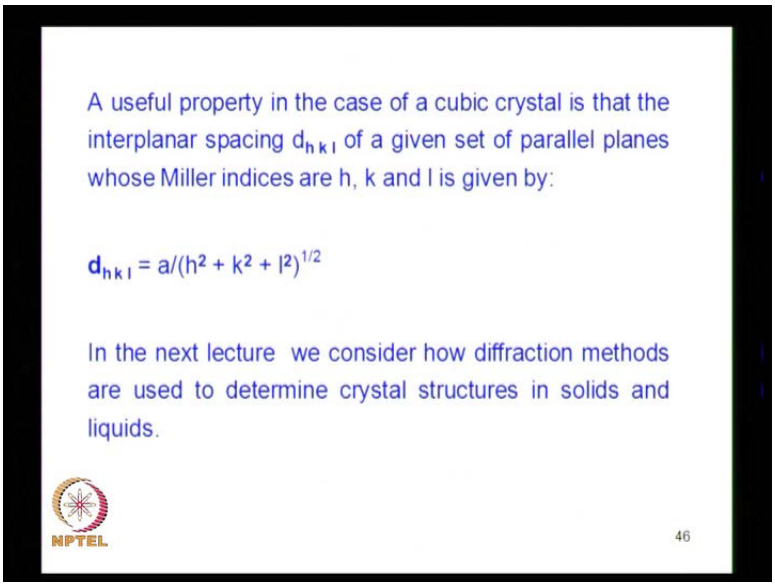

It is one useful property for a cubic crystal is that the inter planer spacing is the lattice parameter divided by h square plus k square plus l square.

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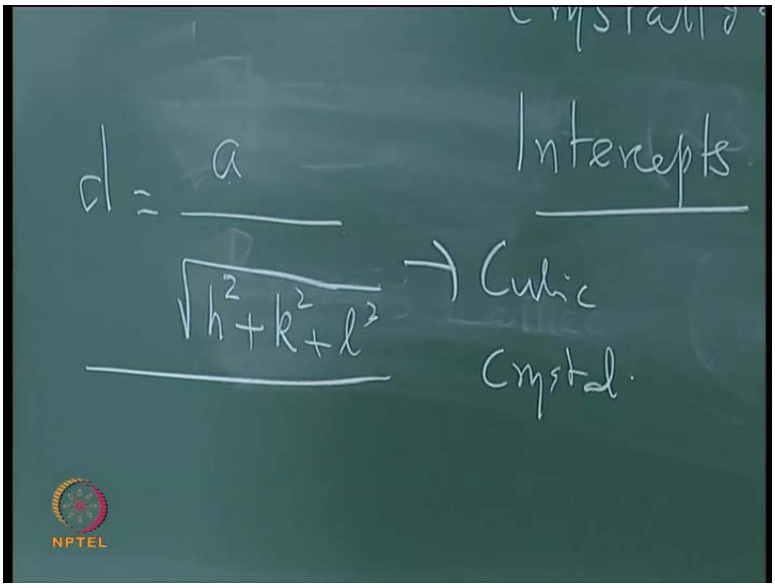

So, this a very useful for a cubic solid is a useful relation to keep in mind. So, we will see in the next class, how do we determine crystal structure experimentally using so called diffraction methods principally by x-rays.