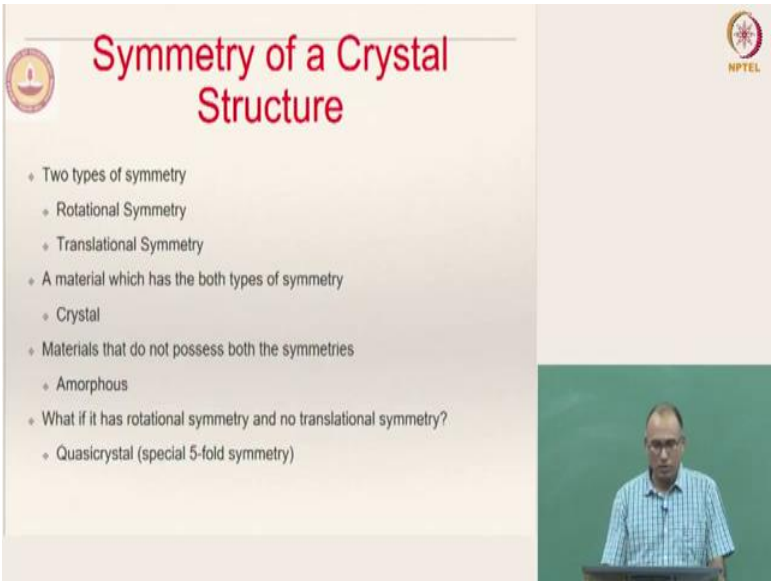
Basics of Materials Engineering
Prof. Ratna Kumar Annabattula
Department of Mechanical Engineering
Indian Institute of Technology, Madras

Lecture - 05
Crystal Structure - 3 (Bravais Lattice, Symmetry in Crystals)

(Refer Slide Time: 00:13)

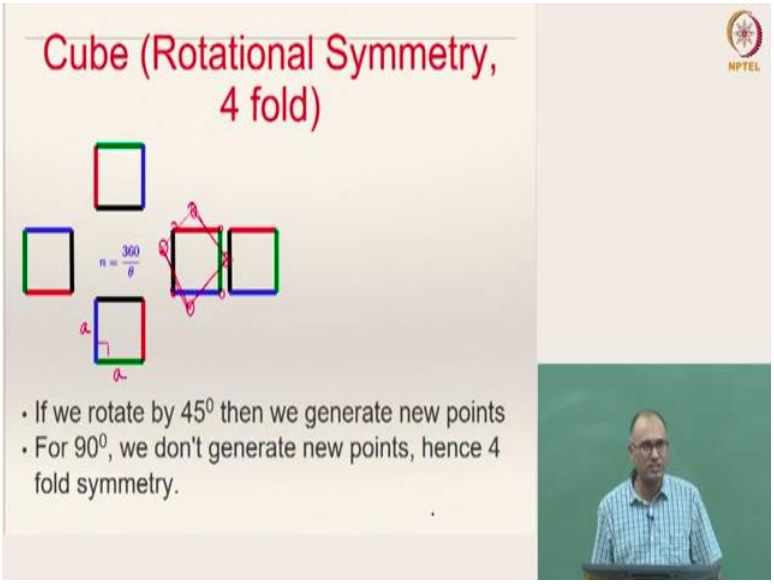


So, now we need to talk about something called symmetry of crystal structure. Whenever you want to call something as a crystal, it can be qualified to be called as a crystal only when it has certain levels of symmetry. There are two types of symmetries, one is called rotational symmetry another one is translational.

So, what is the meaning of that we will see in a moment. You will call something as a crystal only when it possesses both rotational as well as translational symmetry. It should have both the symmetry. If it neither has rotational symmetry nor has translational symmetry, then it is an amorphous material.

But sometimes, you have special class of materials that people have discovered recently, maybe you also had a Nobel Prize for discovering such materials. These materials are called quasicrystals which will have only rotational symmetry, but there is no translational symmetry. That means, there is only partial symmetry. Such materials are called quasicrystals. You can actually Google about quasicrystals and their applications. So, you will understand what is the importance of these materials.

(Refer Slide Time: 01:53)



Now, let us see the meaning of rotational symmetry. I am writing it as a cube, but we are only looking at one view, front view let us say.

That is the front view of a cube. I have identified 4 sides with different colors, so that when we are rotating, we will see that it is actually changing, otherwise it is difficult for us identify.

Now if you rotate this guy by 90 degrees either clockwise or counterclockwise, here we are rotating by counterclockwise direction. I am not showing exactly on the same square, but imagine that this thing is rotated about the out of plane axis, then what happens? This is what you will get. I am showing it separately that is all. I am not actually translating it in order to show the rotational symmetry.

Then what happened to the lattice points? Did the lattice points change their position? So, this is one lattice point, 2, 3, 4, right? When I have rotated this guy by 90 degrees, did the lattice point change the position?

You will have the same lattice point, lattice point positions have not changed.

Now, again another 90 degrees, another 90 degree. So, you will put another 90, that means, you can actually rotate it by 90 degrees and still maintain the same lattice structure. The points will not change whether you take this square or rotated square, it will be generating the same set of lattices. That is what is called rotational symmetry.

A square has 4-fold rotational symmetry. Why it is called 4-fold? Total angle is 360 degrees and when you rotate it by 90 degrees, you are not changing the lattice points. But if you rotate the same thing by any other degree let us say 45 degree, what happens? If you rotate this guy by 45 degree, then you will have something like that.

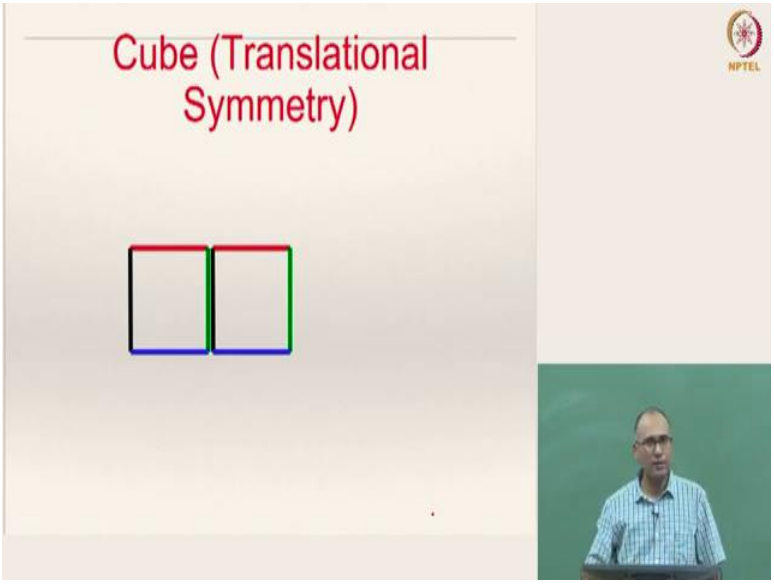
Then your lattice points originally were these. Now, the lattice points have changed. That means, when you are rotating you are actually going out of the lattice point. Then it does not have the rotational symmetry.

So, it will bring back to the same position, right? That is why a cube can have 4-fold symmetry. This is 4-fold symmetry about this axis. If it is a cube how many such 4-fold symmetries can exist? You can rotate about this axis, this axis, as well as -- this one is done, this one is done, and you can also rotate about this.

About three coordinate axis you can rotate. And hence, a cube has three 4-fold symmetries. It also has 2-fold symmetry what do you mean by that? When you rotate it by 180 degrees, it will again give you the lattice position. That means, it has 4-fold symmetry, also 2-fold symmetry, and 1-fold, right? But when you are talking about the symmetry level, you usually look at the highest level of the symmetry that is possible and then that is represented as the symmetry level of the cell.

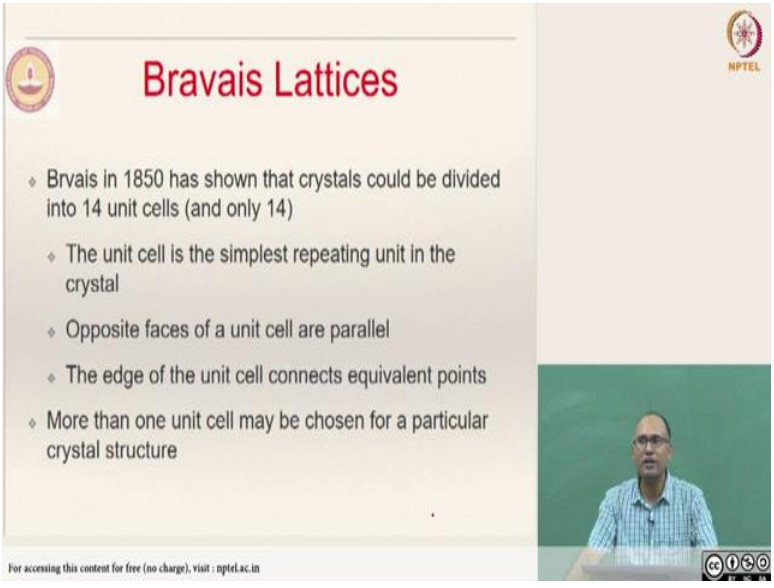
So, that is why whenever you are talking about symmetry level of cube, you only say that it has three 4-fold symmetry. You really do not talk about 2-fold symmetry because 4-fold symmetry is higher level of symmetry compared to 2-fold symmetry. That is about rotational symmetry. What is translational symmetry? For instance, if you take this cube, this is one lattice parameter, this is another lattice parameter, this is another lattice parameter. A cube has α to be 90 degrees, and all the sides (equal to a) are same. These are called lattice parameters, the parameters that describe your unit cell.

(Refer Slide Time: 06:19)



So, what is translational symmetry? If you take this cube, translate it by integer multiples of your lattice parameters, i.e., if you translate it by a distance equal to *a*, what happens? You will reach again a new set of lattice points, because of the translation. And it has both ways, both in x direction and y direction.

(Refer Slide Time: 06:47)



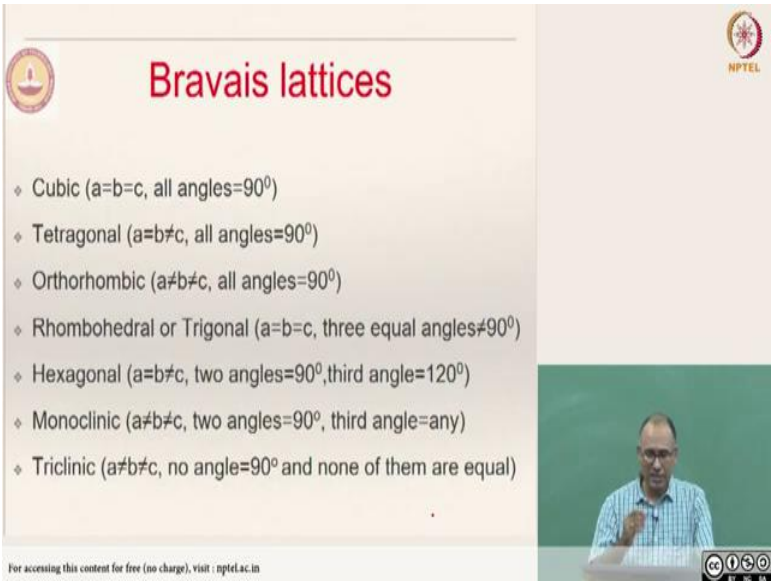
Similarly, for any unit cell you can define the levels of symmetry that is possible. And usually, the geometries of the unit cells are defined based on the symmetry level.

And then, we look at another important concept called Bravais lattices. So, Bravais in 1800's, has shown that crystals would be divided primarily into 14 different kinds of unit cells, and you will only have 14 types of lattices. You will not have anything more. All crystal structures should be falling under one of these 14 categories, i.e., their unit cell geometries should be falling under one of these 14 categories.

And what are the requirements of the unit cell? Opposite faces should be parallel, that is why we said that the parallelogram is the qualified unit cell, right? And the edges of the unit cell should connect equivalent points. What do you mean by equivalent point? If you are on a lattice and if you are sitting on a lattice point in the Cambridge brick wall example, it really does not matter on which brick point you are sitting. All of them are same because all of them have same kind of neighbors, that is what you mean by equivalent point.

So, the edge of the unit cell is actually connecting the equivalent points, opposite faces in 3D and opposite edges in 2D should be parallel. And we have discussed that more than one unit cell maybe chosen for a particular crystal structure.

(Refer Slide Time: 08:51)

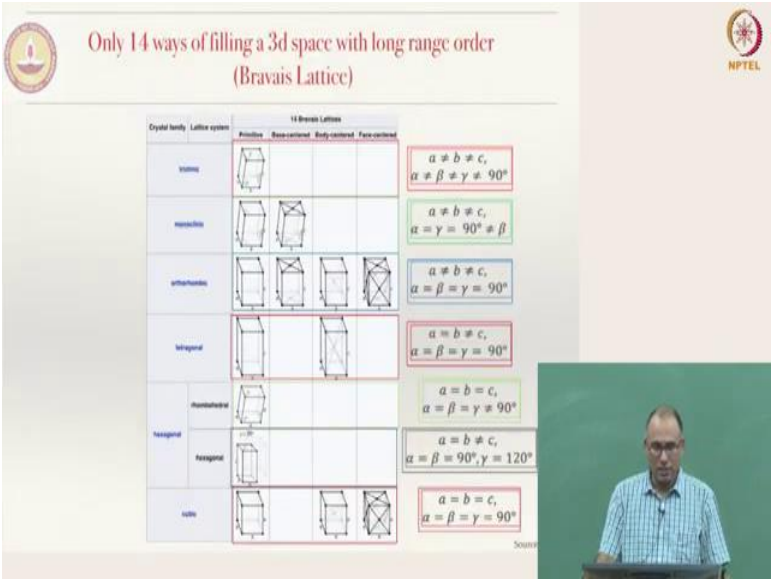


And these are basic seven geometries of the unit cell that are possible. Cubic means a equal to b equal to c, all angles α, β, and γ are equal to 90 degrees. In Tetragonal, two sides are same (a=b). If you take a cube and pull it, then it becomes tetragonal. That can also be a possible unit cell. If you pull in this direction and pull in this direction such that

none of the sides are equal, you will get orthorhombic. And in rhombohedral or trigonal, all sides are equal, but the angles are not equal to 90 degrees. So, they can be anything else, and so on.

So, these are the 7 fundamental unit cell geometries using that you can actually construct different Bravais lattices.

(Refer Slide Time: 09:46)

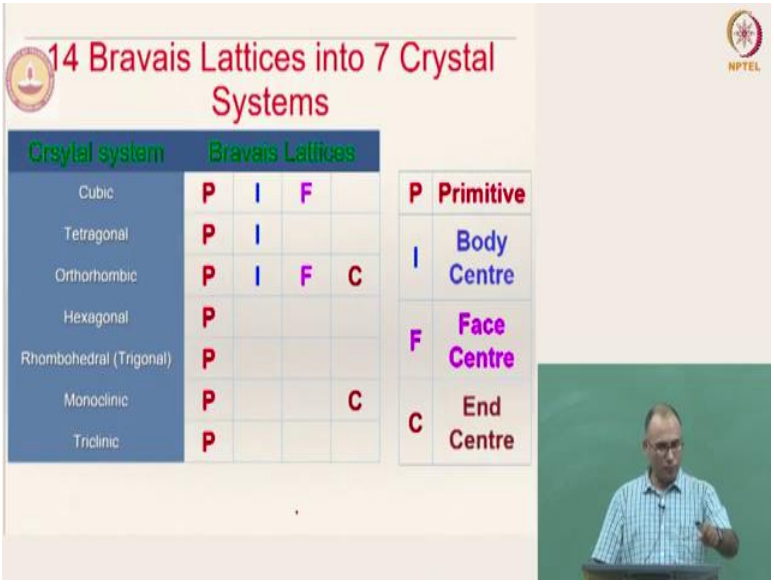


These are the 14 ways of filling a 3D space, these are the 14 possible Bravais lattices. So, you have cubic primitive unit cell and there is something called body-centered cube and face-centered cube. We are familiar with these two things, right? Body-centered cubic and face-centered cubic structure, we have looked at in your previous class.

Bravais has shown that you can only have primitive triclinic unit cell, you cannot have non-primitive. So, all these things are non-primitive, right? This is non-primitive, this is non-primitive, only the first column is primitive in all the cases.

He has shown that for triclinic you can only have primitive unit cell. You cannot have base-centered, body-centered, face-centered, and so on. By doing so, it is shown that there are only 14 possibilities. These blank positions are not possible. You cannot have these things. Why? We will look into it quickly.

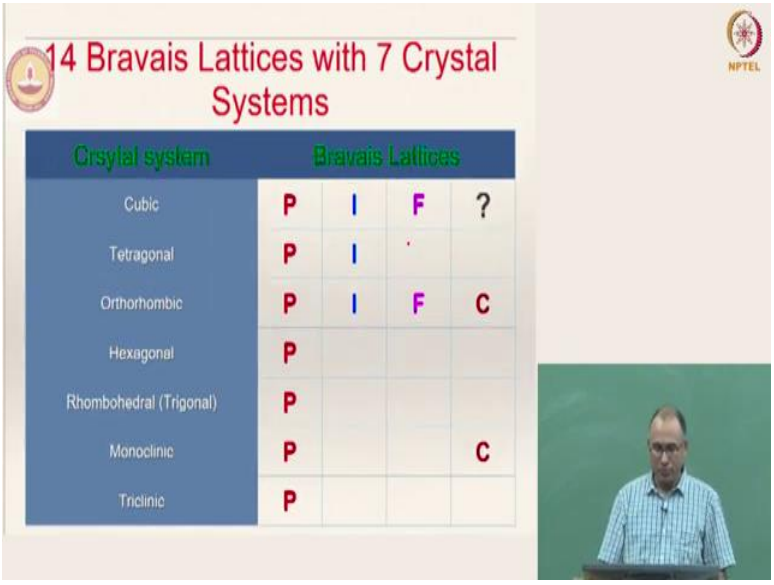
(Refer Slide Time: 11:06)



So, I just have put the same pictorial representation in a textual representation. So, when I say *P*, it means primitive, when I say *I*, that is body-centered, *F* means face-centered, *C* means end-centered or base-centered. So, a cubic crystal will have primitive body-centered, face-centered, but no end-centered. Orthorhombic will have all the 4. So, you will have possibility of all the four unit cell geometries.

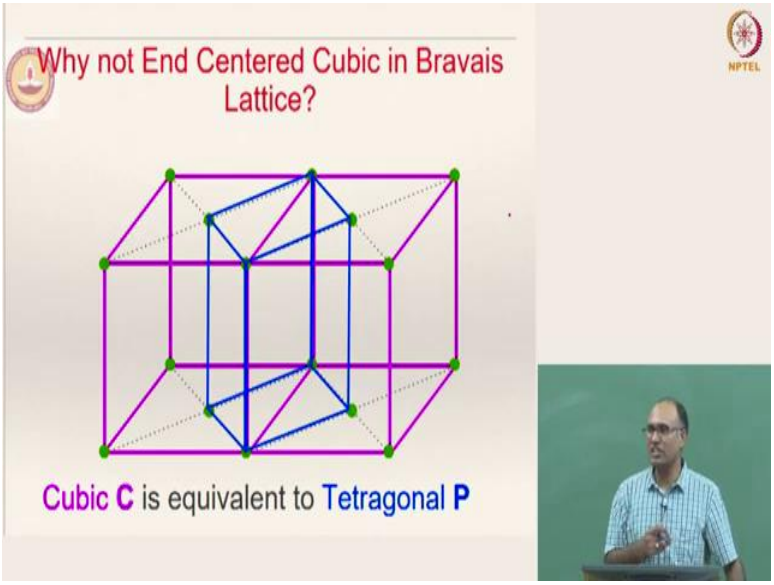
So, together they are totally 14 you can only have these 14.

(Refer Slide Time: 11:47)



Now, through an example we will see why you will not have end-centered cubic unit cell, right? This is primitive body-centered, face-centered, and this is end-centered. That means, only on bases, right? Why will you not have that?

(Refer Slide Time: 12:06)



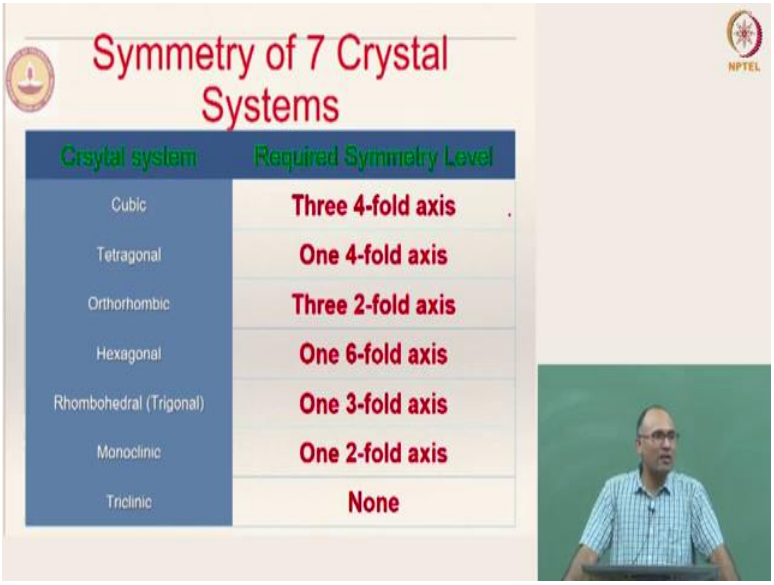
So, this is how an end-centered cubic unit cell looks like, right? When we have this unit cell, when you are constructing your lattice or crystal, what will you do? You translate it in all three directions.

So, let me do it in one direction first. So, you will extend in this way, this way, this way, this way; you will have an infinite system, right? That is precisely what we mean by long range order. Anywhere you see it will have the same structure. Now, in that, you can actually identify another unit cell, right? You could actually fill the entire space using this primitive unit cell compared to these two body end-centered unit cells. Is that clear? That means, an end-centered cubic unit cell is equivalent to? Primitive tetragonal. It is a primitive tetragonal unit cell.

Both are the same. That is why it does not exist. Because both are same, it does not make sense to call that as an end-centered cubic because that actually qualifies as primitive tetragonal. And similarly, you can actually prove for all other combinations where in you do not have an existence of a particular unit cell geometry.

So, in that way you will see that there are only 14 possibilities. So, these 14 lattices or unit cell are called Bravais lattices. So, lattices constructed out of these unit cell are called Bravais lattice.

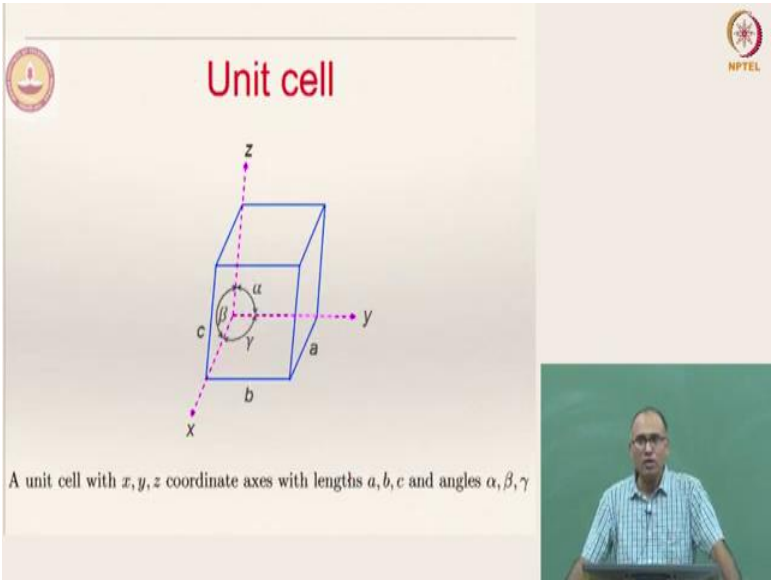
(Refer Slide Time: 13:54)



So, what is the symmetry level of these 7 crystal systems? We have looked at cube and we have shown that cube has three 4-fold symmetry, right? Three 4-fold axis. About each axis you have a 4-fold symmetry. So, you have three axes. So, three 4-fold symmetries. Tetragonal will have only one possibility because along other directions, the dimensions are not the same right, you are pulling in one direction. So, it will have only one 4-fold axis. Orthorhombic will have three 2-fold axis. It will not have a 4-fold symmetry because a is not equal to b is not equal to c, right? That is what is orthorhombic, is not it? a is not equal to b is not equal to c.

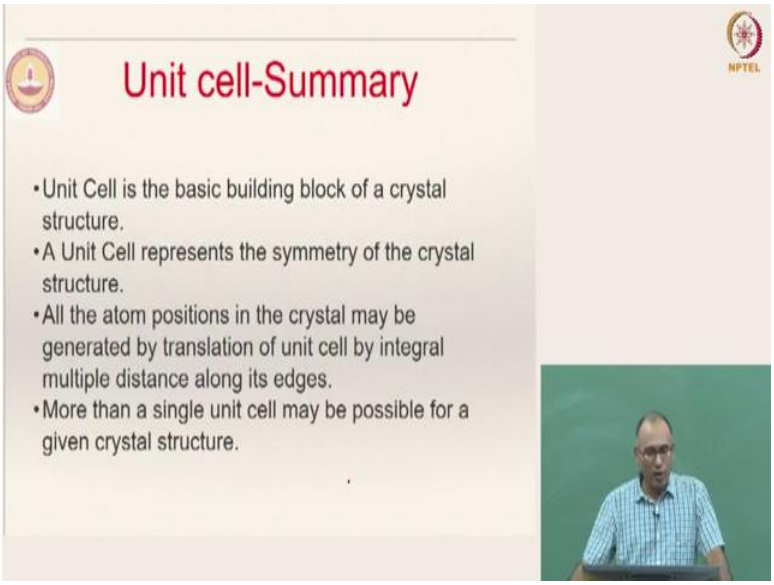
So, you will not able to have a 4-fold symmetry. Like that you can actually define symmetries. And triclinic structure is the one where a is not equal to b is not equal to c, and α, β, and γ are also not equal, right? That is your triclinic structure. So, that means, it does not have any symmetry.

(Refer Slide Time: 15:07)



So, these are your unit cell parameters: a, b, c alpha, beta and gamma, right? So, you define these parameters to describe whatever unit cell that you are interested in.

(Refer Slide Time: 15:21)



The summary of unit cells is a basic building block of a symmetry structure, it represents the symmetry level of the crystal structure that we are looking at. All the atom positions in the crystal may be generated by translation of unit cell by integral multiple distances along its edges called lattice vectors. More than a single unit cell may be possible for a given crystal structure. That is what we have learnt about unit cells.