Structural Biology
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Lecture – 17
X-Ray Crystallography: Journey to 3D land

Hi everyone, welcome to the course of structural biology again we are continuing with structural biology techniques and I am continuing also with X-Ray crystallography. Today is very interesting, we are going to talk about 3 dimensions their unit cells about symmetry about the lattice and all and I always feel that this part is very difficult to understand. So, I have taken a kind of different way to explain those things starting from 1 dimension to further.

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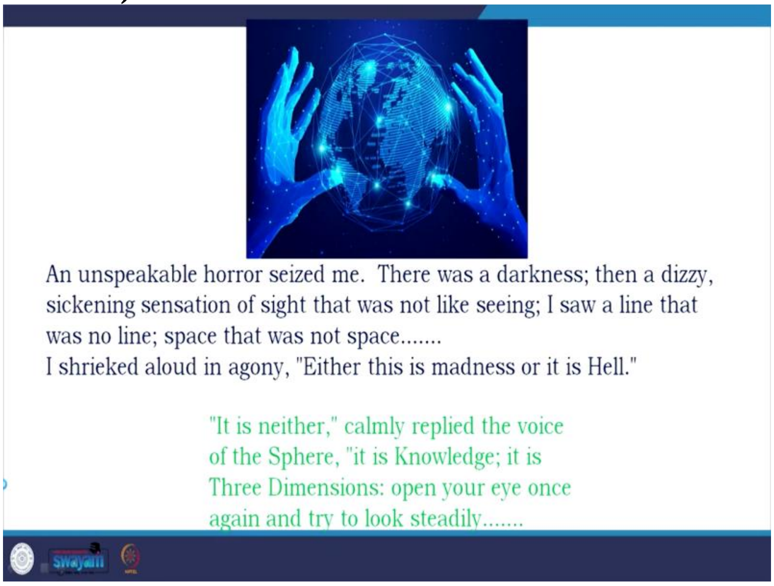

To start with I will start with a small drama about 3D and unspeakable horror seized me, there was a darkness then a dizzy sickening sensation of sight that was not like seeing. I saw a line that was no line, I saw a space that was not a space I shrieked with agony, either this is madness, or is this is the Hell? It is neither calmly replied the voice of the spear. It is knowledge, it is 3 dimensions open your eye once again and try to look steadily.

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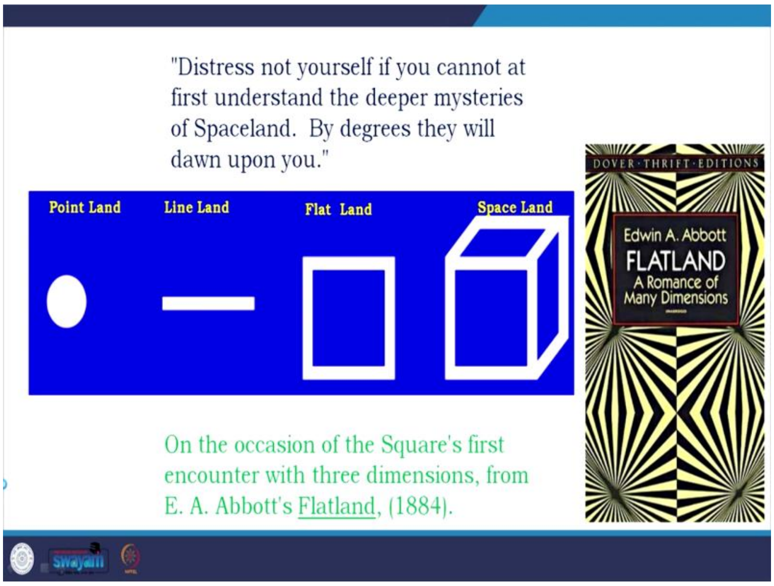

So again, this is taken from a novel called flatland. And they also told distress not yourself. If you cannot at first understand the deeper mysteries of space land, by degrees, they will dawn upon you. As I told this is the thing which came when Square's first encounter with 3 dimensions and in the EA Abbott's flatland the novel. So, you understand the space land as the tool if you have to start with point land a point then you have to go with from 0 dimension of the point land to the 1 dimension which is a line land.

From 1 dimension line land to the 2-dimensional flatland and from the 2-dimensional flatland to 3-dimensional space land that is what they told in the novel, a romance of many dimensions. I am not talking about romance at all. But today, we will talk about many dimensions which reflect the study of protein crystallography. We will start with 1D lattice.

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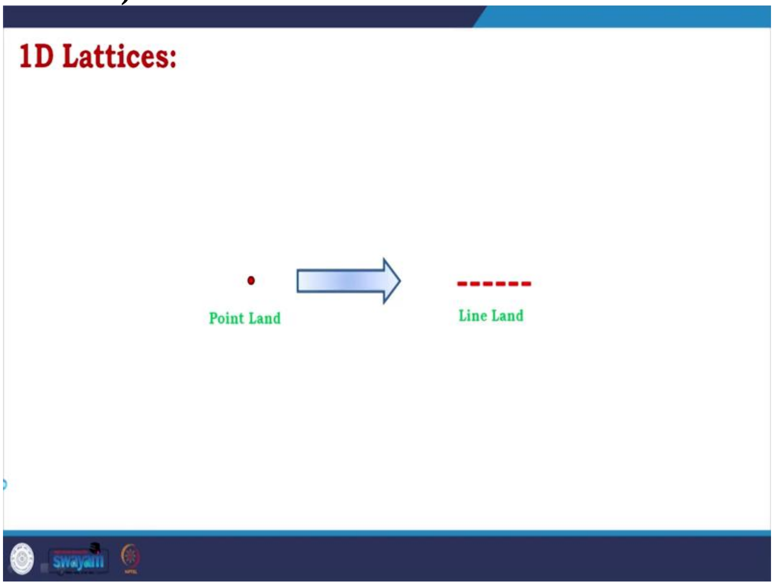

1D lattice is a journey from point land to the line land. So, let us imagine because in reality there is not a 1-dimensional crystal.

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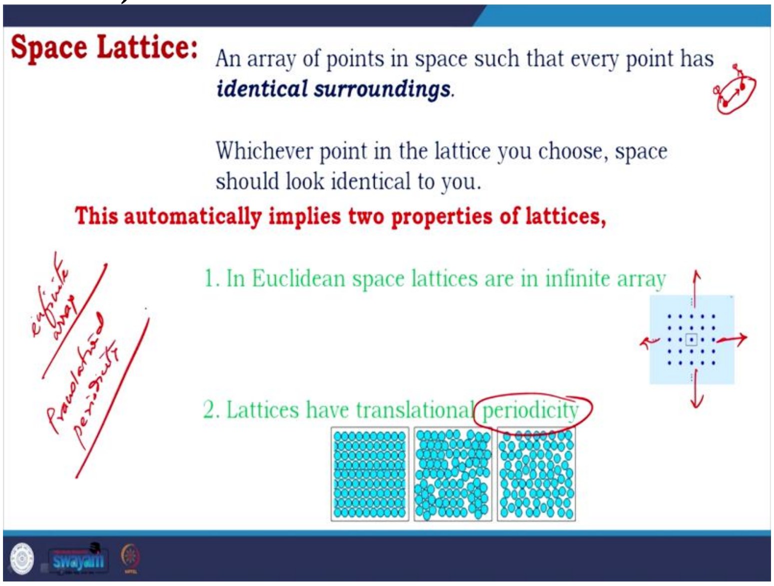

So, we will talk about space lattice first. Space lattices are an array of points in space, such that every point has identical surroundings. So that is what you know, the formation of crystals, if you have a point, you get the other point in an equal distance or identical position. Whichever point in the lattice you choose, space should look identical to you. So, you are sitting here or you are sitting here you should see everything the space the 3 dimension and identical and if that happened, this will automatically implies to 2 properties of lattices.

One is Euclidean space lattices. They are in infinite array, if you see in this direction, in this direction, in this direction, in this direction. It is going in an infinite goal. Lattices have translational periodicity. Here the word periodicity is important. If you look at this is a perfect lattice and you see the periodicity here, translational periodicity. This is a poly crystal, you do not see it as organized like this ideal crystal, but you see local periodicity. And this is amorphous, where you do not see any translational periodicity. So, infinite array and translational periodicity are the 2 things, which connect the space lattice.

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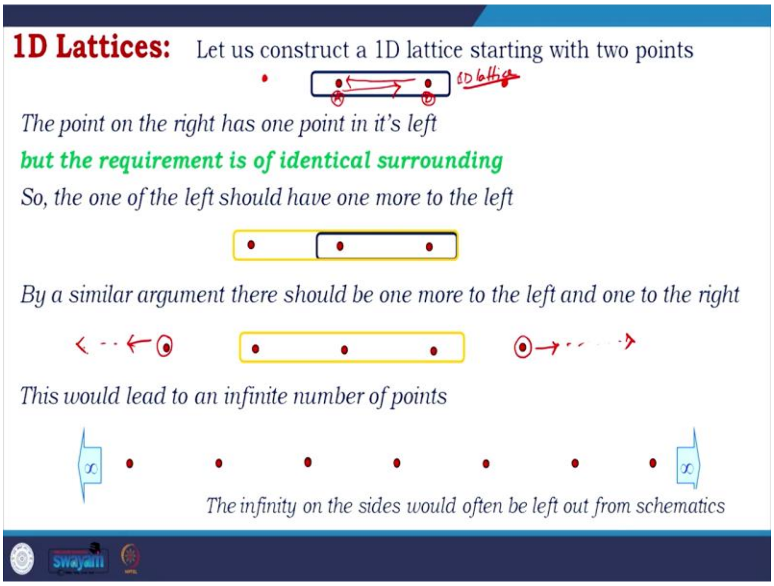

As I told you, let us start from 1D lattices, and as it does not exist, let us construct a 1D lattice starting with 2 points. So, this is one point, and this is another point that develops the 1D lattice. A point on the right has a point on its left. So, one of the left should have one more to the left, and these have one more to the left at the same argument. There should be more to the left and more to the right.

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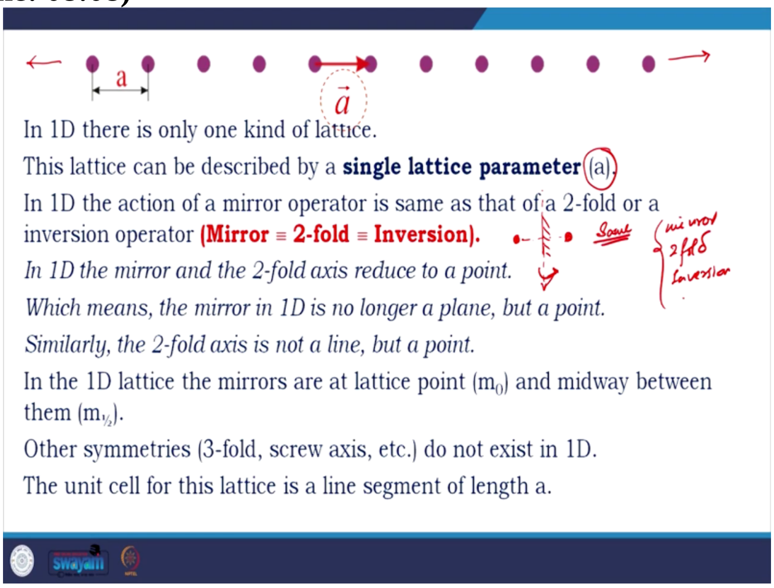

So, this is again the 1D crystal with a distance between the 2 points a. So, in 1D, there is only one kind of lattice, and this lattice can be described by a single lattice parameter, which is a (the distance). In 1D, the action of a mirror operator is the same as that of a 2-fold or an inversion operator. So, here you do not have a difference. If you have a point, you have a mirror, you get 1 point, but that relation is the same with inversion and rotational axis.

So, here the mirror symmetry, 2-fold axis, and inversion play the same result. In 1D the mirror and the 2-fold axis are reduced to a point which means the mirror in 1D is no longer a plane but a point. Similarly, a 2-fold axis is not a line but a point. In the 1D lattice, the mirrors are at that lattice point m_0, and midway between them is $m_{1/2}$. Other symmetries like 3-fold, screw axis does not exist in the 1D lattice. The unit cell for this lattice is a line segment of length a.

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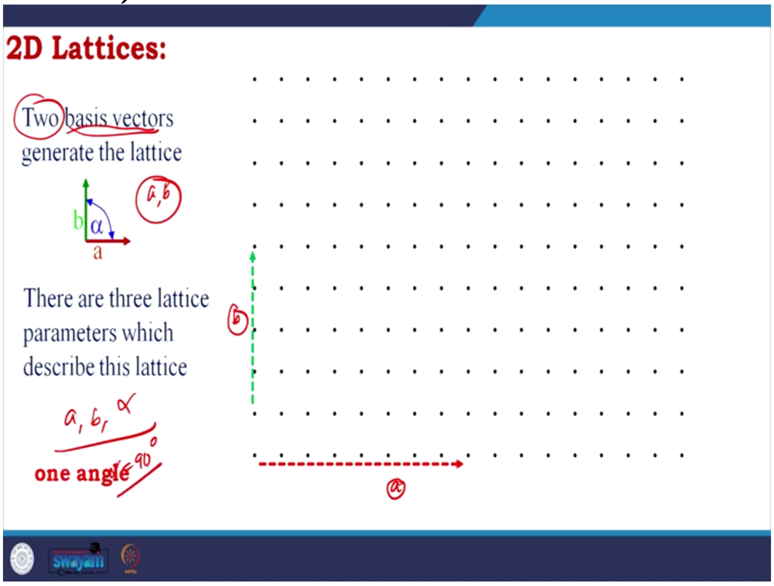

Coming to the next level 2D lattice is a journey from the line land to the flat land. So, a line to a square box represents a 2D lattice with x and y-axis, the two basis vectors generate the lattice, there are a and b, and the angle is alpha. So, there are two basis vectors, a and b. Three lattice parameters described the lattice: a, b and alpha. The angle here for this lattice alpha = 90 degrees.

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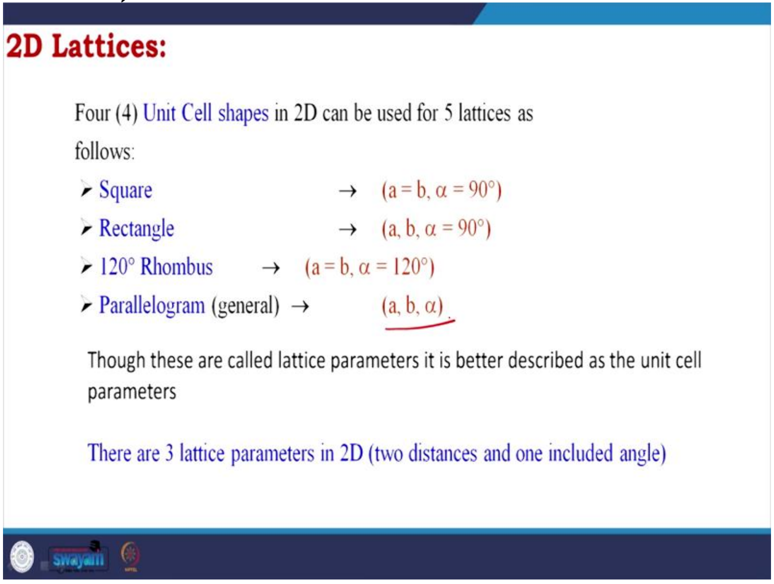

So, in 2D lattice, there are 4 unit cell shapes in 2D. They could be used for five lattices. They have a square, where a = b and angle equal to 90-degree, rectangle, which is a, b and alpha = 90 degree, 120-degree rhombus where a = b and alpha = 120 degrees, and parallelogram where they have a, b, and alpha of any. Though they are called lattice parameters, it is better described as unit cell parameter because they define the unit cell more. There are 3 lattice parameters in 2D, 2 distances and 1 angle, which we showed earlier with a, b and alpha.

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2D Lattices:

Lattice	Symmetry	Shape of UC	Lattice Parameters
1. Square	4mm	1. Square	$(a = b, \alpha = 90°)$
2. Rectangle ✓	2mm	2. Rectangle	$(a \neq b, \alpha = 90°)$
3. Centred Rectangle ✓	2mm	2. Rectangle	$(a \neq b, \alpha = 90°)$
4. 120° Rhombus	6mm	3. 120° Rhombus	$(a = b, \alpha = 120°)$
5. Parallelogram	2	4. Parallelogram	$(a \neq b, \alpha$ general value)

So, suppose you look at the lattices. In that case, There are 5 types of lattice; square, rectangle centered rectangle 120 degree rhombus, and parallelogram. The shape of the unit cell square, Rectangle, 120 degree rhombus, and parallelogram. So, there are 4 lattices with 5 unit cells.

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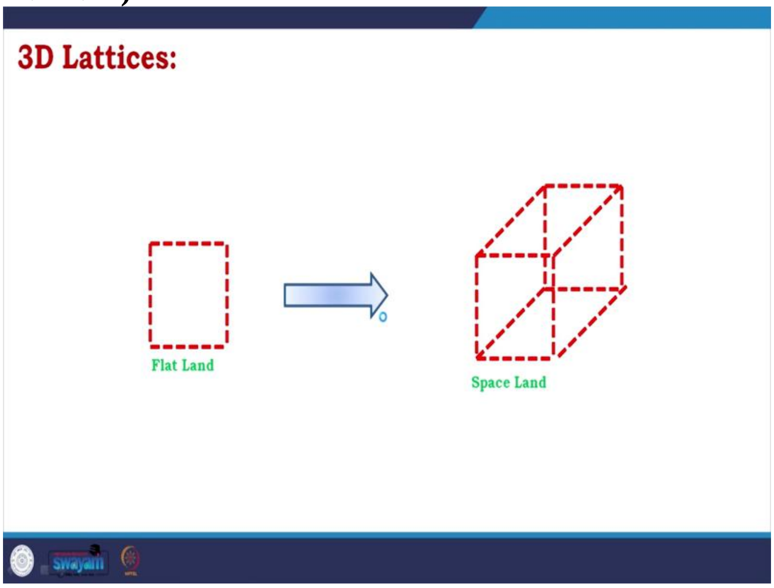

Now, we are shifting to the 3D lattices we want to deal with because 3D lattices mostly define the protein crystals or any crystals we are talking about. So, it is a journey from flatland to space land, which is our dream journey.

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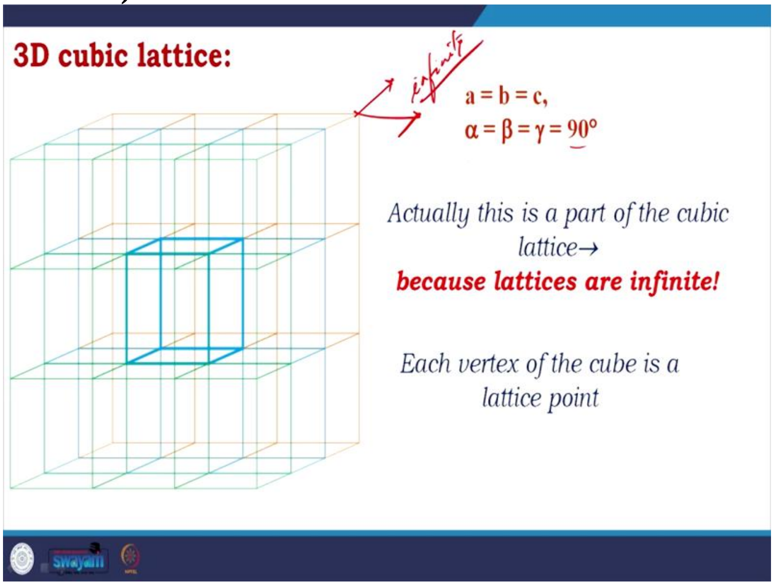

So, 3D lattices could be generated with three basis vectors a, b, and c, showing three axes x, y, and z. 6 lattice parameters describe the unit cell of a general 3D lattice. There are distances a, b, c and three angles alpha, beta, gamma. This is a general 3D lattice. If you see here, a, b and c are not equal, whereas alpha, beta, and gamma are not equal.

The lattice parameters in special cases, some of these numbers may be equal to each other like a could be equal to b, b could be equal to c, or a could be equal to b equal to c or equal to a special number that is equal to b equal to c equal to 90 degrees or something like that. So, we may not require 6 independent numbers to describe a lattice in those cases.

We have a, b, c, three distances, the basis vector, alpha, beta, and gamma angles. So, we have six, but if some special things come like a = b = c, we would have a = b = c represented by s and three angles if alpha = beta = gamma, then we have another angle theta. Such an example is 3D cubic lattice where a = b = c and alpha = beta = gamma = 90 degree. This is a part of the cubic lattice because the lattices are infinite. As I told these could go to infinity. Each vertex of the cube is a lattice point.

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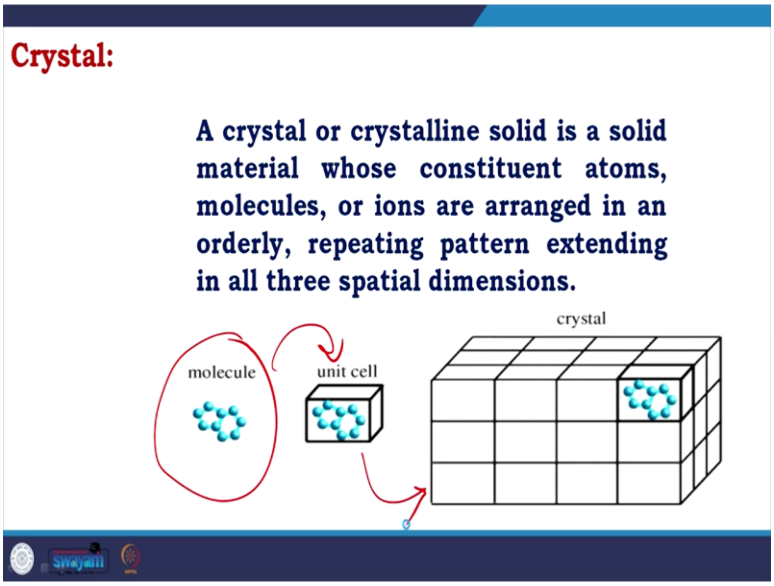

A crystal or crystalline solid is a solid material whose constituent atoms, molecules, or ions are arranged in an orderly repeating pattern extending in all three spatial dimensions. So, we have our molecule, our molecule is going to unit cell, and unit cell is going to crystal.

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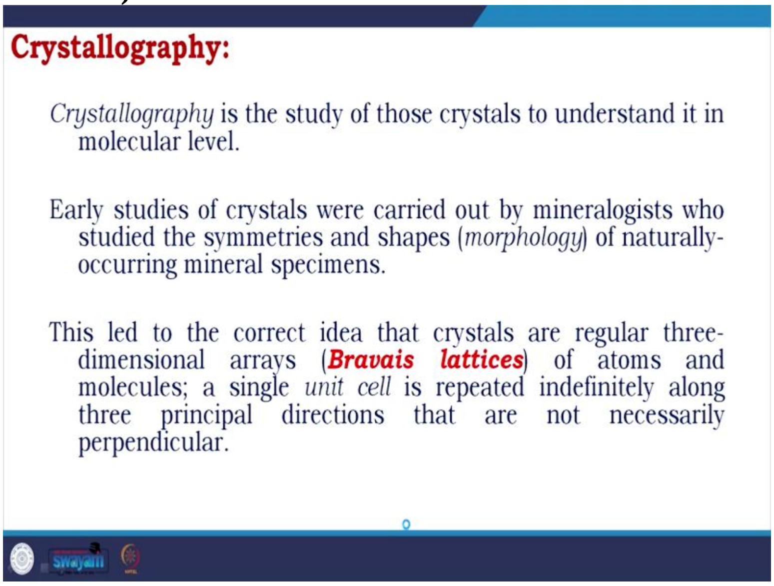

Crystallography studies those crystals to understand them at the molecular level. We want to understand not the crystal here but the molecule inside the crystal because by making crystallography or making a crystal, we just enhance the signal coming from the molecule because the atomic level signal was not possible to find from a single molecule.

A mineralogist carried out early studies of crystal, who studied the symmetries and set up naturally occurring mineral specimens. The starting off or foundation of crystallography is where protein crystallography is indebted. This led to the correct idea that crystals are regular 3-dimensional arrays. These are called Bravais lattices of atoms and molecules; a single unit cell is repeated indefinitely along with three principal directions that are not necessarily perpendicular.

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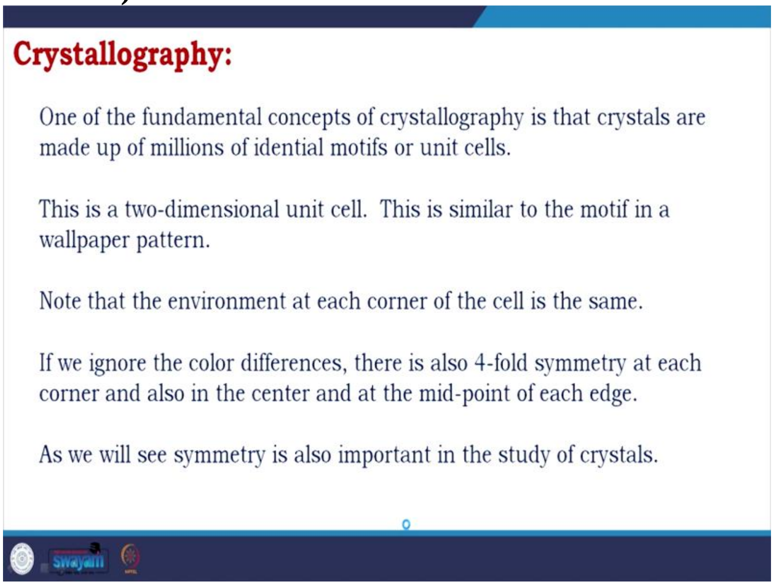

One of the fundamental concepts of crystallography is that crystals are made up of millions of identical motifs or unit cells. For our case, we understand that we do crystallography because we need our proteins to be in millions so that the signal would be very, very enhanced and we could get good signals. This is a 2-dimensional unit cell similar to the motif in a wallpaper pattern.

Note that the environment in each corner of the cell is the same. If we ignore the color differences, there is also 4-fold symmetry at each corner, center, and midpoint of each edge. As we will see, symmetry is also important in studying a crystal where we are coming later.

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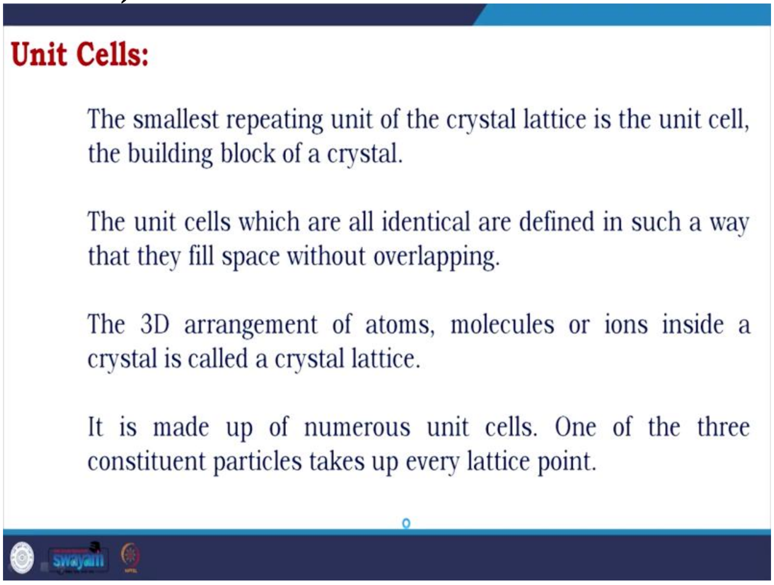

The smallest repeating unit of the crystal lattice is the unit cell, the building blocks of a crystal. The unit cells that are all identical are defined so that they fill space without overlapping. The 3D arrangement of atoms, molecules, or ions inside a crystal is called a crystal lattice. It is made up of numerous unit cells. One of the three constituent particles takes up every lattice point.

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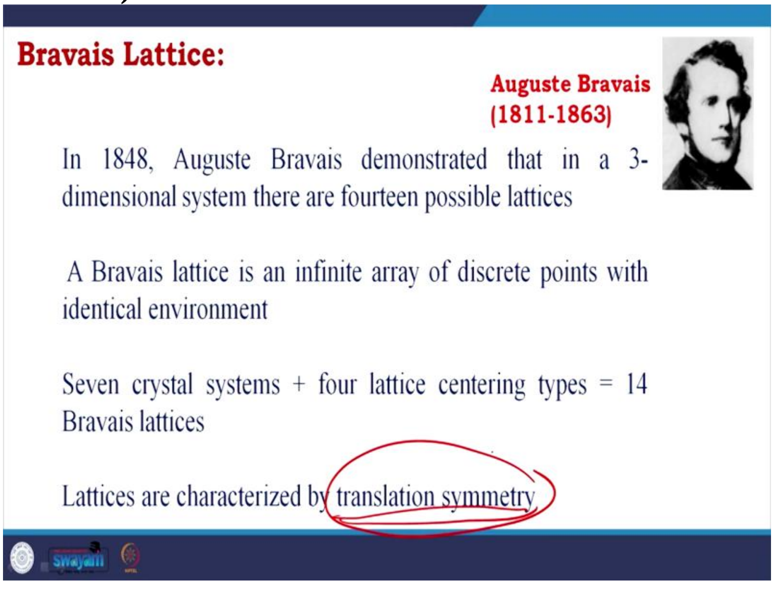

So, coming to Bravais lattice: Auguste Bravais invented the system. Here is the picture of him in 1848. He demonstrated that in a 3-dimensional system, there are 14 possible lattices. Bravais lattices is an infinite array of discrete points with an identical environment. 7 crystal system + 4 lattice centering types equal to 14 Bravais lattices. Lattices are characterized by translational symmetry.

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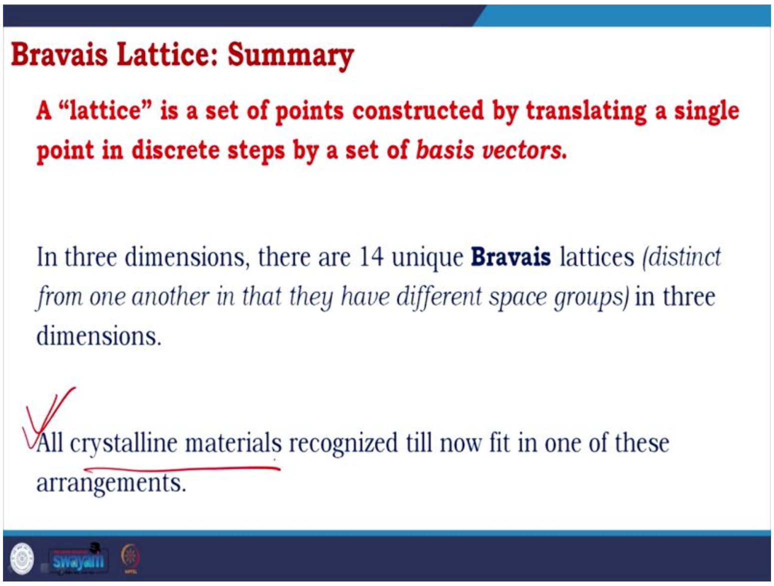

A lattice is a set of points constructed by translating a single point in discrete steps by a set of basis vectors as we talked about when we are talking about 1D, it is the 'A,' when you are talking about 2D it is a, b, and when we are talking about 3D it is a, b, c. They are the basis vectors. In the three dimensions, there are 14 unique Bravais lattices (distinct from one another in that they have different space groups) in 3 dimensions. All crystalline materials recognized still fit in one of these arrangements.

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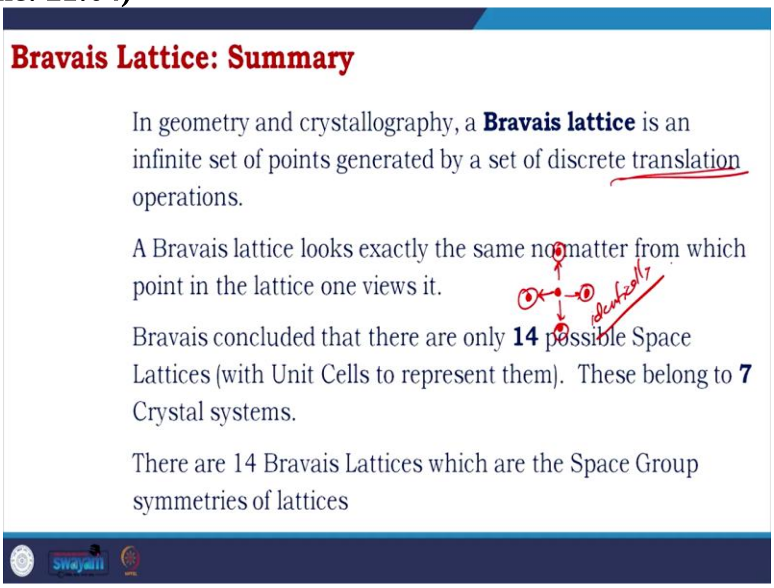

In geometry and crystallography, a Bravais lattice is an infinite set of points generated by a set of a discrete translation operations. A Bravais lattice looks the same, no matter from which point in the lattice one views it.

Bravais concluded that there are only 14 possible space lattices. This belongs to 7 crystal system, there are 14 Bravais lattices which are the space group symmetries of the lattice.

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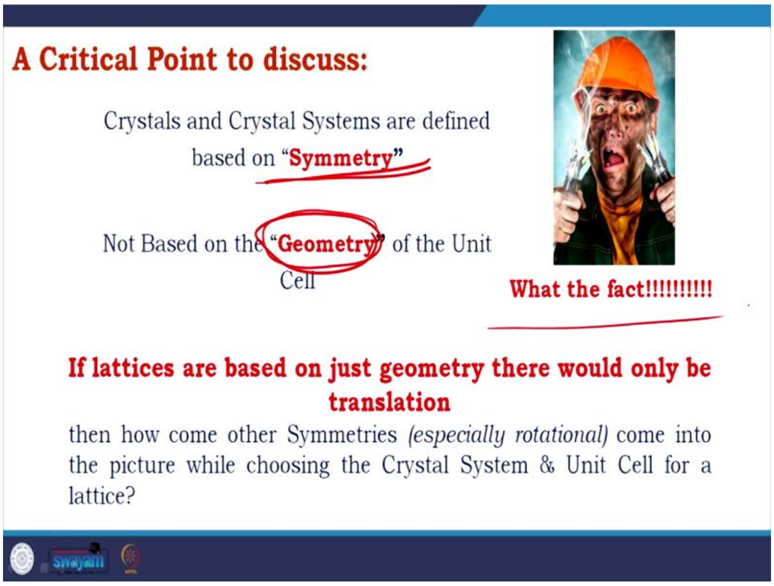

But a critical thing to discuss; Crystals and crystal systems are defined based on symmetry, not on the unit cell's geometry, which we were talking about. So, Bravais majorly talked about geometry, whereas they are defined and properly fit when you consider symmetry as I talked earlier because that is the surprising thing, what the fact?

So, suppose lattices are based on geometry. In that case, there should only be translation. How come other symmetries, especially rotational, come into the picture, while choosing the crystal system and unit cell for a lattice.

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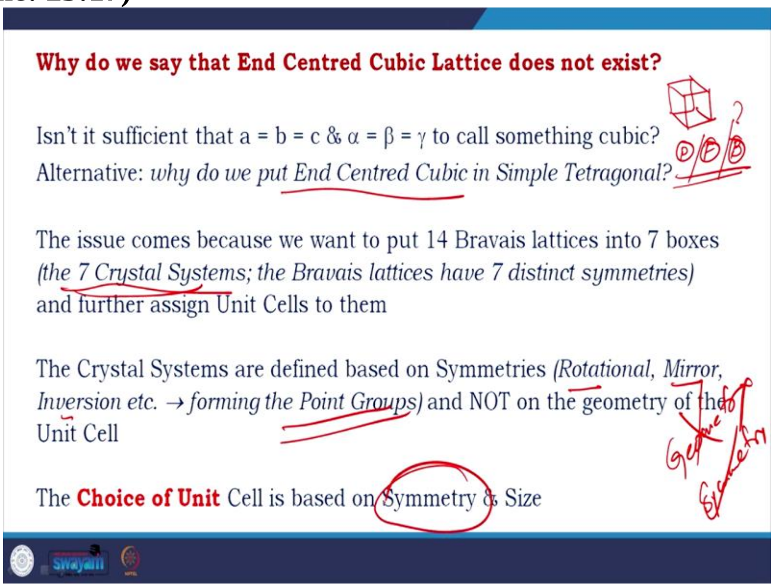

Also, why do we say that end-centered cubic lattice does not exist? So, if you will go further, you will see this is a cubic lattice, and each of the cubic lattices has a primitive face-centered and body-centered but not end centered cubic. So, we do not have the issue because we want to put 14 Bravais lattices into 7 boxes, the 7 crystal systems we are going to discuss the Bravais lattices have 7 distinct symmetries and further assign unit cell to them.

The crystal systems are defined based on symmetries rotational, mirror, inversion extra forming the point groups and not on the geometry of the unit cell. So, first of all, when we knew that the classifications of crystals are not based on geometry, it is not based on geometry. It is based on symmetry, and now we know that this is the point group which is important that the choice of the unit cell is based on symmetry and size. So, symmetry is extremely important.

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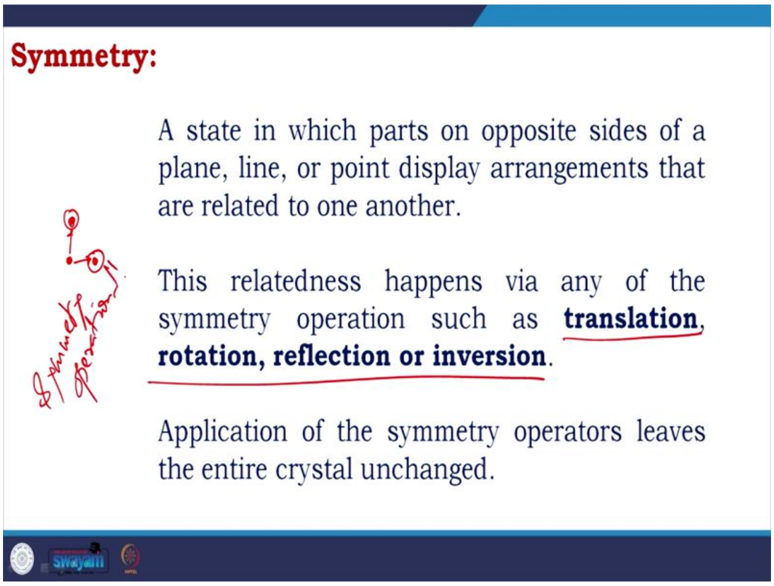

Symmetry is a state in which parts on opposite sides of a plane line or point display arrangements related to one another. This relatedness happens via any symmetry operation such as translation, rotation, reflection, or inversion. Application of symmetry operators leaves the entire crystal unchanged.

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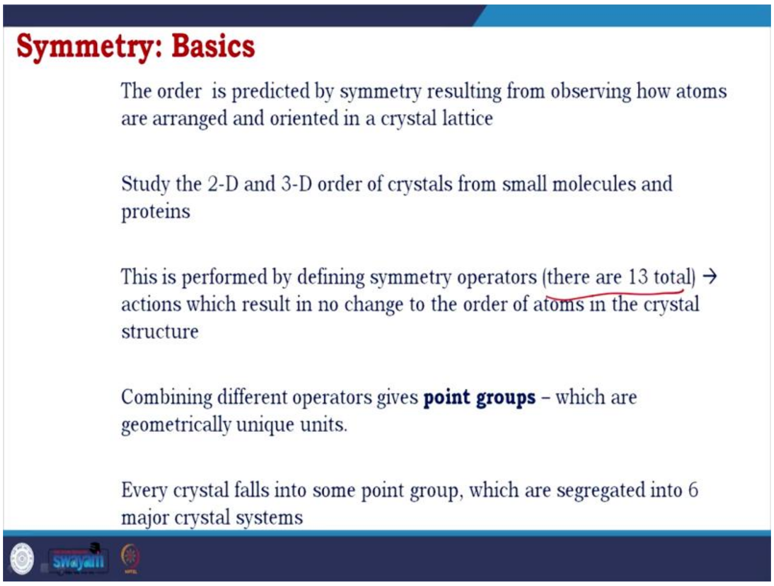

So, what are the basics of symmetry? The order is predicted by symmetry from observing how atoms are arranged and oriented in a crystal lattice. The study that 2D and 3D order of crystal from small molecules and proteins. This is performed by defining symmetry operators. There is a total of 13 symmetry operators not independent. Combining different operators give point groups that are geometrically unique units. Every crystal falls into some point groups, segregated into six major crystal systems.

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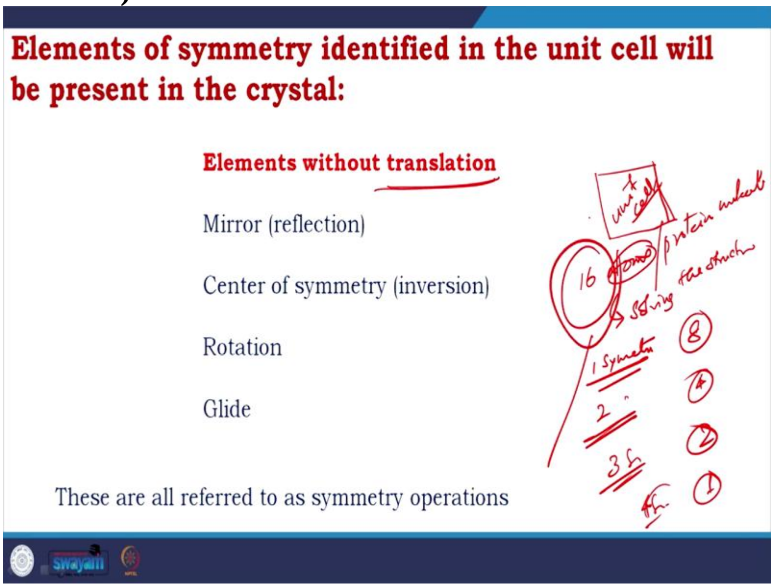

Elements of symmetry identified in the unit cell will be present in the crystal. So, an element without translation, mirror, which is reflection, center of symmetry, inversion, rotation and glide. These are all referred to as symmetry operations. So, we talked about the lattices starting our journey from 1D lattice to 2D lattice and 3D lattice.

And you also understand the upliftment from your journey from point land to line land to flat land and ultimately coming to space land, where you deal with the crystals. We have also looked at Bravais lattice, which we will discuss even more later. We started our concept of symmetry, which is very important in protein crystallography because the more symmetry you get, the more your work is reduced.