Material Science
Professor S. K. Gupta
Department of Applied Mechanics
Indian Institute of Technology Delhi
Lecture No 3
Crystal Geometry

After the introduction of material science now we want to look at the crystalline materials as a told you solid could be crystalline or non-crystalline, so we are going to look at the crystalline solids.

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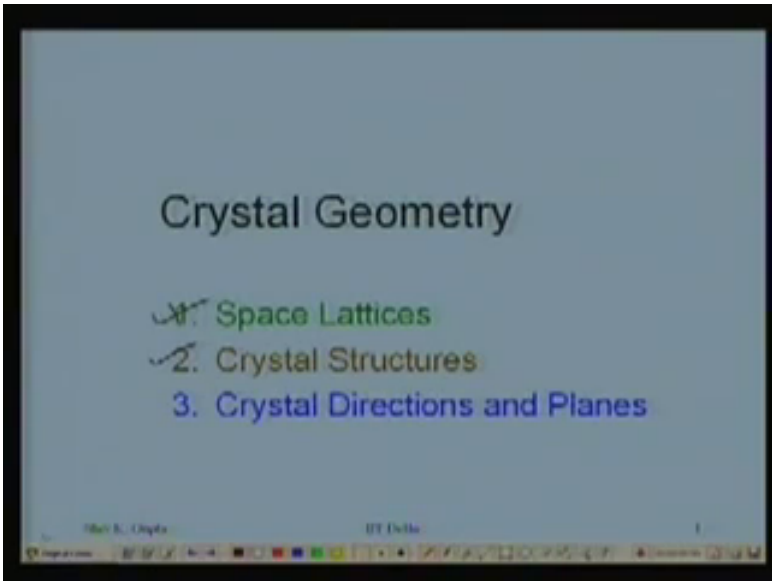

To start with we shall first look at the Crystal geometry because I said while talking about the crystalline solids there is an arrangement of atoms in crystalline solids which is periodically repeating, what is that arrangement, et cetera have to understand that is what I call geometry of crystals. In this 1st of all we shall talk about the space lattices with is arrangement of points in 3 dimensional space which is in periodically repeating manner so that we understand what the periodically repeating arraignment is? Then on this arrangement of points we associate either one atoms or group of atoms or maybe molecules shall be the crystal structure. Once we have understood this we shall look at little more into the volumes of crystals, the directions, then the planes and that shall come the next, so we shall start with today with space lattices.

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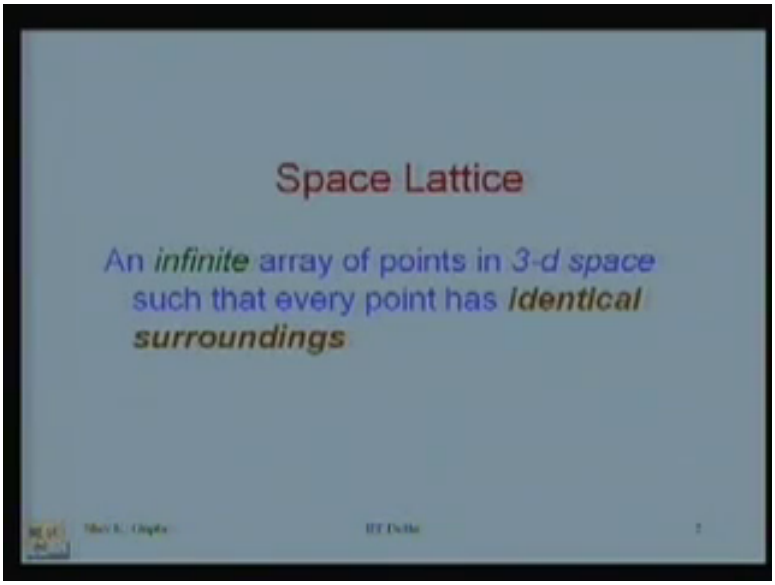

A space lattices can be defined as an in finite array of points in three-dimensional space such that every point has surroundings identical to any other point. We shall try to understand this of course the in finite you understand what is in finite and these identical surroundings we shall try to understand with the help of a two-dimensional picture which is much more easy for us to understand and then we can extrapolate this to the three-dimensions.

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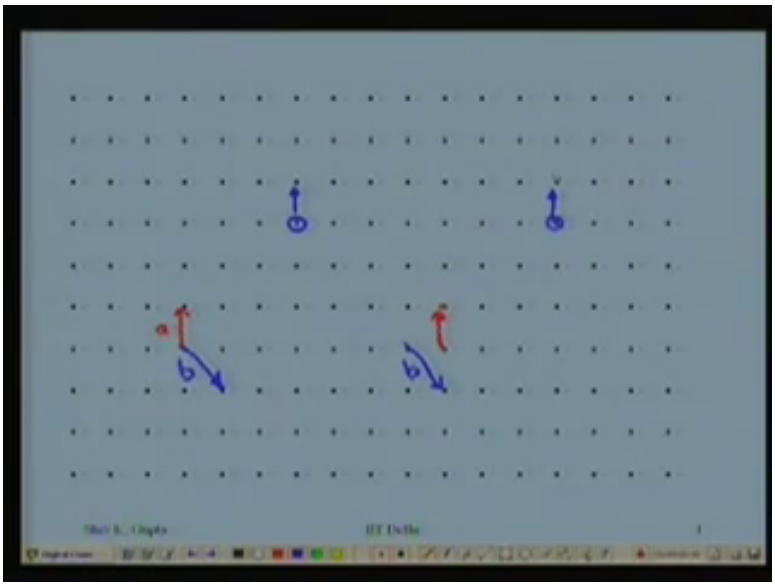

Here is a lattice of points what I am calling is space lattice, just do not worry about the extremities I have already said that it is in finite, right. Let us see the surroundings of a point. Let us consider this point, from this point let us say look upward like this and we see a point at this distance, let us call this distance a. Let us look up another point go in the same

direction, the same distance you see another point there alright from the same point let us go in this direction which is slightly different let us go in this direction, call this b direction I start from this point go in the same direction at the same distance I find another point that you do anyway this is what I mean by identical surroundings.

You stand on any lattice point see yourself in any direction chosen direction to see a certain symmetry to stand on another lattice point see in the same direction you see the same scenery around you, you see in any direction for that matter that is the meaning of identical surroundings. Just to give you an example of identical surroundings another example, let us say I have grown a planned jungle trees which are identical trees and they have grown identically, they look identical which usually is not the case all trees look very different like all human being looks different but let us say they are all identical and I leave you in that jungle you move from one place to another keep moving but after some time you will be lost you would not know where you are where you started from and where you end it because wherever whichever tree you go to you will find you are at the same place unless if you have kept track of your steps you have moved around you will not know where you started from and where you have ended there is the meaning of identical surroundings that is what this is also showing, right.

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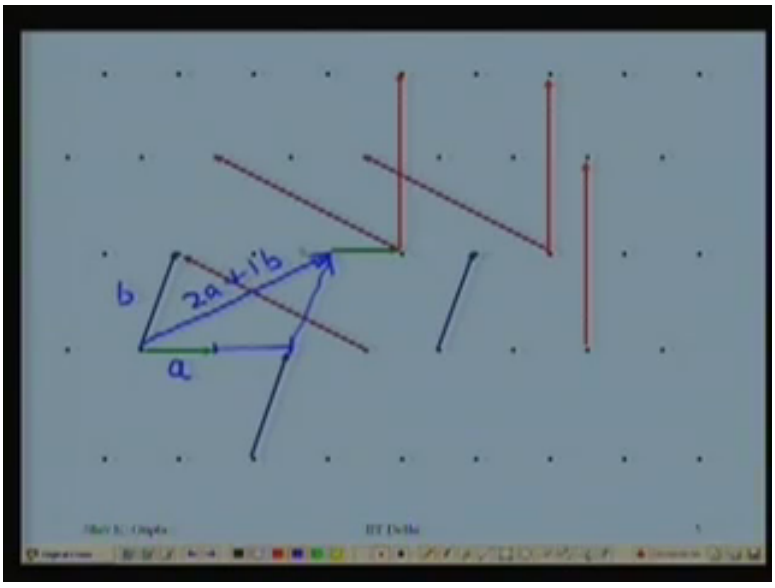

Alright then this is what I have thought to show in a different kind of a arrangement of points it is not similar arrangement which I showed you earlier but there also you can see the surroundings are identical from various points I have gone in various directions and these show that at the same distance you will find the lattice point in that particular direction that is

again also to say it is a periodically repeating arrangement in other words if I am going in this particular direction all the way after this distance every time I shall see a next lattice point, next lattice point and then next lattice point that distances the same that is a period at which this lattice point is repeating this particular direction.

Another thing you will notice that this period is not same in all directions, in this direction the period is this this distance while in this direction I have another period, it is much more longer period, so periodicity would be different in different directions and same thing is 2 and 3 dimensions, right. Now if I have to understand the location, understand these arrangement I should be translating from one place to another in this and my moment have to be defined usually in 2 dimensional space you can define this with the help of 2 vectors which are known collinear, okay.

So for example if you take this one as a and this one as b, any moment you want to define you can define with the help of these 2 vectors, so for example I want to define this moment from here to there it would be one of a, 2nd of a and then I move one of b in this direction, so this 2 of a plus one of b like that I can define if it is a three-dimensional space lattice, what do I need? I need the vectors which are non-coplanar, 3 vectors which are non-coplanar and I can define moment, alright. The next thing is if I want to represent this infinite I already said it is infinite and try to understand as a finite thing I had to take some part of it, a finite part of it and trying to understand it, right we shall look into that, right.

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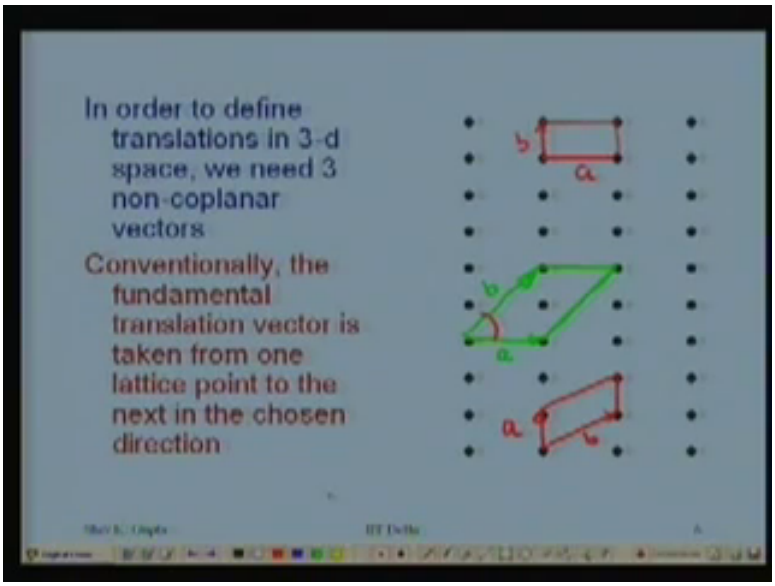

As I already said that in order to define our translations and three-dimensional space we need 3 non-coplanar vectors and this I define as in terms of rather fundamental lattice translation vectors, now since it is a space lattice, lattice I said in three-dimension array of points. Points are geometrical points having no physical dimensions, no physical entities just geometrical points, right, so which to define the translation I just showed you 2 vectors a and b which 2 to be chosen and what is the minimum vector which you choose, so any direction you choose choice is yours but in that direction the distance between 2 nearest lattice points because that is the periodicity of repetition in that direction.

Say for example here let us talk about one vector a in this direction this is the minimum distance between 2 lattice points in that direction and let us take another one in this direction, it is the minimum distance between 2 and let's call it b. You could have chosen any other direction, right? But I have chosen this, now with the help of this is possible for us to define or translation and also possible for us to select from here finite part using these 2 fundamental factors form a parallelogram, right. If you have decided to choose this as a and decided to choose this as b then it would form a parallelogram like this.

This is another finite which is representing this in finite, okay. Similarly somebody decided to choose this as a this as b it can make a parallelogram like that which could be a rectangle plus between these 2 vectors what is this angle (())(12:38) we do not know yet but we once we choose we can define that angle, measure it and define that, right. So that is what how we can try to look at this in finite with the help of the finite part of it. I showed you a parallelogram formed by the 2 fundamental lattice transition vector taken in 2 dimensional spaces.

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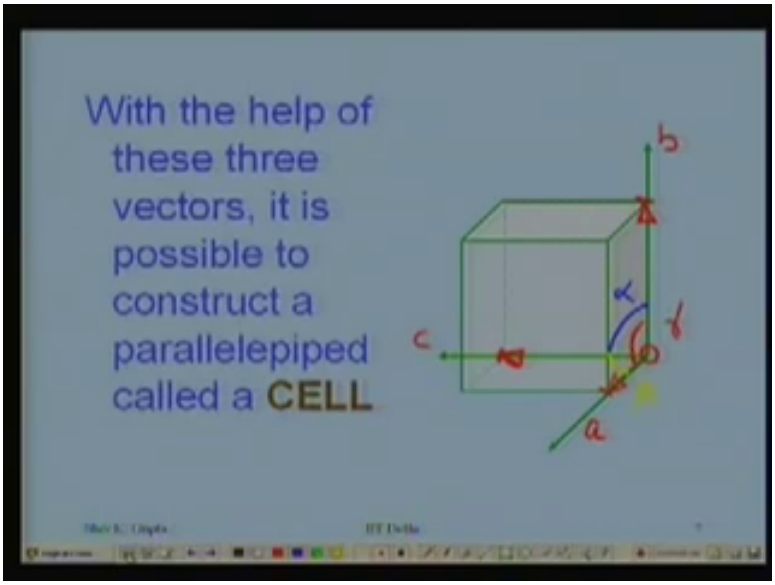

In three-dimensional space the same thing will form a parallelepiped, this is what is called a cell like this case this cell is formed here this is a cell and lattice transition vector direction have shown, their magnitudes are let us call them a here, b there its magnitude is from this origin to there and magnitude of the c is here, so unit vector is from here to there let us put that with a narrow from origin to their these are the unit vectors.

This may not be of the same size because periodicity in a particular direction is different, it need not be the same in all directions, it can be but need not be, okay and then we also define the angles between a and b here is defined as Gama and angle between a and c is defined as beta and angle between c and b is different as alpha it is easy to remember between a and b it is c which is missing. a, b, c is one order alpha, beta, gamma is another order, c is missing so it should be called gamma between a and c, b is missing it should be called beta and similarly between a and c yeah b is missing so it is beta between a and b, c is missing it is gamma and between b and c, a is missing it is alpha that is how the angles are different, right and we have also seen in two-dimensional space in a space lattice I can have more than one kind of cells, more than one shape of the cells, more than one size of the cells which is finite part because I have taken a fundamental lattice transition vector in a given direction and that may give me a either a bigger object or a smaller object, okay right. So there could be a variety of cells out of these all cells are not used for representation we use only some cells at a particular cell to represent usually.

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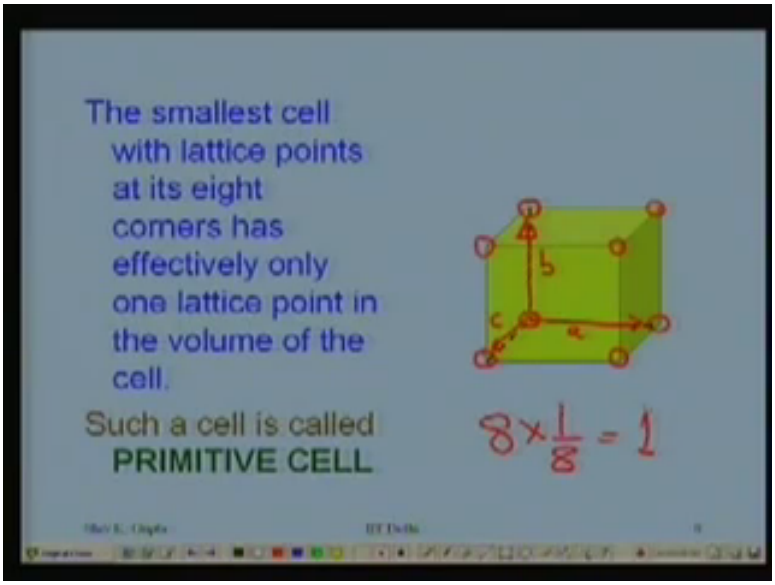

Well before I talk about a particular cell for a presentation, among the cells which is the smallest in the given lattice is called the primitive cells such a smallest cell will have the lattice points only at the 8 corners of the cell nowhere else in the volume of the cell lattice point is there. Such a cell is called the primitive cell it is the smallest I cannot have any cell smaller than this because I said I will choose the 3 translation vectors fundamental lattice transition vector from one lattice point to the next let us say one I have chosen is here 2nd one I have chosen is there and 3rd one have chosen is here I cannot have anything smaller than that but if I have chosen a, b, c such that there are some lattice points lying within the volume of the cells then of course it is not the smallest then it is more lattice points in it.

This one has effectively only one lattice point in it because such piping will be shared at every corner and at any corner of there will be 8 such cells so the 8 quadrants or 8 octants what you call an 8 octants each one would have a cell like this and therefore there would be each corner shared by 8 cells within the volume of the cells the contribution is only one (()) (18:11) and therefore this effectively only one lattice point within the volume of the cell that is another characteristics of the primitive cell there is only one lattice point within the volume of the cell or this is the volume occupied by one lattice point in the three-dimensional space, okay.

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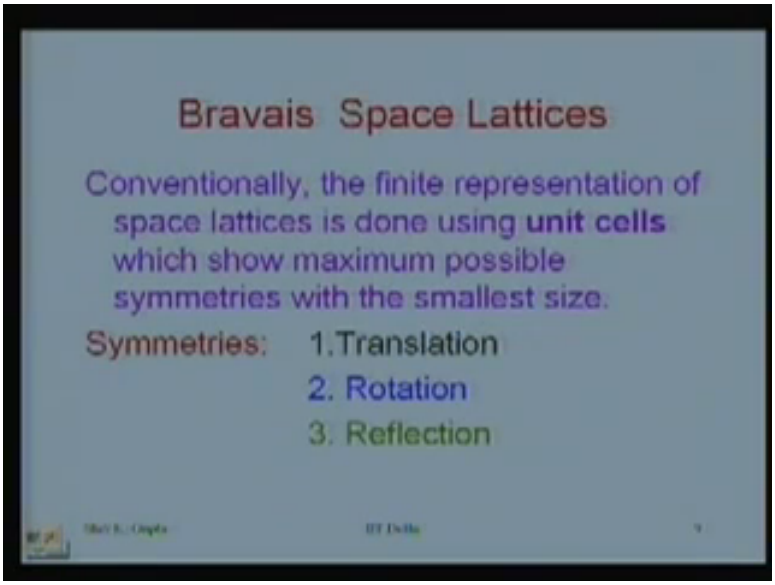

Now coming to choosing a particular cell to represent the in finite space lattice we make use of conventionally Bravais space lattices. In here a unit cell is so chosen that it contains all the maximum possible symmetries of this space lattice and it has the smallest possible size. Before coming to the size I have given some idea but a smallness of the size but I have to talk about the characteristics of the space lattice which are the symmetries of the space lattice, okay. Symmetries of the space lattice if you look at could be translation symmetry, rotation symmetry, reflection symmetry.

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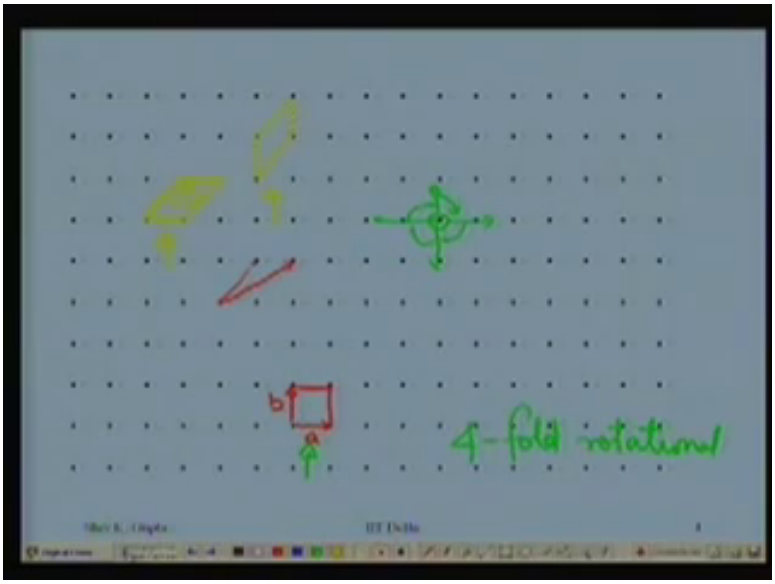

Let us come back here and let me say this is a square space lattice with this is one translation vector another translation vector b here, a is equal to b in magnitude if it is a square lattice

because the cell which is formed will be a square, angle between the a and b should be 90 degrees. In this the translational symmetry is inherent in the definition space lattice, what did we say? Every point has surroundings identical to any other point, so if I travel from this point and translate myself in this position or translate myself to that position I reach an identical place, I reach as if I have not moved at all this is what I mean by translation symmetry. We shall spend little more time on the rotational symmetry and not worry about the reflection symmetry in this course.

If I make a cell like this it is one cell of course and I consider in axis perpendicular to the plane and rotate this square about this axis and standing myself at one place let us say viewing from here. I rotate this square I see the same things 4 times in one full rotation of the square. After it is rotated by 90 degrees what I am going to say is this side is another 90 degree I shall see this, another 90 degree I shall see that and after 360 I shall see the same thing back. Now if I ask you to stand yourself here because infinite is not easy to rotate you stand yourself there and rotate yourself by 360 degrees.

Whatever scenery you are seeing here after 90 degree of rotation you will see the same thing here after another 90 degrees we shall see the same thing there after another 90 degree we shall see the same thing there and after 90 degree we come back to the same place. So in one full rotation you are saying the same things 4 times it is called 4 fold rotational symmetry, it is called 4 fold rotational symmetry. Had it been being seeing the same thing twice it would have been 2 fold rotational symmetry let me show you 2 fold rotational symmetry let us take a cell it is a parallelogram, you rotate the cell about it axis. Let us say like this you rotate, what do you see? You see the same arrangement only after 180 degrees rotation after 180 degrees rotation this side will come here and this side will go there after 90 degrees you do not see the same thing.

After 90 degrees rotation what you are going to see is in this case…right? This is what you will see after 90 degrees this would become vertical that will also become vertical and these sides will be there. This is not the same thing standing here I am seeing this is not the same thing which I see so parallelogram shows only 2 fold rotational symmetry same is true about a rectangle, a rectangle shows only 2 fold rotational symmetry, right. Similarly if I have an hexagon what will it show? 6 fold rotational symmetry, right. So that is what I mean by rotational symmetry it is present and it is there in the space lattice say characteristics of the space lattice.

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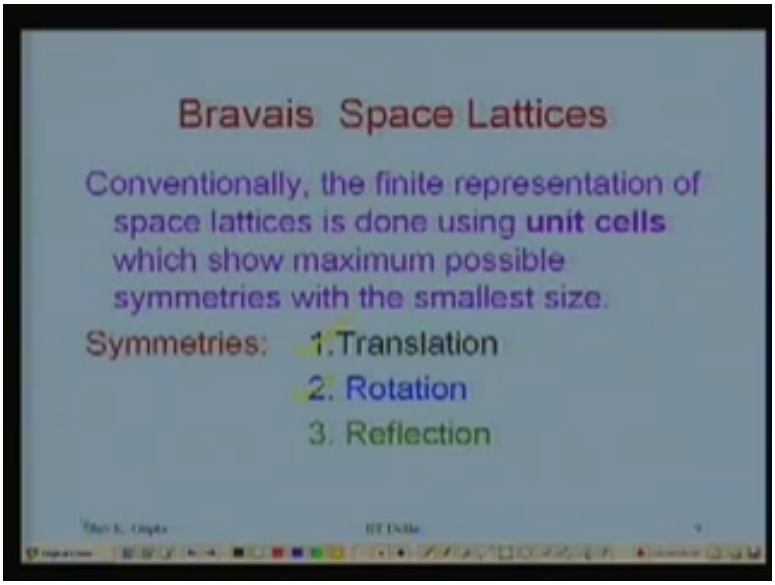

Alright, so we have told you something about the translation symmetry which is inherent in the definition of the space lattice. I have showed you what I mean by rotational symmetry and I said do not worry about the reflection symmetry, so the cell which I choose has to be such that it has the maximum possible symmetries with a minimum possible size and that is what is referred to as Bravais unit cell or Bravais space lattice that is what is used conventionally for representing these space lattice.

Between the cubic space lattice as a square space lattice which I showed you 2 dimensional square space lattice I showed you a cell which is square I showed you another cell which was a parallelogram which one shall be choose? Square. Square shows me 4 fold additional symmetry in the area of the 2 is the same, area is not different, so size is small and I cannot have smaller than that because the primitive… Only the 4 corners of the lattice points it is the smallest and the one which has the maximum symmetry is the square that is what is been done.

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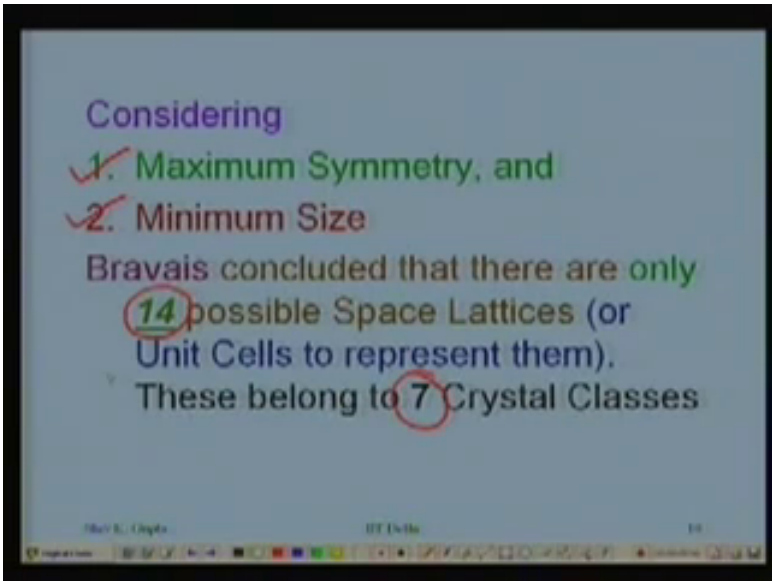

And Bravais found that there are only 14 possible arrangement for space lattices which belong to 7 crystal classes because I have to consider maximum symmetry and the minimum size that is what I have emphasise so far. You have understood the meaning of the maximum symmetry and we have also understood the meaning of the minimum size and then we also have talked about the space lattice it is an in finite arrangement of points where every points has identical surroundings in three-dimensional space, okay. Now we shall look at these 14 possible arrangements in 7 crystal classes one by one.

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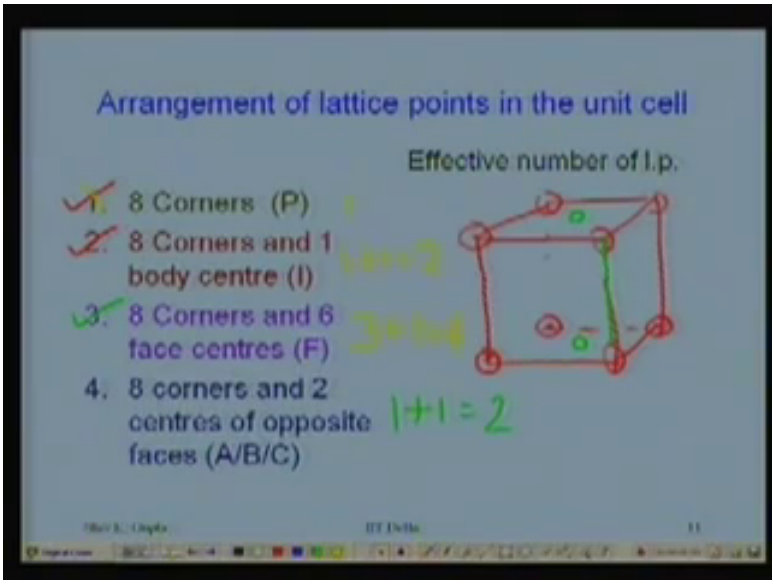

First of all before talking about this 7 crystal classes I am giving you the kind of unit cells we shall see in these 14 space lattices, okay. One is where I have just defined only a primitive

cell where 8 corners are the lattice points. These 8 corners at the lattice points it is called the primitive cells that is one kind of cell will see. The 2nd kind of unit cells we shall see where there is one lattice point also present in the center of the body that is the Centre of gravity of the unit cell, right it has 8 corners and one body centre, right that is the 2nd one.

Now the 3rd one is 8 corners and 6 face centres alright let me put this face centers in a different color so that you can distinguish. Top face center, bottom face center, right side, left side, the front and the back lattice points are located at these locations this is called a face centred cell. All the 6 face center and the 8 corners are there, okay. Then the 4th one will come across lets uhh… The 4th one is 8 corners and 2 face center so the opposite faces like this or left and right or the front and back or only 1 pair such a cell is called encentred or base centre. I have seen simple or the primitive body centred, then face centred then we have seen…seeing now the encentred base or the base centered. From this it is possible for us to find out effectively with the volume of the cell how many lattice points are there, okay. In the 1st one 8 corners I just said there will be only one, 2nd one the one is within the body center that is within the volume of the cell and corners give one so that makes it one plus one.

Student: According to the definition of primitive cell there should be only one lattice point effectively in the volume enclosed.

Prof: Yes.

Student: So there are 2 in this case there are 2 lattice points.

Prof: Alright you are trying to ask me the difference between a primitive cell and a unit cell. Unit cell I said is the one which is going to represent the infinite space lattice and it has to be such that it has all the possible symmetries or the maximum possible symmetries of the space lattice but still the minimum size that means it is not necessarily the primitive, it can be bigger than the primitive as long as it can show me all the symmetries we go in for a bigger size, is it clear? So primitive one is the only one which will have one this has 2. Now the one which has 6 face centres a face is always common between 2 cells, so one lattice points on the face is shared by 2 cells, so therefore 6 by 2 is 3 plus 1 which is coming from the corners makes it 4. You can have 4 primitive cells in this value can have 2 primitive cells the 2nd one you can have 4 primitive cells in the 3rd one, okay. Now coming to the last one how many will be there? One plus one again 2, right alright these are the kind of cells we are going to come across.

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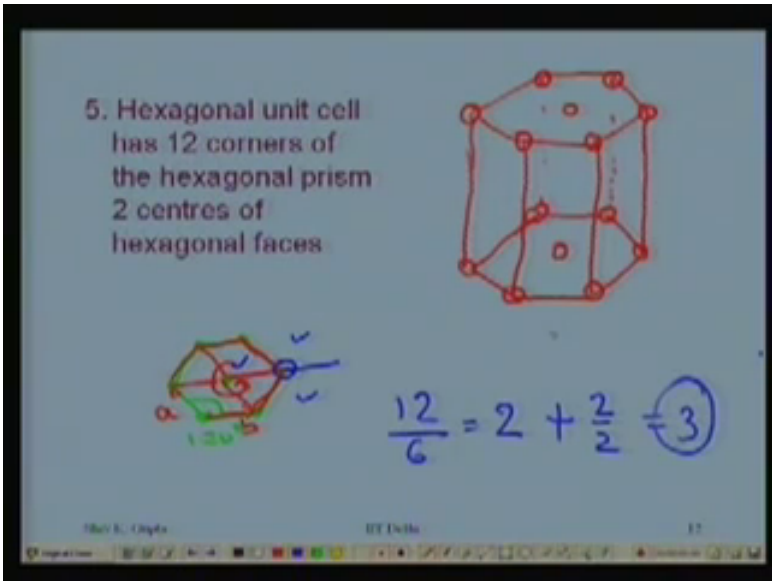

I think there is one more which I would like to say it is normally because I have defined the cells to be parallelepiped electron by taking the 3 translation vectors where the fundamental lattice transition vectors if I do that in a hexagonal unit cell. Hexagonal unit cell let us 1st look at in the 2 dimensional space I make a regular hexagon here is 120 degrees, lattice points are at the corners and lattice points also have to be in the center here without this lattice point which is in the center it cannot define the space lattice or it does satisfy the definition of space lattice because if I start from this place I go in this direction that means distance I find the next lattice point.

If this lattice point is not there here I shall have double the distance, so this is necessary point has to be there, so if I take this as the a vector, this as the b vector then parallelepiped drawn will become parallelogram like this but the parallelogram shows me only 2 fold rotation symmetry it does not show me 6 fold rotation symmetry only when I put some more of these together that is one fellow grams of the same size here and half of that there is another half here I can get a regular hexagon and I can now show the 6 fold rotation symmetry here, right. So we have to make a hexagonal prism, the base is going to be regular hexagon and the c axis the 3rd axis will be perpendicular to this, alright that shall be a hexagonal prism and would be looking like this.

Where the lattice points are going to be? At the 12 corners of the prism and one center in the base here and one center on the base of the hexagon there, can you tell me how many lattice points are there? Yes there are 3 because each corner is not shared by 8 unit cell is shared by 3 unit cells one here, 2nd here and 3rd there because solve the angle of 120 degrees, so 12

corners each shared by 6 unit cells, so 12 by 6, it makes it 2 and then we have to add on to this, this one and this one which is shared by 2 unit cells, so 2 by 2 that makes it 3, so effective lattice points are 3 in this hexagonal unit cells.

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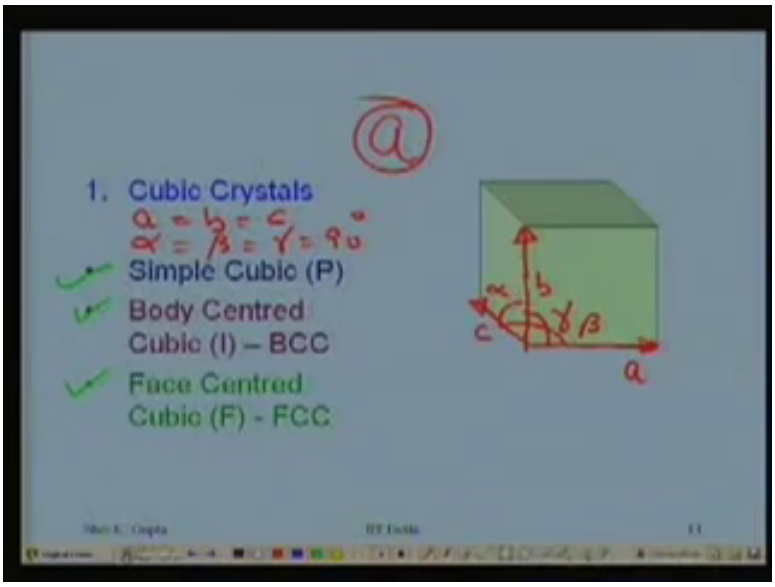

Alright, now the 7 crystal classes and we can quickly go over them 1st one is called a cubic crystal class where we define a is equal to be is equal to c angle alpha is equal to angle beta is equal to angle gamma is equal to 90 degrees. So how many constants a, b, c, alpha, beta, gamma out of the 6 constant which any unit cell is going to have. In case of cubic crystal how many do I have to define? I need to define only one, I need to define only one, angle is already 90 degrees I do not have to define them, now a, b, c definition is left to you, you can define this as unit a, you can define this as unit b alright and you can define this as unit c and angle of course will be calling a and b is gamma, b and c is Alpha and a and c is going to be beta there and here I have 3 cells different cells simple where are the lattice points? Only corners 8 corners. Body center where are the lattice points? 8 corners and one body center and face centred and the 6 face centres. No other cells or no other distribution of lattice points we find I told you 5 out of this only 3 are here, okay. The 5th one we will find only in hexagon nowhere else.

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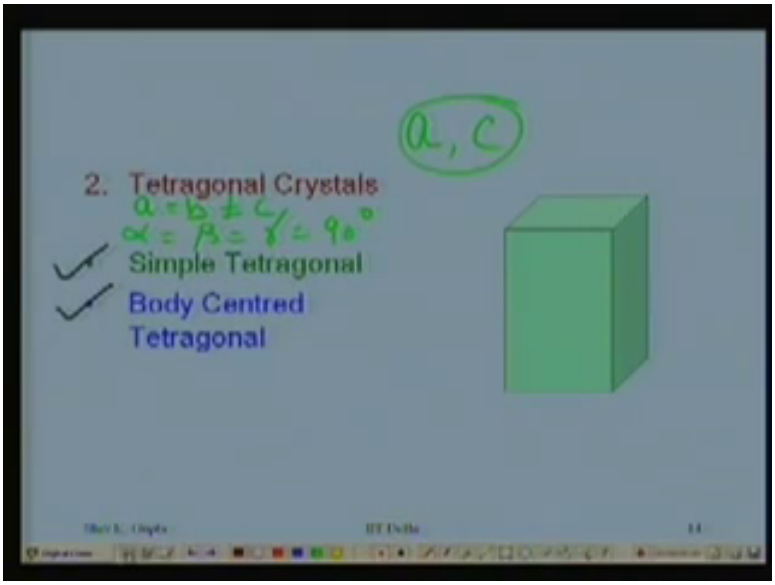

The 2nd crystal classes is Tetragonal crystal class where a is equal to b is not equal to c and alpha is equal to beta is equal to gamma is equal to 90 degrees. Now how many do I have to define? 2, I have to define a and c and in here I have only 2 arrangements one is primitive or simple tetragonal and 2nd one I have 8 corners and one body center which is called a body centred tetragonal. You see space lattices as a told you simple body centred, face centred and center or the base center now what I am doing you can see that simple one simple tetragonal because that gives me the crystal class and crystal class define the 6 parameters then the body centred tetragonal, right so that is the makes its 3 plus 2, 5.

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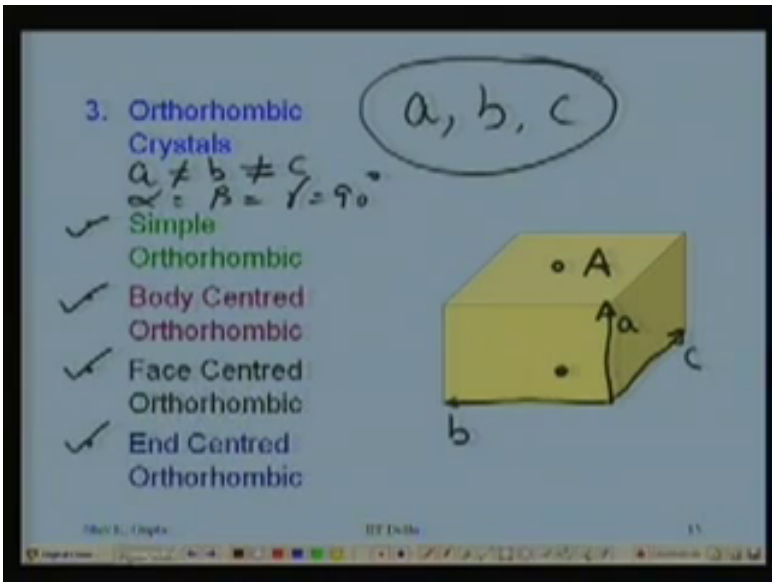

Alright then we have Orthorhombic crystal class in where a is equal to b sorry not equal to b not equal to c, alpha is equal to beta is equal to gamma is equal to 90 degrees. This one is rectangular prism, okay and tetragonal was a square prism. Here I have 4 all the 4 simple orthorhombic means only 8 corners that is a primitive, body centred 8 corners and one body center, face centred orthorhombic 8 corners and 6 face centres, End centred orthorhombic 8 corners and 2 opposite faces.

Opposite faces let us okay define this is the a this is the b and that is the c then if I have face centred here and at the bottom what do I call it? a center or a b center or a c center. It will be called a centre because the plane which or the face which has the center does not have the a axis in it, it has only b axis and c axis, okay. Right so similarly if a face is front, face it will be called the c centred, side faces will be called b center depending upon what you have called a? What you have called b? And what you have called c? And here I need to define all 3 axis and a, b and c their magnitudes need to be defined so I need 3 of them angles at 90 degrees they are already defined. So that makes it how much 3 plus 2, 5 plus 4, 9.

Student: How do we (())(44:47) for a crystal class orthorhombic tells there are 4 subtypes simple orthorhombic, body centred orthorhombic and for the previous (())(44:58) still there were only 2 sub classes.

Prof: Yes you have a question which I was going to leave for you to answer this, the question as he is asking is that we have shown simple cubic, body centred cubic, face centred cubic but when I came to tetragonal I showed a simple tetragonal and an body centred tetragonal, I did not show the face centred tetragonal and either I did not show the end centred cube nor I had shown the end centred tetragonal, why? This I am leaving a problem you have to answer and I can only give the hint, the hint is we are choosing that cell which shows maximum symmetries and maintains the minimum size. Shows the maximum symmetries and maintains the minimum size, is that clear? Alright.

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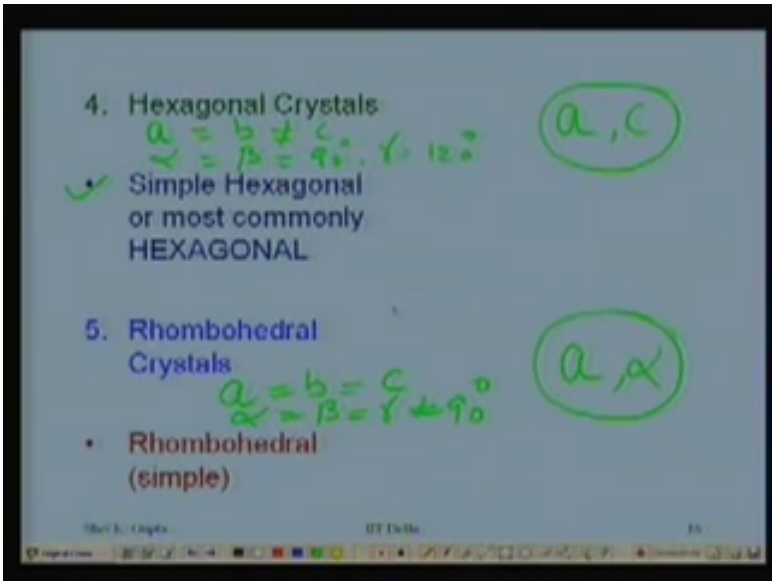

Alright next one is the hexagonal crystal class which I also defined for you a is equal to b is not equal to c alpha is equal to beta is equal to 90 degrees gamma is equal to 120 degrees. How many lattice parameters we have to define here? 2 a and c height of the prism and the side of the prism hexagonal side of the prism. There is only one but simply which I just showed that these simple hexagonal or most commonly we simply call it the hexagonal. Then the next one we have a Rhombohedral crystal class where a is equal to b is equal to c alpha is equal to beta is equal to gamma is not 90 degrees. There is also only 1 primitive in this a Rhombohedral or a simple Rhombohedral unit cell and we need to define only 2 parameters a and alpha.

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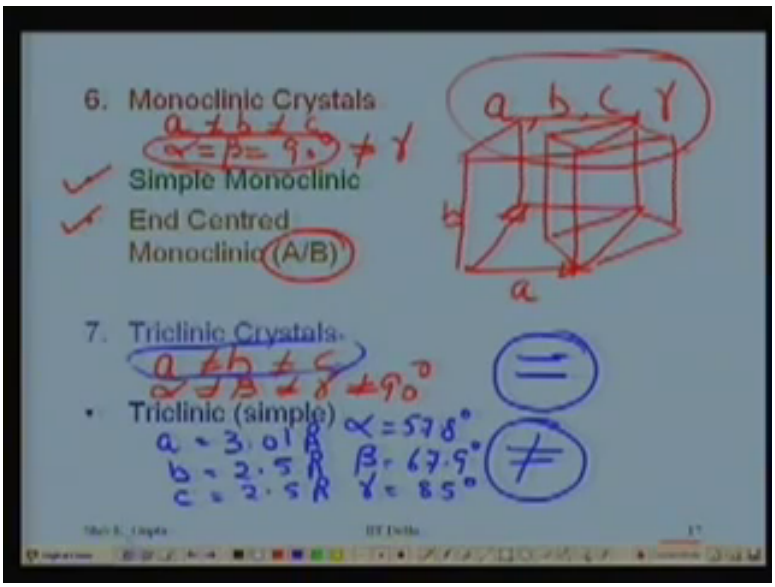

Alright next is 6th crystal class is Monoclinic where… In the monoclinic crystal class we have a not equal to b not equal to c alpha not equal to sorry alpha equal to beta is not equal to gamma sorry hash…alpha is equal to beta is equal to 90 degrees and it is not equal to gamma, so here I need to define 4 parameters a, b, c and gamma. So that is a monoclinic crystal class in this I have one simple monoclinic only at the 8 corners of the unit cell, the lattice points are there 2nd one is the end centred monoclinic where lattice points are 8 corners and there 2 opposite faces but the 2 opposite faces be either A or B it is not the C, okay because if you make it the base will be a parallelogram where this is the a axis that is the b axis, c is perpendicular to this let us draw that like this.

So if I make a center on the c which is here I can make a smaller parallelogram like this it will be smaller cell, so c center is not there a center the front, the back or the left or the right those centres are allowed. They become the end centred monoclinic than the last one crystal class is a tri-clinic where a is not equal to b is not equal to c alpha is not equal to beta is not equal to gamma and they need not be 90 degrees. Now before I proceed further I will count it 14 of these I have to make the difference between 2 kinds of things 1 I have showed here alpha equal to beta equal to 90 degrees and the other kind of thing which am showing as a is not equal to b is not equal to c, so there is one sign is equal to another sign is not equal to… their understanding and interpretation is very important.

For a cube I said a is equal to b is equal to see alpha is equal to beta is equal to gamma is equal to 90 degrees if a, b, c are not equal then a is let us say 3.01 Angstrom and b is 3 Angstrom differences 0.01 Angstrom will it be a cube? You will say 0.01 is negligible when I talk about the crystal in the dimensions of 4 centimetres or 5 centimetres I would have added difference of millions of units cells in one direction with the difference of 0.01 Angstrom, right so equal to is a very rigid relationship but when I say not equal to I am not so very rigid what I am trying to say is these parameters are not related in any way and they can take independent values.

Once they are taking independent values they are not related once such Independent value could happen that to our equal, if that happens and the symmetries of the unit cell do not change, symmetries do not change it shall remain whatever crystal class it is but the moment the symmetries change because something has become equal it will go to a higher crystal class with higher symmetries then only its name would change. Say for example I talk of a triclinic crystal a is not equal to b is not equal to c and alpha is not equal to beta not equal to

gamma and 90 degrees let us say it has no symmetry as a matter of fact it is highly unsymmetric crystal it is.

I say a is 3.01 Angstrom, b is 2.5 Angstrom and c is also 2.5 Angstrom alpha is 57.8 degrees, beta is 67.9 degrees and of course gamma is 85 degrees by making b and c equal has it become monoclinic? (())(55:34) symmetry? It has not, so it is still triclinic it will remain triclinic it does not satisfy the relationship with any other crystal class it does not have the symmetries of any other crystal class it remains triclinic, so you have to be careful with the meaning of this equal to and not equal to. Equal to a very rigid relationship I cannot accept an iota as a difference and not equal to means they take independent values.

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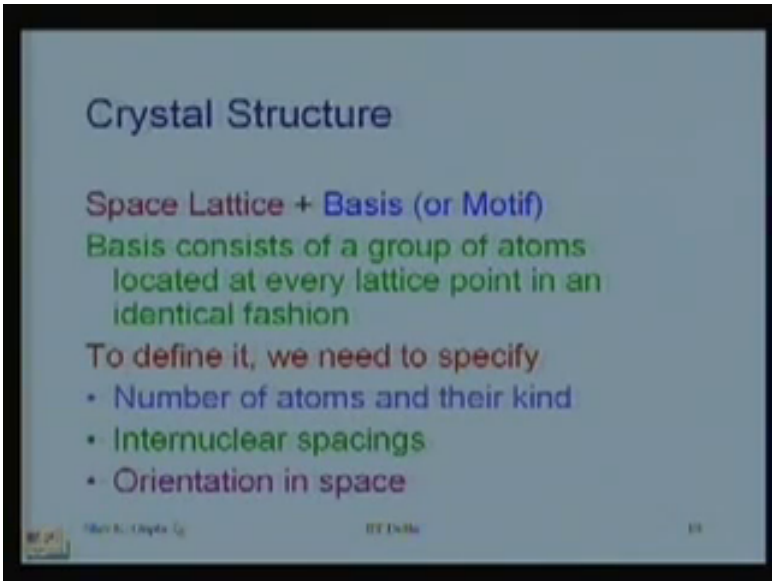

Alright, alright this is what we shall take in the next class.