An Introduction to Materials: Nature and properties (Part 1: Structure of Materials)

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Lecture – 06
Crystal Systems
Bravais Lattice

So, now in this new lecture which is on; which is in which we will discuss Crystal Systems and Bravais Lattices following; what we have discussed in previous lectures on which was a background basically on how do you construct a lattice, what do you mean by lattice? And what is the meaning of a crystal lattice? So, far we have talked in generality so, what we have seen is what.

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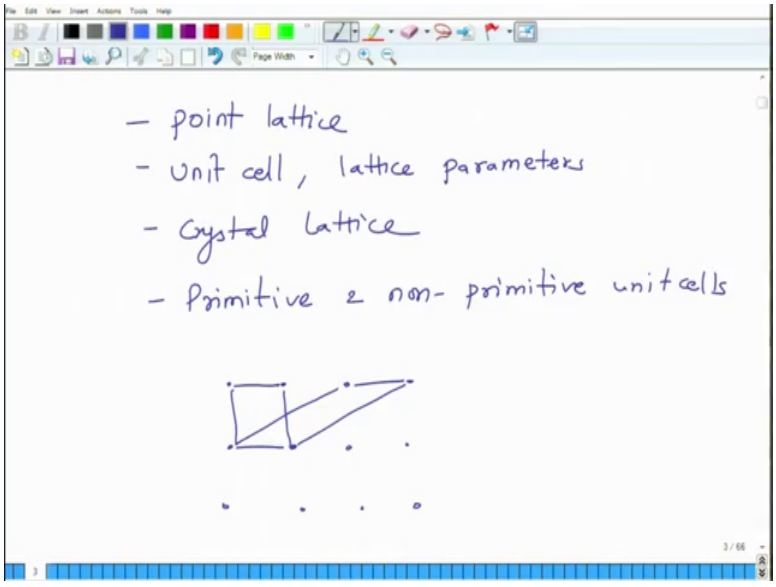

We have seen is you have a point lattice; in this point lattice you can make a unit cell, unit cell has lattice parameters, you can make a crystal lattice by replacing points with atoms or group of atoms and then we talked about primitive and unit cell, but a question is still remains in the unit cell is what kind of unit cell you choose? Can you choose any arbitrary unit cell? Because there are multiple possibilities are there you can see that in this for example, simple example let me remove the other ones which are really far you can choose this as a unit cell, you can choose this as a unit cell.

So, there are multiple possibilities the question is what; which one do you choose or is there a day is there a basis for choosing a unit cell and what is that basis. So, that is what we will discuss in the next few lectures. In this lecture I will just tell you the established mechanisms to identify did these different patterns and then we will get into why these patterns, what is the basis of making these patterns? So, what we basically have here is we call them so, the depending; so, you cannot choose any arbitrary shape first of all the shapes are divided into few categories.

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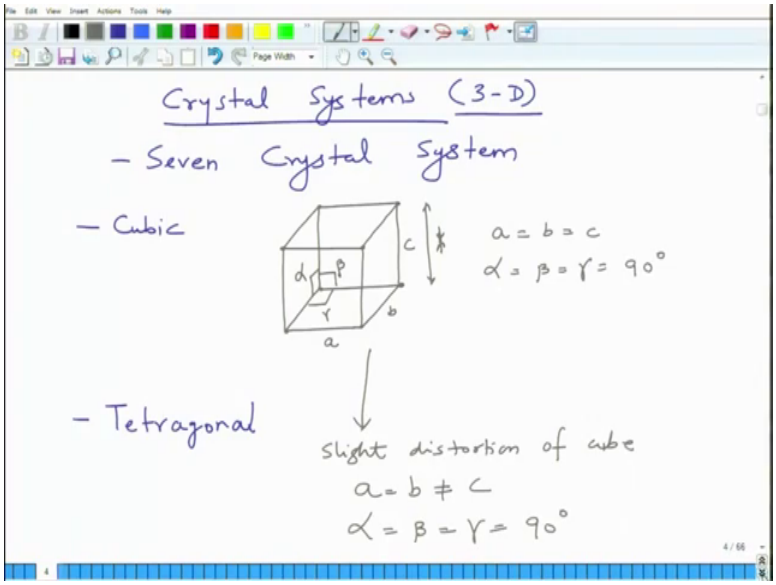

And those categories basically define what we call as crystal systems ok.

So, there are total of 7 crystal systems; starting from the first one we call that is a cubic crystal system. So, in a cubic crystal system essentially what happens is you have you can see that it is nothing, but a cube. So, now, we are talking basically in 3D ok. So, we can say these are the crystal systems in 3D so, you can also have you can you can also ask me a question that what about crystal systems in 2D.

So, I will give you some hints at the end of it let and I will hope that you will be able to tell me how many maximum possibilities of crystal systems can exist in 2D ok. So, let me first give you the examples of 3D. The possibilities of and then we will discuss the origins behind these possibilities.

So, in the cubic crystal system what you have here is; basically the lattice is based on the cubic arrangement of points in space. So, every point will follow this kind of cubic arrangement such that, so you have a, b and c; a is equal to b is equal to c and alpha is equal to beta is equal to gamma is equal to 90 degree. So, this angle, this angle and this angle all the 3 angles are 90 degrees.

So, between so, between a and b you will have gamma between a and c you will have beta and between a and c you will between b and c you will have alpha. So, all these 3 angles it will be equal to 90 degree. So, if your arrangement of points allows you to construct a unit cell you will go with that cubic unit cell, because as we will come to perhaps in next lecture or a lecture after that this is the most symmetric what do we mean by symmetry we will see that in the next few lectures.

So, we will choose a cubic structure when it is present and when the symmetry permits it. Second choice of this is slight distortion of cubic which is called as tetragonal so, what happens here is your unit cell is slightly distorted. So, basically what you do is that you extend the c or compress this c a little bit as compared to the cubic case so, what happens here is a slight you can say it is a slight distortion of cube of a cube.

So, what you will have here is you will still have a is equal to b, but c is unequal ok, but alpha beta gamma still remain 90 degree. So, it is still a orthogonal system cube is a orthogonal system tetragonal is a orthogonal system. So, that is the only distinction that you have. So, the next one is a little bit even worse than that.

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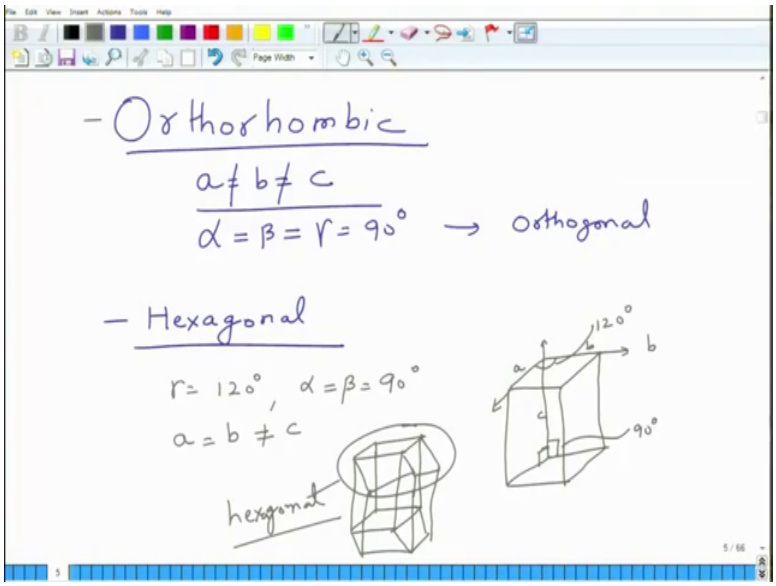

Third one is called as so, basically you have a tetragonal unit cell and you now change the dimensions along a, b and c all the 3 directions without changing the angles. So, what you have here is a is equal to a is not equal to b is not equal to c alpha is equal to beta is equal to gamma is equal to 90 degree. So, it is still orthogonal, but lengths are not at all equal so, this is a third ah variation that you see in this structure.

Fourth one that we talked about is called as hexagonal; in this hexagonal system what you have is basically it is it is it looks like a hexagon. So, what you have here is so, you can say that you have a unit cell like this angle here is 120 degree and these other 2 angles are so, this angle and this angle they are 90 degrees ok.

So, you can say this is you are a this is b and this would be c this is a this is b and this is c let me just alright ok. So, here now the angle between a and b that is gamma. So, here gamma is equal to 120 degree what about alpha and beta? Alpha is equal to beta is equal to 90 degree, what is the relation between a and b? A is equal to b, but it is not equal to c.

So, why this is called as a hexagonal system? Because when you put 3 of these unit cells together they make a hexagon pattern. So, if you if you make something like that you will see let me just try making one for you. So, this will be the first one ok, this the second one so, not a very good drawing, but still you can probably see what I am trying to do here. So, this will be the next one and before I connect it well enough and then you will have this is the second one and then you can draw the third one in front ok. So, third

one would be something like that so, this is these are the 3 unit cells which are drawn so, in a in a hexagonal pattern so, this face will look like a hexagonal face.

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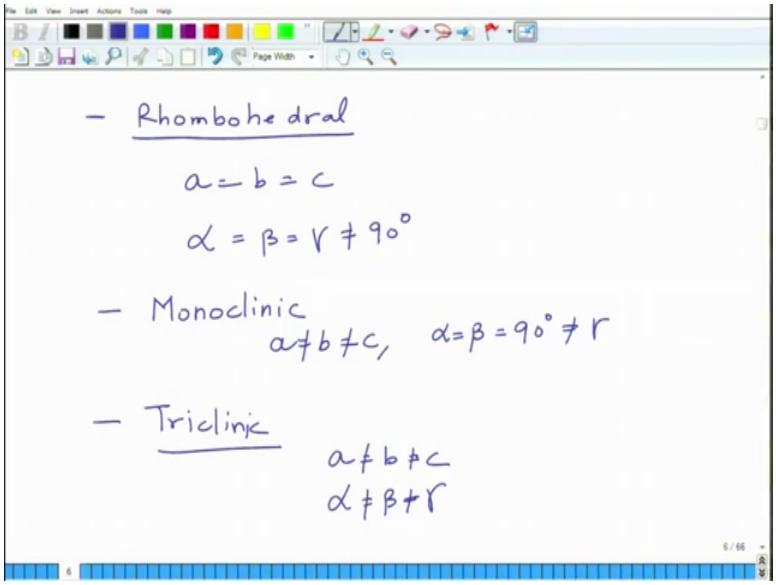

So, that is why it is called as a hexagonal system and now the next one is called as rhombohedral, in this system in the rhombohedral system it is rhombohedral system can ideally be represented from a hexagonal system. What happens in rhombohedral system is a is equal to b is equal to c, but alpha is equal to beta is equal to gamma, but they are not equal to 90 degree. So, this is what makes a rhombohedral system.

So, you can say you can see that it is all of like a cube, but it is not a cube you squeeze the cube in such a in such a fashion so, that a b c are equal alpha beta gamma are equal, but alpha beta gamma are no longer equal to 90 degrees.

So, this is called as rhombohedral, there are 2 more distortions which are there the first one is called as monoclinic and the second one is called a triclinic. In the monoclinic case your a is not equal to b is not equal to c and another difference is that alpha is equal to beta is equal to 90 degree which is not equal to gamma. So, gamma is an angle which is not equal to 90 degree, but it is not necessarily as you can see in the hexagonal case it is necessarily 120 degree, in this case it does not have to be a necessary angle, it is it is just not equal to 90 degree it can be anything else. In the triclinic case this is the least symmetric of them you can see a is not equal to b is not equal to c and alpha is not equal to beta is not equal to gamma this is the worst of them so, in terms of symmetry ok.

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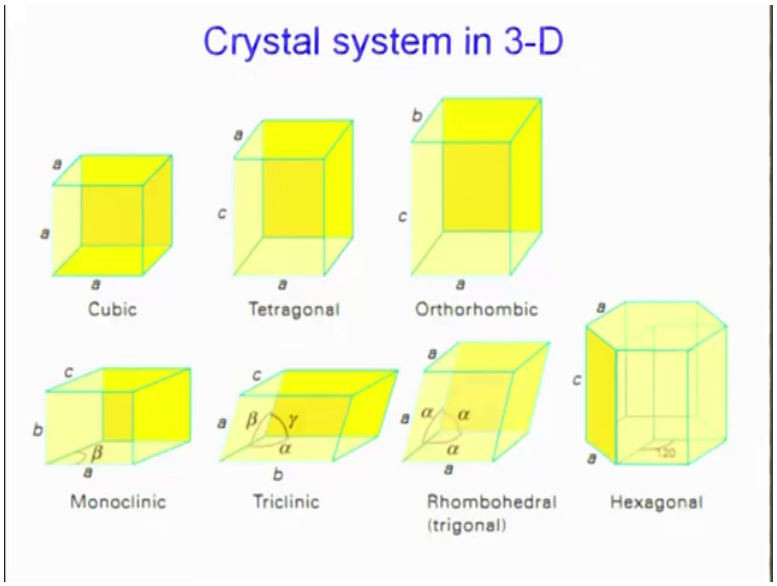

So, these are the crystal systems that you can see in 3D. So, what you have here is ah. So, this is the cube, second one is tetragonal system, third one is orthorhombic, fourth one is monoclinic, you have triclinic, you have rhombohedral.

Rhombohedral often also called as trigonal or trigonal system ok. So, here all the 3 angles are equal alpha, but they are not equal to 90 degrees and a, b, c are all equal and this is the hexagonal system. So, this is the basic unit cell in the light green. So, you can see the gamma is equal to 90 degree a are equal, but they are not equal to c ok.

So, this is the 3 crystal systems in 3D. So, I will I will give you a bit homework you can get back to me in the next class or I will discuss that in the next class that what are the possible crystal systems? So, you have 7 crystal systems in 3D, how many possible crystal systems they will not necessarily have different name same names because remember there is no third direction they are only 2 directions. So, they will have different names forget about the names, but you just have to think about what different geometries are possible in 3D and can you generalize them you see that the point is about generalizing them here we have generalized ah.

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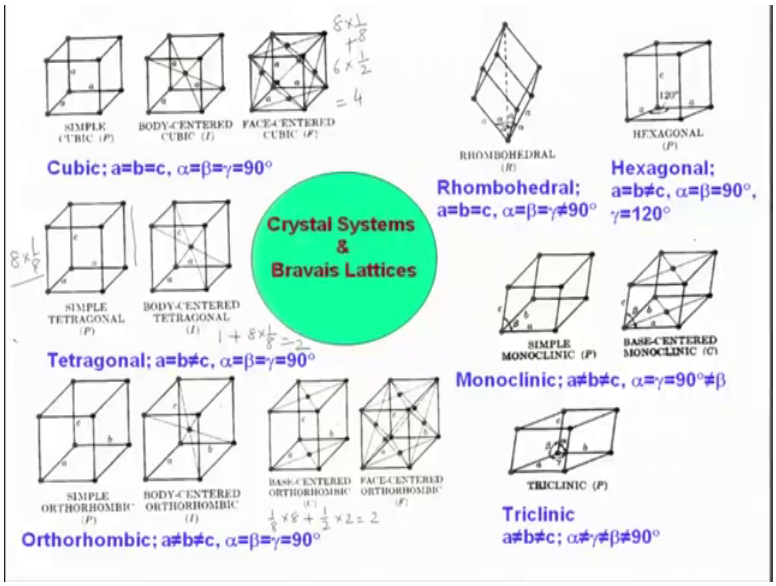

Can you generalize a few crystal system maximum possible crystal systems in 3D. So, once you know about the crystal systems what we talk about now is called as Bravais lattices ok. Bravais lattices are a further up from crystal systems because they now consider whether it is a primitive lattice or whether it is a non primitive lattice. Again the reason for choosing particular type of Bravais lattices will be discussed later on when we talk about symmetry, but let us see just on the basis of primitive and non primitive unit cell what kind of lattices are possible.

So, in case of in case of cubic system you have 3 primitive lattices which are possible first one is called as simple cubic lattice that we have seen. So, simple cubic lattice you can see that how many number of atoms does it have? It has only 1 so, it is a primitive lattice that is why there is a letter against it which is called as p, p means primitive anything which is not p is not primitive.

So, second possible variant in some in cubic systems is that you can make a body centred cubic lattice where you have one lattice point at the corners and the second lattice point is at the centre of the unit cell these 2 are identical lattice points. So, which means if these were 2 different atoms this will not be a this will not be a body centred, what will it become? It will become simple cubic lattice.

So, these 2 points have to be identical if they are identical then this can be called as a body centred cubic lattice. Third possible variation in cubic system is face centred cubic

lattice, where you have where you have points at the centre of each of the faces. So, you have 6 faces in a cube, all the 6 faces will have lattice points at the centre of these faces along with a corners being occupied.

So, total number of lattice points in this system now becomes 4 because you have 1 because you have 8 at the corners which are shared by 8 unit cells. So, 8 divided by 8 is equal to 1 and then you have 6 at the faces, but each face is shared by 2 unit cells as a result you have total of 3. So, 3 plus 1 make it 4 so, you have 4 identical lattice points again in this case if any of them becomes different it does not remain as a face centred cubic lattice that is a take away, but they follow the same definition of cubic crystal system.

Second variation in this case is tetragonal lattice in case of tetragonal you can see that so, in the tetragonal again you can see this c is different than a. So, this is simple single tetragonal you have 8 points at the corners and since you share each of the unit cell by 8 neighbours, a 8 neighbours share 8 unit cells share 1 lattice point as a result this is this is 8 into 1 by 8.

So, 1 lattice point again here you have body centred tetragonal so, you have 1 Lattice point here under here both are identical lattice point. So, you have 1 plus 8 into 1 by 8 is equal to 2 lattice points, in the previous case it was 8 into 1 by 8 plus 6 into 6 into 1 by 2 this will make it 4 ok.

Now, let us see the third example third so, you can always ask me a question now you can see that there are other possibilities also. So, you can ask me a question for example, why do not you have a cubic system in which you do not have at the edges for example, why is why do not you have an edge centred cubic lattice? I can ask a question; why do not we have a face centred tetragonal? And we will answer those questions later on there are crystallographic reasons, symmetry related reasons which do not permit the formation of a body centred tetragonal face centred tetragonal lattice.

So, in case of tetragonal there are only 2 possibilities 2 distinct possibilities simple tetragonal and body centred tetragonal, this is primitive and this is non primitive. Remember body centred systems are represented as I so, whenever you have in the crystallographic terms any lattice represented as p which means primitive, I it means body centred and f means it is face centred ok. So, these are crystallographic notations

which will be useful for you to remember to identify or distinguish between various lattices.

Third one is called within orthorhombic now you have 4 categories simple orthorhombic same as simple cubic and simple tetragonal so, again it is p, you have body centred orthorhombic which is same as body centred tetragonal, body centred cubic in terms of it is understanding. So, it is I you have face centred tetragonal orthorhombic which is which is built in a similar fashion as you made face centred cubic lattice, but within an orthorhombic framework.

The next one you have is base centred orthorhombic so, which means what you have here is on 2 of the faces 2 of the opposing faces you have and an atom or a point sitting at the centre of the faces ok. So, you have one point here, one point here. So, total number of lattice points in this case will be 2 because you have 1 by 8 into 8 plus 1 by 2 into 2.

Now, this option you can see is not available in tetragonal and in cubic and why is it not there that we will discuss later. The next option that we next possible variation that we have is of rhombohedral crystal system. In this case you have only one lattice which is called as rhombohedral although it is a primitive lattice we designated as a R.

So, rhombohedral systems the primitive lattices of rhombohedral systems are designated as R, in case of hexagonal system you have again only one kind of lattice that is primitive hexagonal there are other variations which are not possible. In case of monoclinic lattice you have simple monoclinic which is primitive and you have base centred monoclinic same as base centred orthorhombic where you have 2 opposing faces having atoms so, these so, you have a b face 2 a b faces have atoms or points at the middle of those faces ok.

So, this is a base centred question again you can ask a question you can you can think about can you have any 2 opposing faces? Or do you need to have a specific 2 opposing faces? Ok in case of orthorhombic it is simple to answer it does not need to be only these 2 faces you can have you can have centres of these faces as atoms, but only 2 either these 2 or these 2 or these 2 because it is orthogonal system; however, monoclinic is not a orthogonal system. So, question that arises is.

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Can do only these 2 faces must have should only these 2 faces have atoms at the centre of the these or you can have a these also or these also, but only 2 at a time. So, just think about it and we will answer these some of these doubts in the next few lectures. Third and the next last one is triclinic again only a primitive option is possible. So, you can see that there are various primitive lattices non primitive lattices which can be built, but only in a few systems in cubic, in tetragonal, in orthorhombic and in monoclinic rhombohedral hexagonal and triclinic do not allow you to have any other possibility.

So, how many of Bravais lattices do you have now? So, you have 14 Bravais lattices, 7 crystal systems and 14 Bravais lattices. The number of combinations go down in 2D, in 2D there are different numbers and I will just allow you some time to think about it before I give you the answer in the next class to so, a number of possible.

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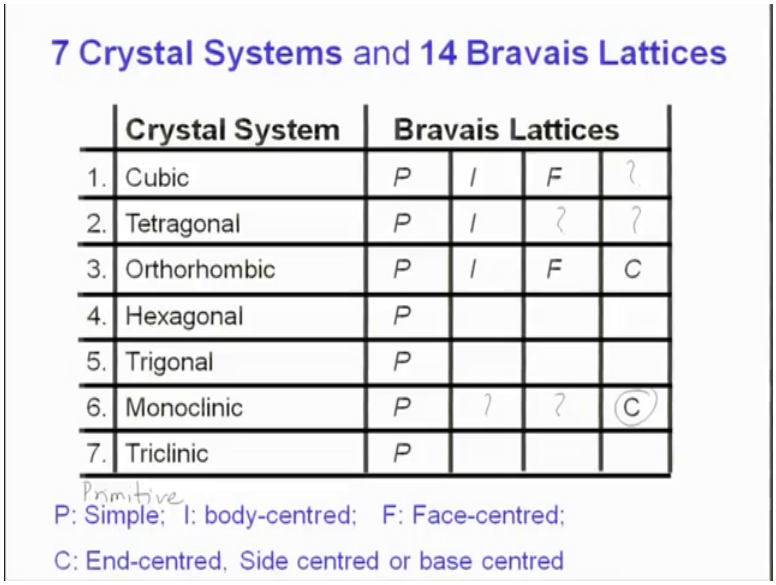

So, this is the sort of summary slides you can see that there are 7 crystal systems in case of cubic you have P I F C, P means simple or primitive I can write this simple or primitive ok. So, P means primitive or simple, I means body centred, F means face centred, C means n centred or side centred or base centred. So, any of these is called as C centred ok. So, you can see cubic has P I F options, but there is no C option, tetragonal has P option and I option, but there is no F option and C option. Orthorhombic is the most versatile, it allows you to have primitive lattice, it allows you to have body centred

lattice, it allows you to have face centred lattice and it allows you to have C centred lattice. Again hexagonal is only primitive, trigonal is only primitive, monoclinic is primitive and C centred triclinic is only primitive.

So, now, the question that arises is why do not you have this? Why do not you have this? Why do not you have this? Let us first discuss these 2 few these few cases and once you understand these cases that everything else will become clear about other cases as well I mean the only thing that you have to worry about then is probably the monoclinic c case. This will this is not possible, but you can see why this is not possible because monoclinic is very least a less symmetry lattice, as a result it is not possible to make a non primitive structure because remember lattice has to be periodic. So, that periodicity of lattice translation symmetry and other symmetry as we will see later on should be obeyed ok.

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	Position of lattice points	Effective number of lattice points per cell
P	8 corners $8 \times \frac{1}{8}$	1
I	8 corners + 1 body centre $8 \times \frac{1}{8} + 1 \times 1$	2
F	8 corners + 6 face centre $8 \times \frac{1}{8}$ $6 \times \frac{1}{2}$	4
C	8 corner + 2 centres of opposite faces $8 \times \frac{1}{8} + 2 \times \frac{1}{2}$	2

So, effective number of lattice points now you can calculate. So, for a primitive systems you have only 8 corners. So, number of lattice points is 1, for body centred system you have 8 corners and 1 body centre. So, total number of lattice points is 2 so, this is 8 into 1 by 8 plus 1 into 1, this is 8 into 1 by 8, in this case it is 8 into 1 by 8 and this is 6 into 1 by 2 yeah sorry and again here you have 8 into 1 by 8 plus 2 into 1 by 2. This gives you the total number of effective atoms in the in itself. So, the questions that we.

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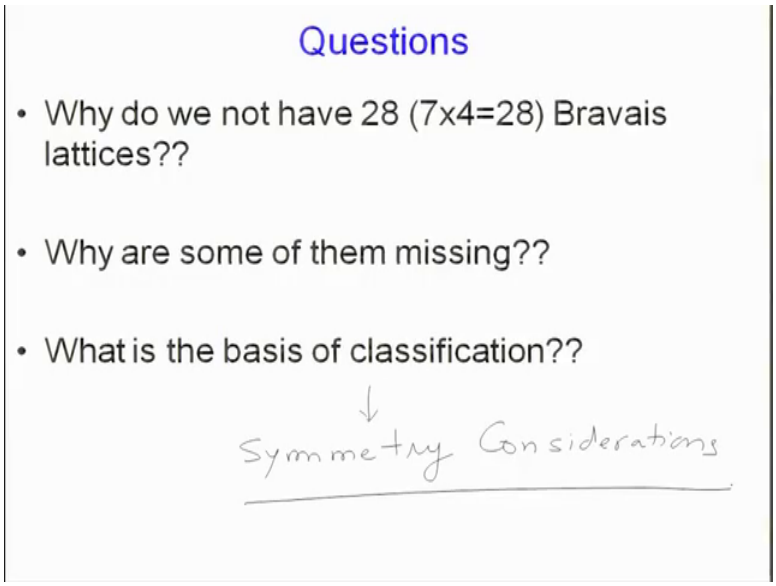

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Now, want to answer is why do we not have 28? Because there are as we saw in case of orthorhombic there are 4 possibilities. So, why do not we have 28 Bravais lattices? Why do we have only 14 Bravais lattices? So, why are some of them missing and what is the basis of classification and the answers will be given in the in that symmetry. So, these answers will lie in symmetry considerations symmetry considerations are typically not talked in any of the standard elementary textbooks of material science. So, this you may not find in the references that I have mentioned in the beginning of the lecture series. So, this is something that you may feel a little bit more attentive to or I will give you some references which are different references to read them about.

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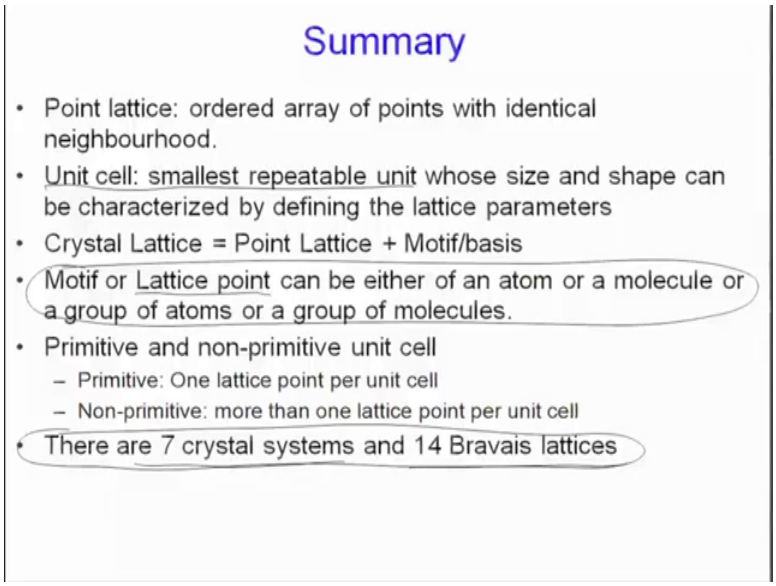

So, to summarize let me just go to the last slide you have a points lattice which is ordered array of points with identical neighbourhood, you have a unit cell which is within a point lattice which can be smallest repeatable unit whose size and shape can be characterized by defining lattice parameters. A crystal lattice can be defined as point lattices with motive or basis this which is a atom or group of atoms. A motif or a lattice point so, we normally call it as a lattice point a motif or a lattice point can be either an atom or a molecule or a group of atom or a group of molecules and depending upon the relative positioning of these atoms and molecules with respect to each other. You define lattice into 2 different types one is the primitive lattice, second is the non primitive.

That definition of primitive lattice is one lattice point per unit cell, we call it lattice point not atom because atom is little misleading the moment you have more than one atom depending upon their relative distribution with respect to each other the definition changes.

So, you may have 1 atom, you may have 2 atoms, you may have 3 atoms, you may have several molecules within one lattice point. So, that is why we refer it as a 1 lattice point ok. So, this is one lattice point per unit cell makes a primitive lattice and this can be very big unit cell within a lattice depending upon the relative orientation and then you can have non primitive one which has more than one lattice points per unit cell.

And then we saw since there are multiple possibilities of unit cell you see you just said earlier we just said that it is a smallest repeatable unit we did not talk about the shape and size ok. So, the question arises is what are the possibilities? Can you have infinite number of possibilities? So, instead of having trouble of finding in this system infinite possibilities let us define certain criteria and that criteria as you will see is based on symmetry it is not a arbitrary criteria. So based on the consideration that we will see later on;

There are 7 crystal systems and based on those 7 crystal systems considering primitive and non primitive considerations and symmetry considerations there are 14 Bravais lattices. So, this is the basic introduction to crystallography, in the next few lectures we will look at what is the underlying reason behind 7 crystal systems and 14 Bravais lattices and that is where you will also understand importance of motif or lattice point. That will become more clearer as you will as you correlate this so, symmetry ok. So, we will end up here.

Thank you very much.