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

Prof. Ashish Garg
Department of Materials Science and Engineering
Indian Institute of Technology, Kanpur

Lecture – 05
Primitive and Non-primitive Lattices

So good morning; today we will start the lecture number 5.

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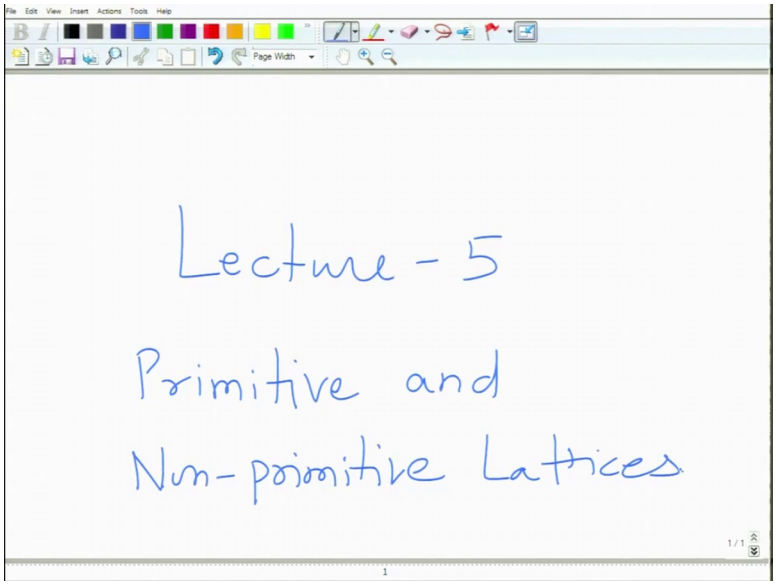

So, and this is again going to be on crystallography. So, what we will talk about and this is the distinction between so, primitive and non-primitive lattices.

Now, this understanding is important, if you want to understand the crystallography to reasonable level. So, let me just give you a recap of lecture 4, in the previous lecture we learnt about what is a lattice.

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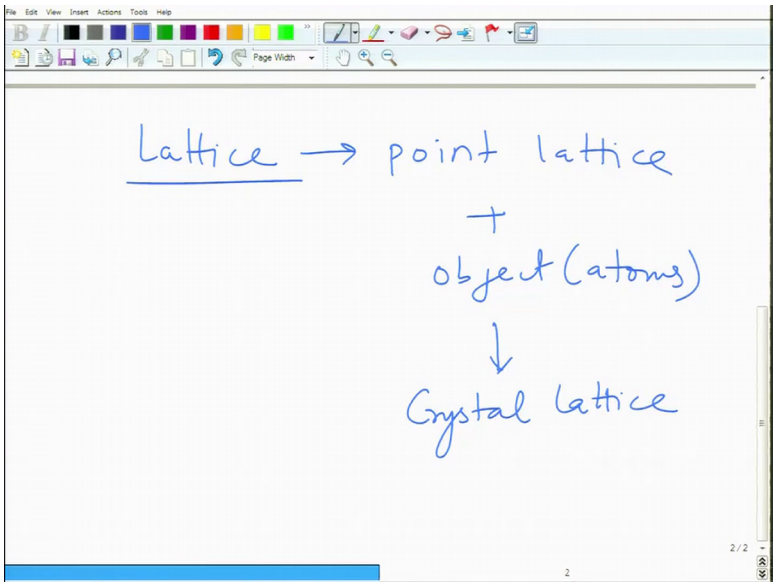

So, lattice is nothing but a 3D arrangement of coins regular arrangement of points in space with the condition that each point must have identical neighborhood. So, this is point lattice as long as you have point it is point lattice. And if you put some object such as atoms to it or it makes as a crystal lattice.

So, basically a lattices a point lattice has 3 arrangement of points in space a crystal lattice has 3, 3D arrangement of periodic arrangement of atoms in a space ok. So, instead of points you have atoms or molecules a group of atoms. And second thing that we considered was, a lattice can be represented by vectors such as so, you can have this cartesian vectors.

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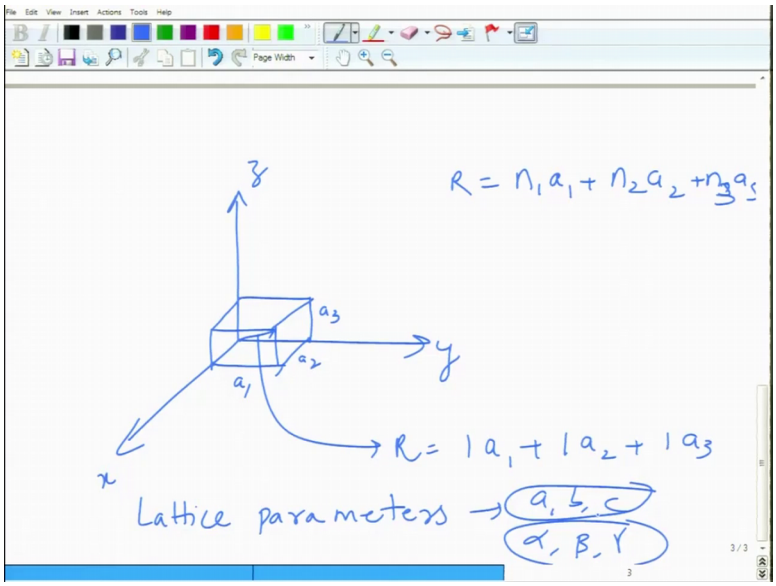

So, let us say this is x, this is y, this is z. So, you can have a lattice which is represented in this fashion ok. So, here I can have a vector such as R, and this R is nothing but n 1 a 1 plus n 2 a 2 plus n 3 a 3. So, n 1 n 2 n 3 are integers, which determine the number of translations translational steps that you take along a 1 a 2 and a 3 axis is so, in this case for example, this is let us say a 1 this is a 2 and this is a 3.

So, this vector R will be; 1 of a 1 plus 1 of a 2 plus 1 of a 3 ok. So, this is what this vector will be. So, and lattice parameters of this can be determined as a lattice parameters are a, b, c; alpha, beta, gamma; a b c are the lengths or unit cell lattice translations. And alpha beta gamma are the angles. Now let me now move to the next topic of this series; which is called as primitive versus non-primitive lattice.

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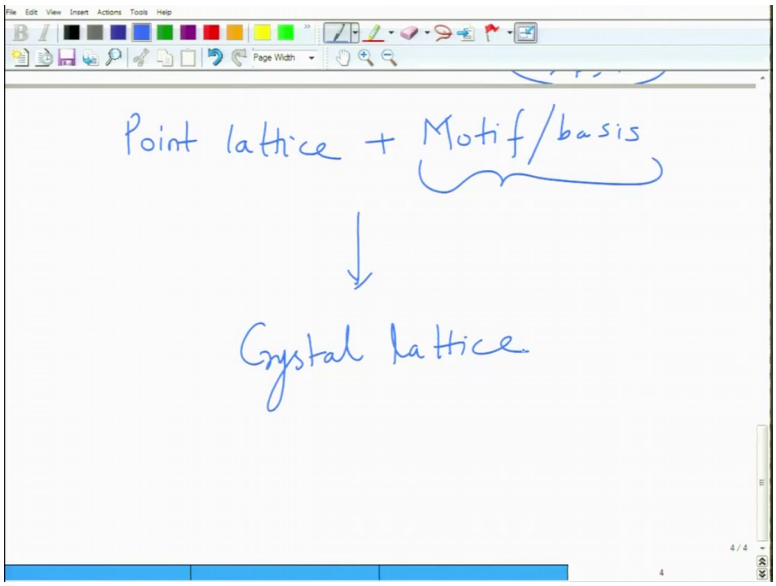

So, earlier we were talking about point lattice. Now I said object earlier I was saying object or atom, in the technical language we call it as a Motif ok, Motif or basis ok. So, when you combine these 2 aspects what you get is a crystal lattice. So, what is this Motif. So, we define this Motif as Motif slash basis now this is loosely used in line in many books and notes.

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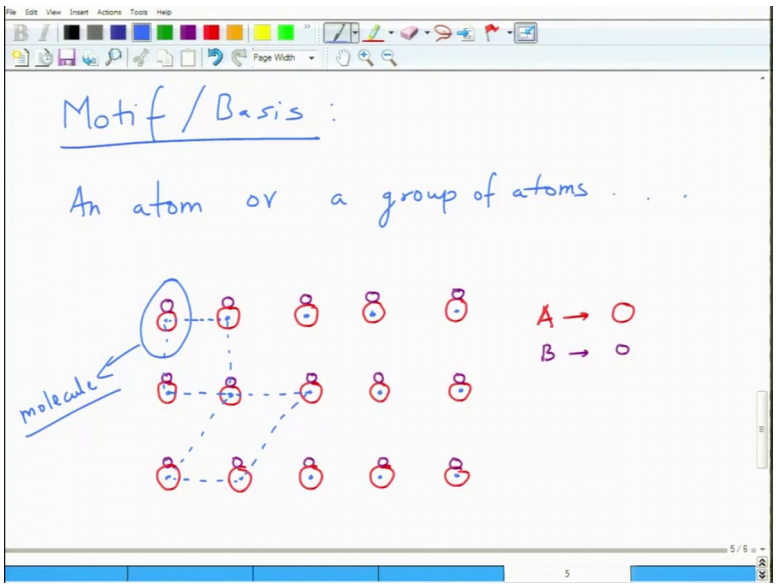

So, either you can say Motif or basis.

So, this is an atom, or group of atoms and so on and so forth. So now, let me just give you a simple example. So, you had a periodic lattice like this ok. So, translations are not exactly equal, but I hope you understand what I mean here. So now, let me replace each of these points by this let us say atom a. So, this becomes a periodic lattice of a, all right. Now for the sake of simplicity we have taken A as a circular or a spherical atom in 3D.

Now, it does not need to be like this for the sake of change or modification, I can convert this a as it could be a molecule. So, for example, if it was a if it was a molecule like this. So, this is A B atom which is attached to A all right. So, this is now so, this is B atom which is the smaller one. So now in this case, this whole thing it is a molecule it is not an atom; I can give you now. So now, this is put on same point you can make it in a different manner.

Now, let me just draw the point lattice again.

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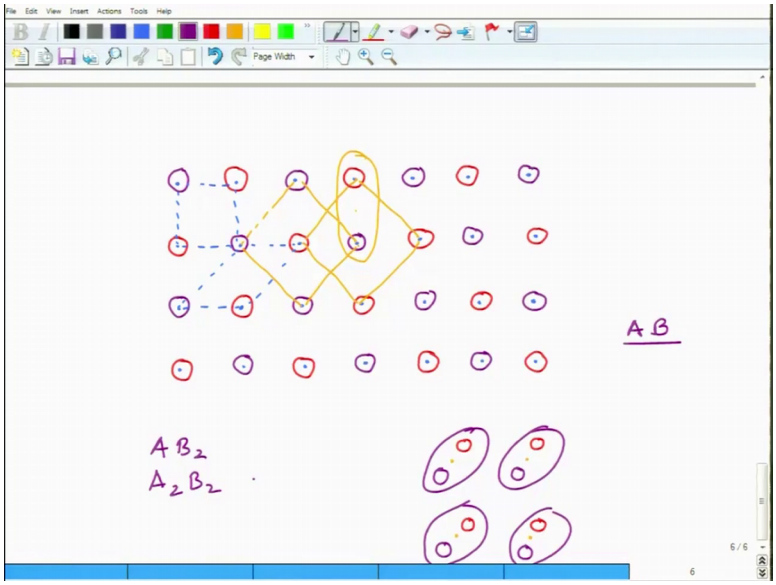

Now what I do here is, I put one atom here, another atom here, another atom here and another atom here ok. And then I put one atom here, here, one atom here, and so on and so forth. And I choose the second atomize which is a.

So, in this case, what is the first of all repeatable unit cell is the repeatable unit cell. So, in the pre-let me just go to previous case, in the previous case the repeatable unit cell is still this one right or you can have this another parallelogram. Let us say this one, but for

the sake of simplest and most symmetric we take the square one or rectangular one ok. So, these are the 2 smallest unit cells, 2 examples of the smallest unit cells.

In this case, what is the scenario? Now is the smallest unit cell same as before this one or is it this one. No, it is not. You can see that it violates the definition of lattice, each lattice point does not have same neighborhood. So, smallest lattice in this case happens to be this one let me draw with a different color this one or that one. So, this is now what is the Motif in this case, what is the basis in this case?

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Basis is this or that.

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Basis is combined right. So, basically the basis is these 2 atoms put together, the unit cell has gotten bigger then what we have been going so far you can just make it smaller and blue remain the same size. But basically, the you can you can now construct this as let us say, this is the smaller unit cell. It is as if you have group of atoms positioned. So, if you look at this unit cell, it is like a dumbbell right. You can move the corner of the unit cell anywhere you want right. The corner can be here, the corner can be here, the corner can be here, all right. Corner can be anywhere.

So, what it will look like is basically you have a dumbbell shaped sort of that representation, one was red. So, let us say this is my red atom. And this is my purple atom somewhere here. So, this is a group of atom or a molecule. This is a simple example of A B kind of molecule. You can have much more complicated one. So, you can have A B 2 you can have a 2 B 3 and so on and so forth.

So, the moment you have more than one atoms. You need to look at the repeatable unit cell very carefully. So, as to ensure that at least one formula unit lies within the unit cell. So, how many formula units are there in one-unit cell, you have one formula unit in the unit cell, you can see that there is one of a and one of B. You can have more than one of more than one as well and we will see that later on, but at least one must be there ok. For a that is the bare minimum requirement.

Now, so, based on this let me now provide a definition to do this. So, you have a lattice like this.

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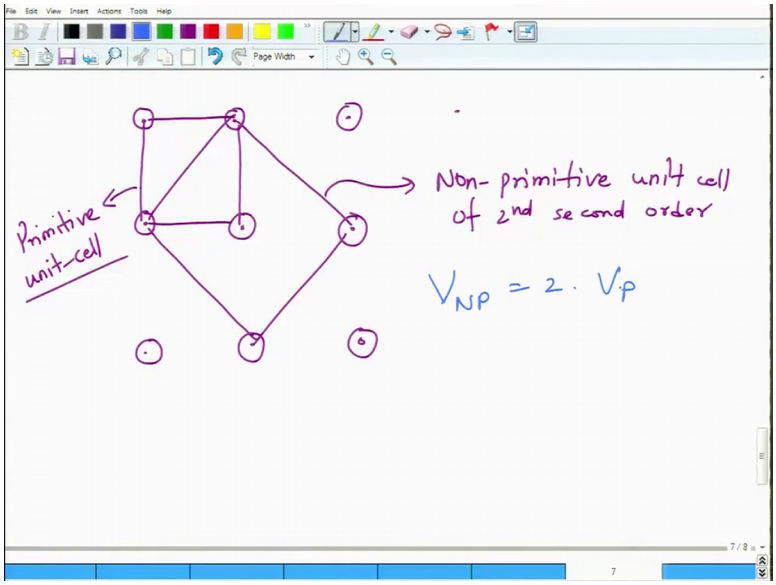

I just draw few of them ok. So, when I said, I have one atom of this, this is one, this is one, this is one, this is one. If I have this off same kind, then I draw a unit cell, this is a repeatable unit cell. This unit cell is the smallest unit cell and how many a atoms it consists of it consists of only one atom. So, this is called as a primitive unit cell.

Now, if I can draw a bigger unit cell which is also the beatable in a space like this, right, how many atoms does it have? It has 2 atoms. So, this is called as non-primitive unit cell of in this case second order. You can go higher and higher, things are simple when you have just one atom things become a little complicated when you have more than one atom. So, I gave you one example last time.

So, if you take the example of more than one atoms. Now of course, you can have some more correlations here. You can see that non-primitive unit cell that is next order non-primitive unit cell contains twice the number of atoms. As the primitive unit cell contains the area or the volume of non-primitive unit cell is area is number of atoms multiplied by the area or volume of the primitive unit cell.

So, you can see that here V N P will be equal to twice of V P all right. So, I can give you little bit more difficult example ok.

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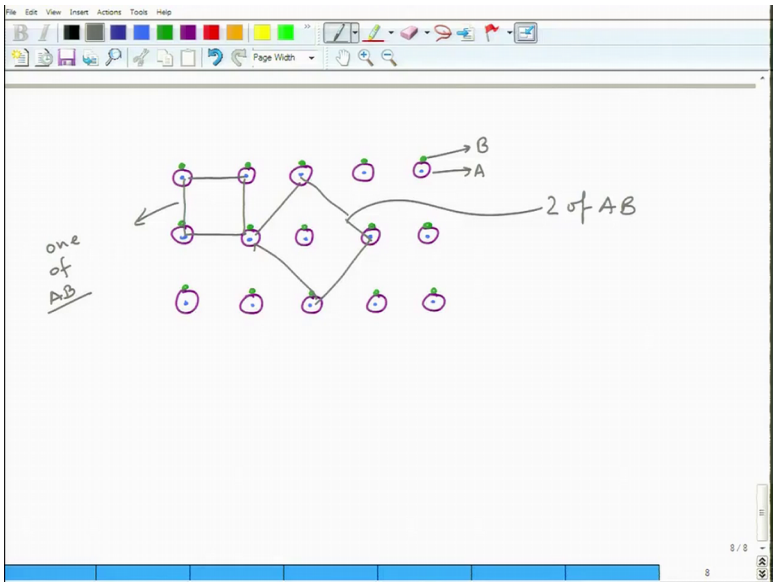

Now let me let me say I my Motif is not a single atom, but it is a group of atom ok. So, let me just throw these little ones here ok. Now first example, I take is I draw this little green dot here ok. This is same as before it again has a primitive unit cell which is like this.

So, this is the primitive unit cell, and it contains now one molecule of A B ok. Because this is A, and this is B. Again, you can draw the non-primitive one, this is the non-primitive one, and this will contain one of 2 of A B. Now let us make things slightly more tricky, with this what I do is that I again draw a smaller simple lattice ok.

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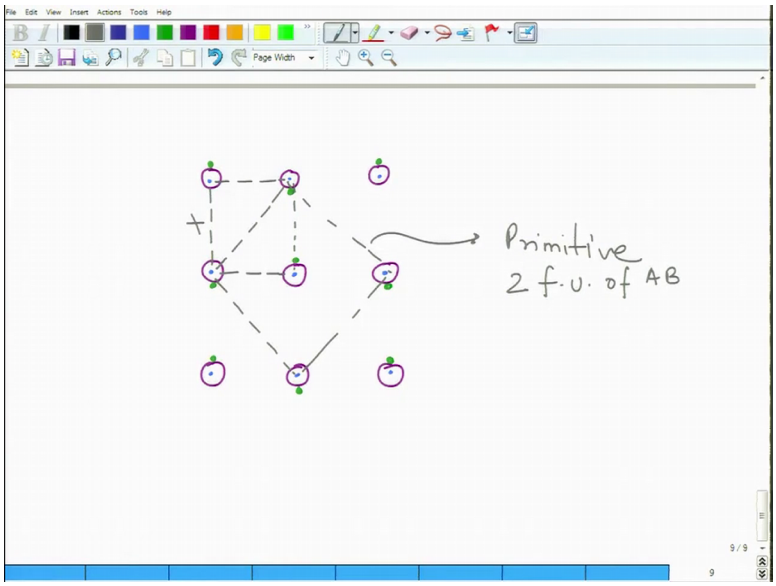

And I put the green atom one here, one there, one here ok. And then one here, one there, one there, one here, one there and one here. So, which is the repeatable unit cell now. Is this the repeatable unit cell? Yes, this is not, right? What about this? So, this is not . So, you will know the straightness, it is not very straight here, what about this? It is so now, this is the smallest unit cell. So, this is the smallest unit cell which means this is the primitive lattice. So, this is the primitive lattice.

But it has,

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Two formula units of A B not just one. So, primitive unit cell does not necessarily have to contain one formula unit in the case of molecules ok. It can contain more than one formula unit, it depends upon the relative orientation of molecules with respect to each other. And then you have to figure out which is the smallest repeatable unit cell, all right? So, again you can find you can make it a little bit more complicated there are several examples of that. So, these are certain illustrations that you can you can do away with.

Now, let me let me give you a few examples of these primitive and non-primitive lattice in a little quick manner. So, we are talking about the parameter non-primitive lattice.

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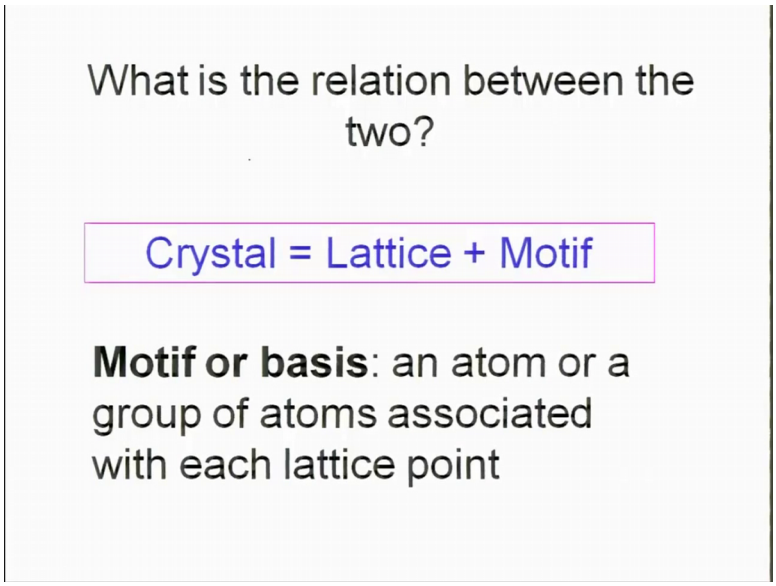

So, basically, we said that the Motif for basis is an atom or a group of atoms which is associated with each lattice point. And I gave you a demonstration of when you put a when the atom is replaced by a molecule that things could be quite different. The definition of primitive a non-primitive unit cell does not remain the same.

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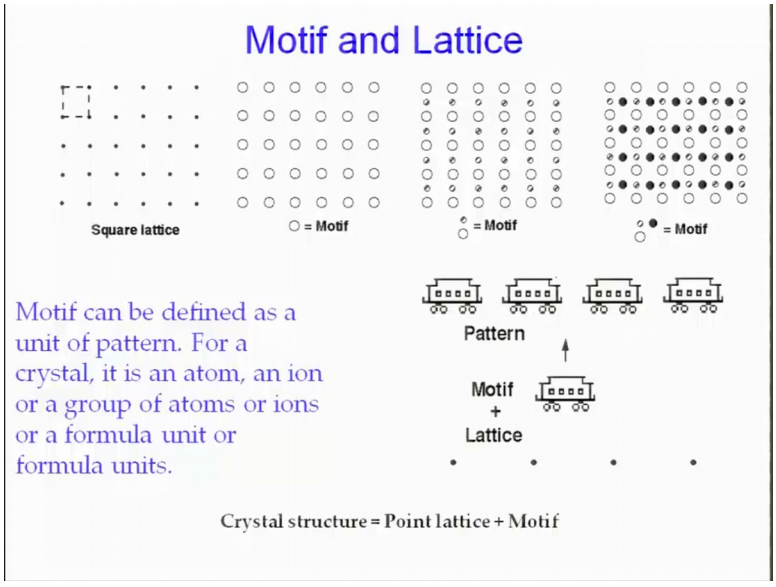

So, basically so, we said that you can have a square lattice like what you see on the left this is the square lattice, and then this could be a Motif, or this could be a Motif, or this could be a Motif. So, this is much more complicated Motif, there you have 3 atoms

instead of having just 2 atoms Motif. Can does not need to be a very symmetric object? It can be a symmetric object; for example, it can be something like that you can have a pattern like these this trolley, and when you when you when you combine this periodic lattice with either with a trolley like that then you get a lattice off trolley.

So, this is sort of a trolley lattice, the only condition is that all these all these atoms or group of atoms or objects should be arranged such a such a manner. So, they make up periodic lattice. So, that there is a distinct there is a distinct distinctness about the neighborhood of each of the lattice point that you see. So, for example, this is a lattice

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which is which professor Rajesh Prasad from IIT Delhi gave me. So, you can have this periodic arrangement of hearts ok.

Now, this periodic arrangement of heart says like it is like a he used to call it a love pattern. And so, this is like a lattice. If you replace each of the point by a heart it becomes a love pattern something like that.

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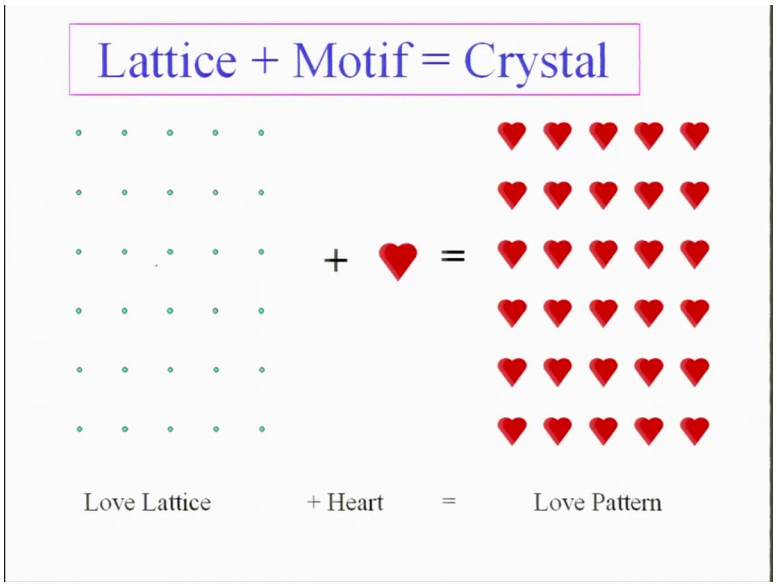

And you can have a monkey pattern, you can have a dog pattern you have provided all the dogs or monkeys are arranged in such a fashion so that you make a periodic one.

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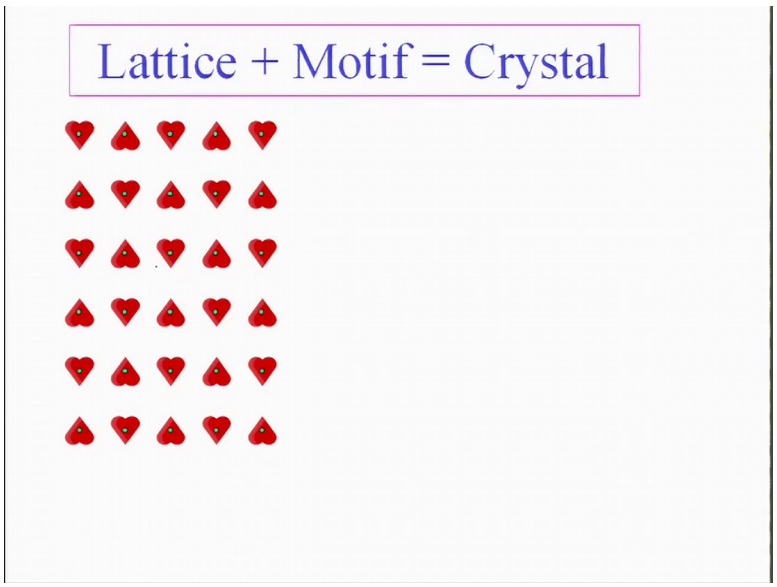

So, this is the illustration of how you can have a primitive lattice with different arrangement of now you can see that each of the heart is arranged in such a fashion. So, that each alternative heart is in same orientation. So, as a result what you have is when you now represent it using the lattice now the Motif is this. So, as a result the periodic lattice does not remain the same as what you had earlier, you need to define it differently.

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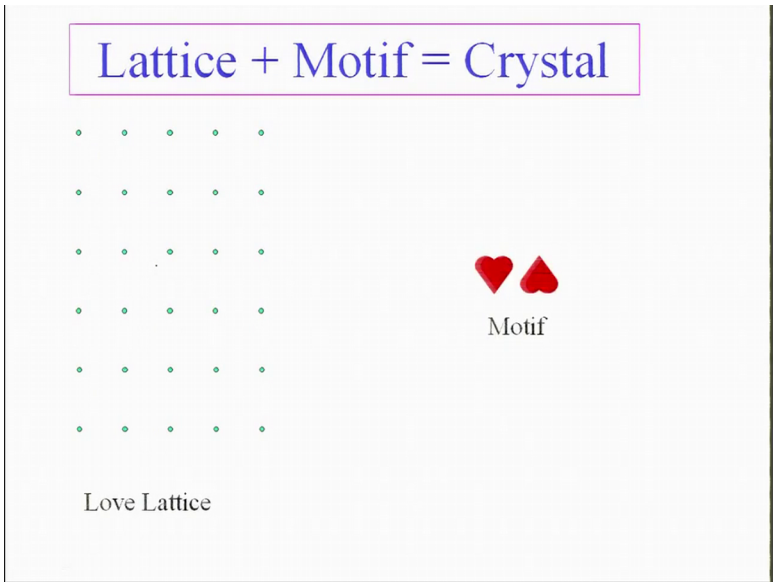

So, I will show you how, you do that now.

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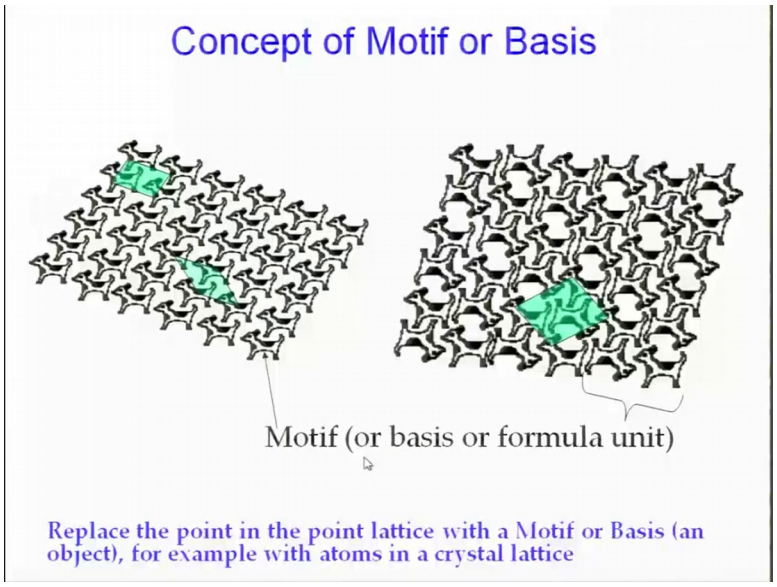

So, this is for example, the set of dogs who are standing, you can make a periodic lattice like this. And this is the unit cell that you draw the green one. So, this one or that one these are all primitive unit cells; however, in this image on the right now what I have done is, I have changed the orientation of each alternating animal.

So, for example, these and let me just change a color of the pointer. Let me just bring 2 arrow. So, so this dog is standing up. This is standing up. This is standing up, and every

alternate one is standing upside down. So, here now if you want to draw a periodic lattice, this periodic lattice, or that periodic lattice on the left cannot be the periodic lattice here. So now, here when you want to now make a lattice is bigger which contains one up side facing up standing animal and one downside facing animal.

So, basically the formula unit in the previous case is this animal one animal, in this case the formula unit is a group of 2 animals. One is standing up, one is standing down. This is what happens with atoms. So, you can consider an animal which is standing up like one type of atom, and the animal which is standing upside down is a another type of atom ok. So, basically what you have to do is that you replace the point in each point lattice with the Motif for basis. And in case of crystal structures, we do that with atoms or group of atoms or molecules.

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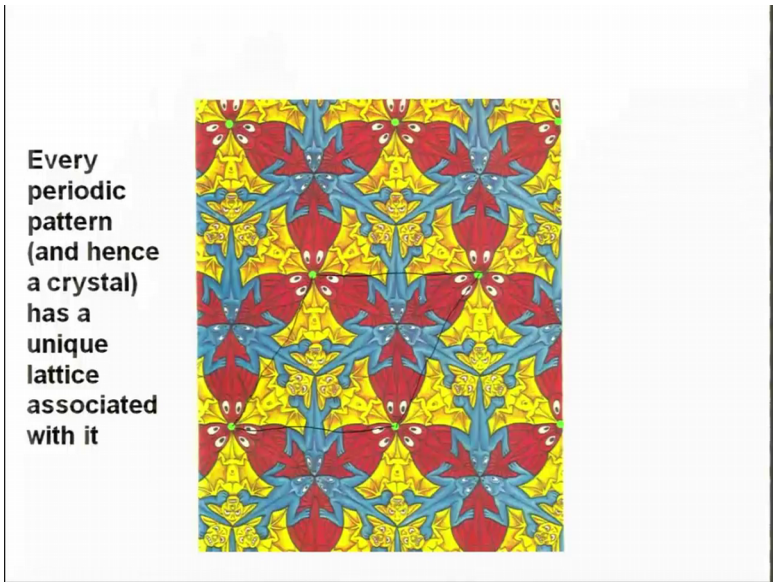

So, this is for example, a very famous picture by mc escher; which depicts air water and earth. So, you can see that there are there are 3 kinds of species here. There is fish, there is bat, and what you have is a lizard right. So, these 3 animals represent the 3 constituents of universe air water and earth.

Now, in this pattern, can you find out the primitive lattice, first of all? So, I put one point here, the first one. The one in the green here, can you see that? And then I put the green points all over the place. So, you can see that there is certain periodicity with it. Each green point has these 3 inward looking fishes, 3 bats and there are 3. So now, 3 lizards

which are not visible. So, what you can do is that, you can move this point somewhere else.

So, basically you can say that every periodic pattern as a result of crystal has a unique lattice associated with it. So, when you now make a lattice out of it, if you go to the previous one this was a previous scenario. So, what is the lattice in this case? The lattice would be if you come from here learn let me now draw it for you yes. So, this, this, this and this ok.

However, as I said, at the point of lattice does not need to be there. So, what is the Motif in this case now? Can you determine what is the Motif? The Motif is how many bats does it contain 3 bats. How many lizards do you have? 3, and how many fishes you have? You have 3 fishes, right? There are some which are being cut here, but there are some which are entering from here. So, overall, they make up 3 fishes. So, overall within one-unit cell you have 3 fishes, 3 lizards and 3 bats. This is the Motif in this case.

You can consider each lizard is one atom each bat is one atom and each. So, it could be just a, b, c; 3 atoms. So, each lattice now has 3 atoms A B and C. And 3 of them, not just one of them, 3 of them. Why 3 of them? Because all 3 of them are differently oriented with respect to each other.

So, as a result, each has 3 of each species in the primitive lattice. So, you can move this lattice, wherever you want and still it remains a periodic lattice. I can put the centre here, and it still remains the same. If I now draw the lattice, the lattice would be this. So, it does not matter where you put the unit cell corner. It still contains 3 of a 3 or B and 3 of c, or 3 fishes 3 bats and 3 lizards.

So, this is just a illustrate of what the lattice could be.

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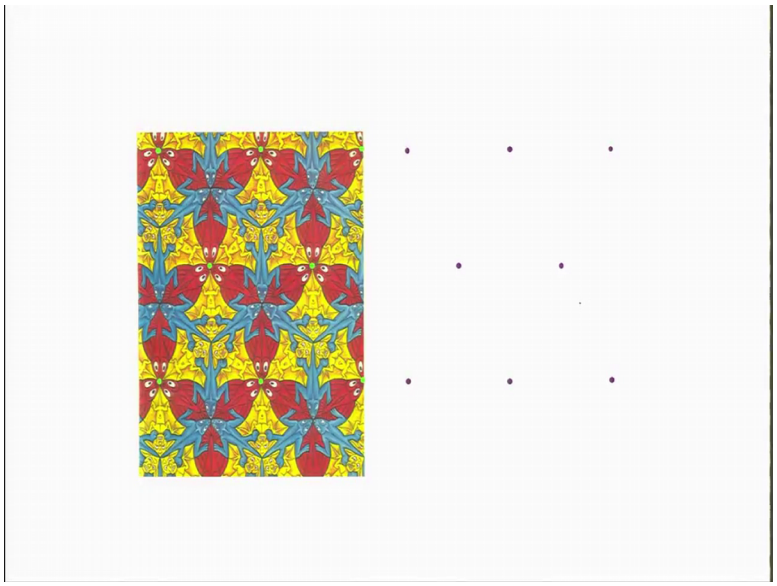

So, this is kind of if I remove the pattern from there. This is how it will look like.

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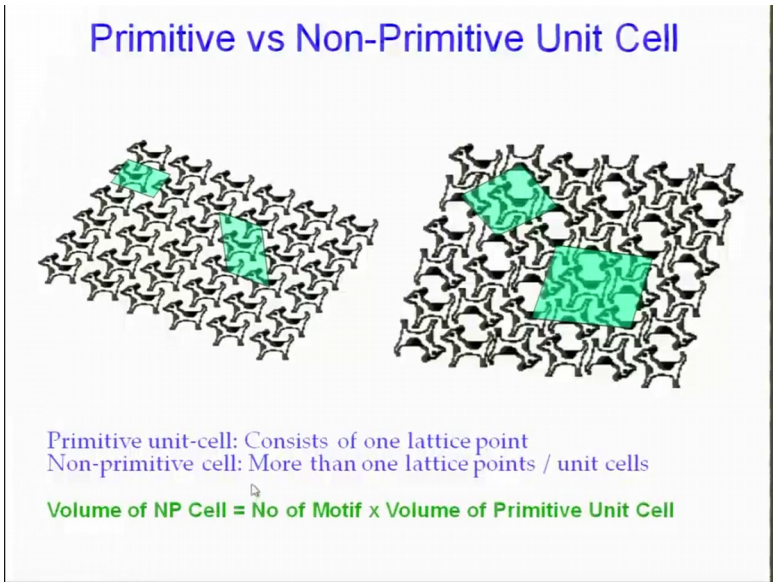

So, I was talking about primitive and non-primitive unit cell. So, basically this is what is the definition of primitive unit cell, primitive unit cell consists of one lattice point. Technically speaking, each atom in this case each animal is a lattice point ok.

However, and for each of them the lattice point is identical ok. On the other hand, if you look at the non-primitive unit cell for example, this is the non-primitive unit cell. So, just go to the pointer. So, this will be the non-primitive unit cell, it contains consists of 2

lattice points. Here in this case again, a primitive unit cell consists of one lattice point; however, one lattice point is now consisting of 2 atoms; A and B of 2 animals, upside down and down side up. And the non-primitive one will contains; consists of 4 animals, 2 upside and 2 down side. That is the difference between the perimeter and non-primitive unit cells.

So, volume of a non-primitive unit cell, as I said will be equal to number of Motif, or number of lattice points; multiplied by the volume of the primitive unit cell. Actually, number of lattice points is more precise definitions, because lattice point can be one atom, it could be group of atoms all right.

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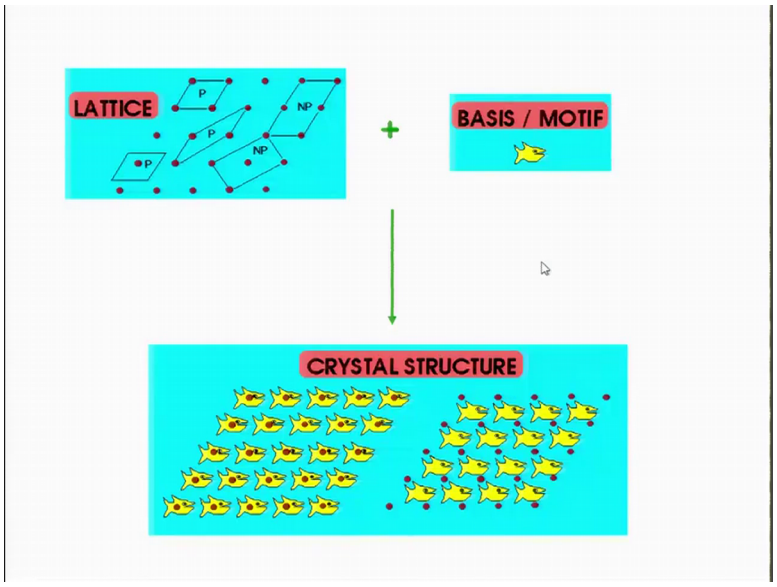

So, this is what the definition of lattice can be summarized as. You can have write your primitive lattices in a periodic pattern. So, this is a primitive lattice, this is a primitive lattice, this is a primitive lattice.

So, you can see that in the first 2 cases, you have chosen to keep the corner of the unit cell at the lattice points themselves, but it does not matter you can keep the corner of the unit cell anywhere in that within the pattern. As long as you have one lattice point within the unit cell. Here the lattice points are shared here; you have one lattice point within the unit cell. This is a non-primitive unit cell, this is again a non-primitive unit cell, you can make the non-primitive unit cell. Likewise, you make different possible options of

primitive unit cells you can make, several options on one-unit non-primitive unit cells as well.

So, this is if you just to somebody. So, this becomes a crystal structure in this case. if you replace a point by a Motif.

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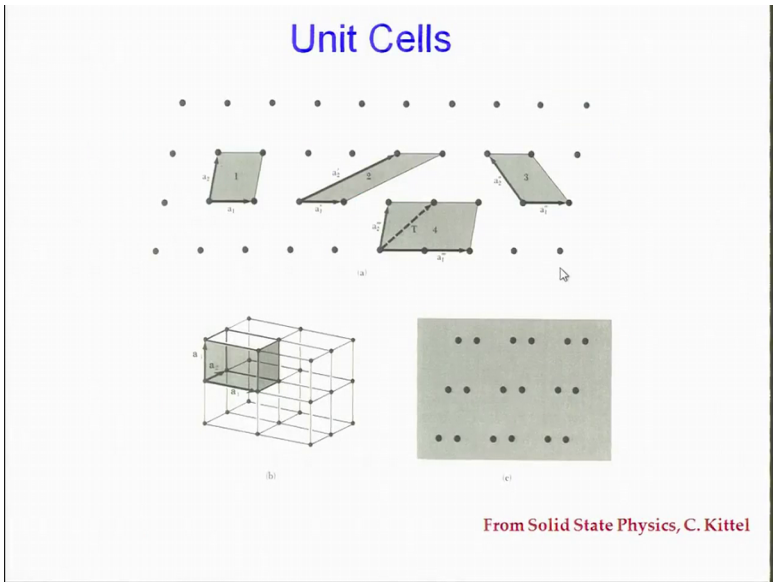

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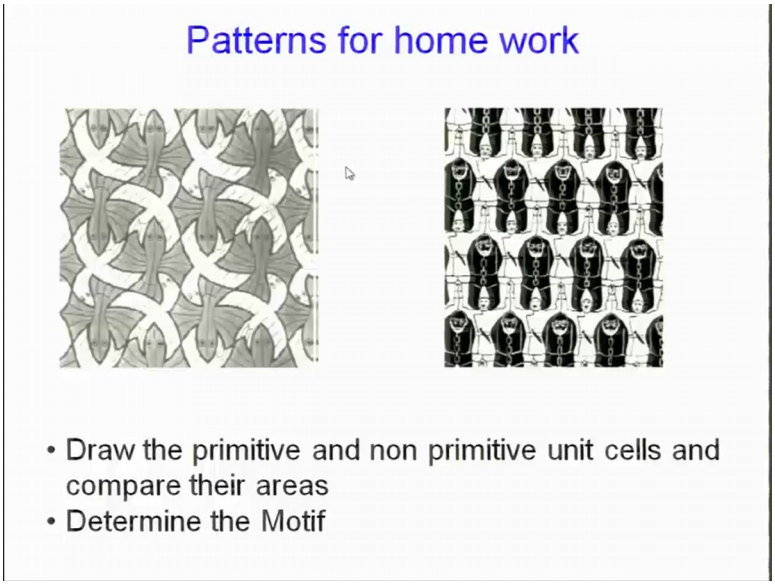

So, I will so, these are some patterns which are which are provided to you can choose these if you go to, if you go online and just google assure patterns ok. And there are a variety of assure patterns which are available not necessarily these, but you can choose

any periodic patterns, and try to draw the primitive unit cells and non-primitive unit cells and compare their areas compare the lattice points what is the lattice point made of determine the Motif in each of these cases ok. So, these are just 2 examples which I am giving here, but you can you take them you can just Google for a share patterns so, all right.

So, this takes us to the to the end of this particular point, which will bring us to the next lecture. So, let me now summarize at this point, you have a you have a point lattice, and when you replace points and the point lattice by atoms or group of atoms or molecules, you make a crystal structure. Now depending upon you can associate incase of in case of one atom it is easy. In case of one atom each unit cell will each smallest unit cell will consist of one atom, and it will it will be called as a primitive unit cell. And we call each of the point and the point lattice or the lattice point.

So, in this case the lattice point is associated with one atom. The things will change when you replace one atom by multiple atoms, multiple different types of atoms or different molecules. That is where the relative orientation of a relative position of atoms with respect to each other will determine, what kind of primitive lattice will you have, and how many lattice points, how many atoms or molecules will be associated with one lattice point. It is possible that one that is mole in may contain one molecule.

But it is also possible that one lattice point may contain more than 1 2 or more than more than even 2 or 3 more molecules. There are several examples of that. So, so essentially it will be governed by relative positioning of molecules with this petitioner provided, they make a periodic pattern. That is ultimate takeaway ok. So now, we will pause here. And we will now go to the next lecture which is on unit cells and crystal structures.