Basics of Materials Engineering
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Lecture - 04
Crystal Structure - 2 (Unit Cell, Lattice, Crystal)

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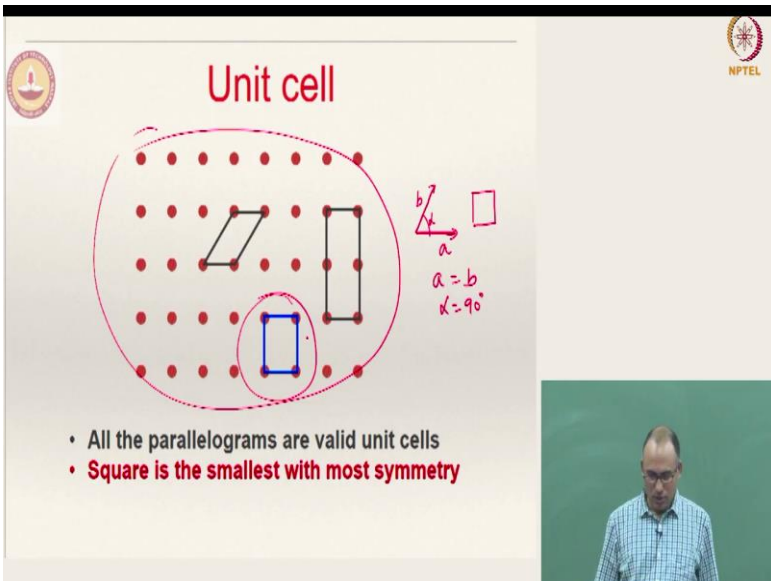

So, in the last class we have looked at the concept of unit cell, and if you are having a lattice you can in principle identify infinite number of possible unit cells that can actually fill the entire space. But then the question is what should be the geometry, alright? What should be the geometry of that unit cell?

For instance, in 2D, should it always be a parallelogram? Can we not have a triangular unit cell and so on? So, the way that the unit cell is defined is the following. Unit cell is an entity which when translated along the lattice vector or along the coordinate direction -- for instance if you are talking about 2D what are the parameters that are required to describe a unit cell? One vector in x direction and another vector in y direction.

So, this is vector let us say **a**. The distance is *a*, and the distance is *b*, and the angle *α*. This side is **a**, that side is **b**, and **a** and **b** have an included angle of *α*. Now, you can define as many unit cells as you want.

If you have conditions like $a = b$, and $\alpha = 90°$, then you will have a square unit cell. If $a \neq b$, and $\alpha = 90°$, then you will have a rectangular unit cell, and so on. You have this small geometry; you take this geometry and translate the geometry in the lattice directions or lattice vector direction.

This is what is called lattice vector, and if you take this geometry and translate it both in x direction as well as in y direction for 2D, then it should fill the entire space. It should not leave behind any voids. Only then such a geometry qualifies as unit cell.

Now, imagine having a triangle. Can you fill the entire space of this particular lattice using a triangular unit cell of your choice without leaving behind any voids? Is it possible? Just by translation it is not possible. You will have to rotate the unit cell. And hence your triangle cannot be a qualified unit cell for filling the space, right?

In general, in 2D, a parallelogram will be a qualified unit cell, and in 3D a parallelepiped will be a qualified unit cell, right? What will be a unit cell in 1D?

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It will be a line. Line will be the unit cell in 1D. And then we have discussed the concept of primitive unit cell and non-primitive unit cell, right?

What is the meaning of primitive unit cell? Primitive unit cell is the one which has effectively one lattice point associated with the unit cell and if it is a crystal then effectively it will have 1 atom or 1 molecule or 1 ion, depending upon what is the point that is sitting -- we will talk about it in a moment ok?

This is the smallest unit cell right with highest symmetry. So, usually the guideline is you choose the smallest possible unit cell as your unit cell of the lattice that you are looking at, but it is not a requirement. In principle you can choose infinite number of unit cells as they we shown and then fill the space, ok?

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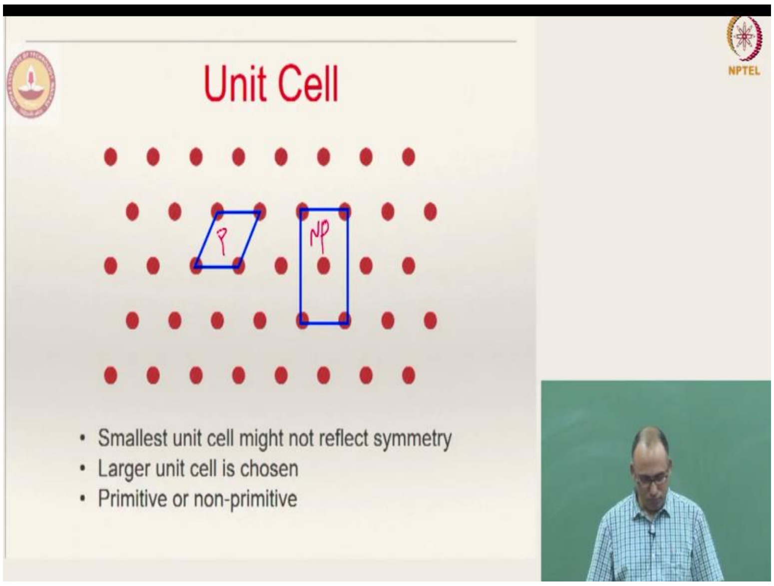

Previously we have seen a rectangular unit cell and hence you have a different set of unit cells that you would get. Here, it is not possible to get square as a unit cell because the way the lattice points are arranged it is not possible to get square as a unit cell. So, you will find something else as your appropriate unit cells and here you have seen this is a primitive unit cell, this is a non-primitive unit cell.

Why is it a non-primitive unit cell? Because effectively it has 2 lattice points per unit cell, and hence it is a non-primitive unit cell. So, you can also choose non-primitive unit cells to fill the space. There is no problem with that.

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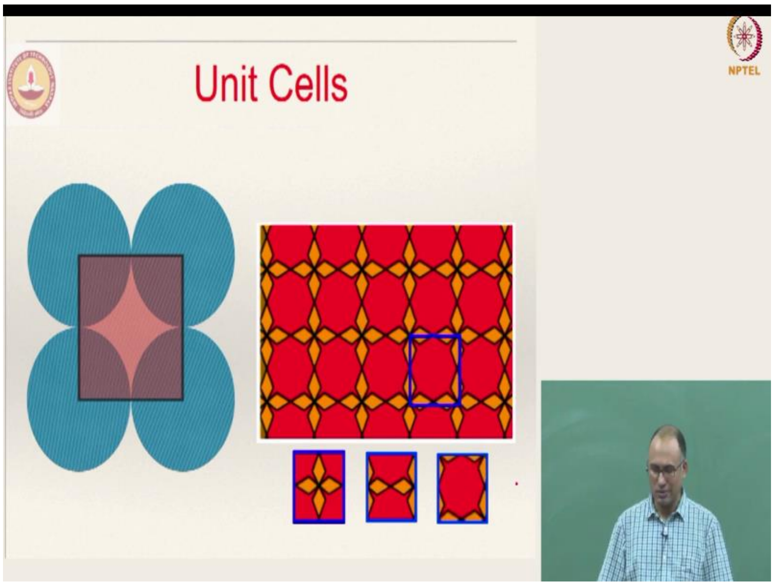

I think we have looked at this concept. You have this tiling and then 2-dimensional map and you are trying to see the different unit cells that are possible. So, we have already identified this as a possible unit cell and then that geometry as another possible unit cell and that geometry as another possible unit cell.

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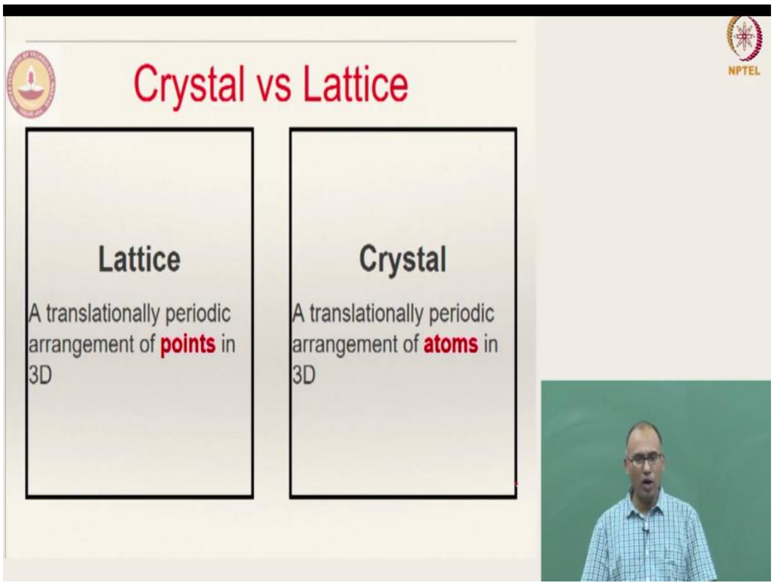

So now, we have only looked at the definition of lattice, right? What do you mean by crystal? What is the difference between crystal and a lattice? So, lattice by definition is a translationally periodic arrangement of points in 3D. That is what we have seen, right?

When we saw the Cambridge wall example, what we did was we have identified bricks that looked identical. It is a 2-dimensional space and we have identified those points and then removed the brick wall. Then the set of points is what we call lattice. So, it is basically a translationally periodic arrangement of points in 3D in general. But, if you are defining a 2D lattice, that will be in 2D. If you are defining 1D, then it will be 1D. Now, what is a crystal?

When we are defining lattice, we only said it is a periodic arrangement of points. These points can actually be occupied by some real stuff. If they are occupied by atoms, ions or molecules, then that becomes a crystal. So, a translationally periodic arrangement of atoms in 3D is called a crystal.

Sometimes, a crystal need not be of a pure metal, but it can be a of an alloy. If you look at iron crystal, so only iron will be there, but if you want to look at iron oxide, then Fe_2O_3 will be there at the lattice point. That is the idea, ok?

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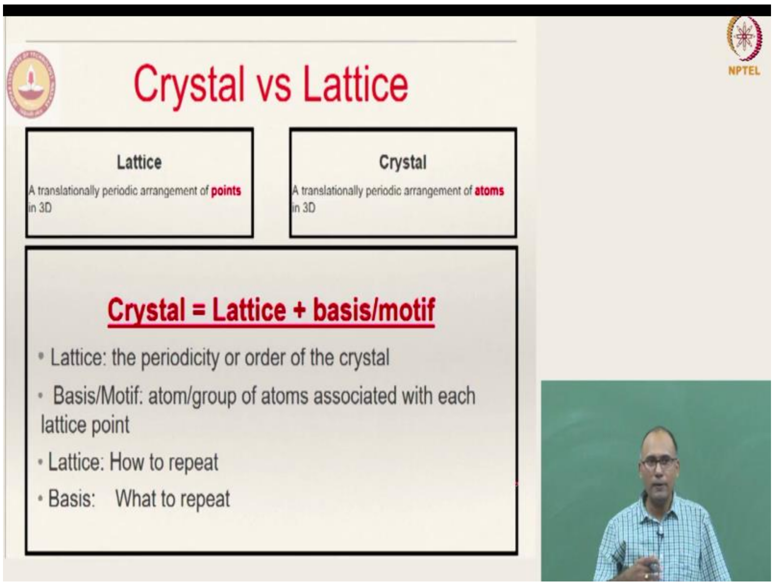

To reinforce this idea of the correspondence between lattice and the crystal, a crystal is nothing but, lattice plus a motif or basis. That means, whatever sits on the lattice points is what is called motif, then the moment you add motif then that becomes a crystal of that motif. So, what lattice tells you is how to repeat the points.

The moment we have removed the brick wall, you have got the points. Now, once you have the points, you can actually construct the entire brick wall it showed you how to repeat these points. So, lattice tells us how to repeat, and basis or motif tells us what to repeat.

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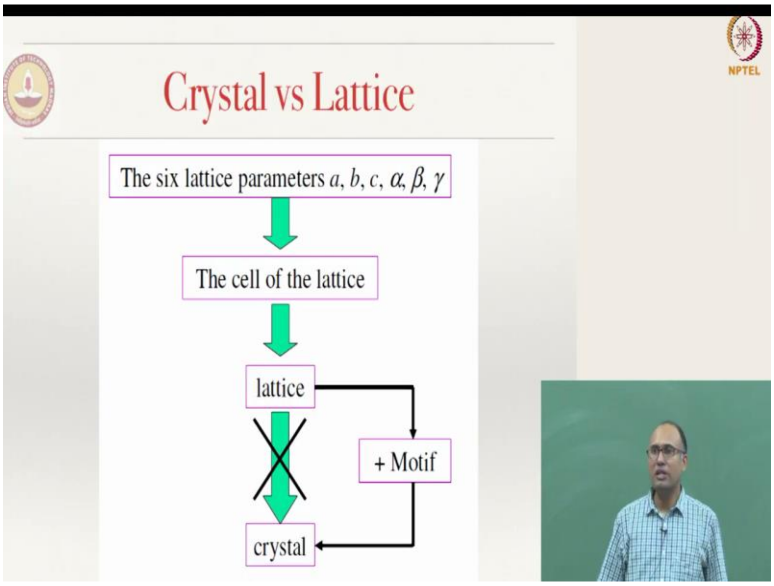

How many lattice parameters are required in 2-dimensional situation to define a lattice or to define a unit cell? Three: a, b and α. In 3D, you have 3 edges and 3 angles. So, a, b, c, α, β and γ, right? You have these 6 lattice parameters and then you get the cell of the lattice, that is the unit cell. Please note that unit cell has nothing to do with the size being unit, ok?

So, unit cell size need not be 1. It is the basic unit that is being repeated, right? It is not about the number 1, it is the basic unit that is repeated, that is why it is call unit cell, ok? Then, you have the cell of the lattice, and from there you can actually construct the lattice. But that will not be called a crystal; the lattice cannot be called a crystal. You can only call lattice as crystal when you add a motif to that, ok?

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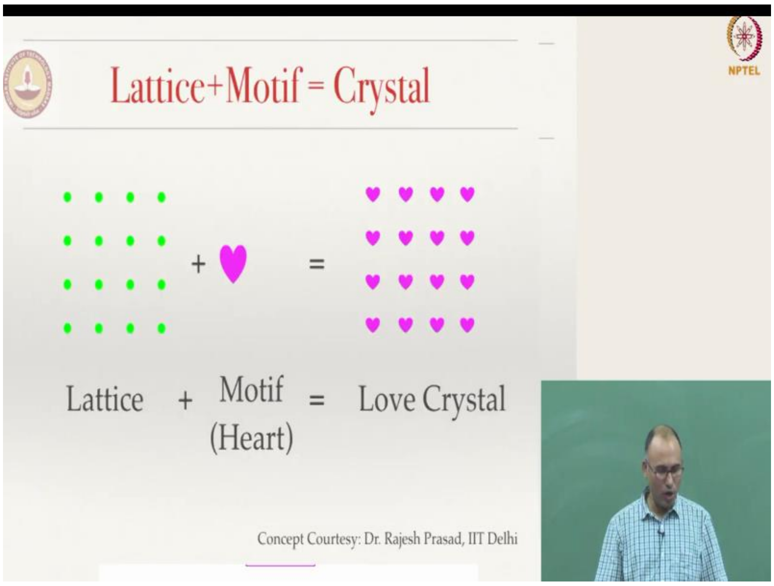

So, how do we understand that? Let us say these are your set of points, lattice points, and then you have your heart as motif. You put heart at each and every position and then you get something called love crystal or heart crystal. If you replace that with football, you will get football crystal.

If you replace that with hatred, you get hatred crystal. You can construct any crystal, right? So, that is the idea. So, now, you replace that and then you know how to distinguish between the definition of a lattice and a crystal, right?

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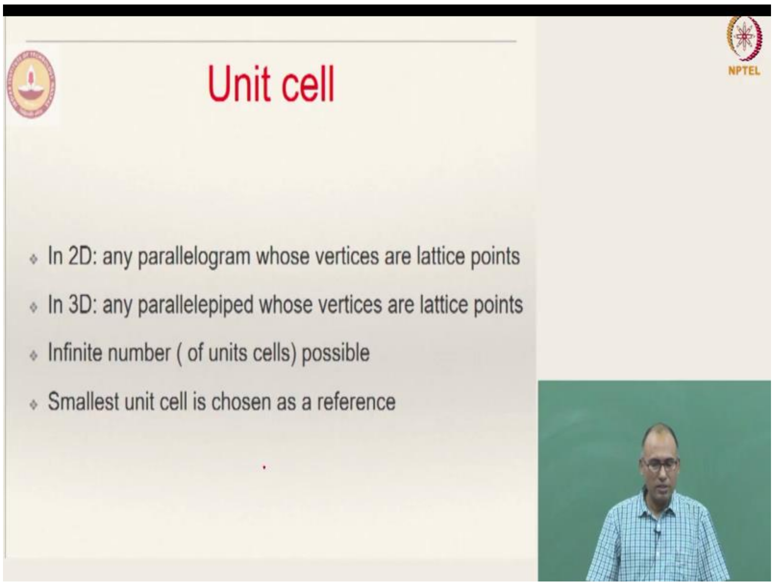

In summary, in a unit cell in 2D, you will have any parallelogram whose vertices are lattice points. If it is 3D, it should be a parallelepiped, and we have discussed that in principle you can have infinite possibilities for unit cells in 2D and 3D.

How many possibilities are there in 1D? How many kinds of unit cells can you generate in 1D? Infinity. How? Very good. How many primitive unit cells can you define in 1D? How many?

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In 2D. Think about it, ok?