Crystal, Symmetry and Tensors
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Lecture 1d
Unit Cell

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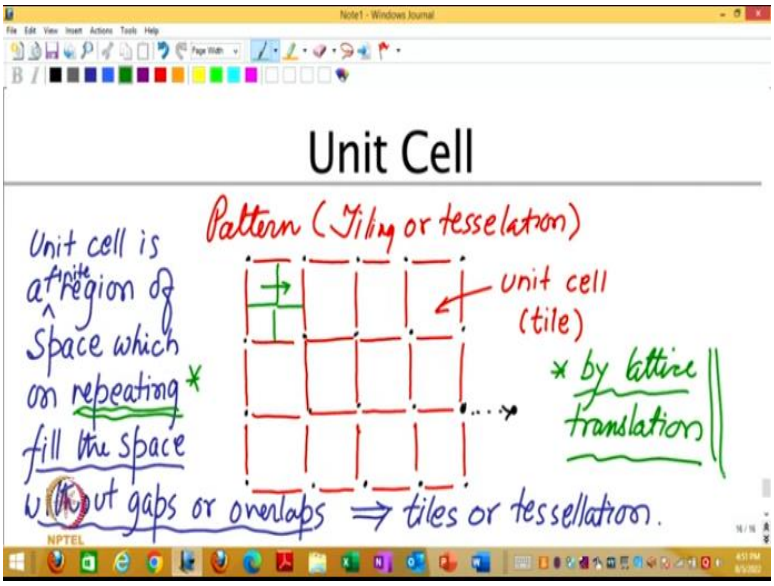

Now we come to the idea of unit cell. Lattice is finite or infinite? Infinite, I am only drawing finite portion of the lattice and leaving rest to your imagination, but you have to keep thinking that points are going in all directions at the same distance otherwise, that definition of periodicity is violated, the definition of equivalence surrounding is violated if I say only this many points, then where is the neighbor to this point? There is no neighbor. So, we are assuming that continues this also has a neighbor and so on so, it will go to infinity. So, it is an infinite structure infinite structure always difficult to handle.

So, we seek for some finite representation of that infinity and that is where the unit cell comes in. That if we select a finite region such that on translations by lattice translations, it fills the entire space or in mathematical sense we call it tessellates the space. So, if we create a tessellation, tessellation just tiling so unit cell is a tiling of the entire lattice or the crystal.

So, the entire pattern can be considered as a tessellation as set of tiles and each unit tile is your unit cell. So, to define it, we will say unit cell is a region of space obviously, a finite region of space let us put that fill the space, in what way? Fill the space without gaps or overlaps. So, filling the space without gaps or overlaps for that, a short word is that it tiles the space or tessellate the space because tiles floor tile, you will not like one tile to overlap on the other tile, you will not like gaps between the tiles, so, the flooring is good only if tiling is satisfying this criterion that there are no gaps and no overlaps.

So, unit cells should satisfy the same criterion, so, unit cell is actually a tile of the whole space. One thing I am missing here, that if you want this, this has to be this repeating by lattice translation, this was required actually is an important part of the definition which I was missing again that a by two example if I do not put this lattice translation then a quarter of this tile also is a tile mathematically it is a tile it will fill the space by repetition, but then the repetition vector is a by two repetition vector is a non lattice translation so that is why the green tile although is a tile, but it is not unit cell of my pattern, for unit cell the repetition has to be by lattice translation.

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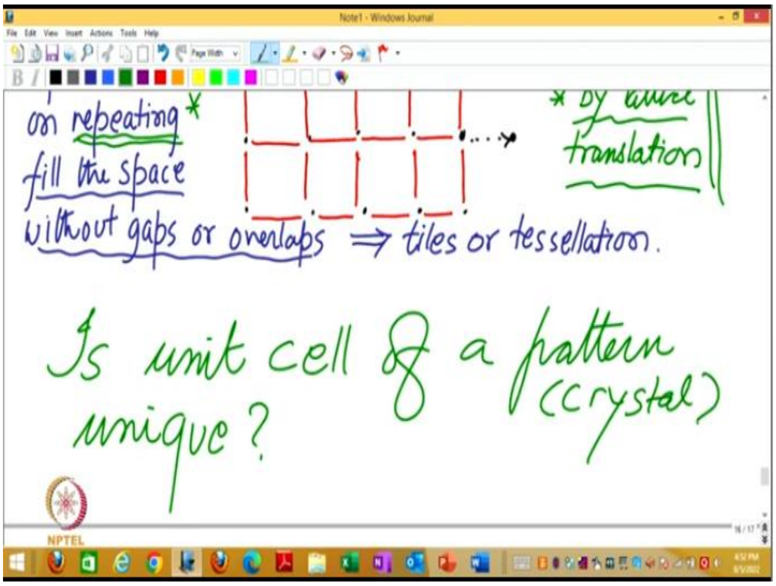

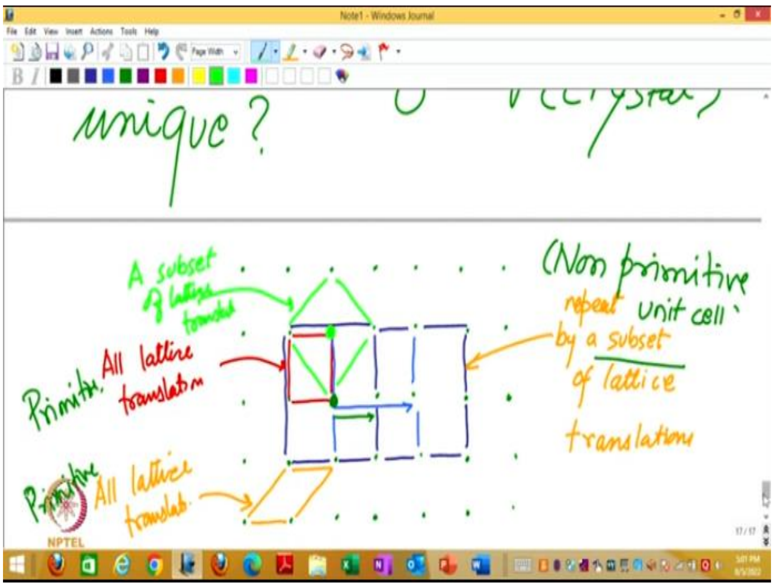

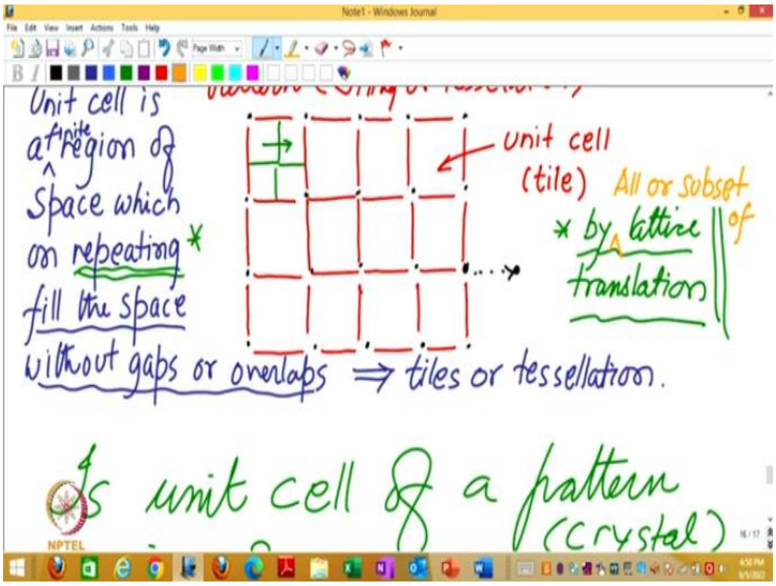

Now an important question pattern and crystal I am interchanging pattern more general it can be pattern of anything, crystal is a pattern of atoms, so unit cell of a pattern unique so, like I drew a square tile a square lattice and I drew a square unit cell. Is there a one to one correspondence one to one relation between unit cell and lattice? That is what I am asking. Yeah, is it unique?

Student: Yes.

Professor: Yes, and no?

Student: I can choose a bigger one?

Professor: You can choose a bigger one, the smaller also.

Student: (())(7:14)

Professor: Smaller okay. So, what we had selected is the smallest, the red unit cell was the smallest one, what you are saying that we can select a bigger one how? What will be your choice of the bigger one? Can you guide me? How shall I go?

Student: (())(7:37)

Professor: 2 by 2, so 2 by 2 of this, this was there in your mind?

Student: (())(7:54)

Professor: Sorry?

Student: (())(7:57)

Professor: Or you can change the orientation, very good. So, let me change the color also to show the change in orientation. You mean something like this?

Student: (())(8:16)

Professor: So, shape so you can change the shape also it need not be perpendicular, something like this. Are all these unit cell or will they qualify as unit cell?

Student: (())(8:40)

Professor: Which two?

Student: Square one and the rhombus.

Professor: Square and rhombus. What is the problem with the blue?

Student: Because points are not covered.

Professor: But did I say that all the points should be covered? Unit cell is a region of space which by repeating by lattice translations fill the space. So, if I repeat the blue one, of course I need to extend my lattice. Am I not able to fill the space? Is there any problem in filling the space?

Student: (())(9:36)

Professor: No, how much I translated? From this center, from this lattice to this lattice, if you say center to center that is the lattice translation. So, I am translating by lattice translations, and I am filling the space, so at as I if we need to (def) change the definition then that is a different matter. But as given the definition as given is accommodating this bigger blue unit cell also no problem because the shift is by lattice translation and by shifting of all lattice translations. No, by shifting by these lattice translation, I just caught myself in saying by all lattice translation, if I shift this bigger unit cell by this there is a smaller lattice translation also in that same direction if I had shifted only by this then obviously there will be overlap, then there will be an overlap.

So, carefully again in my definition or rather carelessly you can say that I did not specify that repeating by lattice translation repeating by all lattice (trans), do I mean all lattice translation or a subset will do? So, a subset will, let us accept that to accommodate we want to be biased towards that bigger unit cell. So, by all, “usko admission dene ke liye school mein, apna kanon badla” all or subset of lattice translations.

So, a blue one will qualify by a subset of translation, non primitive, very good. This is what we will call a non primitive unit cell. So, the same word is coming and the two are connected primitive basis, non primitive basis, primitive unit cell, non primitive unit cell, non primitive basis was giving you only a subset of lattice translations.

So, whenever the repetition is by subset of translation, what is the characteristic of that unit cell in terms of lattice point? Its relation to the lattice point and whenever all lattice translations are being used, what is the relation of unit cell with respect to the lattice point?

Student: There is no point in the, inside…

Professor: No point inside. So, you see here there was a point in the bigger blue unit cell there was a point inside. So, that point inside you cannot reach by, tiling this pattern yeah without overlap. So, you have to overlap it. So, you have to ignore those translations.

So, this is called if you repeat by a subset then we call such unit cells primitive unit cell.

Student: Non primitive.

Professor: Thank you for correcting. I was just checking whether you are awake or not. So, non primitive, non primitive unit cell and all these kind primitive, so primitive is having lattice points only at the corners you can see the way I am I have drawn whereas non primitive is always having some inside this green one also is having one green lattice point inside.

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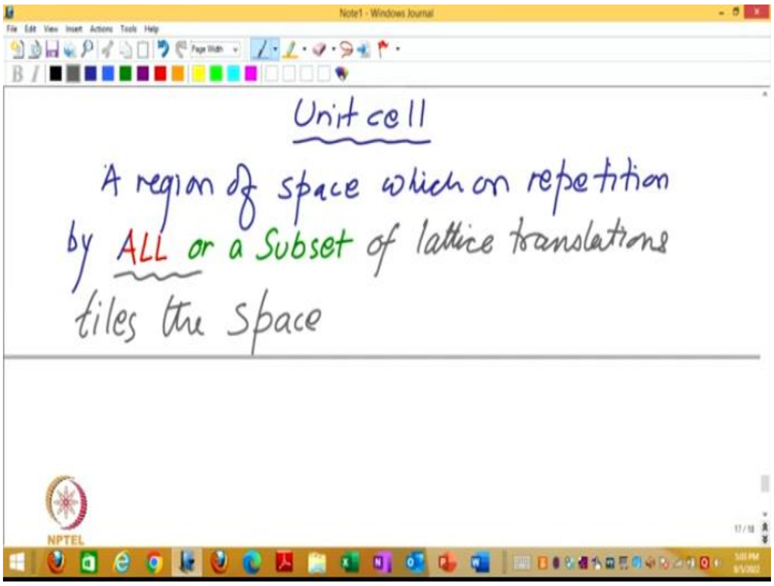

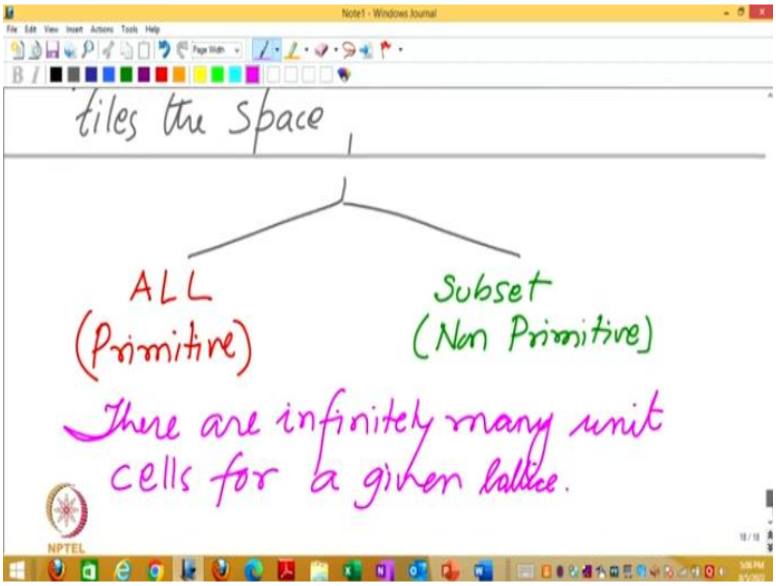

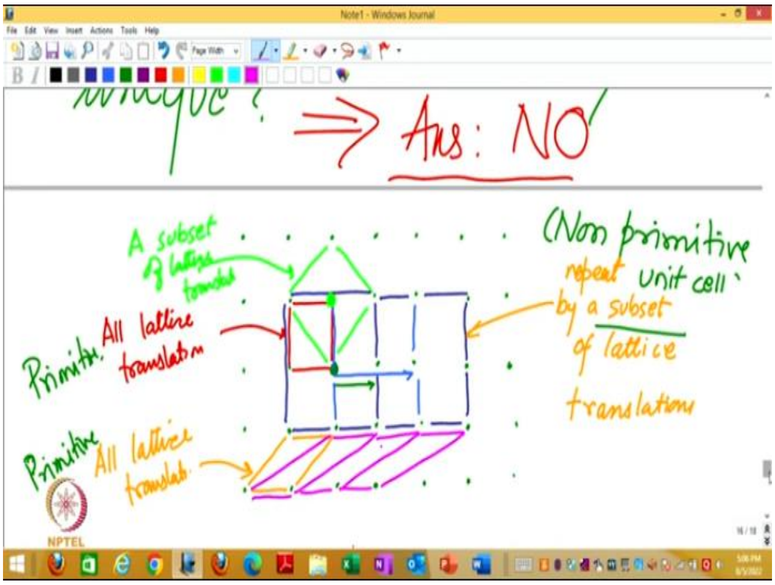

So, that gives us a classification of unit cell. And based on this, that whether you are using all or a subset, you are having two types of unit cell, non primitive and you saw the example. And we had all this and we had, you can see that we had two types of primitive itself. So, primitive also is not unique, the red is also primitive, this whatever color it is? Orange. So, red and orange both are primitive, but they are different shapes, but they are still primitive.

So, it is not that primitive is unique, non primitive also we are having two types may at least in this example. So, in fact, what to talk of non uniqueness? Your answer to this is no of course. Not only it is not unique, there are infinite, it is only depends upon your imagination, it all depends upon how crooked your imagination is? So, from a square you go to this orange one or if I am more crooked I can go this way there is also my primitive unit cell, this also by repetition will fill the space, so infinitely many, you can see.

This is a very-very important thing to keep in mind and that will bring us to an important question which we will deal with the later but it brings us to an important question then what unit cell to use to represent this lattice? And to begin with, I call it a square lattice because points were on a square grid and I selected this red square unit cell, so all was happy and nice, that I have a square lattice and I have a square unit cell, but now if you say that I can represent it by such parallelogram unit cell also, shall I call it square lattice or a parallelogram lattice? That question we will look at in somewhat detail later.