Crystal, Symmetry and Tensors
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Lecture 1e
Voronoi Cell

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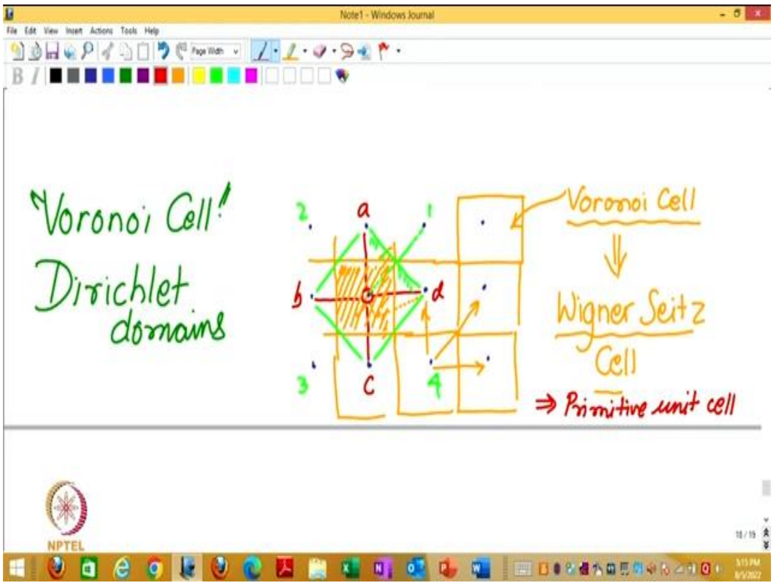

Let me give you one more interesting unit cell which I was requested to include in this course. So, let me, there is one sure short way of getting one unit cell a particular kind of unit cell and it also ensures that you get a primitive unit cell and that is what is called a Voronoi cell, it has many names in mathematics also it has a non unique name, names Voronoi cell sometimes called also dirichlet cells or dirichlet domains and today for preparing for the class when I was looking Wikipedia there are few other names also. So, but Voronoi is quite common and we will use Voronoi cell.

Voronoi cell is that you focus on any you select any given lattice point as your favored point then you draw a line from that lattice point to the nearest lattice point whatever you find then you draw a perpendicular bisector. Why I am doing this? Actually, see the whole space is there and so many points are there, these points are now demanding right, they do not want to be in the community, they are demanding tell me how much of this space belongs to me? Give me my land.

So, now, it was a very democratic government which decided whatever land is closer to you than any other point you take, it belongs to you. So, now, that is why I chose this point and its neighboring point and divided a boundary here perpendicular bisector.

So, everything on the left of this boundary is closer to my central point than the other point to which I have joined it. So, if these two are fighting, what region belongs to me? And what region belongs to you? Then the left region obviously belongs to this because any point in this region will be further to that point, then to this point. Is that fine? So, a fight between these two is decided, but then there is so many fighters, so, many points all around. So, we have to do this exercise for all other points.

So, then we say okay, there is a point vertical above so again we divide the space, so, everything below this line belongs to my central point and then there is this I again divide a bisector, everything to the right belongs to this and everything above belongs to this. So, of course, others are also fighting, but their claims are weaker. So, if I join this and draw the bisector so, that goes exactly through this point. So, that is anyway is on this side.

So, a smallest region of course, yeah, if I do this like should be also there. So, with respect to these four points, the region which belongs to it, to the central point is this green, green square. But with respect to, no sorry, I wrote it wrongly, let me correct it. With respect to these points the green square belongs to the central point but with respect to these points the orange region belongs to the central point.

So, the smallest region which we get from this analysis is the orange square so, we say with the central point this orange square belongs and since all lattice points are identical, all of them will get if I do the analysis for all point, all of them will get identical orange square. What will be the property of these orange square (with)? So, this is what is called a Voronoi cell, Voronoi cell in mathematics, little bit more general because it can be made for non periodic set of points also, but when done for periodic set for crystal, in crystallography a special name is given a Wigner Seitz cell.

So, we have constructed a two dimensional Wigner Seitz cell for a square a lattice, region which is closer to a given lattice point than any other lattice point. So, this square is closer to the lattice point which belongs to the square than any other lattice point so, that is the Wigner Seitz cell. Is it primitive or non primitive?

Student: (())(7:11)

Professor: Primitive, because by definition every Voronoi cell or every Wigner Seitz cell will contain only one lattice point so, when you will go from one cell to another cell the translation will always be by the lattice translation and since each one is having one lattice point all lattice translations have to be included if I want to tile the entire space.

So, Wigner Seitz cell automatically are primitive unit cell, this is a special kind of primitive unit cell. Now, in a square lattice it did not give anything much interesting result because we were anyway we were getting a square unit cell without thinking so hard about these perpendicular bisectors and all also, but when you do it for other unit cells, other lattices then you start getting interesting result.

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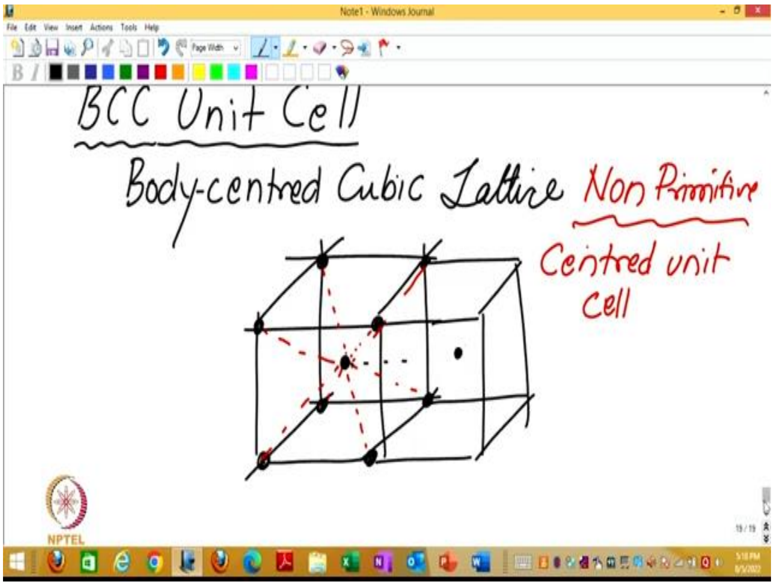

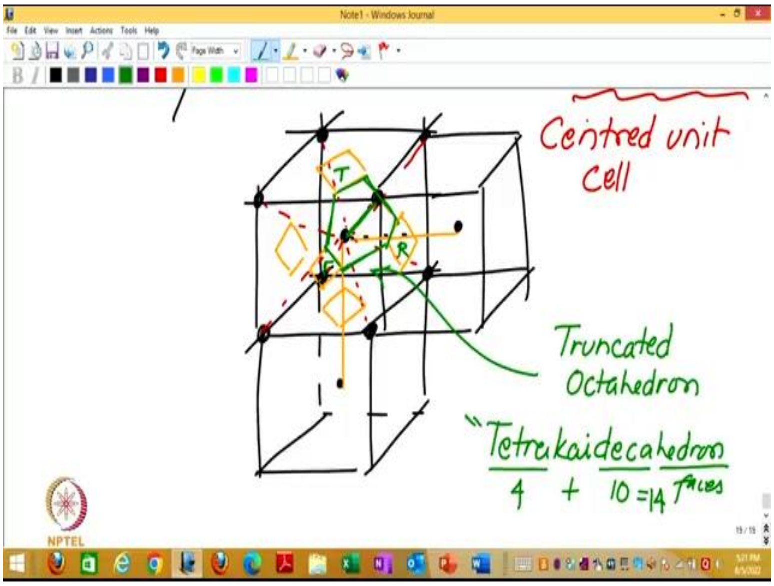

So, for example, now, let us jump I have not given any example till now for 3D, so, let us end with one 3D example, let us say BCC unit cell Body-centered Cubic. Body-centered Cubic is a three dimensional lattice where the lattice points are at the corners and there is a lattice point at the center that is why it is called and by repeating this cube, the lattice which I will generate I will call it Body-centered Cubic lattice.

So, is it primitive or non primitive?

Student: Non primitive.

Professor: Non primitive, because it has a lattice point in the middle, so non primitive that is why non primitive since they will always have something inside also so, often called centered lattice, centered unit cell because they have some centering, either body centering in this case or face centering. How will it is difficult to imagine? How will the Voronoi cell or the Wigner Seitz cell of this will look like? So, you can see that there are 8 near neighbors, if I focus on the central one, 8 near neighbors.

So, I will draw a perpendicular bisector to all these 8. So, I will have some 8 faces perpendicular to these, but not only that there is a cube next to this cube sharing the face so you take that center, there is a cube below this, so on all the 6 faces there are other cubes standing like this top and bottom, left and right, front and back all these 6 also when you bisect so the 3D construction is not easy and I am not able to do but I am only giving you the result so to say.

So, where will be the bisector plane for this? Write the common face, common face itself is the bisector and on the common face, so on the common face because of this cut you will get a square, so, on all the common faces you will get a square on your Wigner Seitz cell. So, you will get six squares and then I am drawing I can understand if you are having difficulty in seeing what I am drawing but these will then be connected like this if I rub this off for a moment the back one. So, this is the top square, this is the front square and this is the right square and in between the square you will get a hexagon which is a face coming by the bisector of this vector.

So, the green near neighbor from the center to the corner is divided by this hexagonal phase. So, this solid which comes out of this analysis is known as Truncated Octahedron sometimes a more fashionable name Tetrakaidecahedron, which does not mean anything more than tetra 4 and deca 10 and kai plus, so and hedron faces, so 14 faces, 6 square faces and 8 hexagonal faces gives you 14 faces. So, the Wigner Seitz cell of a BCC is a Tetrakaidecahedron.

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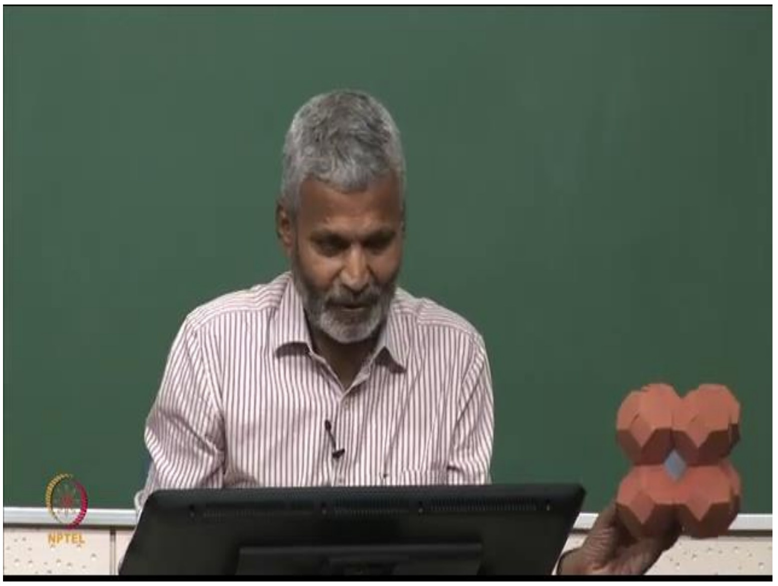

The colored are Voronoi points of Voronoi cells of, the corner eight corners of the cube and the internal blue one of which you are seeing only the square faces, the hexagonal faces are hidden because these other cells are sitting on that, so, that is the Voronoi cell of the central one. So you can examine this, so with that thank you.