Crystals, Symmetry and Tensors
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Lecture 7a
Orthographic Projection of Crystals

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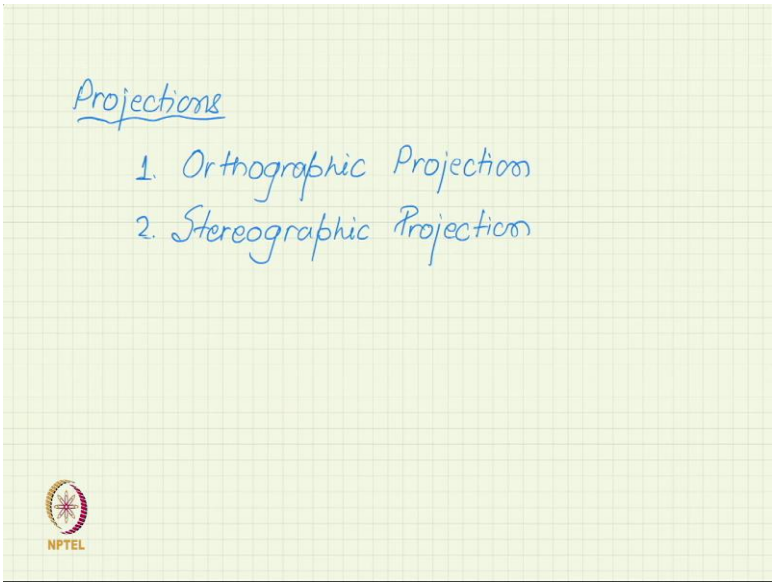

Welcome to this lecture of the course. So, these two projections are very, very important in crystallography orthographic projection and stereographic projection. Orthographic projection certainly you all must be familiar because that simply projection of a point on a plane.

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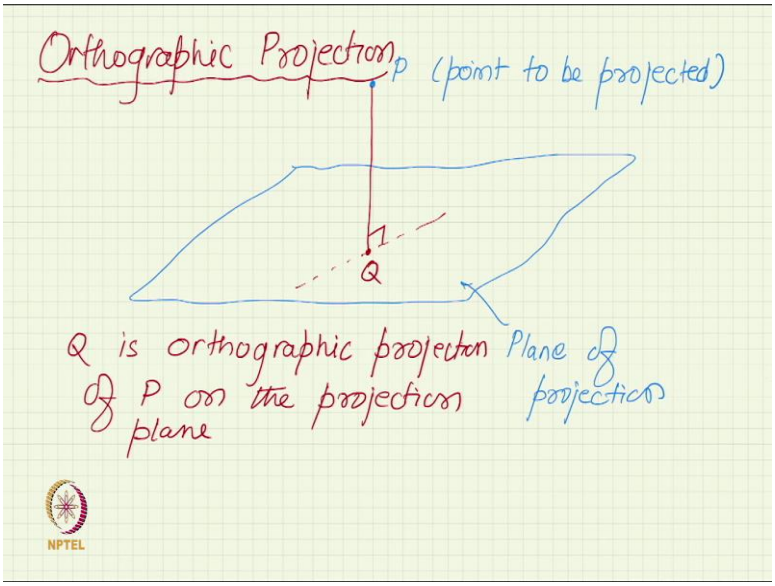

So, if you have a plane. So, that is the plane of projection and then there is a point to be projected then you simply drop a perpendicular from the point to the plane, then Q is orthographic projection of P on the projection plane. So, that is the orthographic projection for you, we all know this for the sake of completeness, I am writing this here because this is the common projection, which we keep doing all the time and in crystallography in international tables, which is one of our goals in this course. So, you will find several orthographic projections.

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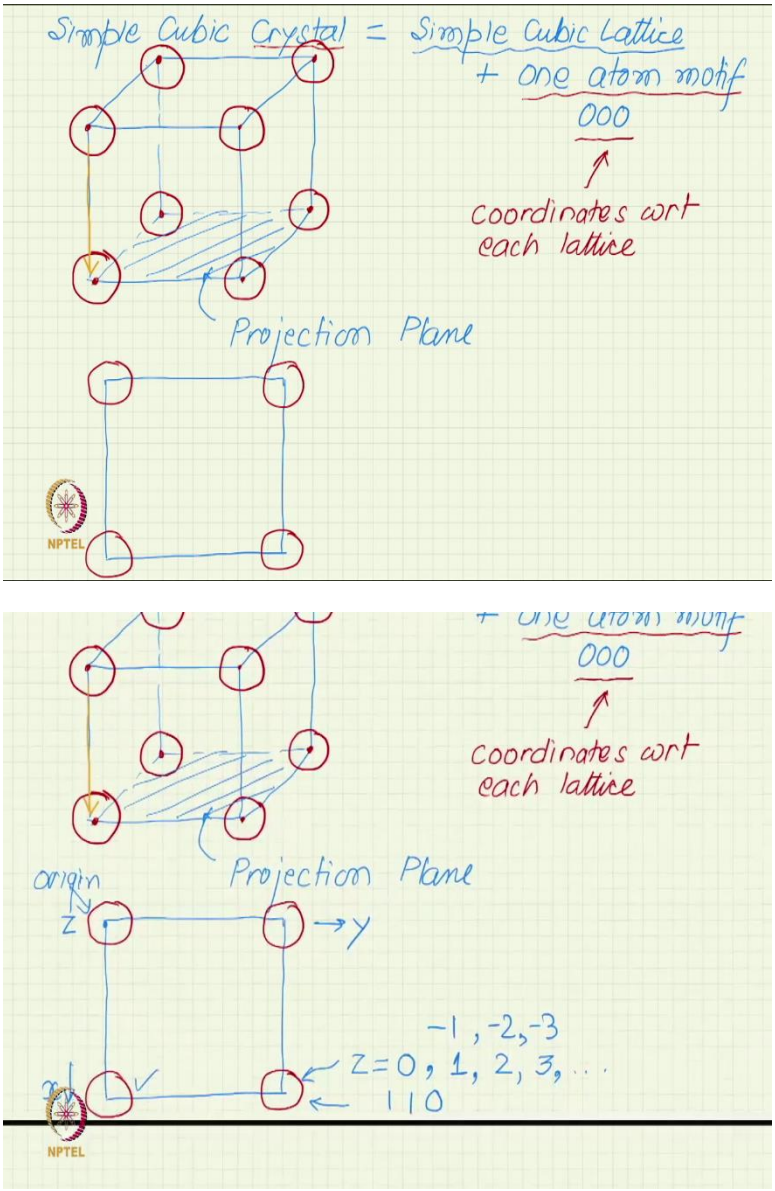

So, in the three-dimensional crystal to which we are interested in are three-dimensional objects. So, let us say simple cubic crustal when we say simple cubic crystal, we mean simple cubic lattice plus one atom motif and that atom is at the lattice point. So, the fractional

coordinate is ooo. So, you have a cubic unit cell, simple cubic lattice means lattice points are at the corners of the cube. So, in red I am marking the lattice points they are still not atoms they are simply points when we say simple cubic crystal, then we will attach atoms to these points.

So, and since we are saying one atom motive so I will attach only one atom to each lattice point. And that atom I am placing at ooo which means, with respect to each lattice point, the coordinates are ooo, ooo does not mean that one fixed origin you place one atom at one fixed origin and be done with it, you will not get a crystal that is not a crystal. So, ooo means, these are coordinates with respect to each lattice point as origin. So, one by one you have to shift your origin and accept each lattice point as origin and then place an atom there. So, when this becomes origin I place an atom there, I placed an atom there.

So, essentially an atom at each lattice point that is what is meant by atom at ooo in the crystallographic language motif atom at ooo means an atom at each lattice point centred at that lattice point. So, this is your 3d cube with and it is a simple structure, if you want to draw a projection of this. So, suppose we select the base of the unit cell as projection plane and we make an orthographic projection. So, since that base is square, so, in the projection it will look like nicely square then four atoms are relying on the plane itself.

So, they will be there, other four atoms which are on the top surface of the cube. So, they will also project you can see in the orthographic projection, they will project exactly on to this point. So, as far as projection is concerned, I will find nothing new. And if I am not writing anything as coordinates of these points. So, x and y coordinate are visible. So, I have to label x and y, let us say this is x, this is y and z is of course, the projection direction and z is going out of the plane normal to the plane.

So, the x,y coordinates I do not write usually, that is the convention in crystallographic projection, because the x coordinate is visible that I have gone all the way to the end of the unit cell edge length. So, the x coordinate is 1 for this atom for example, since I am on the x axis, the y coordinate is 0. So, x and y coordinate should be readable from the projection, but it is usually not written, what should be written is z coordinate, but again the convention is that 0 or 1, z coordinates are not written only fractional coordinates are written.

So, if nothing is written in this projection, it automatically means that the z coordinates are 0, z is 0 nothing is written and what is x and y. So, since this is my selected origin then x and y

for this is x is equal to 1 y is equal to 1. So, this particular atom this particular atom, the full coordinated 1, 1, 0, The z coordinate becomes z equal to o and in the end, I write nothing, I leave that to the intelligence of the reader that they can just by looking at this atom, they can identify that this is a 1, 1, 0 atom.

Usually, as I said that in our convention for coordinates, we will not use the parentheses or anything. So, I just write it as 1, 1, 0. So, this is projection of a simple cubic unit cell what about this is only four atoms I projected eight atoms, so, other top four atoms are also getting projected there.

So, z is not only 0 here, z is also 1 because 1 will also predict exactly at that location and if you really think of the entire crystal. So, it is not only 0, 1. It is also 2 because the next unit cell will give you an atom at 2 and then at 3. So, if you think of it will have you the entire integer sequence 0, 1, 2, 3. There is a unit cell below also. So, that will give you a coordinate minus 1 and then below that is minus 2.

So, really the end with this one single atom in the projection is a representative of the entire row of entire z row of atoms at integer spacing and integer coordinates. So, this is what is meant by and Crystal orthographic projection, why it is useful you will soon see when the simplest example in the simplest example of a simple cubic it may not look so important.

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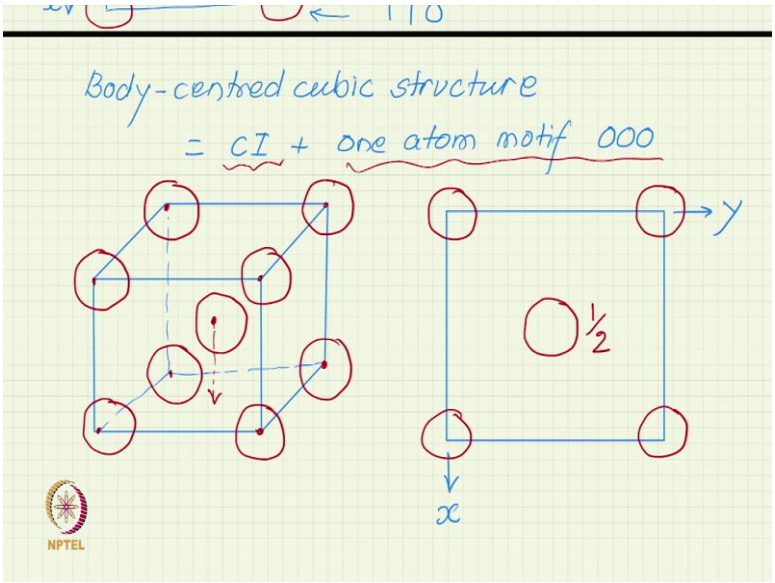

So, let us graduate to slightly more complicated. So, let us say body centred cubic structure. So, this is body centred lattice that is CI cubic I plus one atom motif again that one atom is setting exactly at the lattice point so, ooo.

So, if we now draw our, so again cubic I lattice, so, lattice points are now since it is cubic lattice points are obviously at corners of a cube corners are always lattice points in any unit cell whether it is primitive or non-primitive and then since it is body centred since it is I, there is a lattice point in the centre also and since I am saying one atom motive, so, there is an atom sitting at each of these lattice points.

Now, if you draw the projection of this again on the basal plane or the ooo one plane then like for the simple cubic you will have four corner atoms which as we have seen represent the entire row of infinite row of atoms that integer is spacing, but the central one the I instead the body centred one will now project right in the centre of the cube centre of this square. So, you will have one atom in the centre also. And now, since it is not lying in the plane and not on the planes with integer height. So, the height is not 01 minus 1 or so but height is half.

So, now, we will indicate the fractional coordinate only of this atom. So, as soon as I indicate fraction half here, we know that this is not lying on the projection plane, but at half height above the projection plane obviously half height below the projection plane also by translation translational symmetry because this the fractions themselves are a fraction in terms of lattice translation. So, one is a lattice translation half is half the lattice translation in that direction in the z direction. So, this also was not bad.

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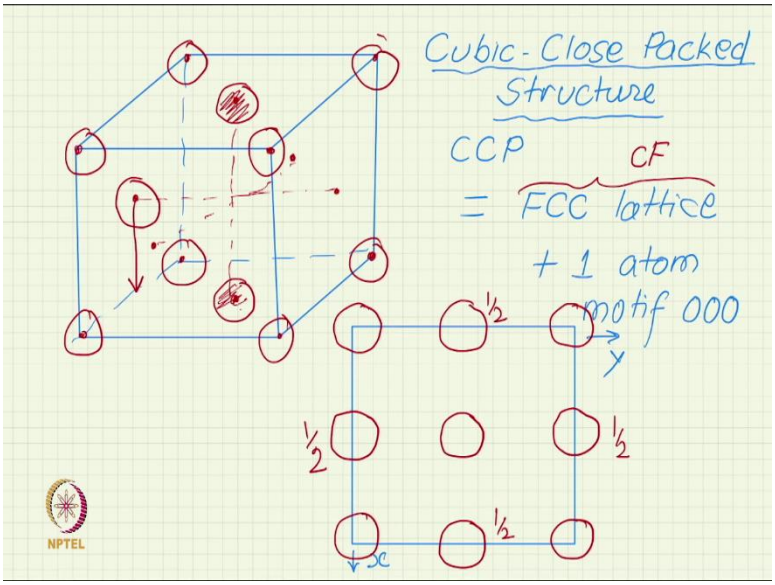

So, next look at next look at the face centred cubic, face centred cubic. So, face centre again face centred cubic structure. So, in this case there is a different name also which I suggest that you use. You call this cubic close packed because we have another structure called hexagonal close packed and the two are related So, to bring that relation out to relate it to hexagonal close packed, this structure should be called cubic close packed structure, it is quite common to call it FCC crystal.

But that is not a good name, and it is not a good practice, and we will avoid that. So, we will not call it FCC crystal we will call it cubic close packed structure that is CCP in the short and this is FCC lattice plus again 1 atom motif at location 000. So, the lattice points now, since it is FCC, FCC lattice, we can also write cubic F. So, that means lattice points are at corners as they should always be, but they are also in the centres of all phases. So, all the six phase centres will have now lattice points.

So, if we now draw the projection of this. So, the eight corners will project into these four locations but there are six phase centres also this bottom faced centre is right on the face itself, but in the centre. So, this is again at 0 height but it comes there. So, there is additional point there which was not there in simple cubic and in body centred cubic it was there but was at half height. But now at 0 height we have an atom there the top face centre projects at the same location. So, as we know that if there is an atom at 0 there is obviously an atom at 1.

Now, the left face centre let us look at left face centre where will that project at the left edge. So, it will project exactly there and its height is half. So, since we have decided to indicate the z, z height is shown because that cannot be read from the projection unless and until somebody tells me that it is half height or is it in the same plane or at three fourths height? I cannot know there is no way of knowing for me, whereas x and y coordinate I can read as I told you. So, that is why there is this convention that the z coordinates are always indicated.

Similarly, the front face centre that will project here again at half height the right face centre will project there at half height. So, this will look like the projection of cubic close packed. Now, let us go to still the next level of complication and let us consider what is called what is called sodium chloride structure, NaCl structure.

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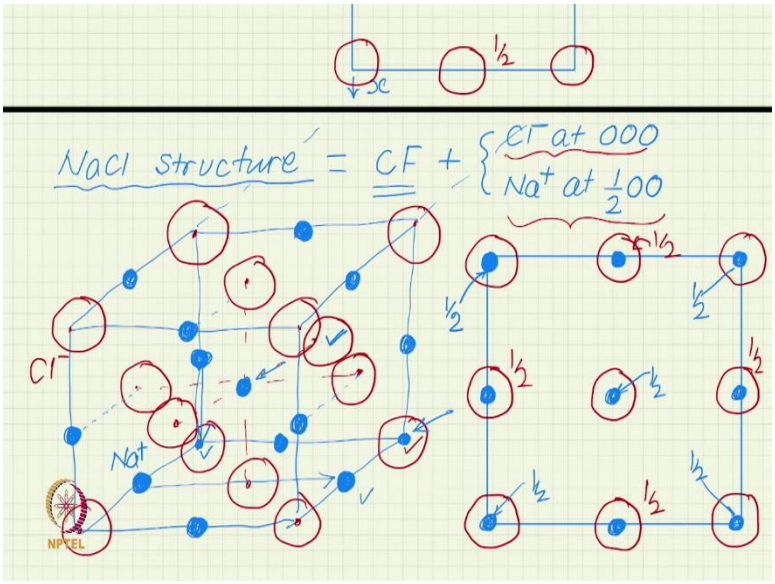

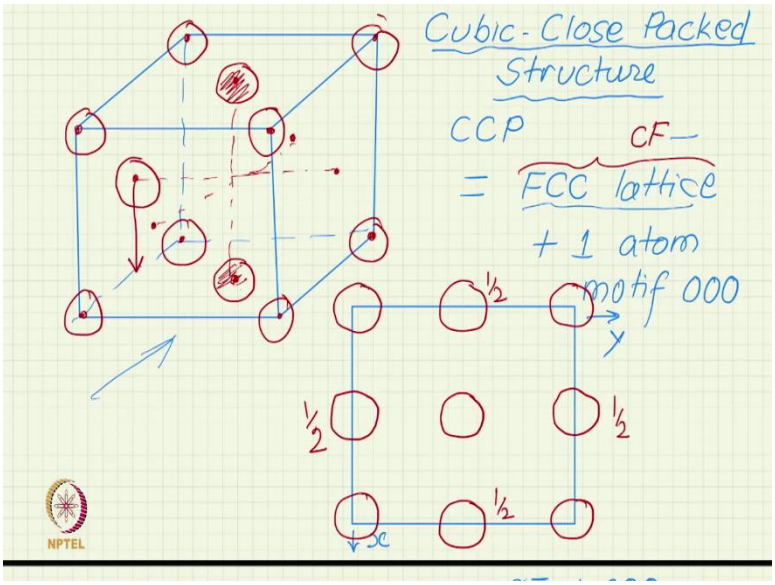

So NaCl a structure if you see this is cubic F. Now for the first time you are going to see that motif need not be one atom motif can be more than one atom. So, motif is two atoms. Let us say sodium let us say chlorine at ooo, to be more precise chloride ion, Cl minus at ooo and sodium ion Na plus at half ooo. Now how, how does that work? Let us see. And that is why see, when I am saying the lattice, this is also face centred cubic CF. See if this will also face centred cubic CF. So, by lattice cubic closed packed structure and sodium chloride structure or diamond cubic structure, all of them have the same lattice.

So, lattice wise there is no distinction. But still, they are different structures, cubic packed structure is not the same structure as sodium chloride structure just because they are both FCC lattice. That is why the reason to insist that the structure should not be called face centred cubic structure.

So, a centred cubic is a lattice. And on that, there can be different structures can be based. One example is to be close packed. The second example is sodium chloride. So, where are the lattice points exactly, again at the corners and at the face centres, top and bottom, left and right, front and back.

Now, this is the skeleton, and I want to construct the structure out of it. So, I will have to start placing as per the recommendation of the motif. So, motif is chloride ion at ooo. So, I start putting the chloride ion at each lattice point at ooo means at each lattice point exactly like we did for the CCB structure, the back face centre for me is now overlapping with others, but I can put it there. So, there are 14 atoms now.

So, you can already see that now, the three-dimensional visualization of the structure by trying to draw perspective diagram does not appear to be a very nice strategy. And I have wondered put chloride ions, I still have to put sodium plus ions, and when I start putting at the sodium plus ions, then I have to put them at half oo.

So, with respect to any lattice point as origin, I go half along the x axis. And put, I do not have to move along y and z axis. So, I come exactly at the middle of the edge. So, with respect to this lattice point, half oo is there and I place a sodium ion there. So, I put a sodium plus there, then when I come to this lattice point, I put another oo.

Now, with respect to this lattice point as origin, my half oo comes there. So, that is how I am generating the second sodium plus ion, I could have also thought of generating this by

translating this iron by one unit and along the y. That is also possible we know that each edge of the cube are translation the directions in those are parallel to those edges.

So, if there is a sodium there, translating it by one unit along the y axis, I should get a sodium plus ion there. But, in the motif description, I am associating with each lattice point in turn. So, when I associate with this lattice point, this particular lattice point then I get half oo there.

Similarly half oo with respect to each lattice point if you start doing you will get these from this vertical left vertical phase will give you an edge centre there. The right vertical face centre will give you an edge centre there and the top face centre will give you ion there, and the bottom face centre will give you an ion there. What about this back edge because there will be a unit cell there in the back and the face centre of that when taken as origin and you move half oo, you will exactly get there.

So, actually you have an ion at all edge centres that is what is the sodium chloride structure. If you can see the power of projection now, because if you now convert this into a projection you will find that it is actually much much neater and easier to understand. So, if I create a projection of this the chloride ions at corners give me this chloride ions at face centre give me this and four others here at half sorry yes, thank you, thank you Harsh. So, this will come by attaching half oo, from this particular back face centre which I was missing. So, thank you for pointing that out.

So, there is a with the back face canter if I go half oo I exactly get in the centre of the cube also. So, there is one atom at the centre of the cube also one sodium plus ion is at the centre of the cube.

So now, wherever you had ions at 0 height, you also have a have another ion at half height. So now you have to be a little bit more careful. By giving your z coordinate you have to clearly indicate that which one is half. So, either by colour coding, as I am doing here or by arrow, which also am doing here, you have to clearly show that it is the blue one, which is at half white and not the red one, because both are projected at the same location because this one this ion and the red ion will both projected the same location.

Similarly, where you have half of chloride ion there, you have also at the base 0. So, this is 0, 0 we are not writing anyway half we just want to make it clear that the half is for the red one

there. So similarly, you can complete the projection. So, looking at this projection also you should be able to construct your three-dimensional unit cell.

So, that is about orthographic projection and a sort of review also of what is meant by lattice and motive and also an alert or warning that lattice is different from a structure. So, I have shown you two different structures the cubic close packed and sodium chloride structure, both of which have the same lattice FCC. So, what is the distinction, distinction is coming from the motif, CCP will have a single atom motif ooo, whereas sodium chloride will have two atom motif ooo and half oo.