Solid State Physics
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Lecture - 08
Crystal Structure (Contd.)

Let us continue the calculation of coordination number. So, you have calculated packing fraction, now we will calculate coordination number.

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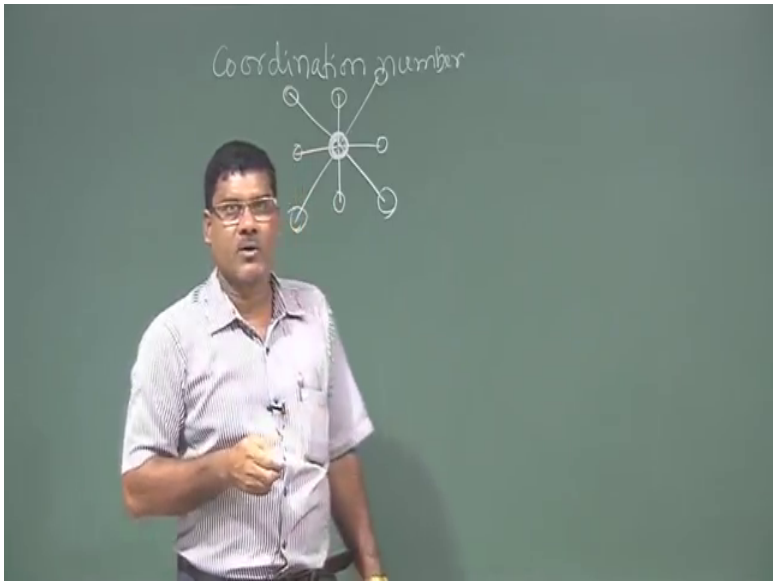

What is coordination number? Coordination number is basically number of the atoms or lattice point from number of the atoms or lattice point which are the nearest way to another atoms or lattice point. So, I want to calculate the number of coordination numbers means I want to calculate a; count the number of nearest neighbor atoms or lattice point of this lattice point or atoms.

And nearest neighbors; there are many neighbors, but nearest neighbor of equidistance. So, if it is the arrangement of these atoms in crystal of lattice points. So, what is the nearest neighbor of this lattice point or atoms? So, immediately, I can say these 4 are nearest neighbor and there they have equal distance, there are other neighbors and they are also equal distance, but their distances are higher than this one. So, that is why not

only neighbors; nearest neighbors of equidistance; how many atoms are; lattice points are there around this lattice point? So, that is the basically coordination number.

So, again it depends on the crystal structures and mainly, we will calculate this coordination number for cubic system. So, for cubic system, we have again 3 Bravais lattice simple cubic.

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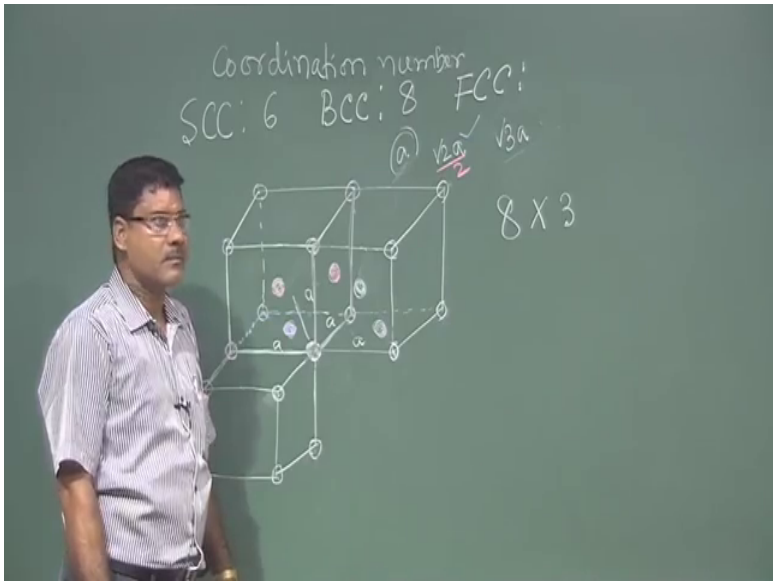

And then other 2 are there. So, let us calculate coordination number for simple cubic system. So, simple cubic let us; let me draw it. So, these are the simple cubic. So, it has atoms at the corner only at the corner. So, if I can consider any lattice point for which I want to know the nearest neighbors or coordination number.

So, let us consider this point; this lattice point. So, what is the coordination number of this lattice point? So, that is the task we want to do. So, here; obviously, the distance between these 2 atoms is basically a; these 2 also a, these 2 also a and so, this let me complete this one. So, it will be slightly; so, all mode is there. So, except this 3, except this 3; this, this and this one other atoms that distance are different, next nearest neighbors if I say, then it will be this along the along the phase diagonal.

So, that distance we have seen that it root 2 a, right and next neighbor or nearest next nearest neighbors which will be along this one; this atoms, this and this is the along the body diagonal. So, that distance will be root 3. So, along the axis the distance between

atoms; 2 atoms or 2 lattice point is a along the phase diagonal distance is root 2 a and along the body diagonal it is root 3 by a. So, we can say that this is the smallest distance. So, this with this distance; so, we have to find out; how many atoms or lattice points are there at this distance because we need the number of atoms or lattice point at equidistant.

So, that that number is basically coordination number. So, I think you can find out easily; you can find out easily. So, here immediately, I can see this, this is one nearest neighbors, this is another nearest neighbors and this is the third one and from this cubic, there is no that this other are not at this distance a, right. So, in crystal, this is one unit cell. So, this crystal is full of unit cell unit cells are arranged periodically in 3 sides, in 3 sides. So, you fill the space. So, immediately you can see if we. So, there will be another unit cell; say in this side. So, I can do it I can draw it. So, this is another unit cell. So, these are the lattice point.

So, you can see that these distance also a. So, from this unit cell; so, it will have another nearest neighbor. So, that is this one. So, I have. So, its nearest neighbor is one can see that it is along the axis. So, along the a axis for these 2 their nearest neighbors. Similarly along this axis along this axis; so, I will have another unit cell below right. So, I will have another nearest neighbor and this other axis, we have another nearest neighbor. So, basically if you if you draw because these corner this corner this point is attached with 8 unit cell that you know, it is attached with 8 unit cells, right, it is attached with 8 unit cell if I complete this one. So, it is like this.

So, these 2, these 2 and these 2; these are the nearest neighbor in simple cubic crystal when you will draw this 8 unit cell attached with this. So, you will find you will find that this only these 6 are the nearest one having the distance a. So, in case of simple cubic crystal we tell that the coordination number is 6 coordination number is 6. Similarly you can calculate for BCC; body centered cubic crystal. So, what is the coordination number of this one has to find out. Again, I think now easily we can tell this for BCC the smallest distance was root 3 by 2 root 3 a by 2 that during calculation of radius we have seen.

So, if I consider again this point again this point this lattice point and what will be the coordination numbers for what will be the coordination number for body centered cubic crystal. So, I can put I can put. So, this is the body diagonal. So, at the center of this; at the centre of this, there will be atom, right and these distances is root 3 a by 2, right. So,

these distance is root 3 a. So, this distance will be 3 by root 3 a by 2. So, these are the nearest distance and other optimization.

Next one; this distance will be a see in body centered cubic all distance; this, earlier this we have seen the distance area. Now, we are getting in case of BCC we are getting even one lattice point that is sitting, it is at the body centered. So, that distance is smaller than this one. So, for BCC we have to find out how many lattice points or atoms are there or at distance at distance root 3 a by 2 that we have to find out. So, that same way if one can push it. So, this one; this corner point this; what we have considered second these this one is attached with this point is attached with the 8 cube. So, this is 2 and on top this side to right and in again bottom will have this what about top 4 and bottom will have 4.

So, 8 unit cell attached with this one. So, 8 unit cell will have 8 unit cell, we have this, this is the body diagonal of this unit cell I think. So, yes; so, here this body centered atoms are there here, I think. So, I think this the body center. So, distance of this between the body centered and this lattice point is a root 3 a by 2. So, this is 1, you will get another 1, 2 and this side again will get the 2 more unit cells are there. So, we will get this is a third one and this will get the fourth one; right if I go down. So, this is the fifth one, this side if I go. So, that will be the sixth one right and 2 modes are there, this below of this one. So, we will have seventh one and eighth one.

So, 8 unit cell attached with this one, each unit cell have the body centered one and the distance of all this 8 body centered atoms from this point is same. So, they are equidistance and smallest distance equidistance are smallest distance and the distance is this root 3 a by 2. So, this is the 8 number of nearest neighbor in case of BCC lattice and does the coordination number is 8, right. So, this way one can calculate for FCC lattice; this also, this is similar way, we can proceed and find out, right. So, what is the coordination number for FCC lattice? So, let us use this same figure in case of FCC; so this in case a; this FCC the additional lattice point act at each phase at the middle of each phase. So, this each cubic has 6 phases. So, we will have 6. So, this phase; so, here, this one too I can use probably and then. So, I have many more this one and this face. So, it will be middle of these, right and this one at the center of this.

So, 1, 2, 3, 4, 5, 6: so for this unit cell 6 faces are there. So, we will get 6; 6 atoms or lattice point at the center of each face. Obviously, if you see this from this lattice point,

what will be the nearest neighbors? So, that one has to find out first. So, again we have seen this the smallest distance between. So, this along the along the along the faces along the face diagonal; so, this distance is basically root 2 a. So, here if we see this root 2 a this distance. So, now, in middle one atom are there. So, distance will be half of it. So, it is root 2 a by 2, right.

So, now let us find out how many numbers are there at this distance root 2 a by 2. So, that is the task we had to complete. So, for I think; so, this faces attached with this faces attached with these corner that atoms on that face will be the; at this distance, but atoms on other faces will be having the higher distance. So, I will just remove these points for. So, then picture will be clear I think. So, this is one face attached with this, this point, this is another face this is another face attached with this one this is another face attached with this one right. So, here and this is the third phase attached with this, this point.

So, from this unit cell there are 3 nearest neighbors having the equidistance of this one root 2 a by 2, right. So, similarly from other unit cell; so, we have 8 unit cell, we have 8 unit cell. So, from each unit cell 3 phases 3 phases will be attached with this one. So, 3 phase will have 3 face centered atoms or lattice point. So, here just we can see. So, this phase is attached for this unit cell. So, this face is common. So, it is attached to with this and then I can see this face is attached with this. So, we will have in this case say here and I have to complete it then this face is attached with this one. So, I will have another face centered atoms.

So, again from this unit cell these 3 are attached with this; these 3 atoms they are having the same distance. So, again from here we are getting 3 nearest neighbor, right so, but one thing you can observe that as you know in case of face centered lattice point per unit cell when we calculate it then we consider that it is 4 why now each face shared with the 2 unit cell right. So, that is why; what we have considered there. So, this we have taken the contribution half to this unit cell. So, 6 faces half contribution 6 faces half contribution. So, thus basically for that unit cell it was 6 into half equal to 3, right and from corner point 8, corner point is shared with 8 units cell. So, one eighth from each corner; so, it has one.

So, 3 plus 1; so that is 4; you know 4 4 4 lattice point per unit cell. So, from there we have learned that each face shared with 2 unit cell. So, when here we are seeing that

nearest neighbor are 3 from each unit cell nearest neighbor are 3 from each unit cell nearest neighbor are 3. So, I have. So, this is attached with the 8 unit cell this is attached with the 8 unit cell right and from each unit cell 3 or from each unit cell 3 or the nearest neighbors right and again this each one this out of this 3 each one is shared by 2 unit cell is shared by 2 unit cell.

So, basically for; so, contribution is half contribution is half for one unit cell. So, 3 from each unit cell, but these 3 are not fully from this; it is this 3 are shared with other unit cell. So, basically per unit cell this 3 the contribution will be 3 by 2 half of it because these 3 are shared each one is shared by another one; so 3 by 2. So, how many nearest neighbor then the nearest neighbors from here you can see this is just 12. So, thus the coordination number or FCC that is crystal; they say one can calculate the nearest neighbor this is the first nearest neighbor if you say then if I ask you to calculate the what is the coordination number of second nearest neighbor what is the I do not know whether we should call coordination number.

Coordination number generally indicates the smallest distance nearest neighbors are situated at the smallest distance, but for cubicity you want to find out the how many numbers are numbers are there for next nearest neighbor.

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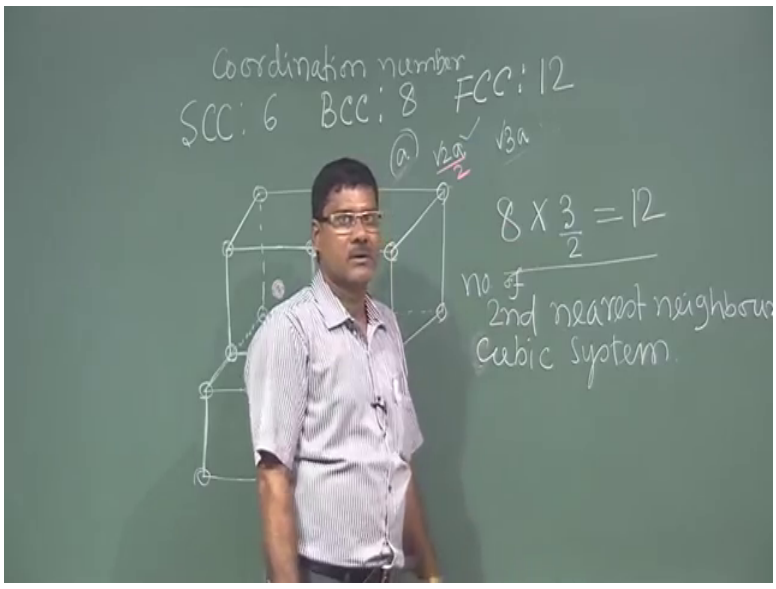

So, take as a homework, calculate the second nearest neighbors, second nearest neighbor, number of second nearest neighbor; number of secondly, nearest neighbor are for cubic system.

So, that homework you can do yourself and this not for only cubic system one can calculate for other cubic system other crystal system. So, you have orthorhombic crystal hexagonal tetragonal; so, for other cases. So, one can calculate and I think you should practice or learning the things and more in practice more you learn and concept will be clear because geometry is involving in crystallography. So, if you do more homework your concept will be I think more clear.

So, I will stop here today, we will continue the other aspect of the crystallography crystal structure. So, next class, we will start this crystal about crystal planes and how it is identified. So, then we use miller indices. So, I will talk about that crystal planes and miller indices in the next class.

Thank you very much for your attention.