Solid State Physics

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Lecture - 07
Crystal Structure (Contd.)

So, we continue calculation of some parameter in last class we started.

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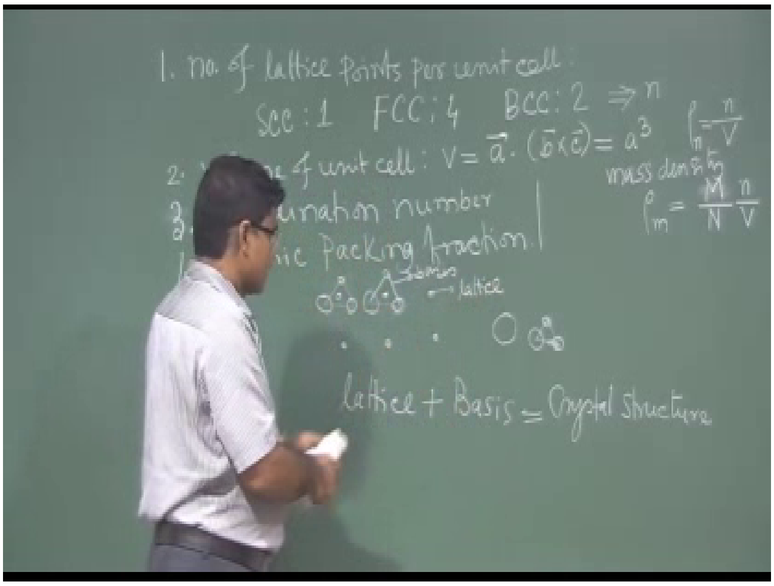

So, this we have seen the number of lattice point per unit cell, so for mainly we will deal with the cubic system, so for cubic, simple cubic crystal. So, for that we have seen this number of lattice point is one or unit cell for say FCC face centred cubic. This we have seen this 4 and BCC body centred crystal that is we have seen this 2.

So, let see it represented by this number small n. And then we have we have calculated volume of unit cell say V equal to a dot b cross c, so for cubic system is basically a cube. And then today we will try to calculate the coordination number, and coordination number going out of this range. So here let me write here itself. And other parameter is atomic packing fraction.

So, see yesterday also we have seen this number density. So, that is nothing, but number density we have seen this say rho n that is basically number of lattice point per unit cell and that divided by volume of that unit cell right. So, we know about we can calculate number density. So, if you want to calculate mass density that also you can calculate.

So, say mass density say rho m. So, for that you know these one contains Avogadro number of atoms or molecules; so mass of one. So, this atomic mass this capital M divides by N. So, that will be the mass of 1 atom. So, here how many atoms are there per unit cell these. So, that will be the mass of this n number of atom divide by volume; so mass per volume. So, that will be mass density.

So, for coordination number and atomic packing fraction; so I need basically need to place atom in lattice. So, as I mentioned that, that lattice is basically the purely mathematical concept, but real crystal has atoms. Now question is how atoms are arranged in in lattice. So, that we have to know. So, we have to know the difference between the lattice and atomic position in lattice. That I need for calculating of this 2, so lattice have some points in space right.

Now, in real crystal, we have to put atoms in this lattice. So, basically this as I mentioned earlier this lattice is nothing, but a framework or skeleton of a crystal. So, when we will put atoms in this skeleton or framework. Then we get the real crystal. So this is lattice. Then we have to put atoms or group of atoms attached to the to each of the lattice point. So, that is called basically basis. So, basis is a atom or a group of atom attached with each lattice point in same manner. So, then we will get the resultant one is the crystal structure real crystal structure real crystal structure.

So, basis can be just one atom like this or it can be a group of atom, so this type of group of atom. So, whatever it is. So, we have to attached to each lattice point in such a way that center of this atom or group of atom coincides with the lattice point. So, I can put if one atom I can put like this or if it is a group of atom. I can put like this as if the center of this is coincide with this, so similar way with each one.

So as if this atoms or groups of atoms are at the position of the lattice point. So these are basically basis and this is the lattice or lattice point. So, then we get the crystal structure. So, atom generally is considered group of atoms considered say as a spherical shape. So, express the size of this atoms or groups of basis size of the basis we express in terms of a radius, say radius r.

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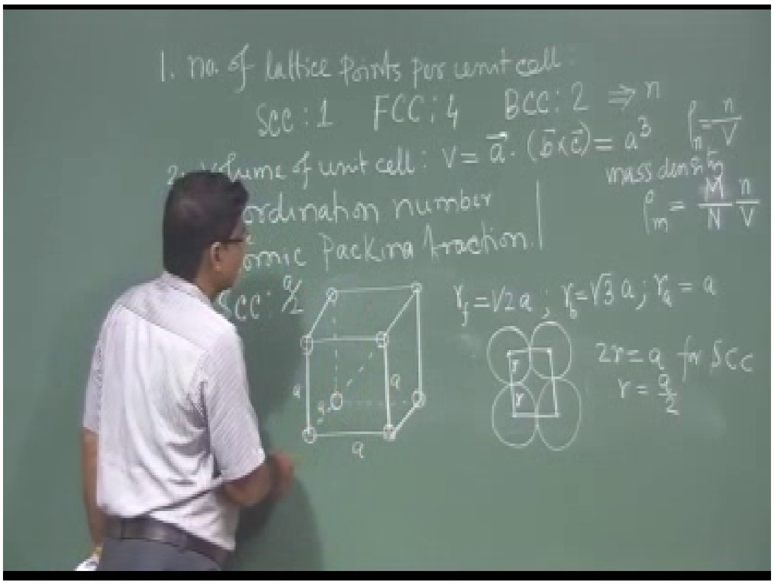

So when basis, let us called this atom, when atom is in a lattice, then the size of the atom or radius of the atom in terms of lattice parameter we can find out so for that to find out the radius of the atom how to proceed. So, for again we will take simple case for cubic system; for cubic system say if simple cubic say for simple cubic, what is the radius of the atom that would be like to calculate.

So, simple cubic; so it has, say it has 8 corner and say in each corner 8 atoms are there. So, here we assume that these atoms are compact in this unit cell. So, nearest 2 atoms we will touch each other. Then we can find out the distance between the 2 atoms in terms of radius. So, for simple cubic what is the nearest 2 atoms that smallest distance between 2 atoms.

So, they will touch each, other atoms may not touch; so in case of simple cubic. So, these are the, this here the distance between atoms is basically a distance between 2 atoms is a that is the smallest distance. So, distance between this 2 atoms along the face diagonal what will be the distance. So, the distance will be one can calculate. So, if it is a. So, this will be square root of a.

So, this we can write that distance between 2 atoms along the face diagonal say r f. So, that is root 2 a. What will be the distance between this 2 atoms along the body diagonal. So, that one can find out, one can calculate and show that show that. So, it is r b body diagonal. So, distance between this 2 atoms it will be square root of 3 a, whereas for simple for this along distance between 2 atoms along any axis. So, say this is r a along any axes. So, that will be a.

So, here in case of simple cubic, we can see that is the smallest distance. And so this 2 atoms along the axes this 2 atoms will touch each other. So, that will assume. So, basically if I just it is on a surface, one face, only one face. Think I can draw smaller one or just let me draw this way so on a face 4 atoms so on any face if once this 4. So, they will touch each other if this radius of atoms is r. So, then 2 r will be equal to a for simple cubic right and r will be a by 2.

So, in case of simple cubic; so we got this radius of atom is will be half of the lattice constant a.

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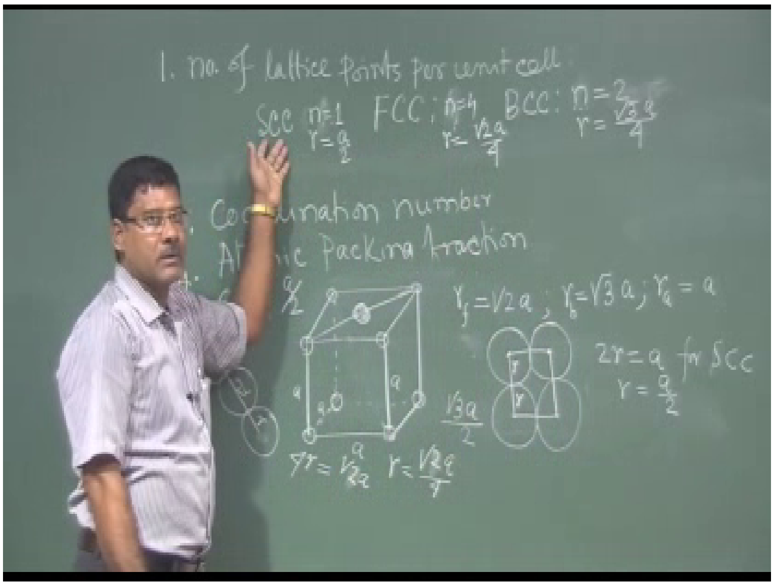

So, now, in case of say BCC, one atom will be at the center of the of the unit cell. So in case of BCC the distance between this 2 corner atom is root 3 by 2; when one atom in middle. So, then the distance between this 2 atom will be 2 3 by root 3 by 2 a.

So, in this case we will get the distance between this 2 atoms is root 3 a by 2. So, another distance are there. So, this distance of this one it will be a, and in case of this 2 it will be root 2 a. So, distance, these will be then this will be the smallest distance in these BCC lattice. So, root 3 a by 2 is the smallest one among this this root 2 a and a right. So, this will be the smallest distance.

Now, in this case, we will assume that this 3 will touch each other, right? This 3 will touch each other. So, this is r, then this 2 r, then this is r. So, total is 4 r. Right and this 4 r is root 3 a right.

So, this a root 3 a by 2 that I have I have calculated to find out the smallest distance between 2 lattice point or 2 atoms. So this from here one can get r equal to root 3 a by 4. That is the radius of atom in BCC lattice. So here let me write here; so for SCC this this basically for SCC n equal to 1. And r atomic radius it is a by 2. And then for BCC if I write n equal to 2 and then this r equal to root 3 a by 4 right. And for FCC when one atom is on one each space in middle of each space there will be atom. And one can easily see that the if I just.

So, these distance is basically root 2 a right. So, distance between these 2 corner atom and this middle atom, it will be root 2 a by 2 means a by root 2. So, again a by root 2 will be the smallest distance. Because this other 2 distance are higher. So, then in this case this will be the smallest distance. So, this 3 atoms will touch each other and corresponding radius will be again similar way this 4 r will be equal to in this case root 2 a. So, r will be root 2 a by 4.

So, in this case it will be root 2 a by 4. So, radius of atom, radius of atom will be different for different bravais lattice. So, for cubic crystal system we have 3 bravais lattice. Simple cubic face centered cubic and BCC body centered cubic. So, the radius of the atoms will be different. And now if I know the radius I can calculate the atomic say let us calculate first one atomic packing fraction.

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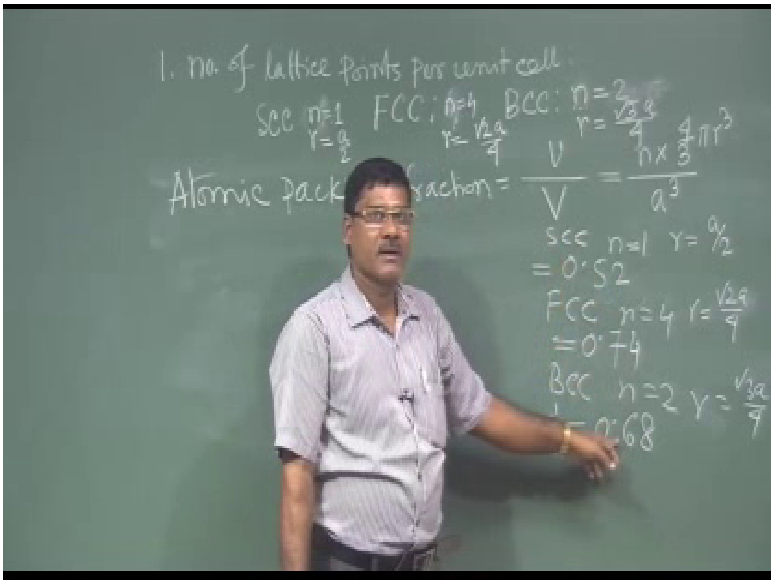

Atomic packing fraction is defined as atomic packing fraction is defined as the unit cell atoms are there. Unit cell itself has a volume V. And now in this unit cell how much volume occupied by the atoms.

So, let say small v volume is occupied by the atoms; so this ratio of this 2 is basically is called the atomic packing fraction. So, now, for cubic crystal, we have seen that volume of unit cell is a cube and for simple cubic the volume of the atoms in that cell. So, those basically if a number of atom per unit cell or number of lattice point per unit cell into volume of each atom. If it is radius is r. So, it is 4 by 3 pi r cube right. So, now, for FCC this packing fraction you can calculate; so n equal to taking, n equal to 1. Taking just putting n equal to 1 and putting the radius r equal to a by 2, we can calculate packing fraction and you can find out it will be 0.52. Because a cube here it will go only you will have pi and n equal to 1. So, this is for FCC.

Similarly, for FCC n equal to 4 and r equal to root 2 a by 4, so then you calculate then this packing fraction you will get 0.74. Similarly, for BCC n equal to 2 and r equal to root 3 a by 4; if you put there you will get this 0.68. So from this packing fraction one can one can tell how compact the crystal. So, from these data one can say that 74 percent of this unit cell is occupied by the atoms, whereas in case of simple cubic it is 52 percent and for BCC that is 68 percent.

So, in next class we will continue the calculation. Mainly these one more calculation is left that is coordination number. So, let me stop here.

Thank you very much.