Solid State Physics
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Lecture - 06
Crystal Structure (Contd.)

Today we will discuss about some of parameters, which are useful for Crystal Structure.

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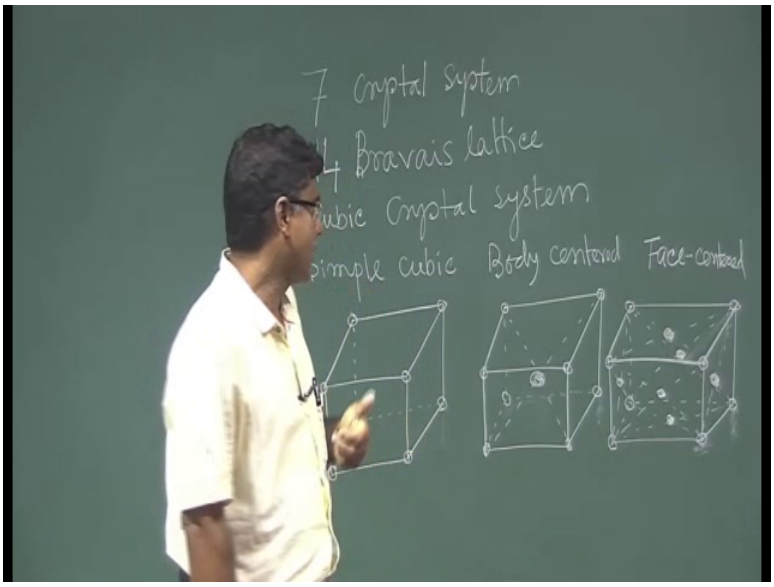

So, we have seen that 7 crystal system, where this lattice points are considered at the corner of the unit cell of this pattern in it. So, what bravais considered the of center, of corner or some lattice points which satisfy the condition that the surrounding of those additional of corner points satisfied this. The surrounding will be same as the surrounding of the corner points.

So far considering this of corner points; so this 7 crystal system basically it is a 14 bravais lattice. So let us consider the cubic system cubic crystal. So, for cubic crystal system have 3 bravais lattice. So, one is simple cubic crystal. So, this simple cubic, this corner has lattice point each corner has lattice point. So, 8 corner, 8 lattice points.

So, another bravais lattice is body centered cubic. So, in this case 8 converts is or have having this 8 lattice points. In addition, along the body diagonal there is a one more

lattice point. So, along the body diagonal if you this and I think if I just take this one. So, here there is additional lattice point. So, this is the body centered cubic crystal. And then face centered another bravais lattice face centered. So, in this case, so 8 corner will have 8 lattice point as in case of simple cubic and at the in each phase. So, there are 6 phase phases.

So, in each phase at the center of each phase there is a there are additional lattice points. So, it will be here and 2 more from this phase. And this other one is this phase; so 6 additional 1 2 3 4 5 6 additional up corner points. So, it forms the it is a face centered cubic crystal. So, this for other crystal system also there says additional bravais lattice. So, like orthorhombic it has 4 bravais lattice. And these 3 simple body centered face centered orthorhombic and in additional base centered.

So, that we have discussed. So, today basically what we want to find out that some parameters, so which are useful to study the crystal. So, this, if we want to calculate some parameter say one is number of lattice point per unit cell.

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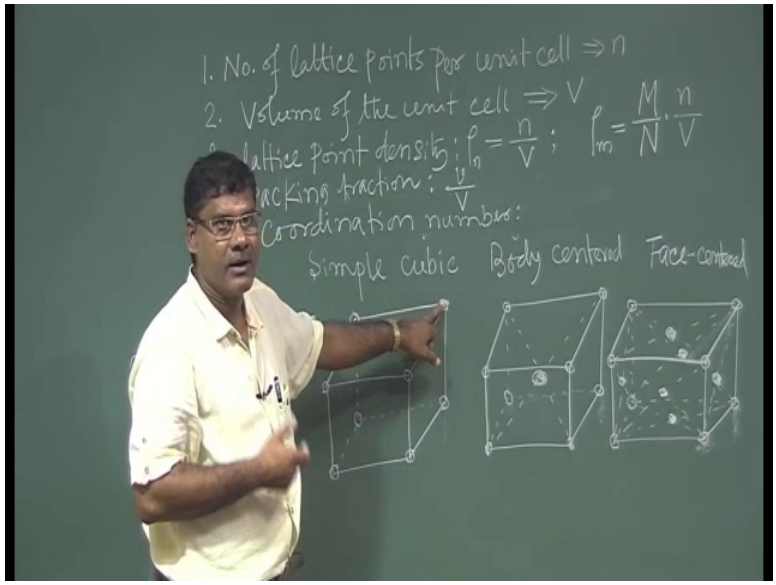

So, how to calculate that we want to see; then what is the volume of the unit cell, how to calculate that one volume of the unit cell? Then also one can calculate the number density of unit cell. Means how many number of lattice point per unit volume.

So, basically if you calculate these 2. If I this will be the n and volume of unit cell is v. So, lattice point density in the initial or in the crystal lattice point density, that will be say it is rho n, lattice point density say rho n it will be n by v right. So, for if we want to know the mass density, in terms of mass if you want to know the density of the crystal, so then if say it is rho n. So, how we can find out? So, you know this one gamma of any material contains Avogadro number of atoms or molecules. So, here say that atoms are at the lattice point.

So, mass of Avogadro number of atoms; so mass of one atom will be this molecular weight divided by Avogadro number. So, this is for one. So, if n number of per unit cell n initial in number of lattice point of atoms are there; so in 2 n. So, this is the total mass of the atoms in a unit cell. So, volume of the unit cell is v. So, divided by v so that will be the mass density; so then other parameters also, there is are like packing fraction of the crystal. This basically unit cell have volume now. What are the ratios of proportion of the volume occupied by the atoms? So, volume of the say v volume of the atoms in a unit cell divided by the volume of the unit cell.

So, this ratio will is called basically packing fraction. So, how much packed with the atoms in that crystal. So, from that this data one can understand this other parameter is there. These coordination numbers coordination number that is basically for any lattice point how many nearest neighbors are there which are equidistant from that lattice point. So, that is called the coordination number. So, that also we will calculate. So, let us calculate first this number of lattice point per unit cell; so in case of simple cubic. So, in this unit cell 8 corners are there. So, 8 lattice points are there, but now this.

So, this it is not that 8 lattice point per unit cell, because these each corners because we said this is a one in unit cell in a crystal. So, crystal basically is formed or lattice is formed just translating this unit cell in all directions. So each corner will attach with how many unit cell that we have to find out. So, you can see that. So, this side there will be one. So, on top of it 2 more. So, these 4 will have this corner. So these are on this plane, if you think that is one is here and 2 more are on top. Then this side 4 more unit cell will be there. So, basically each corner will attached with the 8 unit cell. So, this is it will share with 8 unit cell. So, for each unit cell this it is a heat will contribute one-eighth of each lattice point.

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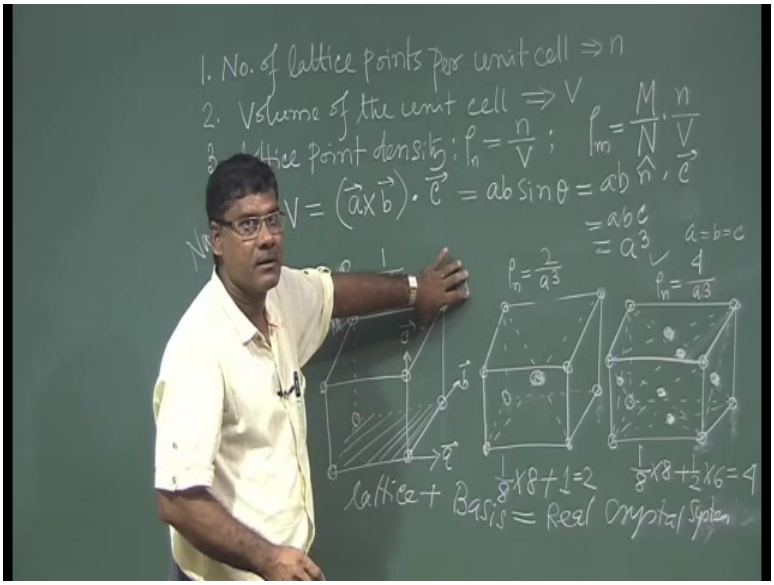

So, we have 8 lattice points. So, basically effectively it will be one lattice point per unit cell. So, similarly for other cases we can calculate. So, let us I think it will be easy to understand if we see some model. So, we have model for simple cubic crystal. So, this is a simple cubic crystal. So, these 8 corners, 8 lattice points. So, now, if we see here, just think this one, each one is one unit cell right. This is 1 2 3 4, then below product there. So, total 8 unit cell. Now if we consider just one corner, just if you consider this corners right, so these corners. So, these corner is attached with this unit cell, this unit cell and this this top 4 as well as this bottom 4.

So, similarly if you extend this; so you will find that each corner point will attach with 8 unit cell as it is. So, it is obvious that it is it will have one 8 contribution to each unit cell. So, thus that is what I have written, 1 8 into 8 corners. So, it is effectively one unit cell per unit volume. So, this it also expressed nicely here. If you see this this is a simple cubic. So, 8 corners are there see just in each corner. So, this is the lattice point this portion is that is one-eighth; so this one-eighth. So this one it will be half and top of this 4 parts. So, that will give half. So, this is a total will be for the 8 corners, 1 8 into 8 corner 8 lattice points that effectively will give of 1.

So, similarly other one, if we consider the body centered cubic. So, this is the body centered cubic right as I have drawn and in model you can see. So, this is the cubic unit cell 8 corners are there 8 lattice points; so one more at the center of the body. So then

easily you can calculate how many lattice points per unit cell. So; obviously, 8 corners will give you one contribution effectively one lattice point per unit cell and one more there in body. So, it is not sharing within unit cell. So, total will be 2. So, for body centered it will be one-eighth. So, I can write one-eighth into 8. So, there is a from the corner plus this one in body. So, it is a effectively 2.

So, 2 lattice points per unit cell. Similarly, for face centered cubic how many will be there. So, from model we can see. So, these are face centered cubic. So, you see 8 corners are there; so one-eighth from each corner. Now if you see this each face will basically attached with the 2 unit cell. So, on top of it, on top of a another unit cell one top of another unit cell. So, these this face centered that lattice point. So, it will share with the 2 unit cell. So, it will contribute half to each unit cell. So, that is I hear this you can see this half of the lattice point in this scene unit cell.

So, I have 6 faces. So, this from opposite faces. So, one these 2 opposite faces one more. So, other 2 opposite faces; so one more, so total 3 plus from corner one. So, total will get 4 unit cell, 4 lattice point per unit cell. So, here basically we are getting one 8 into 8; so from corners plus half from each face. So, into 6 face. So, equal to 4. So, in face centered cubic. So, we have 4 unit cell 4 lattice point per unit cell. So this n basically for this simple cubic is one n equal to 1 for this n equal to 2 and this for face centered n equal to 4.

So, next let us calculate the volume of the unit cell. So, let us concentrate for this case for cubic or basically you can construct it octagonal as well as atomic also higher these crystal axis are mutually perpendicular to each other. So, in this case, volume we calculate taking the dot and cross product of lattice crystal axis. So, crystal axis if it is a b c, if it is a that is say b and it is say c. So, what will the volume? Volume we can write in this case, I will write a equals b dot product with c.

So, a cross b is basically the you know the I mentioned probably. So, this tells about the area. It tells about the area. This is the area equals v. So, this is b axis; so this parallel to this. So, this b and this is a. So, this area is a b. So, here if I can write a b sin theta, I can write a b sin theta, but if it is cubic crystal of tetragonal orthorhombic, so this theta is 90 degree. So, it will be 1. So, it will be for cubic system or this orthorhombic system, it is a b and if it is cubic. So, it will be a square. So, there a equal to b. And direction this is the

plane. And direction will be say unit vector n. So, that will be perpendicular. That will be basically perpendicular on this plane.

So, then I can write this. So, in this case if it is cubic or orthogonal system means this all 3 axis are mutually perpendicular to each other. So, this n it is the direction will be c direction. So, this n is basically c direction unit vector towards this towards c. So, this cross product if I take a b c, and this cos theta say if I write just one angle. So this theta is 0 basically right, because they are in same direction. So, it will be cos 0 is 1. So, it would be a b c. So, for cubic crystal it will be a equal to b equal to c a equal to b equal to c for cubic system. So, it is a cube. So, volume of the unit cell cubic unit cell is a cube.

For tetragonal, orthorhombic it is a b c. I think tetragonal, it is a square a square c and orthorhombic it is a b c. So now, you can. So, this volume is same for simple cubic for body centered cubic and this face centered cubic right. So, easily I can calculate density. I can calculate density; so rho n for simple cubic. I think I write here, this for simple cubic rho n equal to n by v n is 1, v is a cube. So, that will be the lattice point density for simple cubic. Lattice point density for body centered cubic it will be 2 by a cube and lattice point for lattice point density for body centered cubic will be sorry for face centered cubic will be 4 by a cube.

So, if you know the mass of one gamma material, then Avogadro number is known to us. So, for that material just we can get the mass density. So, that way if we can calculate this parameters and this is a very important parameter that we see later on. So, similarly this others to this packing fraction as well as the coordination number we can calculate. So, for packing fraction, to calculate the packing fraction we need the radius of the atom. So, here we have considered the lattice point. So, actually it is not representing the real crystal; so to get the real crystal. So, these are just mathematical concept. So, for real crystal basically I have to we have to add. So, with lattice we have to add basis; this is called basis. Then we will get real crystal system, right.

So, this basis is basically atom or group of atom attaches to the each lattice point in same manner. So, that if it is one atom it can be just at the position of lattice point. If it is 2 atom say sodium chloride in case of sodium chloride in case of sodium chloride. So, each basis will each basis will, consist one sodium and one chlorine atom. So, that sodium and chlorine just it is I am not putting exactly just one can put this way; so here

one sodium here one chlorine. So, then we have to put attach this group of atom in same manner. So, these are called basis. So, lattice plus basis with each lattice point will give the real crystal structure.

So, now this in real crystal structure there these atoms are there a group of atoms are there then to know the packing fraction. So, we have to find out the radius of the atoms. And we have to assume that in at the smaller distance smaller distance between the lattice points along that this atoms we will touch each other. So, from that assumption from that concept one can calculate find out the radius of the atom. And from there we can get the packing fraction of the unit cell as well as it will be adequate for calculating the coordination number of the lattice point.

So, I will stop here.

Thank you, for your attention.