Semiconductor Device Modelling and Simulation
Prof. Vivek Dixit
Department of Electronics and Electrical Communication Engineering
Indian Institute of Technology - Kharagpur

Lecture - 04
Crystal Concepts (Contd.,)

Hello, welcome to lecture 4 so, we will continue our discussion on crystal concept. So, today's topic is unit cell description. So, all the crystals they can be described through certain unit cell, which has certain characteristic properties related to the symmetry. So, different crystals we discussed in last class, they were 7 crystal types, and then we had around 14 previous lattices. So, here we will consider the cubic lattices and they are unit cells.

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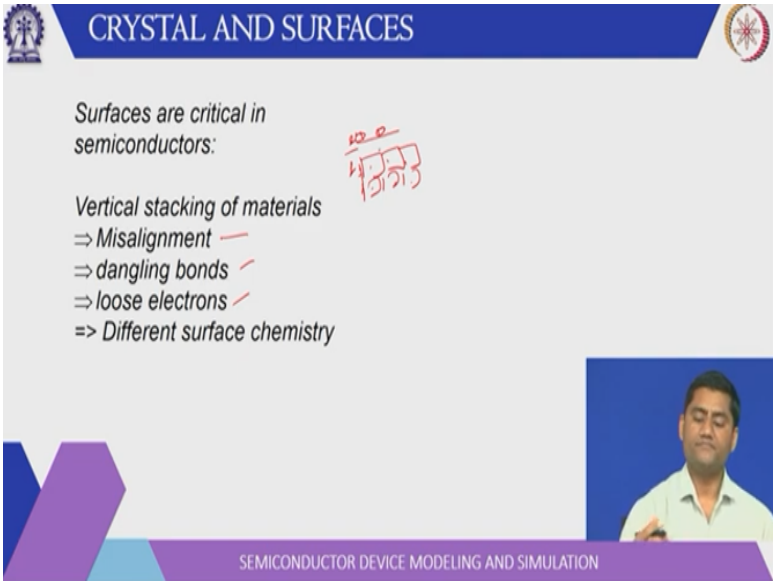

Now, why it is important to understand the unit cell because, if you look at the semiconductor crystal, it is made up of the unit cells and these unit cells can be repeated in 3D space. So, this is 1 unit cell, then is in 2D and then you can stack up so, you can have 3D structure. Now, it is possible that an engineer can put different materials on top of another material. So, let us say this is material 1 on top there is a material 2.

And in that case, if they are lattice constant that it means, the inter atomic distance is different, then there will be some misalignment up to certain thickness of course, the top material will try to comply with the bottom material, but after that there is a possibility of misalignment at the surface, there is a possibility of having dangling bonds. So, number of atoms per unit area on the surface will determine the density of these dangling bonds.

That will affect the chemical properties then, the constituent atoms are the basis a group of atoms, they will decide how many loose electrons are there. So, that means, in overall the crystal and the surfaces they determine what is the property? What is the property of semiconductor? What is a property of the surface? What will be the quality of the surface? How it will respond to different chemical substances?

And these crystals have different properties along different directions. So, those properties can be found from the unit cell. So, let us consider them one by one.

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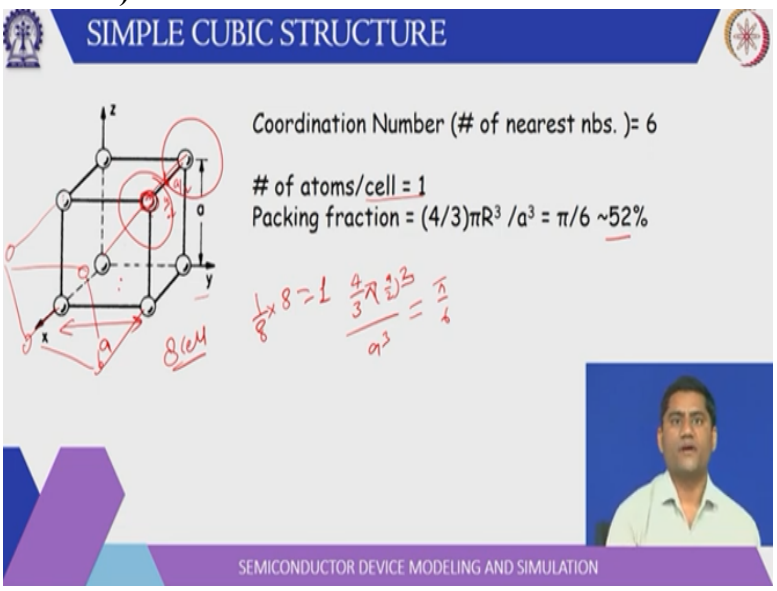

The very first one is a simple cubic structure. So, simple cubic structure basically the unit cell is of the nature of cube, where atoms, they are occupying the 8 corners of the cube. And the distance between these nearest atoms is also called lattice constant. And if you reconstruct it, then let us say this is x direction, so in x direction, there will be another cell here, then there will be another cell in y direction here, here.

And so, there are total 4 unit cells in this plane, you will see the plane which is parallel to xy plane, 1, 2, and on right, 3, 4, then on top there will be 4 at the bottom also there will be 4. So that is this one corner is shared by the 4 in the plane and 4 above the plane. So, 1 corner is shared by 8 cells. So, that means each corner atom is shared by 8 cells. So the contribution to the unit cell will be 1 / 8.

And there are such 8 atoms so that means this unit cell contains 1 atom. So there is a number of atoms per cell. Now, this diagram is shown for the convenience. But in reality, the atoms

are much bigger and they are touching each other. So, this is the middle of the side length. So, up a / 2 here and a / 2 this and a / 2 this side. So, you have some atom like this, and you have another atom like this.

They are touching each other so, the radius of the atom will be a / 2. So, the volume occupied by 1 atom is 4 / 3 pi r cube and r is a / 2 / a cube. So, that comes out to be around 5 / 6. So, that is around 52% so, that is a packing fraction. So, out of the total space of the unit cell 52% is occupied by the atom the rest is the space.

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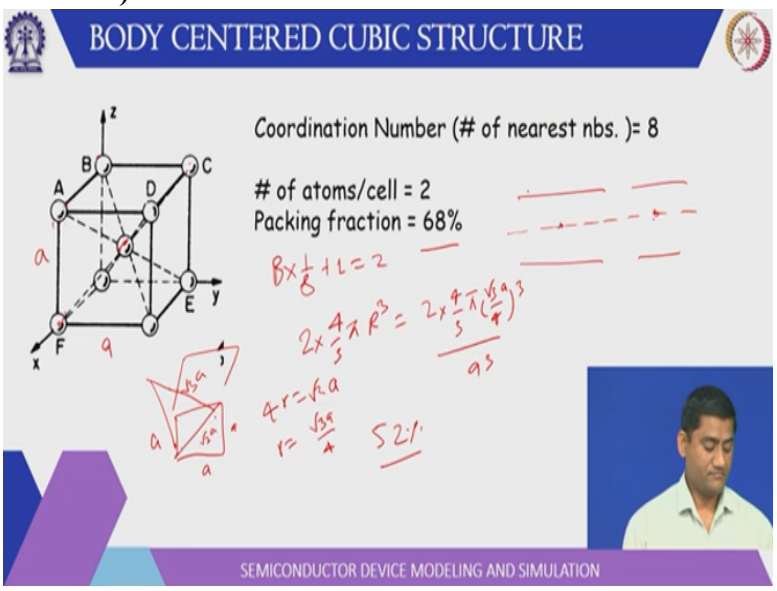

Next one is body centered cubic structure in body centered cubic structure apart from the case similar to the simple cubic structure there is one atom at the center of the cube. So, you can draw a body diagonal and they will intersect at one point that is the center of the cube. So, total it will have there are 8 corner atoms shared by 8 unit cell plus one body atom shared by no other unit cell so, there are total atoms are 2 per cell.

And then of course, you can multiply. So, these 2 atoms their volume will be 4 / 3 / r cube. So, what will be the radius of these atoms? Now, if you see the nearest atom, the distance between these 2 atom is a, these 2 atom is a whatever the body diagonal, body diagonal will be you can determine like this. So, this is one side then you can build the surface so, this is a, this is a so, this will be root 2a then if you construct in 3D.

So, this height is a and this will be root 2a square + a square so, this will be root 3a. So, root 3a is the length of the diagonal. So, this is now atoms here there are 3 atoms. So, this is r, this

is r, this is r and this is r. So, this is basically 1, 2, 3, 4 there are 4r so, 4r = root 3 times a so, your r = root 3a / 4. So, that means, you can write 2 times 4 / 3 pi r cube, so, root 3a / 4 cube / a cube. So, that will come around 68% so, that is the packing fraction of body centered cubic.

So, if you compare this thing with the simple cubic where the packing fraction was 52%. So, that means, the BCC is more densely packed compared to SCC simple cubic structure you can also find different properties if you look at the surface the top surface there are 4 atoms then at the bottom surface there are 4 atoms or 4 lattice point per unit cell, then if you compare with the simple cubic, this is one layer this is one layer.

Now in BCC you have one atom here. And let us say this is another cell that there is one atom here. So, that is there is an extra layer in this case is present right and then if you see the atom density, so, it is something like middle plane where there is a presence of atom. So, number of layers are basically you can say they are different and the properties are the number of items per unit area that we can calculate basically and that is called surface density of the atoms.

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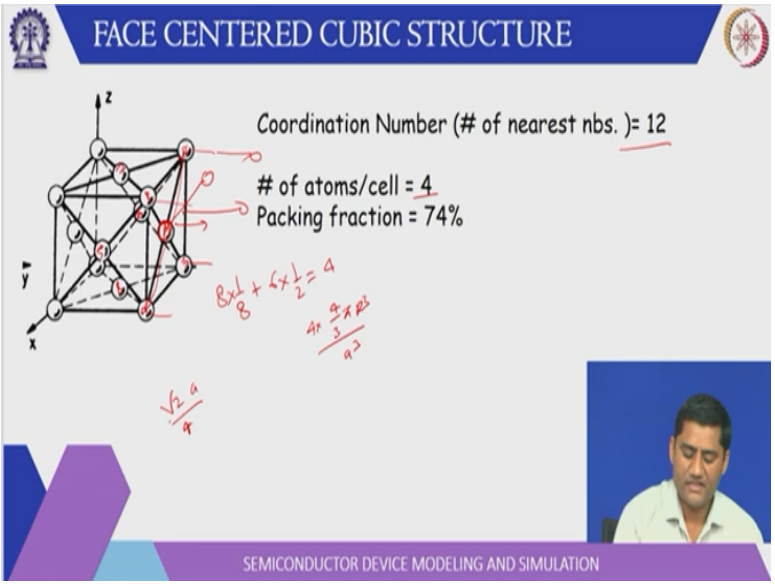

The next one is the face centered cubic structure in case of FCC apart from the atoms at the 8 corners of the cube there are atoms at the 6 surfaces. So, an atom at the surface will be shared by the side unit cell. So, all the 6 surface, so, that is this atom at the surface will be shared by the 2 unit cells. So, its contribution will be half, so, now you can write number of cells, there are 8 corners, there are 8 atoms at the corners and each contribute 1 / 8 plus a cube has 6 surfaces so 6 and each contribute half.

So, that comes out to around 4. So, you have 4 atoms per unit cell the nearest neighbour of atom you can count here in case of BCC and simple cubic it was simple here, you have to basically do little imagination, you can see that there is a atomizer surface. So, how many neighbours does it have? There are 4 neighbours at the corner. So, we can number it 1, 2, 3, 4 and what are others?

If you see the surface atoms of the 2 sides, so, this will be your 3, 4 this is 5 and this is 6 and on the top 7, 8 now such atoms will exist in the cell beside it. So, there will be atom at the front surface back surface top surface bottom surface of the cell nearby. So, this is one cell and same thing will repeat here. So, this is also neighbour and the distance is basically same. So, totally it will have 12 nearest neighbours.

And there are 4 atoms per unit cell and packing fraction you can calculate four times 4 / 3 pi r cube, that is a volume divided by a cube what will be the radius here you can calculate because these 2 atoms are nearest neighbours. So, this diagonal is root 2a and this will be r this will be 2r this will be r so root 2a / 4 so that is the radius. So that comes out to around 74%.

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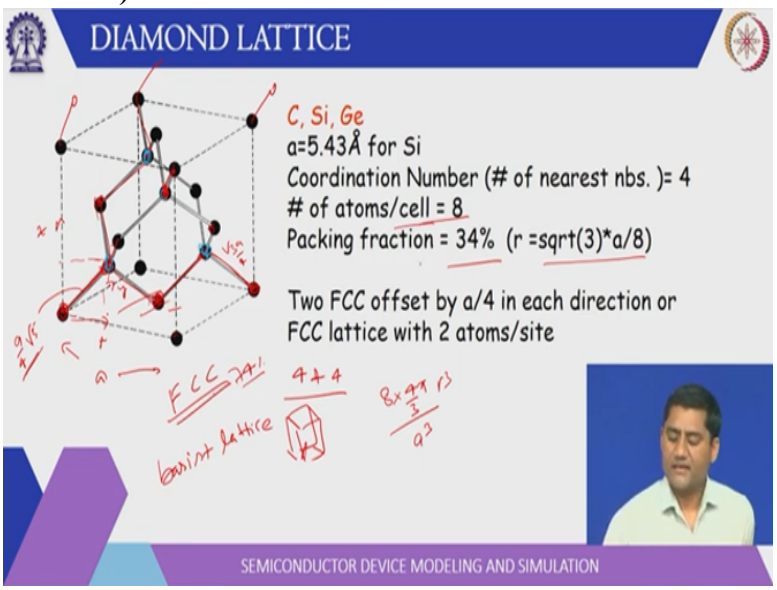

Now the popular elemental semiconductors silicon germanium, they are found in diamond lattice diamond lattice is nothing but a slightly modified version of FCC. So, this is actually FCC lattice, FCC crystalline structure, the difference is now the lattice site is occupied by 2

atoms instead of 1 atom. So, there are 1 atoms this one and this one, the line connecting them is along the diagonal.

So, let us say this is x axis, this is y axis, this is z axis and let us say this side length is a. So, this will be at a / 4x, a / 4y, a / 4z. So, the length this is a / 4 times root 3. So each lattice side is occupied by a group of 2 atom that we discuss is called basis. A crystal is basis plus lattice. So, we have given it a name called diamond lattice. So, and please remember, this diamond lattice will not be a previous lattice, FCC is a previous lattice.

So, an FCC is occupied by where FCC sides are occupied by 2 atoms, we call it diamond lattice. So, or you can think of it as a 2 FCC lattices. And they are staggered by length a / 4 along a diagonal. So, or you can say root 3a / 4. So, in each direction x direction a / 4, y direction a / 4, z direction a / 4 this a staggered basically. So, if you see here, there will be 2 atom like this, this will actually go to outer cell, this will also go to outer cell, there is a middle one.

So, this will also have 1 atom along the length and this will be outside this will also be outside and this face will have along this line then the face here and this is the bottom one, this is a side one, this will also go out so, if you see here the left one and the right one. So, this is the basically the bottom face, this is the bottom face, and this actually is same length at the same distance from the opposite atom. So, let us say this is side 1, this is side 2.

So, this is it, this is also root 3a / 4. So, there are 2 atoms in this layer, then if you look at the top, this is one atom and this is first corner so, there is another atom here. So, these 4 atoms are and that we use different colours, this one, 1, 2, 3 and 4 these are the atoms that are inside the unit cell and rest are basically the part of the FCC lattices. So, how they are related the first one is related to this corner, second one is related to the bottom face.

The third one is related to the side face, the fourth one is related to the front face, this is the front face and others will have associated the atom but that will be outside this unit cell. So, that will contribute to some other unit cell. So, if you find out how many atoms are there in one unit cell here, so, FCC has total 4 plus there are 4 atoms inside, so, there are total 8 atoms.

So, this is a number of atoms per unit cell then if you find out the nearest neighbour, these 2 atoms are the nearest neighbour, these are the nearest neighbour, these are the nearest neighbour, these are the nearest neighbour, so, it is a tetrahedral structure. So, in 3D, you know, you have to have a 3D view basically. So, there are popular sites for showing that crystal you can see the structure in more detail and this nearest neighbour distance.

So, this distance is root 3 a / 4 so, the radius will be root 3 a / 4 / 2. So, that is the radius root 3 a / 8, then if you calculate a packing fraction, it will be there are 8 atoms times pi 4 / 3 pi r cube / a cube. So, that will come around 34%. So, you notice FCC has around 74% packing fraction but the diamond lattice which is FCC having 2 atoms per side the packing fraction is reduced. So, it is less densely packed.

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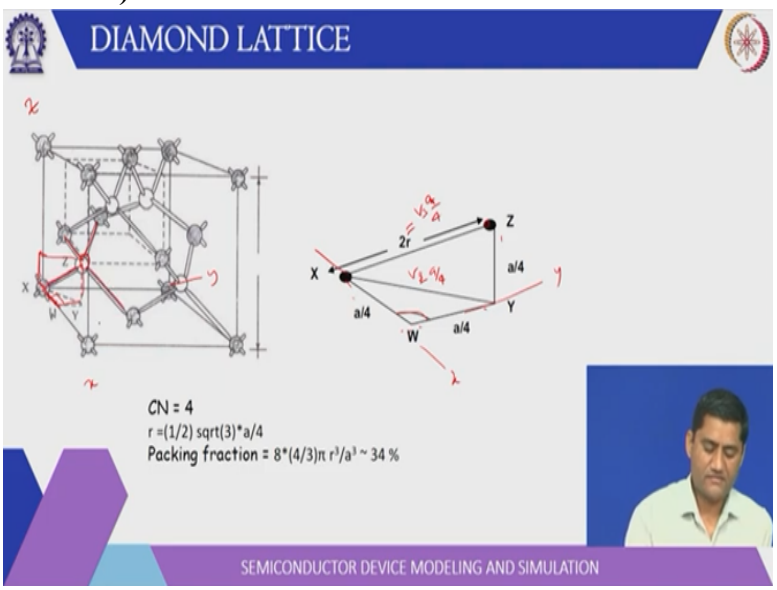

You can see further view of this diamond lattice. So, here this corner atom you can see this distance is W this is Y and this is Z. So, this is basically a Z point W point Y point. So, this is let us say X axis this is Y axis this is Z axis. So, you can think like this, this is X axis and there is a one Y axis here. So, this is parallel to Y axis, so, you can see the Y axis and then the top is the Z axis.

So, if you see here at W there is a 90 degree angle it is not properly shown here, but we will see this angle is 90 degree then this will be this is a / 4 this is a / 4, so, this will be root 2 times a / 4, then this height is also a / 4 this is here, this is the point Z the side is a / 4. So, this will be 2r will be root 3 times a / 4. So, accordingly you can find that coordination number is

around for this atom you can see there are 4 nearest neighbours and the packing fraction is around 34%.

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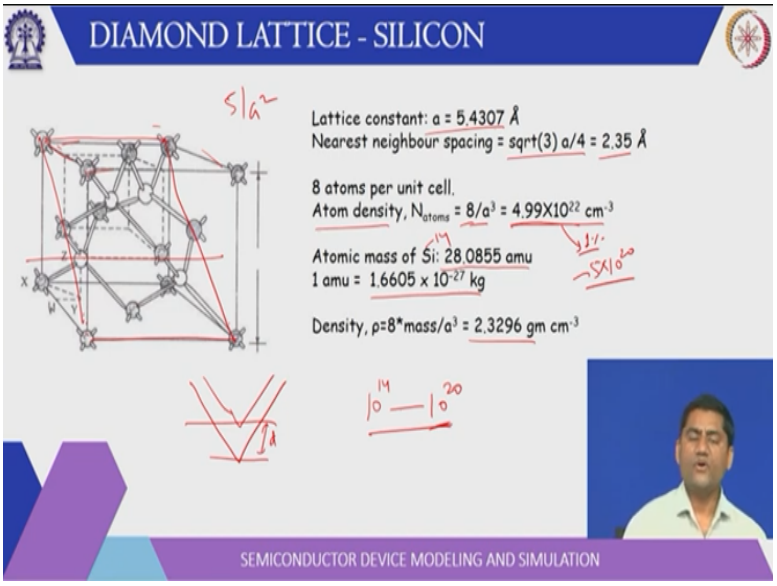

We can actually calculate other properties of the lattice if we know the lattice constant. For example, if you consider silica which is FCC with a basis of 2 atoms you can find in the literature there are tables which lists the lattice constant and the bandgap of the semiconductors. So, for silicon, the lattice constant is 5.4307 Angstrom and these lattice constants are actually calculated through x ray diffraction techniques.

So, x ray basically they assign on it and then they are deflected. So, this is a relationship and this distance between the plane so, this 2D sine theta will a phase difference and then based on the constructive and destructive patterns, we can estimate what is the distance between these 2 planes. So, from this we can determine the lattice constant. So, if the lattice constant is 5.43 angstrom the nearest neighbour is spacing is root 3a / 4.

So, that comes around to 2.35 angstrom so, please remember the inter atomic distance need not the same as the lattice constant and there are 8 atoms per unit cell. So, of course, we can calculate that atom density this is the atom density so, there are 8 atoms divided by a cube. So, that gives you around 5 into 10 is to power 22 atoms per cubic centimeter. So, you might have seen that doping levels in semiconductor doping tables.

So, it may start with something 10 is to power 14 or something and it goes to around 10 is to power 20. So, you see, if you go to 10 is to power 20 there is a limit. So, if you go to 5 into

10 is to power 20 that is a total number of atoms. So, if you take 1%, the 1% is of this number will be 5 into around 20. So, if you go to 5 into 10 power 20, that is the 1% so, that will be your basically it will be some things like compound basically it has 1% contribution from foreign atom.

So, generally we keep the doping below 10 is to power 20, 20 is very high doping. And of course, when you dope there are some activation issue also that how many of those dope and atom will actually be active now, each silicon atom has some mass. So, if you look at the periodic table, it lists the atomic number. So, atomic number for silicon is 14 atomic mass is 28 the unit is AMU atomic mass unit and one AMU is 1.66 into 10 is to power -27 kg.

So, if you know the crystal structure, you can also find the density and if you calculate the density it comes out to around 2.3296 gram per cubic centimeter. So, this is not you know just one case you can find multiple properties. If you can find out how many atoms are there in this surface, the top surface there are 5 atoms per unit area the top surface at the bottom surface then, if you take this layer here, you can find that number of atoms.

If you take another plane, let us say along the diagonal, the diagonal here. So, if you take this diagonal here, how many terms are there 1, 2, 3, 4, 5, 6. Then, there will be this body diagonally around here 7, 8. So, you can calculate this 8 atom per this will be a root 2 times a. So, root 2a square that will be the area. So, you can find out the atomic density. So, this atomic density plays a role.

Let us say if you choose certain surface let us say 100 surface 111 surface, these will of course discuss in the next lecture, but, you know from the crystal point of view, you can find out that how many atoms are there in a particular plane. So, if the number of atoms per unit area is more in certain plane, that plane will be more active or more reactive, because it has more number of atoms and it will affect certain properties of the semiconductor device made from those materials.

So, when we choose the material, we also choose you know which orientation of the lattice we are using we also choose the doping level.

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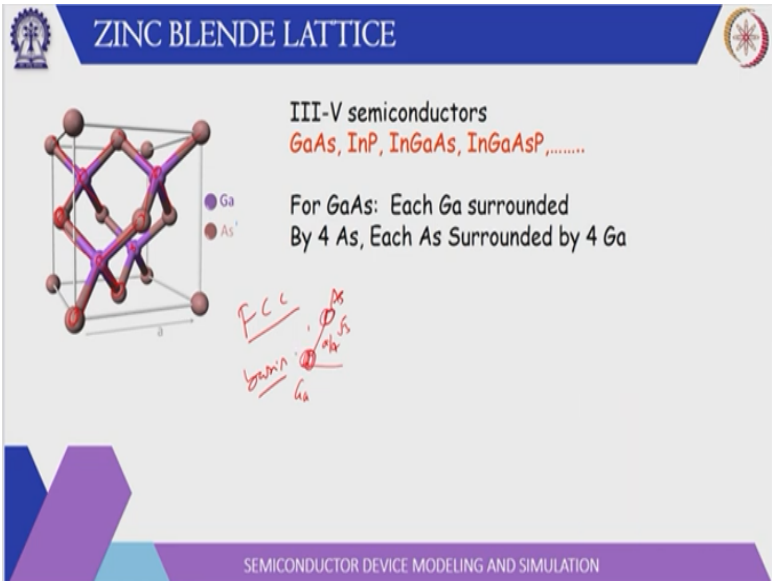

So, for zinc blende structure this is very similar to the diamond structure, the only difference I,s it is an FCC lattice with a basis of 2 atoms and the same orientation, the length is a / 4 root 3, so, x axis a / 4, y axis a / 4, z axis a / 4. The only difference is these 2 atoms are different, let us say if it is gallium arsenic, so, this atom is gallium this atom is arsenic. So, each gallium atom is surrounded by 4 arsenic atoms.

This is a corner these are the face, here front face, the side face, the bottom face and the corner and then again this is here. So, this is in the body then this corner, the top face the right side face and the front face near the corner, the top face the side left side face and the back face and similarly here so, this is the name is called zinc blende structure this is zinc blende lattice.

So, generally the 3-5 semiconductor they are found in zinc blende lattice form. So, this is very similar to a diamond the only difference is in the basis atom in the basis there are 2 atoms which are different the rest of the properties are similar.

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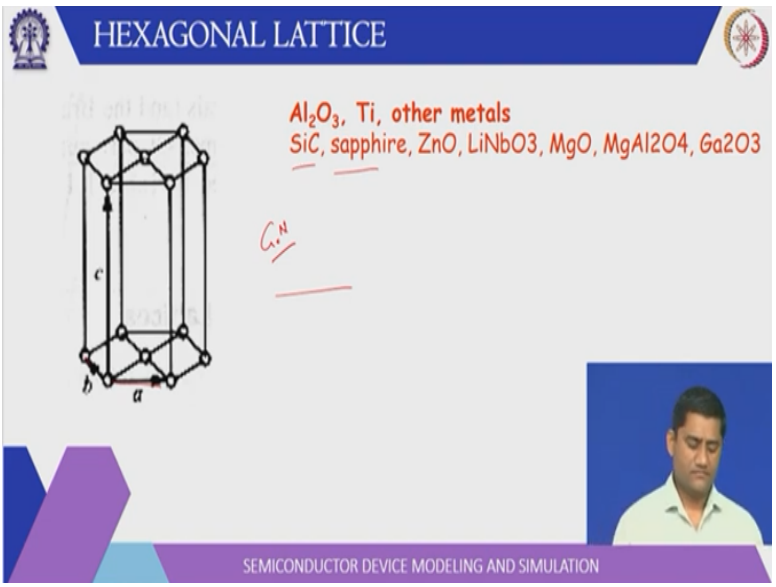

The next one is the hexagonal lattice so, in hexagonal lattice, these atoms are arranged in the form of the hexagon. So, each hexagon has a site length a another b and the height is c and the typical materials that are found in hexagonal lattice are silicon carbide, sapphire, zinc oxide. Now, some materials like gallium nitride they exhibit both the forms they may be found in hexagonal lattice or they may be found in zinc blende lattice.

So, that depends on the growth technique that is used. So, by tailoring the growth condition and substrate below you can grow gallium nitride into either zinc blende or wurtzite that is hexagonal lattice. So, that basically depends on the substrate material on which we are growing the layer and the growth condition.

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So, in this lecture, we have discussed about the common unit cell is specifically the cubic crystal unit cells, their structures and their coordination number held by the individual atoms,

we also discussed the diamond lattice and we also discuss how to calculate the atomic density on a particular layer or the density of certain crystal. So, thank you very much and in next class we will discuss about we will further continue our crystal concept and we will discuss about how to quantify this unit cell lattices. Thank you.