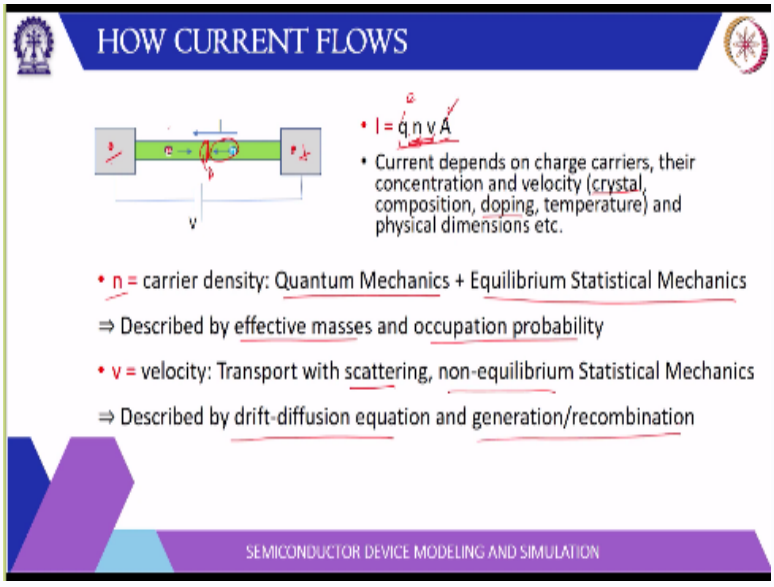
Semiconductor Device Modelling and Simulation
Prof. Vivek Dixit
Department of Electronics and Electrical Communication Engineering
Indian Institute of Technology – Kharagpur

Lecture – 03
Crystal Concepts

Dear students, welcome to the third lecture on crystalline structure. In last class we discussed about nanostructure and the heterostructures. And we also discuss the process of simulation first we do process simulation input of the process simulation is a semiconductor material output is a device structure, then device simulation output is an IV characteristic from there we get a compact model.

Then again supplied to the circuit simulation tool and they are the output is the system performance. Now, the basis of the semiconductor is the crystalline structure that is there and we will try to understand this crystalline structure from the point of view of how the current actually flows?

(Refer Slide Time: 01:22)



So, if you take a simple piece of material here can be semiconductor can be any other material. So, let us say this is a piece of material and then there are 2 contacts here contact 1 contact 2, so, this is less a positive this is negative. Now, these positive negative are basically relative so, when

we write positive that means, it is at higher potential with respect to the other terminal. And if it is negative.

Then it this terminal is at lower potential compared to the other terminal and there are carriers here that there is a conception of 2 carriers electrons and holes, these electrons will move from lower potential to higher potential and these holes will move from higher potential to lower potential. So, when this potential is applied, a current will flow and the expression of current can be given by q times n times velocity times the area.

So, q is the charge on individual carrier and n is the number of carriers per cubic centimeter or per unit volume. So, q, n is basically the charge per unit volume that is present and that charge is moves with the velocity v and amount of that charge crossing an area, area of cross section. So, this is the structure it will have certain cross section. So, cross section area is a (()) (03:03) that is a current.

Now, in this expression q is the charge on the carrier which is e 1.6 into 10 to the power -19 Coulomb that is fixed. A is again the area of the cross section which is again physical dimension. So, 2 things that are remaining is the number of carriers per cubic centimeter or the volume and v the velocity of these carriers. So, these 2 parameters actually determine the current that will flow. Now, number of carriers depends on the crystalline structure velocity also depends on the crystalline structure through the bendy structure.

So, of course the crystalline structure then of course, what is the composition of their crystal what are the different constituent atoms of that crystal or for a given a constituent, what is the doping what is the level of doping and what is the temperature? So, they will determine the n and v the carrier concentration and the velocity and physical dimension is of course, they control the length and the area. So, your carrier density is actually given by this concept called quantum mechanics. So, it actually comes from the crystal.

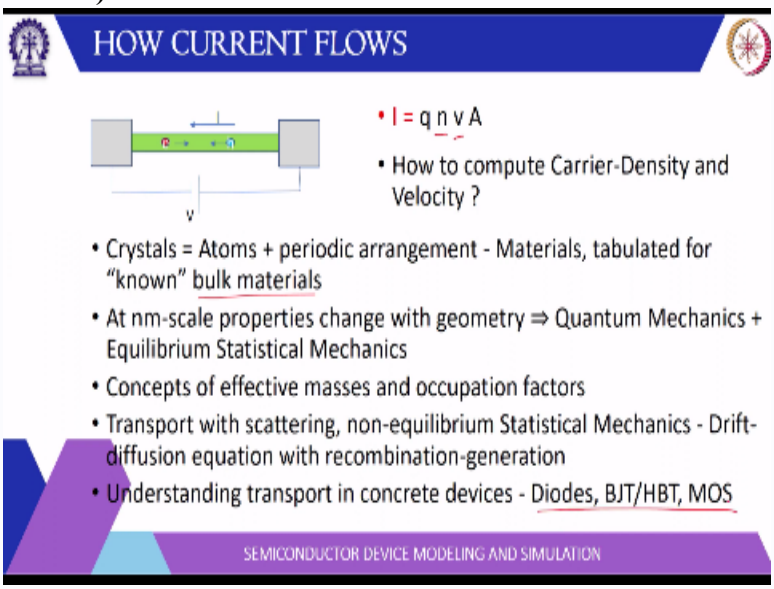
So, because in the crystal atoms are spaced at order of nanometer distances so, that means, the quantum mechanics principle will be applicable there and that will give rise to certain allowed

energy states for the electrons. So, these electrons can only occupy certain energy states and from that we can find out what is the probability of these electrons filling those states? So, how many electrons can occupy certain energy level and from that if you calculate number of a state times probability that is called equilibrium statistical mechanics.

We can estimate the number of carriers and of course, the concept of hitting mass and occupation probability. So, that determine the carrier concentration, velocity of these carriers is determined by the hindrance that these carriers experience. So, once you apply a field these carriers will move, but in the process they will get scattered. So, scattering is a non equilibrium process. So, then you have non equilibrium statistical mechanics.

And generally this movement of carrier is described by drift and diffusion equations and these carriers can generate and can disappear also. So, that is called generation recombination mechanism. So, these things will actually describe the velocity.

(Refer Slide Time: 06:07)

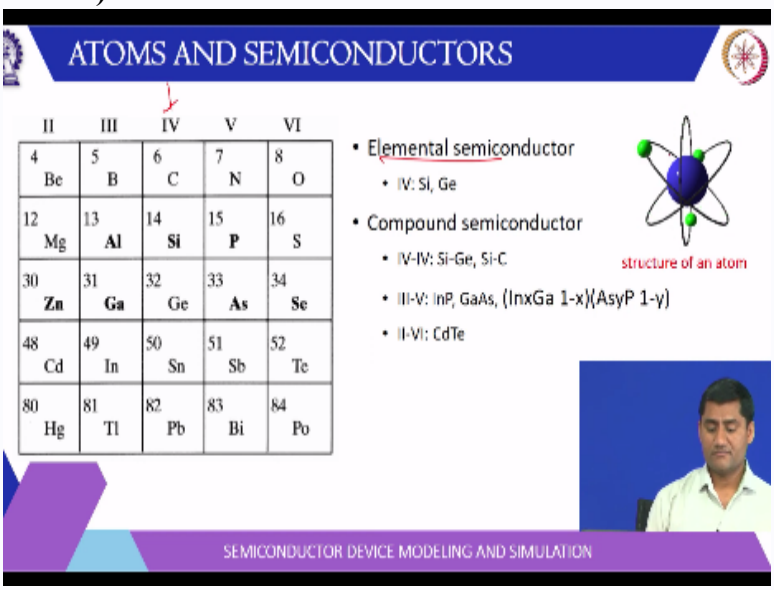


So, now, how to compute the carrier density and calculate the velocity of electrons or carriers? So, for that we need to understand about the structure of the semiconductor. So semiconductor is a crystal and crystal consists of atoms, atom placed at periodic locations. So, there is a periodicity and these material parameters are actually you know tabulated in the well-known texts. So, for different bulk materials like silicon, germanium, gallium arsenide, so, these material parameters are tabulated.

Because the in the crystal the atomic a student the distance across atoms is order of nanometer. So, quantum mechanics and equilibrium statistical mechanics are applicable here and the concept of active as occupation factor we will discuss and transport with scattering non equilibrium statistical mechanics those also we will discuss and together with the crystal physical mechanisms will help us to understand the flow of current through the semiconductors.

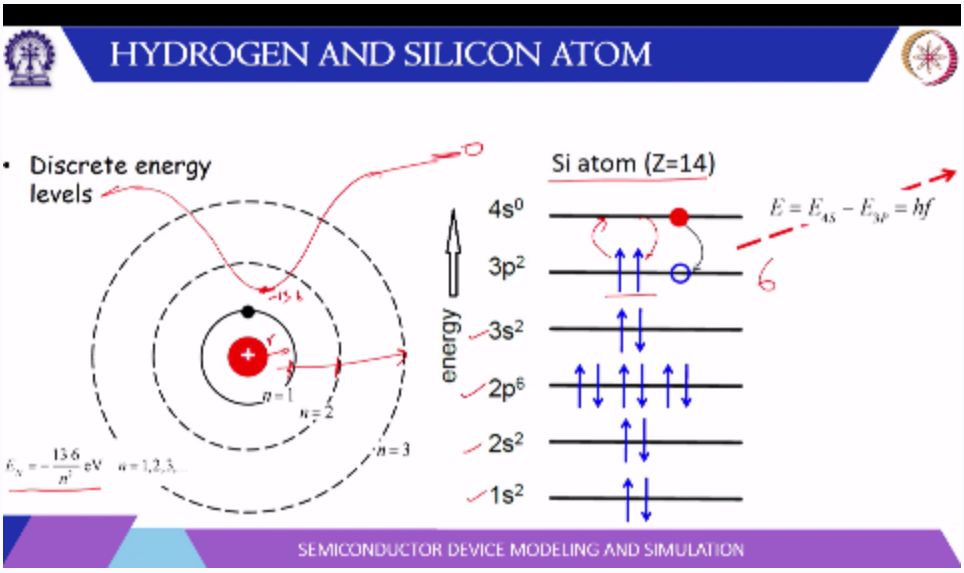
And of course, once you know about the carrier concentration and velocity of these carriers we can understand how these different devices work diodes, bipolar junction transistor, heterojunction bipolar transistor or MOS or MOSFET.

(Refer Slide Time: 07:55)



So, this you already know that 3, 5 semiconductor group for semiconductor 2, 6 semiconductor so, group 4 semiconductors are called elemental semiconductor and others are called compound semiconductor. So, this is a typical structure of atoms that you know as a nucleus here and these electrons are moving around the nucleus when these atoms come together what happens?

(Refer Slide Time: 08:22)

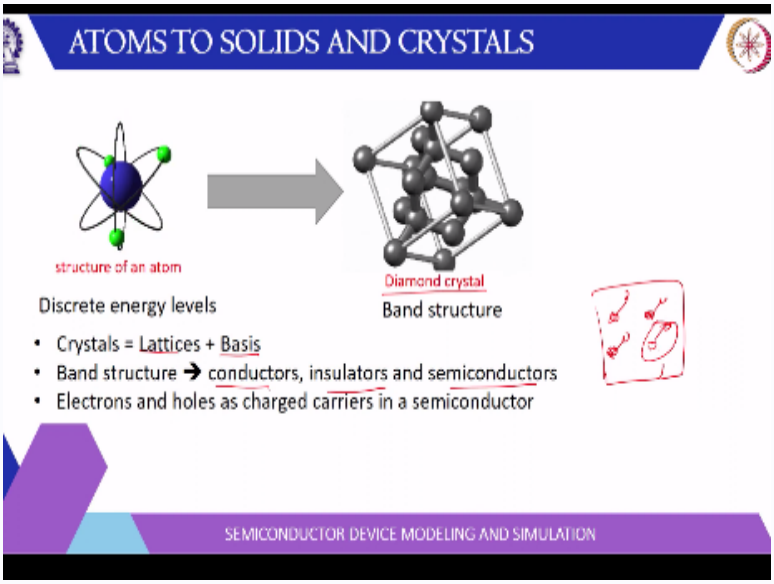


So, if you look at the individual atom this is the silicon atom so, the silicon atom is number is 14. So, you can represent the energy of these electrons through the states 1s state, 2s state, 2p state, 3s and 3p state. So, the states are fully filled and 3p is partially filled it can occupy 6 what it has 2 and it is also possible that these electrons can move to higher state or from higher state an electron can come from some other atom another electron can come the hydrogen of this atomic structure is actually done through the hydrogen atom.

So, for hydrogen atom there is only 1 nucleus 1 proton so, and the class 12 text actually describes what is the energy of this electron in different states. So, the energy of this electron is -13.6 by n square electron volts. So, for first energy level the energy is -13.6 for second energy level the energy of electron is -13.6 divided by 4. So, that means, this energy is actually increasing. So, if you plot this energy structure it will look something like this. So, here it is -13.6 and it is increasing.

So, if you move away from sufficient level from the atom this energy is 0 basically. So, you can think of it as some kind of quantum well nucleus is situated here and these electrons here have different energies at distance that this has some radius. So, that also you can calculate when such atoms they come together they form the crystal.

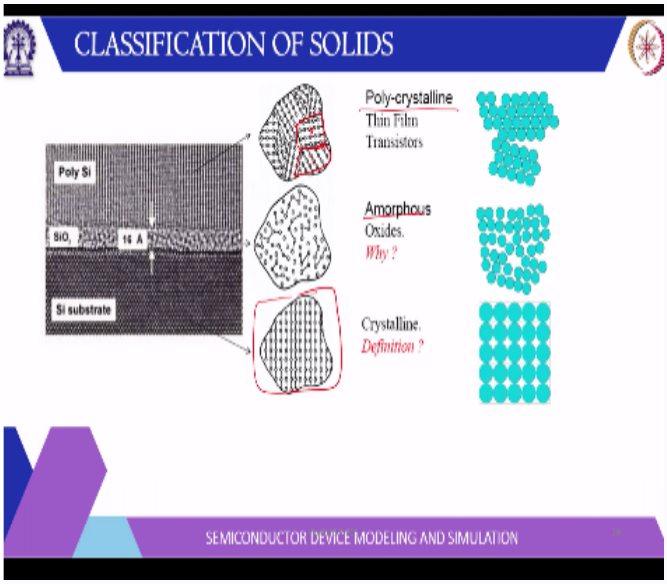
(Refer Slide Time: 10:22)



So, for silicon the crystalline structure is basically called diamond crystal the crystal actually consists of 2 things one is a lattice other is the basis so, lattices you can say let us a cubic crystal or cubic lattice, lattice is basically by definition a collection of points in periodic form. So, they are periodically arrange points is a mathematical concept basically and at these lattice points atom can sit there or group of atom consider there let us say 2 atoms are sitting there. So, this is group of atom is called basis.

So, the combination of lattice plus the basis is called crystal and this atomic arrangement will give rise to certain when they structure and that when the structure will decide whether a particular material is conductor, insulator or semiconductor and of course, in all of them there are electrons which are a charged particle and we have the concept of hole that also we will discuss.

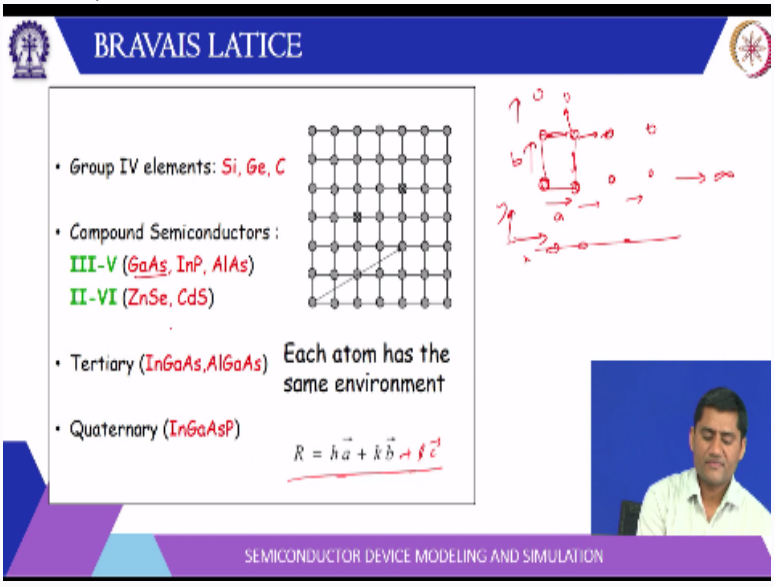
(Refer Slide Time: 11:39)



It is also possible a material or semiconductor material may not be single crystal. So, if whole chunk of material is following the pattern then we call it single crystal, but if there are blocks of single crystal like this here, this is 1 block of single crystal is another block of single crystal. So, that means it is not totally crystalline, but there are a number of crystals small crystals, which are randomly arranged.

So, then we call it poly crystalline. So, they have order but only up to sort length so, they have short range order and of course, if there is no such order, we call them MRFS. So, generally oxides, silicon oxide designer for MRFS material.

(Refer Slide Time: 12:37)

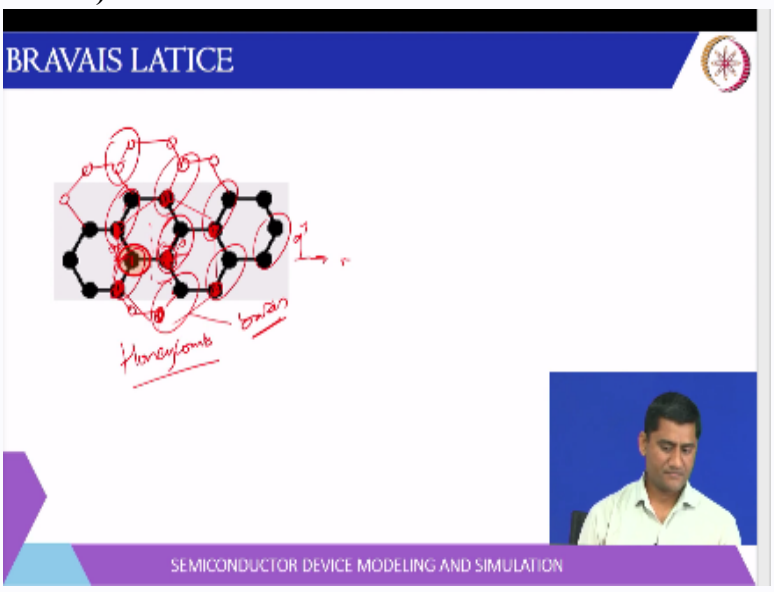


Now, these lattice we have a concept of Bravais lattice so, Bravais lattice is basically a lattice with a basis so, for example if you consider 2d lattice. So, these dots actually are the circles so, the location of individual atoms then you can define 1 vector here a you can define 1 vector here b and you can choose let us say you choose this set of these 4 atoms then you translate it by a n number of a or and then y direction. So, this is x direction this is y direction, in y direction you translate y b 2b, 3b like this.

So, that way you can cover the whole region of space with the crystal. So, this is called translation vector. So, it is h times a + k times b is for 2d. In 3d of course, if you have another diamond set then you can put l time c vector. So, that will use translation vector. So, by different combinations of h, k and l which are integers starting from 0 to any number or negative number you can cover the entire space and this a, b, c becomes the lattice vectors.

Another thing you notice here that each atom here has the same environment. So, number of nearest neighbors it is same for all atoms. By definition this is a bulk semiconductor or bulk material where this is extending up to infinity because at the area of course, if this is terminated then the environment will be different. But as far as the atoms in the bulk are concerned, they see the same environment. Now, even further compound semiconductor which has 2 atoms or 3 atoms, they will also have the same environment that you will see through their individual crystalline structures.

(Refer Slide Time: 15:17)



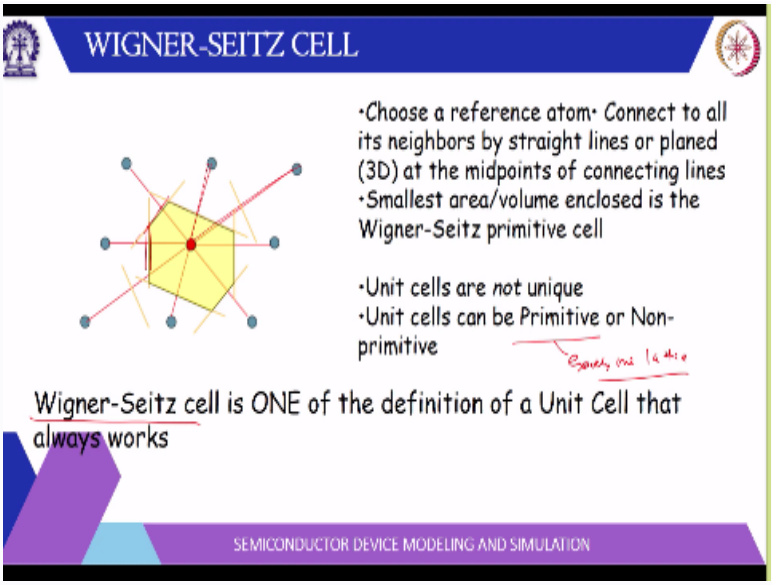
Now, sometimes we have this complex structure this is called honeycomb lattice now, if you look at this structure you can complete it like this now, here the environment seen by 2 atoms may not resemble if you see this 1 atom is less so, this is 1 and this is atom number 2 the environment scene is not same because we are there is a some kind of mirror symmetry is there. So, this is less the x direction this is y direction. So, here it the number 2 actually sees in the -x direction and at certain angle in x direction.

But one actually sees another atom in x direction instead of -x direction and another atom certain angle theta 2 - x axis here it sees another atom at angle theta 2 the x axis. So, environment scene is different. So, we cannot say this is a Bravais lattice, but, we can construct a Bravais lattice from here also if you choose an appropriate basis. So, you can consider lattice group of these 2 atoms then group of these 2 atoms if you consider these are group 2 atoms group of 2 atoms, atoms, atoms.

Now, you see that the environment is actually same here surrounded by these 4 groups so, the environment is same so, then you can describe this as a Bravais lattice with a lattice structure something like this maybe I can write a solid circle here and another atom is attached to it. So, these are the lattice points basically and group of these 2 atoms is the basis so, this is a basis and this is the lattice. Now, this lattice actually called triangular lattice and here the; environment seen what each lattice point the same basically.

So, it is something like this you see and then send this there so, we call it honeycomb lattice with a basis of 2 atoms then it becomes a Bravais lattice. So, otherwise it did not have the same environment for each atom, but if you choose the basis, then each basis has the same environment. So, I hope that clarifies the concept of basis and the crystalline structure. So, crystal is basis plus lattice.

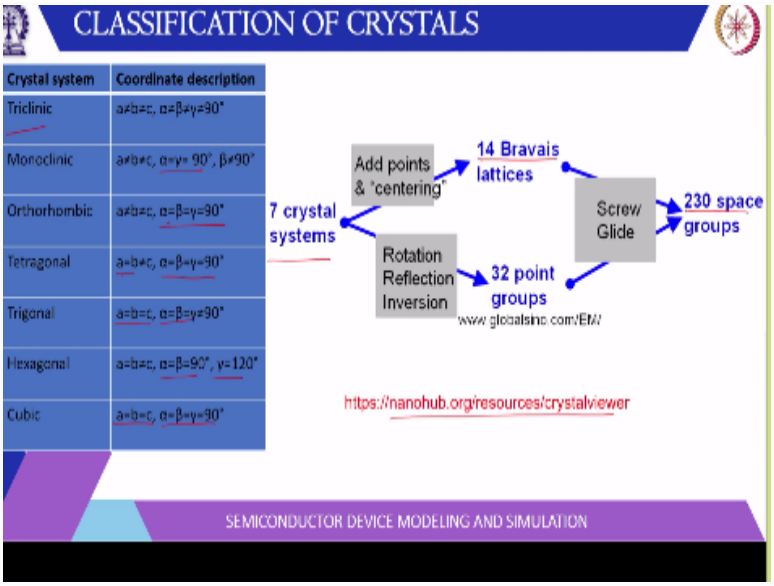
(Refer Slide Time: 18:34)



Now, there are different ways that one can formulate the unit cell in fact, one can have infinite number of unit cells and they are not unique, but there is a concept of called primitive unit cell. So, primitive unit cell is basically which has exactly 1 lattice point. So, exactly 1 lattice point so, it contains exactly 1 lattice point. So, for example, if you see any crystalline structure and this is 1 lattice point and there are nearest neighbors.

So, what we can do we can draw a line connecting these individual lattice points and do perpendicular bisector and where the perpendicular bisector crossed this and they formed the region that we call the Wigner Seitz cell. So, this is a primitive unit cell and primitive unit cell is also not unit you can have number of primitive unit cells. So, this is one cell which actually helped us to find out the further concept like reciprocal lattice and when the structure so that we will see later, but this is 1 unit cell and this is one of the primitive unit cell.

(Refer Slide Time: 20:10)

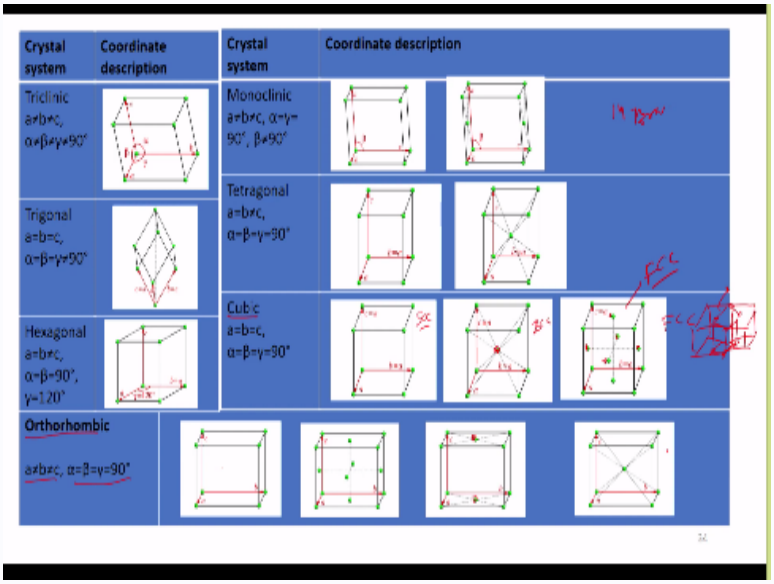


Now, there are total 7 crystal systems and that basically gives us around 14 Bravais lattices so, a modification of these 7 crystal system will give you 14 Bravais lattices, if you further modify it, then again you will basically due to symmetry you will come back to the same lattice. So, there are total 14 Bravais lattices are there and based on the symmetry there are 13 point groups and total 230 space groups out there. So, there is one website here and nanohub where you can see those crystals.

So, I would recommend that you go to the site and have a view of these crystals by rotating at different angles. So, you get some idea now, these 7 crystal systems are triclinic, triclinic is basically a more general or more general means its angles are not 90 and the side lengths are not equal that means, it will have a minimum amount of symmetry properties then of course, monoclinic here sides are not equal but 2 angles are 90 degree then orthorhombic all the angles are 90 degree, but sides are not equal.

Tetragonal 2 sides are equal and all the angles are 90 degree, trigonal all the sides are equal but angles are not 90, but equal to each other. Hexagonal here angles 2 angles are 90 third dimension angle is 120 degree and the 2 sides are equal third one is not equal. In cubic all 3 sides are equal and all 3 angles are 90 degree.

(Refer Slide Time: 22:20)



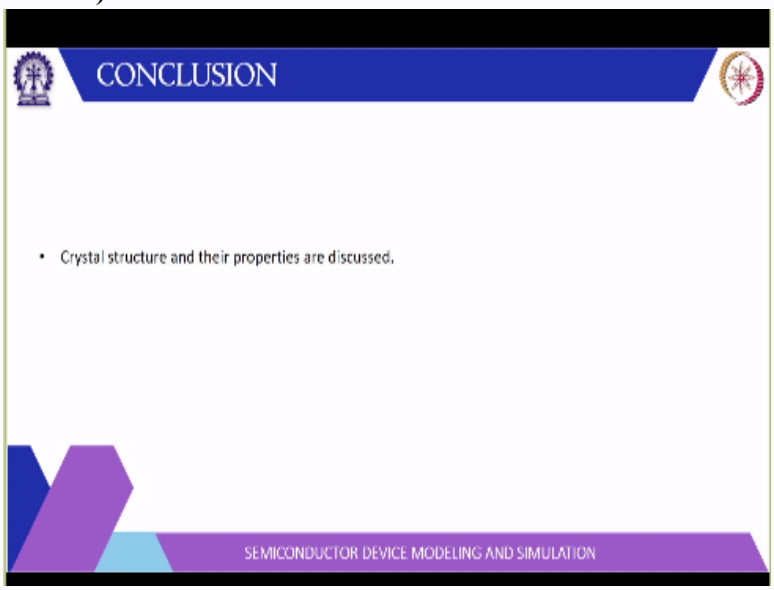
So, for example, let us consider the cubic system there are different variations of this cubic system you can have. So, this is called simple cubic SCC simple cubic crystals. So, all the corners have 1 atom each or 1 lattice point each and the side lengths are equal a, b, c all are equal then of course, you can have a 1 lattice point in the middle of the cube basically. So, that is called body centered cubic or also called BCC.

Another various and you can have the lattice point on the faces. So, there are 6 face of this cubic crystal. So, this is called face centered cubic crystal. So, the 3 variation so, there are 3 Bravais lattice with cubic crystal then for orthorhombic all angles are 90 but side a, b, c are not equal. Here also have simple orthorhombic, face centered orthorhombic, body centered orthorhombic there is another variation here called base centered orthorhombic or the end centered orthorhombic.

You can have similar thing here in cubic also you can have this cubic crystal and then you have this 2 atoms are the top and bottom. But, if you look closely let us say you have another cell here than these atoms are all the corners a lattice point and if you come connect these cells, what do you have here? You have a tetragonal we are a, b are equals c is not equal where the angles are 90 degree. So, this therefore, the cubic has only 3 variations not 4 variations.

Similarly for others for tetragonal your simple tetragonal and a body centered tetragonal for monoclinic your simple monoclinic and the 2 end base centered monoclinic and you have 2 hexagonal 1 trigonal and 1 triclinic. So, this basically this total comes to around 14 Bravais lattices. So, we have 14 Bravais lattices with 7 crystalline structure. Now in case of semiconductor that mostly we are going to deal with like silicon and gallium arsenide. So, they are all face centered cubic they all are FCC with a basis of course. So, it is also called interpenetrating FCC lattice.

(Refer Slide Time: 25:43)



So, in this lecture, we have discussed different crystalline structures and their properties and how we actually though they relate to the current flow in the semiconductor. Thank you.