Semiconductor Optoelectronics
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Lecture - 2
Energy Bands in Solids

So, good morning and we start with lecture 2, energy bands in solids; as I mentioned our objective will be to review the essential semiconductor physics.

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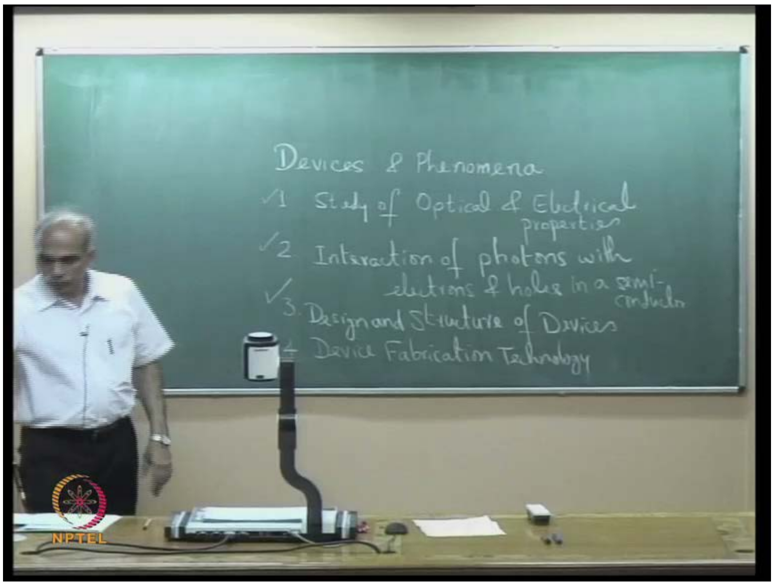

In the last class, we discussed about the subject matter, the subject matter of semiconductor optoelectronics comprises of, it deals with devices and phenomena, devices and phenomena and phenomena which involve interaction of optical processes with electronic processes.

Therefore, this will intern involve study of study of optical and electrical properties optical and electrical properties properties of semiconductor optoelectronic materials, optical and electrical properties. It will involve interaction of a study of interaction of photons, photons with electrons and holes in a semiconductor, electrons and holes in a semiconductor. The technology will further involve design, design and structure and structure design and structure of devices, design and structure of devices. And of course, fabrication technologies; that is device fabrication technology device fabrication technology device fabrication technology. In this course, we will consider these three aspects including design and structure of the devices, their performance, characteristics of the devices, but not the device fabrication technology; because there are other courses which cover device fabrication technology. So, these are the three aspects which we will cover in this course.

So, we start with the first one; that is to study optical and electrical properties of semiconductors, optical and electrical properties. So, we start with the formation of energy bands all of you would have studied about this. So, I am just recalling formation of energy bands in a semiconductor. So, most of the semiconductors of practical importance are crystalline in nature; crystalline (( )), most of them gallium (( )) all the binary semiconductors that I have written silicon, germanium all are crystalline.

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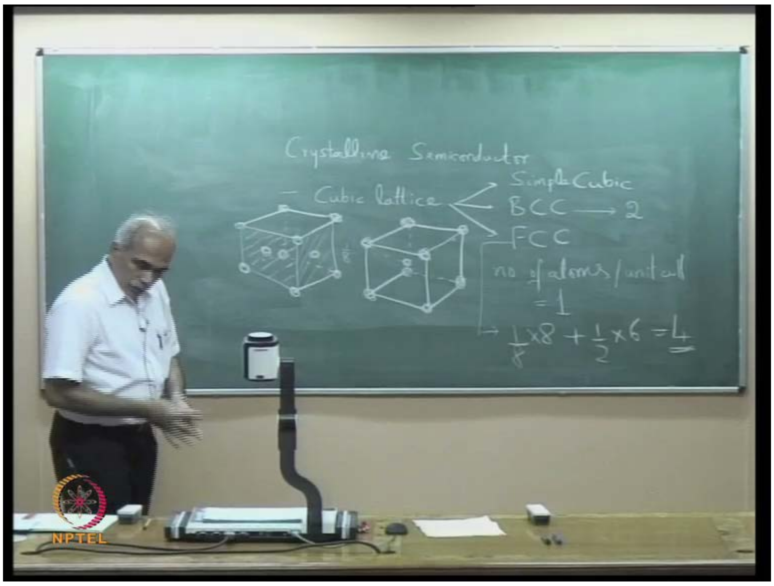

And most of them are also are characterized by a cubic lattice. They may have different structures like diamond structures, zinc blend structure, but most of them are characterized by a cubic lattice. In cubic lattice, as you are aware that there are simple cubic, body centered cubic BCC and FCC face centered cubic. So, simple cubic, if you draw a cube the atoms are located at the corners of this cube. So, naturally there are 8 atoms, 8 corners; the simple cubic. But as you know in the entire crystal structure, each cubic cell here is shared for example; there are further cubes on this side, further cubes on this side. So, every atom here is shared by with eight other cells. And therefore, the contribution of this atom per cell is one-eighth and there are 8 atoms forming one cubic cell here and therefore, number of atoms per number of atoms per unit cell per unit cell is equal to 1.

If you take a body centered cubic, then there is one more atom at the center here one more atom at the center and therefore, number of atoms for BCC, number of atoms per unit cell is 2. If you take face centered cubic; that means, as you can see it comprises of 6 faces. 2 up and down, 2 on these sides and 2 on the other sides; so there are 6 faces. At the center of each face, if you wish you can draw another one, another diagram. So, these 8 atoms are in at the 8 corners plus on this face if I consider this face one in the middle of this face, so first face here, second one here; each face there is 1 atom here and so on. So, we have 6 atoms sitting on 6 faces, in addition to the 8 atoms at the corners. But each face is shared by 2 cells on one on this side and one on this side; which means every cell, the atom contribution per cell is half per face.

So, half into 6 faces; so we have 3 additional atoms which means for FCC we have 1 that is 1 by 8 into 8 plus 1 by 2 into 6 which is equal to 4. Number of atoms per cell is 4, 3 coming from the 6 faces and 1 coming from the corners; so number of atoms per unit cell is 6, is 4. Now, why do I need this numbers we will come to know in a minute. My objective is to have an estimate of number of valence electrons. So, to know the number of valence electrons I must know the number of atoms per unit cell and number of electrons per unit cell. So, I want to calculate how many number of atoms are present per unit volume of the material.

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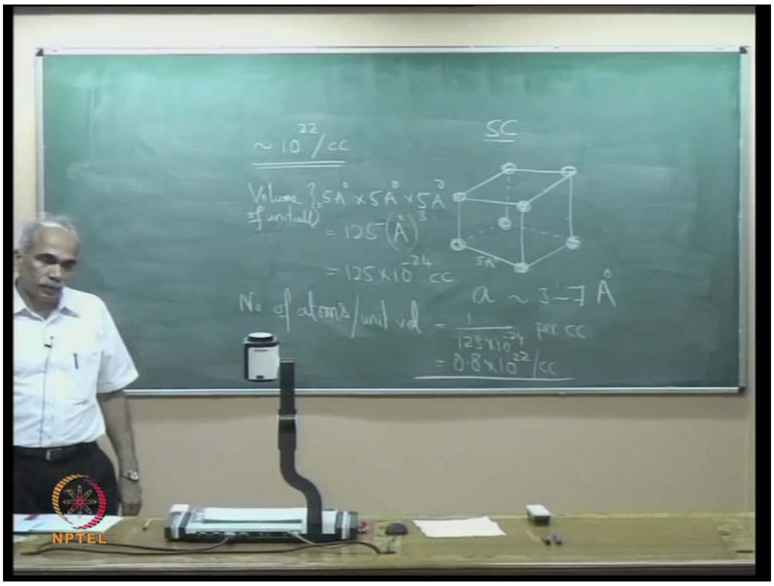

So, simple engineering estimates; so you take the cubic cube again. So, one atom; if I take simple cubic S C, simple cubic, then one atom per cell. I want to finally calculate the number of electrons or density of electrons which means number of electrons per unit volume, number of valence electrons per unit volume because we would require the carrier concentration to determine the electrical properties. And therefore, I am starting with fundamentals.

In a semiconductor, typically the inter atomic spacings that is inter atomic spacing a is anywhere in the range 3 to 7 angstroms, 3 to 7 angstroms is the inter atomic spacing; this one or this one approximately of that atom. If you take gallium arsenide for example, it is about 5.65 angstroms; so 3 to 7 angstrom. So, if I want to estimate what is the volume occupied by one unit cell volume occupied by 1 unit cell, let me take this as 5 angstroms; some intermediate value just can estimate 5 angstrom which means what is the volume of this? The volume is 5 into 5 angstrom. So, volume of unit cell which is equal to 125 angstrom cube. So, that is equal to one angstrom is 10 to the power of minus 10 meters or 10 to the power of minus 8 centimeters. So, this is 125 into 10 to the power of minus 24 CC or centimeter cube is the volume; volume occupied by one unit cell.

What is our interest is to find out the number of atoms per unit volume. So, what is the number of atoms per unit volume? Therefore, number of atoms per unit volume unit volume is equal to 1 divided by 125 into 10 to the power of minus 24 per CC. So, this is nothing but 0.8 into 10 to the power of 22 per CC 0.8 into 10 to the power of 22 per CC or the number of atoms per unit volume is of the order of 10 to the power of 22 per CC. Number of atoms per unit volume in a semiconductor is typically 10 to the power of 22 per CC. If each atom contributes one valence electron, then the number of valence electrons per unit volume is of the order of 10 to the power of 22. What is the number of valence electrons typically that we have? So, it is a quick calculation to get and estimate. So, I would like you to have this kind of practices to estimate very quickly starting from fundamentals.

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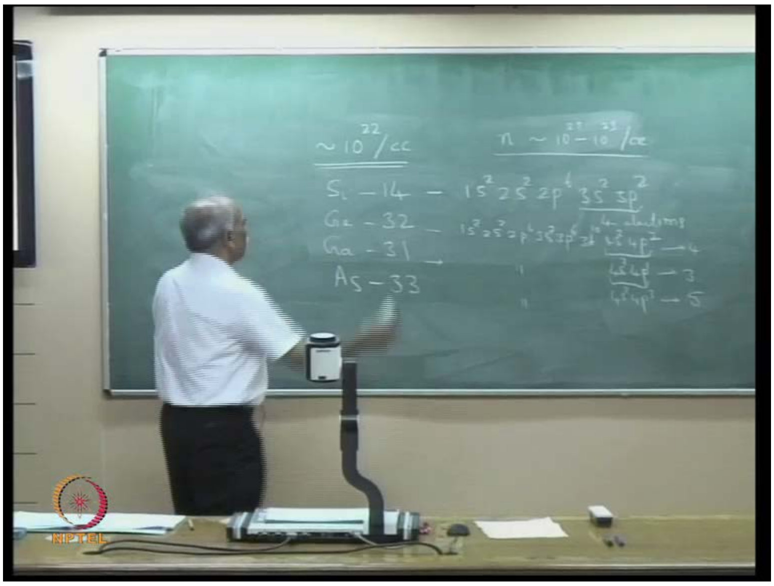

So, number of atoms. So, if you take silicon for example, you know that the atomic number of silicon is 14, germanium most widely used semiconductors atomic number is 32, gallium 31 and arsenic 33; atomic number Z. So, if you write the electronic configurations this is 1 S 2 2 S 2 2 P 6 3 S 2 3 P 2, you see 14. Valence shell by definition is the outer most shell which is either filled or unfiled, but the outermost shell where electrons are occupied; so 3 S 2 3 P 2. So, there are 4 electrons in the valence shell; so 4 electrons. That is why it is in group 4 right, germanium 32 1 S 2 2 S 2 2 P 6 3 S 2 3 P 6 3 D 10 4 S 2 4 P 2; you see the fourth shell is the outermost shell and again you have four valence electrons. If you see gallium here which is 31 it has the same structure, same electronic configuration, but 4 S 2 and 4 P 1. So, this has 3 valence electrons, this has 4, this has 3 valence electrons and here as you know that gallium is a group 3 element.

Arsenic on the other hand will have the same configuration up to this, here we have 4 S 2 4 P 3; so 5 valence electrons, the arsenic is in group 5. Silicon, germanium, gallium, arsenic, yesterday as I mentioned is the 3 5 compound, very important semiconductors in optoelectronics. Therefore, one atom has in this case 5 valence electrons, here 3, here 4 and so on. In other words therefore, the number of valence electrons per unit volume is this number multiplied by number of valence electrons per atom; which means in general n, the number of electrons in the valence shell is per unit volume is of the order of 10 to the power of 22 to 10 to the power of 23 per CC.

Let me come to the second issue. So, I have in this discussion I have made use of the fact that most of the useful semiconductors are crystalline; of course, there are amorphous semiconductors. But most of the useful semiconductors in optoelectronics are crystalline in nature. Let me use another fact, that our topic as you can see is energy band in solids.

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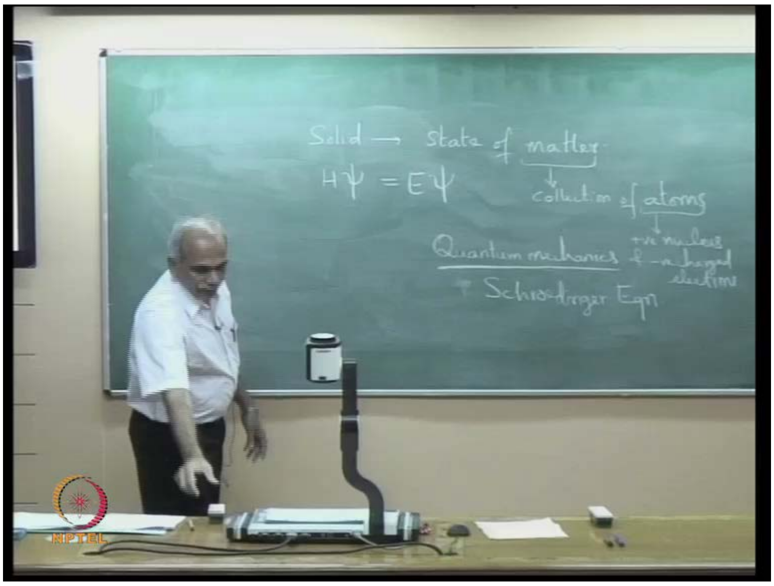

So, solid is a state of matter state of matter. Matter is basically a collection of atoms collection of atoms and atoms comprise of a central positively charged nucleus nucleus and negatively charged electrons. The motion of constituents of an atom are described by quantum mechanics the laws of quantum mechanics. In particular, the motion of constituents are described by the Schrodinger equation. The spelling actually either you have to put two dots or Schrodinger Schrodinger equation I do not know how many of you are familiar with this, but basically Schrodinger equation is defined by H psi is equal to E psi H psi is equal to E psi where H is called the Hamiltonian.

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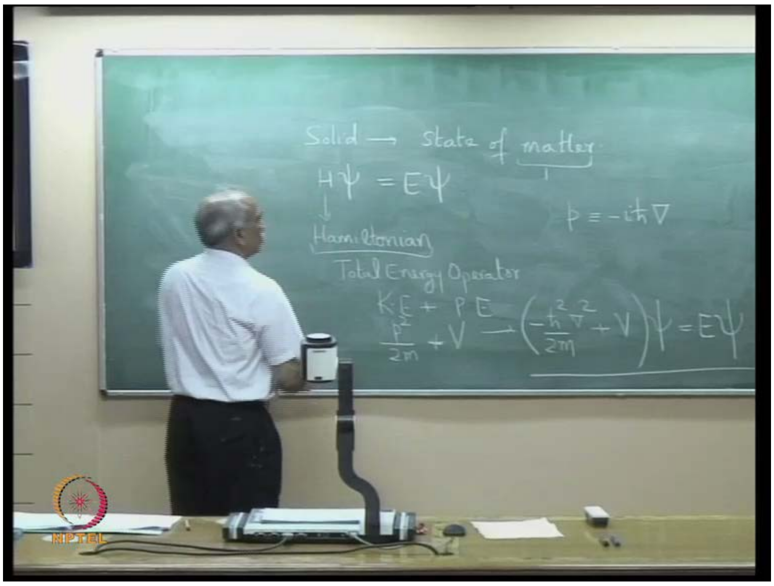

H is called the Hamiltonian which means it is basically total energy operator total energy operator, which means it is an operator corresponding to the kinetic energy and potential energy; which means it corresponds to P square by 2 m plus V. Where P is momentum, m is the mass and V is the potential energy. If you replace this momentum here by the corresponding momentum operator part of the basic quantum mechanics, momentum operator which is minus i h cross del and substitute here. Then you will get the Schrodinger equation. So, this gives you h cross square by 2 m with a minus sign into del square plus V. So, this is H, multiply this by psi, the wave function which is equal to E time psi; where E is the energy Eigen values, psi are the Eigen functions and E are the energy Eigen values. There could be more than one Eigen energy values and therefore, E represents.

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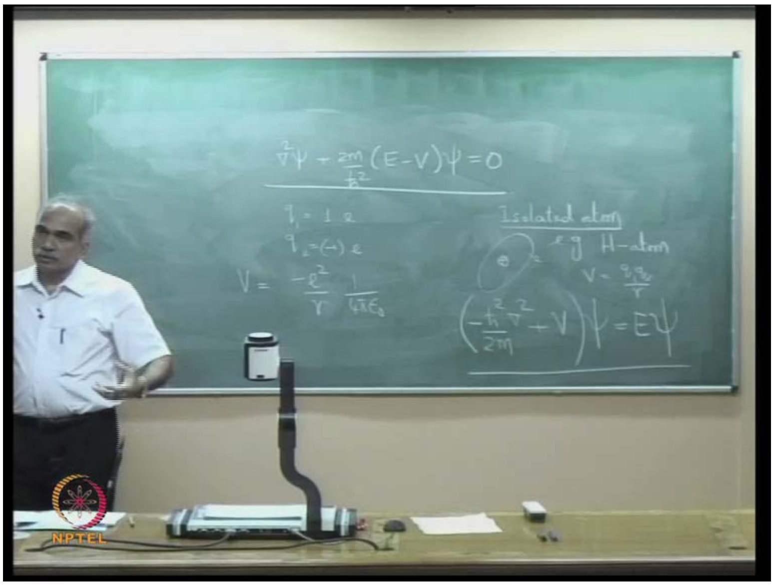

So, this is nothing but the Schrodinger equation which you can rewrite you can rewrite in the form del square psi plus 2 m by h cross square into E minus V psi equal to 0. For every given potential variation V you can find out an energy Eigen value, which gives the energy of the particle under consideration and psi being the wave function, H is Plancks constant, h cross is h divided by 2 pi H is Plancks constant and m is mass of the electron. If you are finding energy of Eigen values of electrons then m is the mass of. If you take an isolated atom isolated atom; for example, hydrogen atom.

I am very quickly recalling all the basics that you have already studied. If you take the hydrogen atom it has a central positively charged proton here and electrons surrounding it as a cloud. So, the potential energy V is given by q 1 q 2 by r q 1 q 2 by r which means in the case of hydrogen, q 1 is this q 1 equal to 1 e; the quantum of electric charge and q 2 is minus 1 into e, charge of an electron. Therefore, q 1 q 2 by r is minus e square by r; v is equal to minus e square by r. In C G S system you have an additional factor which is 4 pi epsilon 0. If you substitute this v here you can find out the energy Eigen values for hydrogen atom.

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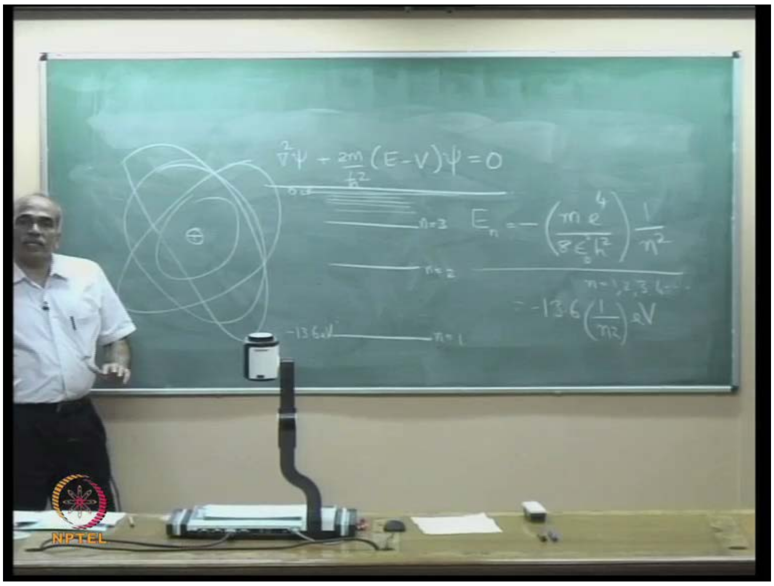

So, this gives you the solution for hydrogen atom, gives you energy Eigen values which are E n is equal to minus m e to the power 4 divided by 8 epsilon 0 square H square into 1 divided by n square. These are the energy Eigen values where n is equal to 1, 2, 3, 4 etcetera correspond to the principle quantum number or energy levels of a hydrogen atom. Since, n is discrete it immediately means that E n is discrete. So, for hydrogen atom if you put values for this, these are all constants; mass of electron, charge of electron, permittivity free space, H is Plancks constant. So, this will come out to be minus 13.6 into 1 over n square e V. If you put n is equal to 1 that is the ground state, then you know that ground state of hydrogen atom is minus 13.6 E v is the energy of hydrogen atom. You may be wondering why I am discussing this. The point is if you take an isolated atom it is characterized by discrete energy levels.

So, this is n equal to 1, n equal to 2, n equal to 3; actually the separation should increase because n square is in the denominator, it is n square, it goes as n square and finally, it goes to 0 which when n becomes very large this goes to 0. 0 is the free state vacuum state. So, as you go here they come closer and closer and closer and finally, that is the vacuum state. With respect to the vacuum state here you are saying that this is minus 13.6 E v, these are the bound states of the atom. So, you have the positively charged nucleus which is surrounded by various orbits just showing randomly some orbits and energy corresponding to various shells and energy corresponding to various levels are what is given here. So, the ground state of hydrogen atom is minus 13.6.

What we are interested is from this discussion is to see that an isolated atom is characterized by discrete energy levels; this is the point. So, I have taken just an example which already you have studied is the hydrogen atom. Let me recall the argument again, matter is a collection of atoms and solid is a densely packed collection of atoms.

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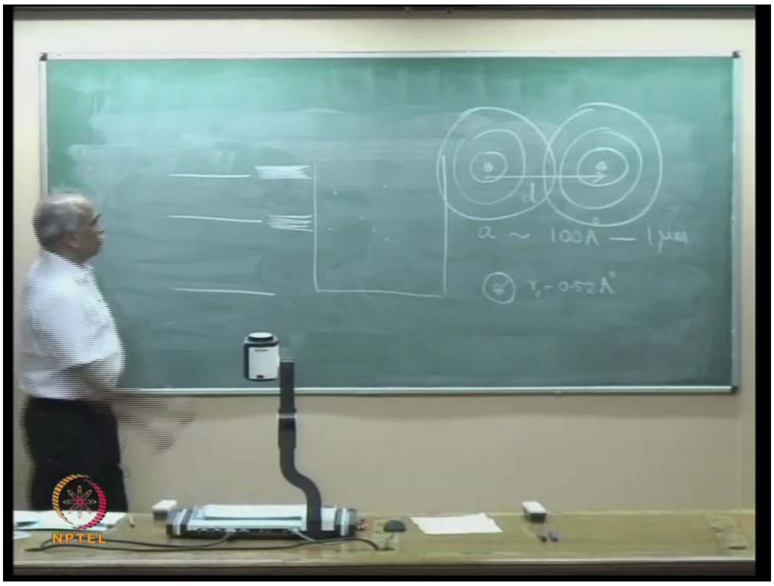

If you take a gas at low pressure, the inter atomic separation you know that if you take a container, the gas at low pressure; then the gas molecules are continuously in a state of motion. The average inter atomic spacing depends on the pressure of the gas, lower the pressure larger is the inter atomic spacing. So, typically the inter atomic spacing a, if I want to call the inter atomic spacing a, is anywhere from the of the order of 10 or 100 angstrom to 1 micron typically the inter atomic spacing that is between atoms in a gas.

What is the size of an atom? The size of an atom, there is no fixed size of an atom, but the size can be estimated if you know that the ground state of hydrogen atom here has a radius here, which is called the bore radius is 0.52 angstrom. Which means the size is typically about 1 angstrom, you can say that the size of an atom is approximately 1 angstrom. Of course, higher orbits will be, that is higher electrons will have the larger spatial extent but the size is typically 1 angstrom. When the inter atomic spacing, if you now consider 2 atoms, 1 atom sitting here and 1 atom sitting here. The inter atomic spacing here, the separation between these; when this separation d is large, then the electrons here do not see any effect due to the electric field. The electro static field here, the field here does not experience the field due to the other atom. Because that is quite far, there is hardly any interaction.

But if they start coming closer, then the field here gets paltered because of the field here or the electrons here start seeing the second atom or they get influenced by this. The influence leads to splitting of the energy levels. The energy levels which were originally discrete, if you start bringing two atoms together then the energy levels split into 2. The outer ones are the more affected ones, because the inner electron shells are inside here; they are not seeing the influence of other atom. The outer electrons, I am just showing circular orbits like this, as you can see the outer orbits or outer electrons start seeing each other or the interaction is stronger there or the perturbation felt by the outer electrons is more. And therefore you start seeing splitting of the outermost electron energy levels.

This is considering two two atoms, if you have a large number of atoms the levels here split into multiple levels. First point, when two atoms are well separated there is very little interaction between them and therefore, the entire collection of atoms are characterized, the entire collection is characterized by discrete energy levels. Because each atom has this energy level. Therefore, the entire collection is characterized by this discrete atomic energy levels. But if you start bringing them closer and closer, then the energy levels get paltered or splitting of energy levels take place; a loud levels become more than one; corresponding to one you now have several energy levels. And therefore, if the number increases this goes over to a band; so they go over (( )). As you decrease the inter atomic spacing the energy levels go over to bands; this is illustrated by the nice diagram which you generally see in books. So, this is the inter atomic spacing a inter atomic spacing versus the energy.

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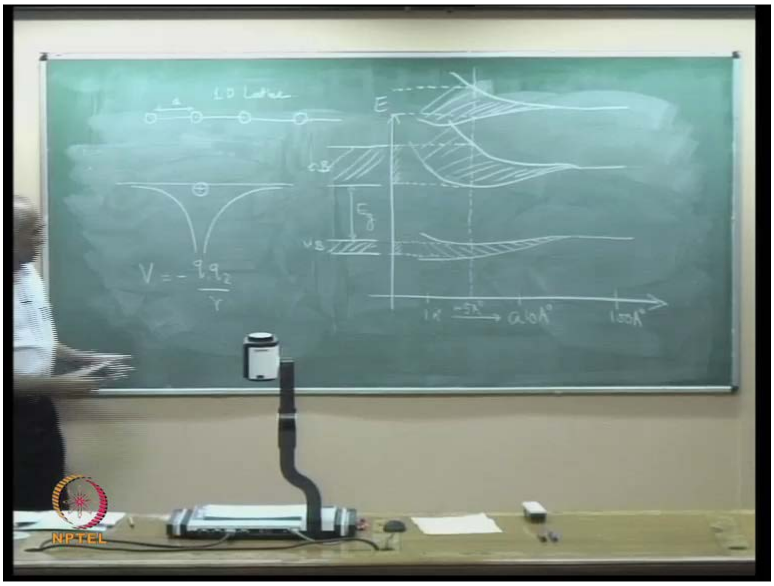

So, when the inter atomic spacing is very large. So, let me put some number, I will put the number 1 angstrom 10 angstroms; this axis is energy E. So, when the inter atomic spacing is sufficiently large, you have energy levels which are discrete. They are not equally space, I am just qualitatively illustrating. As you reduce the inter atomic spacing, the levels start splitting. You would have seen this diagram in mini books. So, what you have is a range of allowed energy levels.

A qualitative explanation I am offering there are. So, semiconductors have an inter atomic spacing approximately 5 angstroms. So, if you go here let say 5 angstroms, what are these? These are the allowed energies, please see these energy levels correspond to allowed energy values. As the inter atomic spacing reduced, the allowed energy values became more, that is the there is a range of energy values corresponding to each level; a range of energy values. And as you reduced it further it started splitting further and in for some values they may also start over lapping with each other.

Typically, for semiconductors where inter atomic spacing is of the order of 5 angstroms you can see therefore, in this energy axis if I draw the range of energy values which are allowed; please see this is the range of energy values allowed here. This is the range of energy values allowed here and this is the range of energy values allowed here. So, what do I have? I have a range of energy values, a range of allowed electron energy values inside a semiconductor and this is nothing but the bands. So, what you have are the band diagram that you see is basically this and the separation here where there are no allowed states correspond to the forbidden gap forbidden gap.

I have written E g, but please remember the highest band which is completely filled is called the valence band. The highest band which is completely filled is the valence band and the next band is called the conduction band. And the energy separation the energy separation or the forbidden gap between the valence band and the conduction band is the band gap. There may be many more bands, but there are no electrons there and therefore, we have not concerned with that. So, a semiconductor is characterized by energy bands. I have given a qualitative explanation here. Let us make it little bit more quantitative, little bit more rigorous and see whether this is really true or not.

Those of you have studied solid state physics, you have studied the kronig Penney model. If you consider a 1 D lattice if you consider a 1 D lattice. So, what I am showing? These are the atoms which are separated by an inter atomic spacing of a. Consider a 1 D lattice. If you consider an isolated atom, single atom what will be the potential energy variation? V is equal to minus q 1 q 2 by r. So, if you plot the potential energy variation, where r is the distance from the nucleus; then the potential energy variation looks like this. It is 1 by r variation, r is equal to 0 here at the nucleus; r equal to 0 so this is the potential energy variation, this is the 1 by r variation and minus. At r equal to 0, it tends to infinity; that is why you see I am sure all of you have seen this potential energy variation, this is for one atom.

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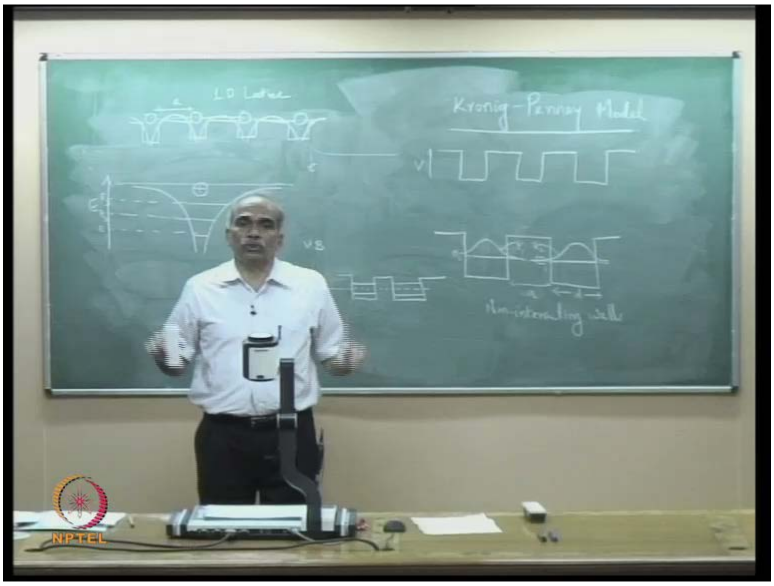

If you have a series of a 1 D lattice of periodically placed atoms, then you will have a corresponding potential energy variation potential energy variation. If you solve this problem like in hydrogen atom you will get. So, this is the potential energy here E and you will get different discrete energy levels, permitted values of energy levels. So, this is E 1 E 2 E 3 are permitted values of energy levels. These are the discrete energy levels of the isolated atom but now what I am showing is a 1D lattice separated by a.

When you have an isolated atom like a hydrogen atom with one electron, it is exactly soluble you have analytical solutions. But if you have many atoms with many electrons then it becomes a multi body problem and you cannot have analytical solutions for many such problems. But you can solve them numerically one or you make certain approximations. So, you may be familiar with the kronig Penney model; we just recalling what you have studied those of you have not studied do not worry. Basically we are interested in the concepts and results; finally, we are interested in the concepts. Because this is not part of this course; so we will not go into the analysis of this. But in kronig Penney model what he did was he approximated this potential variation by a potential well, a rectangular potential well, a periodic potential well and then you have this. So, a periodic potential well. So, potential energy variation here this is v and this is the separation between them.

If you consider a single potential well, this is a particle in a potential box problem we study even in first year under graduate engineering. If you take a potential well here, this supports, analytical solutions this supports different discrete solutions E 1, the ground state, the second state and it may support depending on the height and the width it may support many solutions. For simplicity, let me take a potential well which supports only one solution. So, there is one solution here E 1, one allowed solution which is the fundamental mode, fundamental solution or fundamental state which is the ground state. And if you see the wave function it typically looks like this, it has a oscillatory behavior inside the well and evanescent well behavior outside the well. This is the ground state of particle in a potential well, a single well.

If I bring a second well close to this, reasonably close to it so that they start interacting; if the separation here this is the separation, let me call this as d the separation. If this or let me call this as a, the well is of width d and separation a. If a is sufficiently large much greater than d, then the two wells are non interacting wells. So, this will have one solution here, this also has the same solution; if it is identical size and identical height then this also has a solution corresponding to the same energy value for non interacting wells, non interacting wells. Two potential wells which are non interacting or you you can imagine as it as two atoms which are well separated, non interacting. So, this is the potential well which is approximating this potential, actual potential varies like this. But it is approximated by a box, equivalent box because this has analytical solution, easily you can solve this.

If you when a is much larger than d, there is no interaction between them. But if a starts reducing so each one of these is characterized by the Eigen state here, the fundamental solution or the ground state. When you start reducing this, that evanescent tail of this field here, this psi interacts with the evanescent tail of the psi here; if I want to call this as psi 1 and psi 2 they are actually same states, but the tail start interacting. They start overlapping which means there is an interaction between the wells. This is originally when a was much larger than d, they were non interacting wells when a started reducing they started interacting when they start interacting if you solve this double well problem, then you will get two solutions corresponding to this interacting double wells, now you get two solutions. That is one here this was the original level, let us say this was the original level E 1. Now, the new values are one above that and one below that. So, there are two allowed energy values, you have two solutions. Earlier there was only one solution, now you have two solutions; I do not wish go into the details because there are symmetric solutions, anti symmetric solutions and so on. However, what is important is if there was only one energy level initially when you have two interacting wells there are two solutions. If there are three interacting wells there will be three solutions and if there are n interacting wells there will be n solutions, n allowed states.

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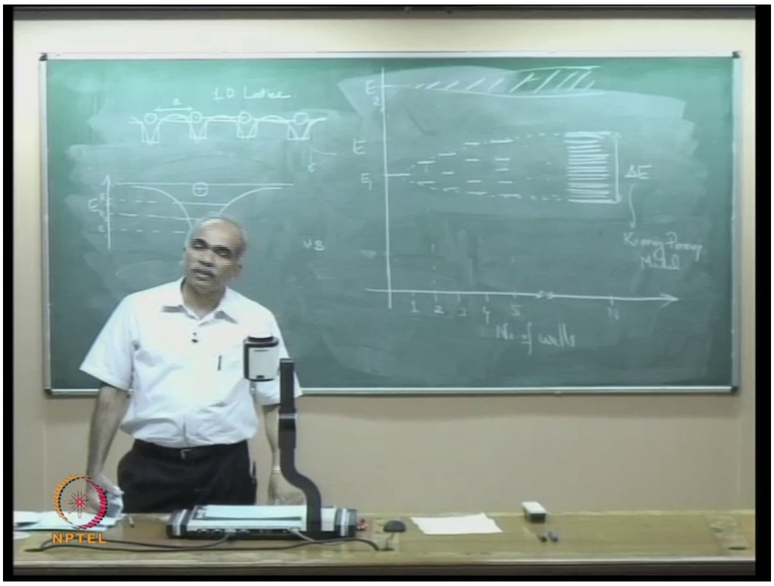

And therefore, if I plot if I plot, so what I am going to plot? Let me erase this. If I plot the number of wells here this is number of wells versus energy allowed energy E allowed energy e this is some state I am discussing about E 1. So, this was my E 1, original E 1 when I had only one value of energy I had this; this is E 1. When I have number of wells two, then I have two allowed values; one slightly below and another slightly above; so two allowed energy states, if I have three wells. Please see the relevance I have considered a 1 D lattice where atoms are sitting along a line; they are like interacting atoms. So, equivalently each atom is characterized by a potential well. So, I have a series of interacting potential wells and I am now writing depending on the number of wells how many energy states are permitted. So, the allowed energy state for this three is here; one above, one below when I go to 4 then it is here one two three four. This is exactly numerically solvable this is not so you solve a Schrodinger equation for the four interacting wells; you will get the four solutions.

These are solutions which are actually you can calculate the solution. As the number of cells increase so you go to 5 it becomes 1 2 3 4 5 and so on. So, the number of cells increase and when the number of cells become very large some n, then you see that this saturates to a very large number of allowed states; the number of allowed states here. Please see there is a discontinuity here in the axis because the number is very large, where I have shown discontinuity. Let me show this again 5 and this is number of wells this is some large number N; there are large number of states. So, this varies something like if I draw it leads to saturation and this separation here delta E is the width of the energy band. The corresponding width of the energy band that you get now there is a range of allowed energy values; because you have N interacting atoms, there is a range of allowed energy values.

This delta E comes out to be the same that you get from kronig model, kronig Penney model. This calculation was not from kronig Penney model; this is calculation from quantum mechanics. So, the quantum mechanical calculation gives this separation as the same which you get from the kronig Penney model. So, what is the point in this discussion is that when you have a closely packed arrangement of atoms, periodically arranged atoms in a lattice, they are characterized by discrete energy band. This is corresponding to one energy level.

Similarly, for the next energy level, if I had the next level E 2 there also I would have had I would have got this splitting into the band; corresponding to E 2. Before this discussion I qualitatively I have drawn that has to reduce the inter atomic spacing it increase the width of the energy level, discrete energy levels split into band; that indeed takes place. That if you calculate with number of wells, there is a range of allowed energy values. In other words corresponding to this energy level of a single atom in a solid you have energy band. So, these are the energy bands in solids.

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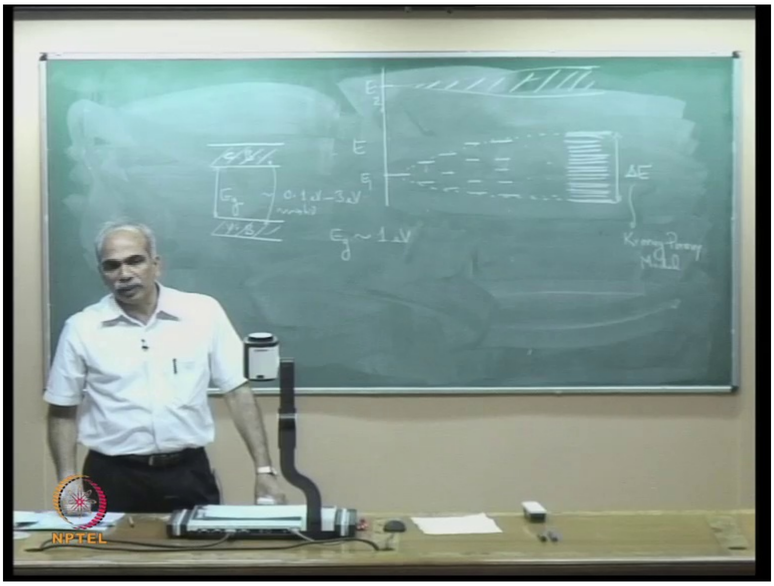

We will stop here for the day. So, as you know ones we have the picture of energy bands in solids which I am sure you have studied. Then we tend to focus on the band diagram, energy band diagram where the semiconductor is characterized by a valence band and a conduction band valence band and a conduction band with an energy gap E g energy gap E g anywhere lying typically from about 0.1 E v to 3 electron volts for a semiconductor. Of course, there are wide band of semiconductors which have even more than 3, gallium nitride is a wide band gap semiconductor which has a band gap greater than 3, within 3.4 electrons volts.

Most of the semiconductors which we use in optical communication have an E g which is of the order of 1 electron volt, plus minus 1 electron volt. I am sure you are also familiar that the electrons in the conduction band, we will discussed more of this subsequently; combine with holes in the valence band to give out photons. In the next lecture, we will discuss about the E k diagram and see what are direct band gap semiconductors and what are indirect band gap semiconductors and why we need direct band gap semiconductors to realize sources.

Thank you.