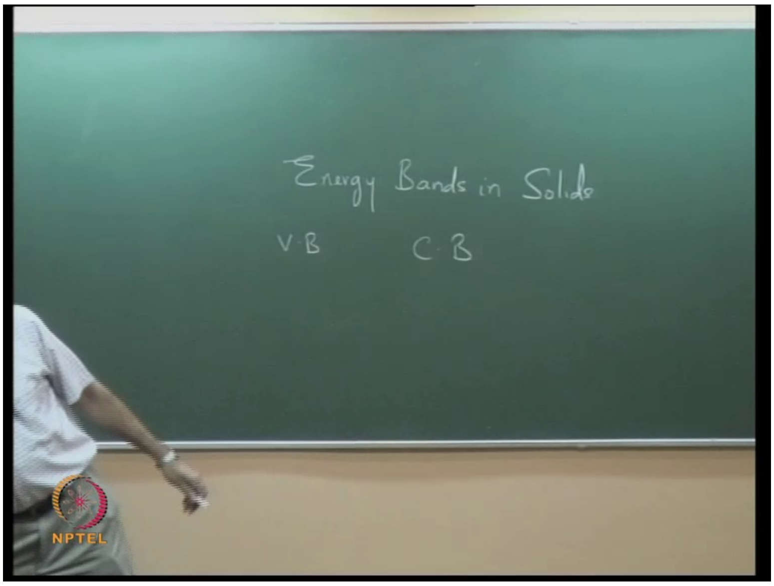
Semiconductor Optoelectronics
Prof. M. R. Shenoy
Department of Physics
Indian Institute of Technology, Delhi

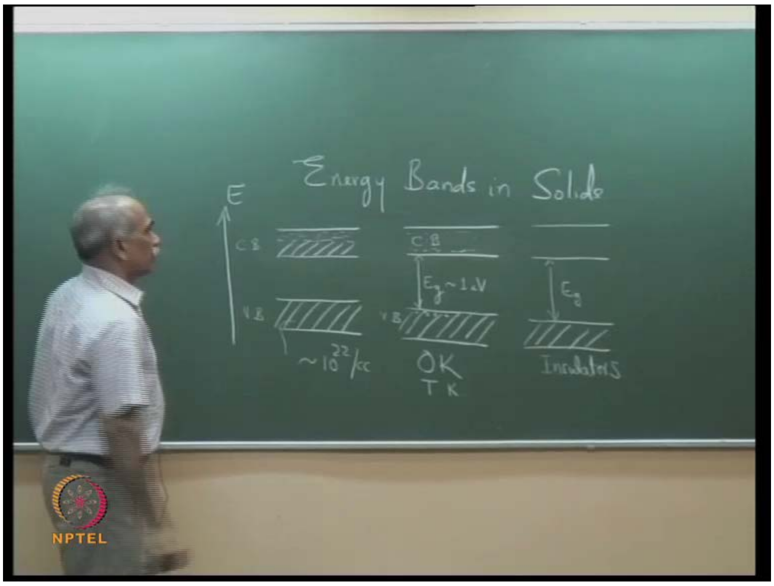
Lecture - 3
"E-k Diagram"

(Refer Slide Time: 00:28)



Let me first recall what we have studied, in the last class in the last lecture we had studied energy bands in solids. And therefore in general solids are characterized by energy bands. The highest band which is completely full or nearly full is called the valance band, and the next band, the next higher band is the conduction band. It does not mean these are the only two bands, there are many more bands which are below, but the electrons in those bands rarely participate in any of the electronic processors, unless you use high energy x-rays to knock them off. So, normally the electrons which participate in optical and electronic processors are those in the valance band and the conduction band. Therefore, if I draw the band diagram, which you have seen in almost all books, metals, semiconductors, and insulators are basically characterized by band diagrams, so let me draw the band diagram.

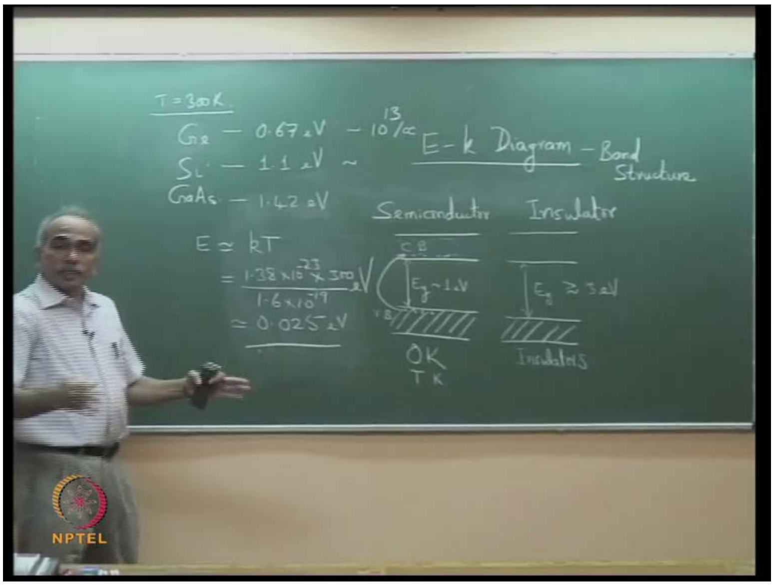
(Refer Slide Time: 01:45)



Although, I am plotting the bands at the same energy level, so this axis in all through the course, the vertical axis will be energy. In metals we have either a completely full valance band, and almost half field conduction band. This is conduction band, this is valance band, if it is almost half full, it means rest of the half is empty or there are free states which are available for occupation. There are filled states and free states, and we have already seen the typical number of electrons, is of the order of 10 to the power of 22 per c c, which means very large number of electrons present, and large number of free states present, which will facilitate movement of electrons in the presence of an external applied electric field, and that leads to very good conductivity of the material. It could be like this, or it could be overlapping bands. In some cases the conduction band and valance band overlaps, and then also you have large number of electrons, and large number of vacant states in the same band, and therefore electrons can move very easily. In the case of semiconductor, at 0 k valance band is completely full, and the conduction band is completely empty. Typically the band gap here E G.

Now we talk of band gap E G, because electrons have to go up E G is of the order of one electron volt, as I mentioned that anywhere from 0.1 electron volt to 3 electron volts, is the band gap of semiconductors, but let us say one electron. At any finite temperature a finite temperature T, there are electrons which go to the conduction band, which lead to conductivity the electrons can then if some electrons from here, then there are free states vacant states and the electrons can starts moving through the band, in the presence of an applied electric field. The electrons which go here leave behind holes, which are nothing but vacancies in the valance band, holes exist only in the valance band, and not in the conduction band. The vacant states in conduction band are different from the vacant states here, these are holes which are vacancies created in an otherwise field valance band. In the case of insulators, the band gap here energy gap is very large. I have shown them all at same level, but we see that these gaps are different for the three different materials. So, what I have drawn, is energy bands in solids.

(Refer Slide Time: 05:24)

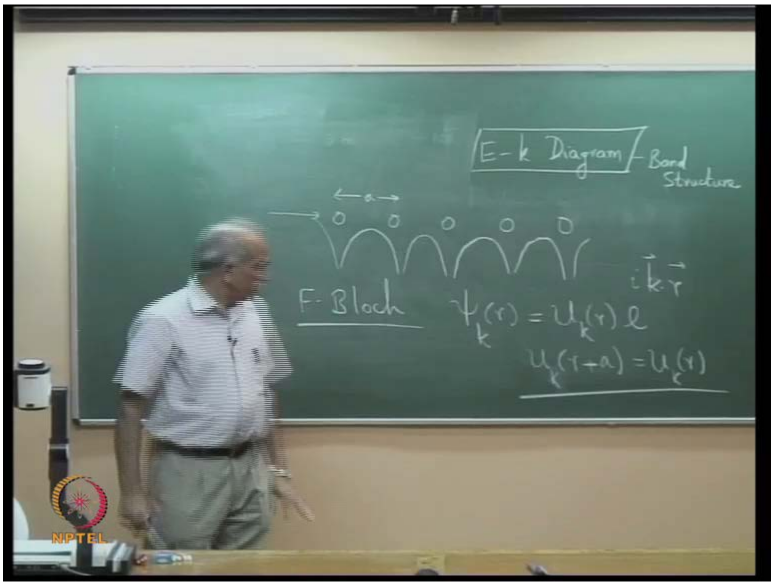


So, metal, semiconductor, and insulator, because the electrons in the conduction band have gone up, or have made an up transition from the valance band. Naturally the number of electrons present at any temperature is given by, is depends on the gap. Smaller the gap, larger will be number of electrons which can make upward transition, and larger the gap smaller will be the number. In general when E G is greater than of the order of 3 electron volt 4 5 6 and all, then the number if electrons which can make an upward transition become extremely small, and therefore the conductivity of such materials is very low, and these are nothing but the insulators.

So, from the band energy bands in solids, the generally characterized metals semiconductors insulators, in terms of this energy band diagram, but these energy band diagrams do not tell anything more beyond this. So, to know more optical and electrical properties of the semiconductor or any material, you have to go to the E k diagram, which is called the band structure, so E k diagram. It is the E k diagram, and it will tell you many more things. So, let us discuss the E k diagrams, or this is called the band structure. Just before I go or there you know that at room temperature, let say around at room temperature; T is equal to 300 k, we have let me take silicon, germanium. Let me take three semiconductors, germanium silicon, and gallium arsenate.

The energy band gap is 0.67 E v, for silicon it is 1.1 E v, gallium arsenate has a band gap of 1.42 E v, which means if this band gap is about one electron volt, then an electrons which wants to make an upward transition here, must have energy of the order of 1 E v or more, but in general we know, that the energy of electrons average kinetic energy of electrons E, is of the order of k T, at a temperature T, where k is boars man constant. So, this is 1.38 into 10 to the power of minus 23 into let say 300 divided by 1.6 into 10 to the power of minus 19 E v, and that is approximately equal to 0.025 E v. We are familiar with this, average kinetic energy of electrons. How is it that the kinetic energy is or when the energy of the electrons, is of the order this. How is it that the electrons, is able to make an upward transition. Think over this, you know that at room temperature germanium has typically of the order of 10 to the power of 13 electrons per c c, silicon this is not dope, and this is intrinsic pure material. The intrinsic carrier concentration due to temperature is of the order of 10 to the power of 10 per c c, and for gallium arsenate, it is of the order of 10 to the power of 6 per c c.

(Refer Slide Time: 09:57)

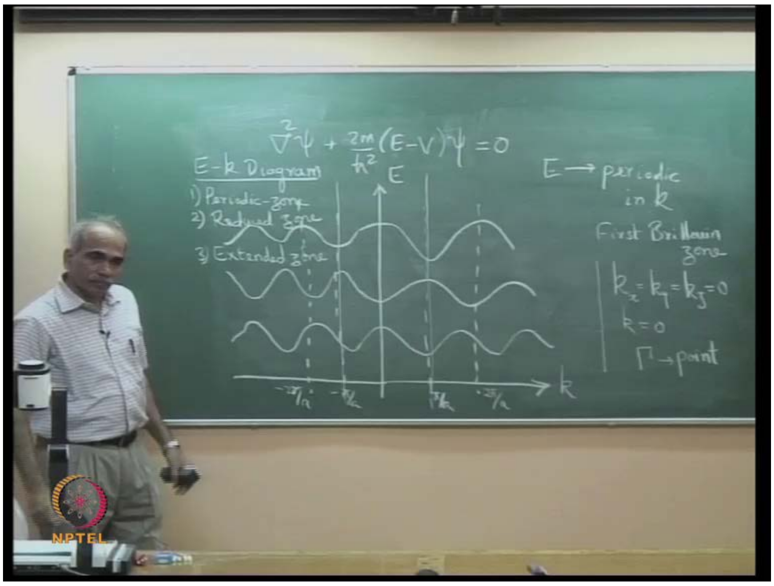


How is it that so many electrons peak an upward transition at room temperature, at 0 k semiconductor in a semiconductor the valance band is full and the conduction band is empty. How is it that such a large number of electrons exists in the conduction band at room temperature; give a thought about this, then we will discuss further. So, let me go for the to discuss the E k diagram, energy versus k. In the last class we discussed that most of the useful semiconductors are crystalline, and in crystalline semiconductors atoms are erased periodically in a lattice.

The periodical arrangement, if I take a 1 d arrangement for simplicity, periodical arrangement leads to a periodical potential variation, periodical variation of potential, potential energy here, but the motion of electrons, the motion of electrons in a crystal, is govern by the loss of quantum mechanics. If you have one electron one proton system like the hydrogen atom, it is very easy to solve the so dinger equation. In a solid when there are large number of electrons and atoms present, it is extremely complicated and difficult to solve the so dinger equation, but Bloch F Bloch, I am sure you have heard of Bloch. Bloch observed that his observation was, since the potential varies periodically, the probability of finding an electron should also vary periodically.

Remember the probability of finding an electron should also vary periodically, which means the wave function should also vary periodically. We see probability of finding an electron is equal to mod chi square, where psi is the wave function. And therefore, he postulated that in such periodic medium, the wave function should be of the form psi k of r, is equal to u k of r, into E to the power of I k dot r; that is the wave function is a product of a plane wave. This is the plane wave E to the power of i k dot r is a plane wave, and multiplied by a periodic function which is called the cell function, u k of r is periodic, u k of r plus a is equal to u k of r. Sometimes I writes is the same k, sometimes I would written like this, sometimes I write like this, please, although I should have been careful, so i k dot r. So, this is a periodic cell function, this is a periodic function, where a is the inter atomics spaces. So, he postulated that the wave function must be of this form; a plane wave multiplied by a periodic function.

(Refer Slide Time: 14:13)

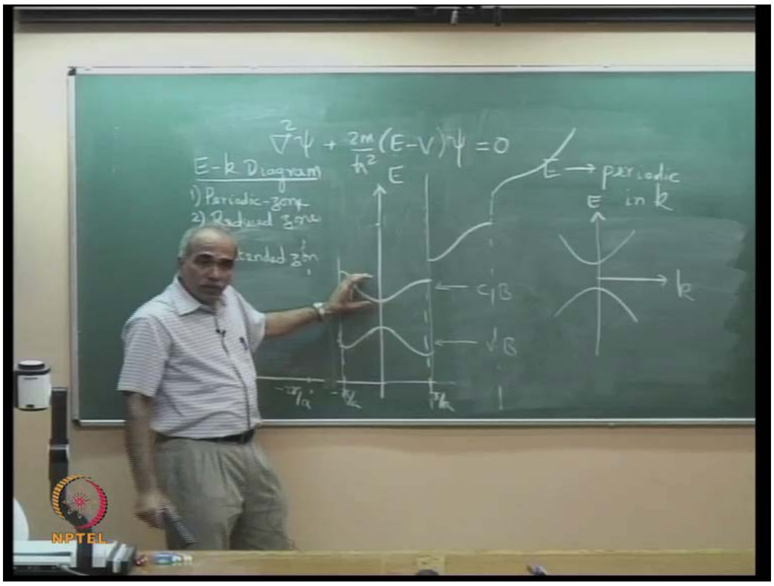


If you substitute this, this form of the wave function in a so dinger equations, dell square psi by 2 m by h cross square into E minus v into psi equal to 0. Then it turns out that, this can be solved several numerical and analytical techniques, or several methods by which you can solve this. If you substitute this form of psi in this, then you can solve this, and you get energy values, icon values. We see here E is the energy icon value, v is this periodic potential, and m is the mass of the electrons, psi is the wave functions. So, you get energy icon values E also turns out to be periodic in k, which means if you plot I am directly giving you the result of this. If you plot energy versus k, E versus k, then for each allowed energy level, each allowed discreet energy level, you get periodic functions. So, always the vertical axis is E, and this axis is k. This is E versus k, which means for every given value of k. This is k is equal to phi by a, k is equal to 2 phi by a, k is equal to minus phi by a and minus 2 phi by a. Corresponding to every energy level of the single potential well, you have now a periodically varying energy value.

If you see the first boundary here, between minus phi by a and plus phi by a, which is called the first brillouin zone, these are the borders of the first brillouin zone, the first brillouin zone, but I will not go into the details and origins of brillouin zone, because this is in the reciprocal lattice. There are some important points, but what we are mainly focusing is on k is equal to 0; that is k we will see shortly, that k x k y k z is equal to 0, which corresponds to k is equal to 0, and this is called the gamma point. If you are not come across these, you may go through, but we are not very, in this course we are not very much key non the brillouin zone, gamma point, x point, L point there are different various points, but what I want bring to your attention is, that energy versus k is periodic, because the potential is periodic.

Since it is periodic it is sufficient for us to restrict our self to one period, minus phi by a to plus phi by a. If you know the values to minus phi by a to plus phi by a, then we know everywhere, because it is periodic. And therefore, in a reduced zone picture, in the E k diagram there are. So, E k diagram there are three pictures. I am sure one of them will be the picture that you have seen. So, the first one is periodic zone picture. The second one is called the reduced zone picture, and the third one, is called the extended zone, extended zone picture. There are three pictures for the E k diagram. What I have plotted is the periodic zone picture. In the reduced zone picture, you simply reduce this up to the border of the first brillouin zone, because you know that if you know up to this, you know beyond this. So, this is the reduced zone picture.

(Refer Slide Time: 20:45)

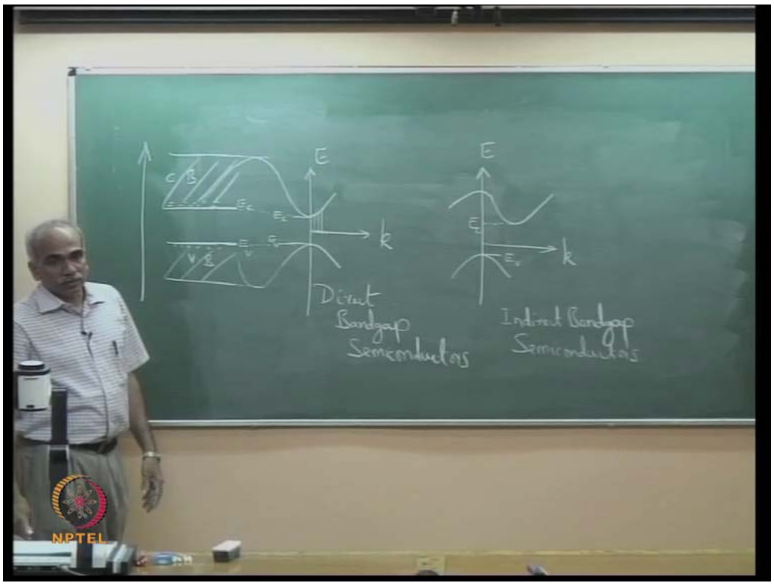


So, normally when we see E k diagram, we look at the reduced zone picture, these corresponds to different levels. And if you see that reduced zone, reduced zone picture, and the highest filled energy level, is the valance band, and the next one is the conduction band. And if you look at this bands and draw the reduced zone picture, then we focused only on this part of the E k diagram; k versus E. Why are we focuses only on this part, I will tell you in a minute. Now let me complete what is this extended zone. In the extended zone picture if you know up to this here, and then there is a. Please we this could have drawn like this, so in the extended zone picture you show this discontinuity and white this. So, you have come up to, this is at phi by a and this is at two phi by a, and corresponding to the next band who have discontinuity, and then again going like this.

So, this is the extended zone picture, where you show from 0 to phi by a for one level, phi by a to 2 phi by a for the other level, corresponding to other level and so on. So, this is the extended zone picture, which you normally plot from the conic penny model, from the result of the conic penny model, you will see that there is a discontinuity, then you see the extended zone picture, but here for this course on a semiconductor optoelectronics, it is sufficient for us to see the reduced zone picture, and more importantly it is even sufficient for us, to focus only at the bottom of this, and at the top of this. The bottom the top of this valance band, and bottom of this conduction band, it is sufficient for us to focus on this; why I will tell you in a minute, that when we calculated at the density of states which will be our next topic.

We will see at the density of a states in a band is extremely large, and the number of electrons or the carrier concentration, which is responsible for the flow of current is extremely small, and only a small portion of this E k diagram; that is only the lowest portion of the conduction band, or only electrons which are holes, which are closed to the top of the valance band, participate in all processors, all electronic processors. Therefore, it is not even, you rarely meet this ends, the ends of the brillouin zone. All the practical devices almost all the practical devices utilize carrier, which are close to the bottom of the valance bands, and close to the bottom of the conduction band, and close to the top of the valance band. And therefore, if you see a simple device, a device oriented book they will draw E k diagram only this much, although the E k diagram continues. Let me plot the that lowest portion of the E k diagram, the relevant portion of the E k diagram and discuss further.

(Refer Slide Time: 24:43)

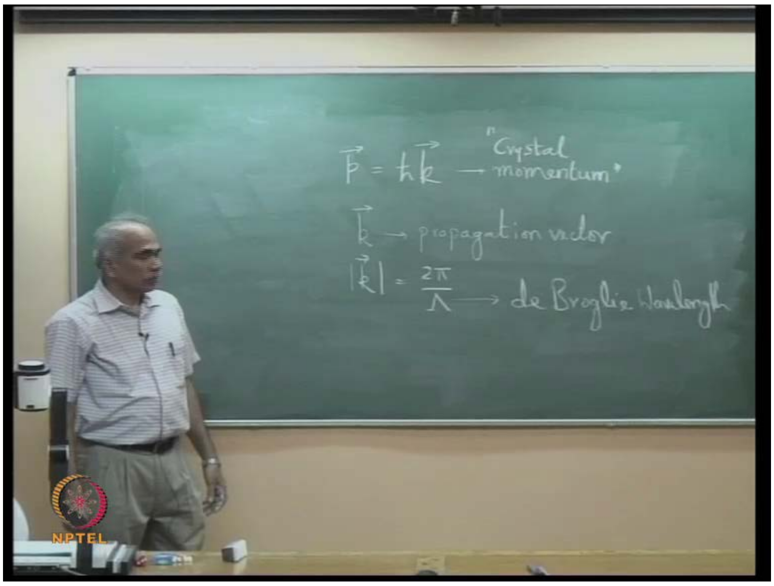


So, now, we have the E k diagram, when you plot the E k diagram, so this is k, you could draw it k here also, vertical axis is always is e. So, what does this represents, this represents, for every value of k we will see shortly that the k values are discreet, for every value of k here, what is the corresponding allowed energy; that is a solution of the so dinger equations. So, what you are plotting, is allowed energy values, as a functions of k. We will see that the k values are discreet, but the numbers of values are so large that you plot a continuous curve. So, materials in which, there are materials in which, the top of the valance band here, coincide with the bottom of the conduction band, and there are materials in which the top of the valance band does not coincide with the minima of the conduction band. So, materials in which for E versus k, for materials in which the minima of the conduction band, and coincides with its top of the valance band; coincide means occurs at the same value of k are called direct band gap semiconductors. And materials in which the minima of the conduction band E c is denoted by E c E v.

So, this value here is E c, the band h E v, coincide does not coincide are called indirect band gap semiconductors. So, two things to note that k can take large number of values. What is this k, we will see shortly we again recall this, what is this k, and corresponding to each k value, there is an allowed energy value. Allowed energy means an allowed solution of the so dinger equation, and we plot energy versus k and that is the E k diagram. Also please recall that we have drawn an energy band diagram, the familiar energy band diagram, where you show that this is the valance band, and this is the conduction band, so this is the conduction band and this is the valance band. This is the band at which is E v, and this is E c, have to the clear picture that this E c is the same as this. The bottom of the E k diagram here, the bottom of this here E c is the same as this, and the top the band at here is that same as this, and this was going up and then turning like this. So, the maximum allowed value was this, and this was going down and turning like this.

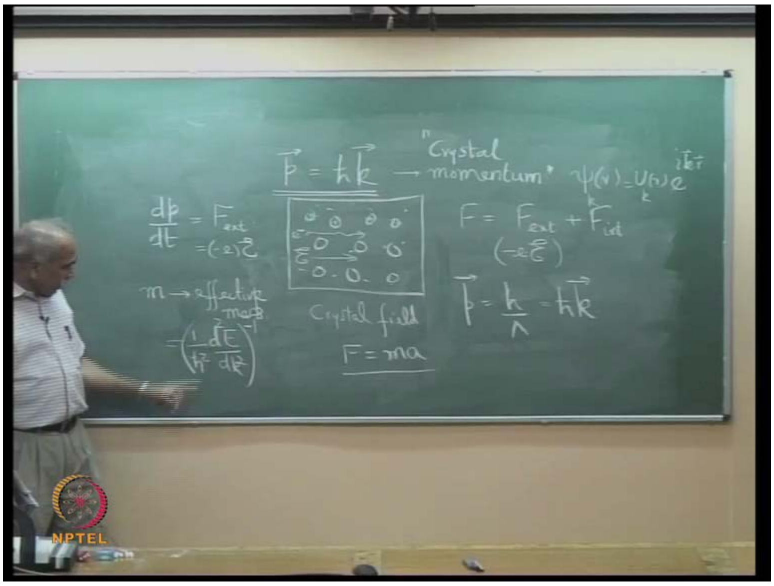
So, the minimum energy value is this. So, the point is the basic energy band diagram, which we have studied in basic classes, is exactly it corresponds to the E k diagram, but this does not tell anything further, other than the band gap, but you will see that it is the E k diagram which will tell us more about the optical and electronic properties of the material. So, this is one to one, usually the holes which are close to the top of the valance band, and the electrons which are close to the bottom of the conduction band, participate in all the electronic transition processors, and that is why I had mentioned that it is only the top of this, and the bottom of this, which are in practice relevant to the optical and electrical properties. I proceeded little bit further to see what is this k.

(Refer Slide Time: 30:20)



This k is the propagation vector of the electron wave function is propagation vector, whose magnitude k is the propagation vector, whose magnitude is given by 2 pi by lambda, 2 phi by lambda where lambda is the de Broglie wavelength of the electrons in the medium, in the semiconductor. This k is such that the momentum p is given by h cross k, the momentum p of electrons in the semiconductor is given by h cross k. This momentum is very often called the crystal momentum, the crystal momentum

(Refer Slide Time: 31:49)



Please see an important concept here, this comes from you are familiar with the de Broglie wavelength lambda is equal to h by p lambda is equal to h by p, where h is the planks constant and p is the momentum, or p is equal to h by lambda. So, if you divided and multiplied by 2 pi this is nothing but h cross k, so momentum is nothing but h cross k. Momentum is a vector, therefore this is h cross k, this is how you get this. Now this is called the crystal momentum. See this picture, if you take a semiconductor, there are large number of atoms and electrons, the ions and the electrons. Any electron here, any electron E is moving through this medium under the influence, when there are positively charged nuclei and negatively charged electron, there is an electro static field.

So, any electron which is moving through this, moves under the influence of a electro static field, which is inside the crystal, this is called the crystal field; this is a crystal field, internal field. Electron is moving through it, it is not moving through this free space, but it is moving through the medium, and there are large very complex crystal field which is present. If you apply an electric field to this, you apply an electric field, so the electron starts moving. This is an external electric field, so you have; now apply an external electric field. Please see there is an internal electric field, the electron has to move in the presence of an internal field, and an external field. So, the force, the net force on this on the electron, net force on the electron will be due to F external plus due to F internal.

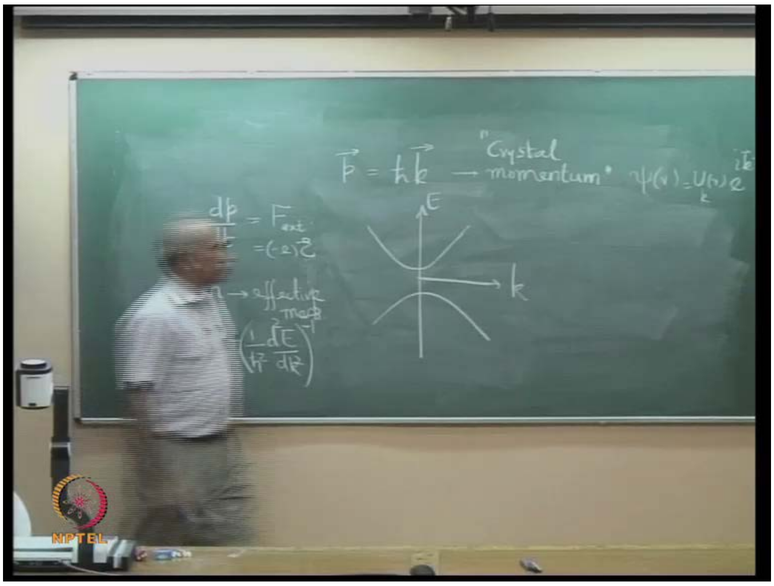
F external is because of the applied electric field, which means you know that it is minus E into E, this is the external field. I applied an electric field out from outside, which means there is a electric field e, so the force is charged into e, so minus E into E. What is the internal field, it's really very complicated, if you define the momentum by this expression, where this k is the same k which appears here; psi k of r into u k of r into E to the power of i k dot r. It is the same k which is the de Broglie wavelength 2 pi by lambda. If you define that then this is called the crystal momentum, which means this momentum is as if it is responding only to the external field. In otherwise you have d p by d T, what is this, rate of change of momentum, is equal to F external.

Normally that if p of the total momentum, it should have been F must have been equal to d p by d T, force equal to rate of change of momentum, but if you define p by h cross k, which is called the crystal momentum, then the crystal momentum is responding only to the external force, and you can write this equation d p by d T is equal to F external. This F external we know, because this is very important, what you know is E, you do not know the internal field. And therefore, it is as if the electron is responding to the external force as if it is a free particle. Please see this, and then it moves with the mass, which is equal to the effective mass of the electron. The effective mass which is defined by 1 over h cross square d square E by d k square to the power minus 1.

I have actually skip the derivation of this, there is a very complex derivation, and also there is a simple heuristic derivations, both I have skipped at this moment, but what I would like you to appreciate is this; that if I define the electron mass by this effective mass of electron, effective mass, it is as if this is an electron, it is a free electron which is directly responding to the external force, which is directly responding to the. When we write F is equal to m a, this is the mass of the particle and this is it's accelerate. This is for a free particle, F is equal to m a.

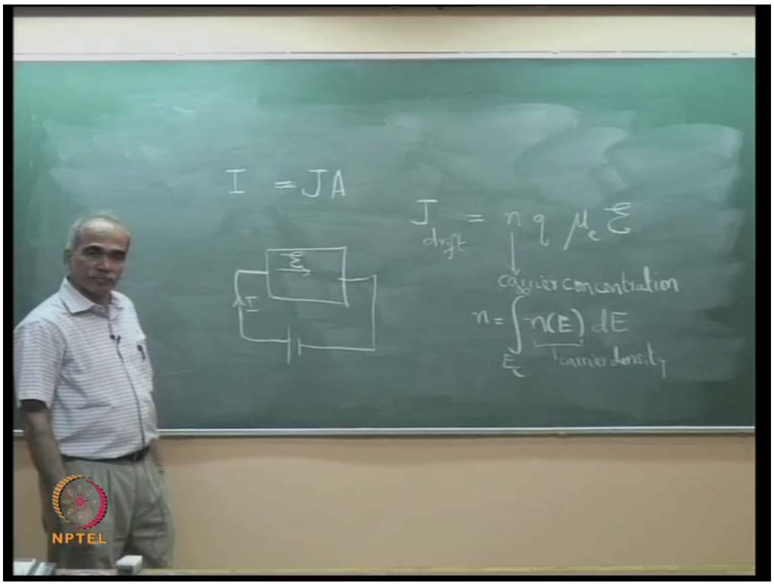
So, if you define an effective mass for an electron, which is given by d square E by 1 over h cross square into d square E by d k square to the power minus 1. Then this electron inside a semiconductor can be treated as if it is a free electron, moving under the influence of the field. You do not need to consider the internal forces within the semiconductors. It is as if the electrons respond directly to the external force; that is why. Now what you see here, is this is d square E by d k square, where do you get this form. I skip the derivation, but to get d square E by d k square, you need the E k diagram.

(Refer Slide Time: 38:28)



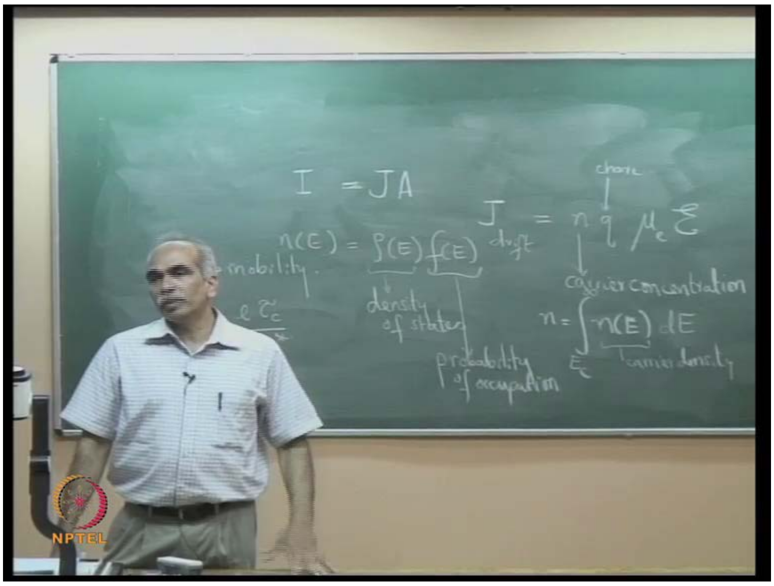
So, you have the E k diagram here, so this is the E k. And the second derivative is you d square E by d k square, and this is the effective mass. So, it is the E k diagram, which will tell you to what is the effective mass. Come up to give a few numbers of effective mass, and why this is important, why am I discussing all these, you are engineers why all these details are required. Please see this.

(Refer Slide Time: 39:14)



If you are a device engineer, usually the control parameter is i the current; i is equal to J into a, J is the current density multiplied by area. If this is your device, we are applying an external field, and then you want to see what is the current i, J drift, because of an applied field. So, what you have is J drift, is equal to n the carrier concentration charge multiplied by the mobility E into the external electric field, because of this there is an electric field here e. So, the drift current density is equal to this, because you need this to know what is current generated in this medium. So, what are all the things you need to know, n carrier concentration, carrier concentration in the conduction band, is given by n is equal to n of E; that is at every even value of E n, this is carrier density into d E. If you are looking in the conduction band, it starts from E c to infinity. So, this is carrier density. Why you all this physics for engineers; that is the question. So, engineers' talk of current, current is given by this, so this is the carrier density n.

(Refer Slide Time: 41:28)



n of E, the carrier density n of E. Please see the context of this discussion n of E is equal to rho of E into F of E, rho of E is the density of states, which will be our next topic, density of states. Almost every course you will come across this density of states, whether it is optics, semiconductor physics, quantum mechanics, density of states multiplied by F of E, what is F of e; probability of occupation. So, density of states multiplied by the probability of occupation will give you carrier density, an integrate over the entire band, that will give you the carrier concentration. That carrier concentration you need to substitute here, if you want to find out the drift current. What is q, q is the charge, and this is the electric charge, mu E is the mobility of electrons, mu is the mobility.

This mobility is given by charge E into tow c divided by m star, where this is the effective mass, mobility is given by charge E or q charge, multiplied by carrier recombination time, divided by m star, where this is the effective mass. So, we need to know effective mass, to know the mobility. To know the effective mass, it is essential to know the E k diagram, band structure, only that will tell you what is this? So, I will give you in the next class, some values of mobility and effective mass in various semiconductors, and you will clearly see, the smaller the effective mass larger will be the mobility. So, for a given applied electric field, you need to know mobility which depends on m star. You need to know the carrier concentration which depends on the density of states and the probability of occupation. So, to know m star, you need to know the E k diagram alright.

We will see that E k diagram is also the one which will determined the optical absorption and emission processors, radiative processors and non radiative processors, there probability of occurrence is determined by the band structure, is very important in optoelectronic devices. So, I will stop at this point, and in the next class we will continue with the density of states, and then probability of occupation, and then we will go out to semiconductor materials, and then come to the interaction of electrons and holes in semiconductor devices. Next class we will also have a quiz, at the end of the class I will give you a quiz questions, and it is basically, it could be one word answer one sentence answer, or a very small questions. So, just a keep a piece of paper ready, and write on that and give it to me and then you can leave.

Thank you.