Semiconductor Optoelectronics

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Lecture-3
E-k Diagram-The Band Structure

Let we first recall what we have studied in the last class in the last lecture we have studied energy bands in solids.

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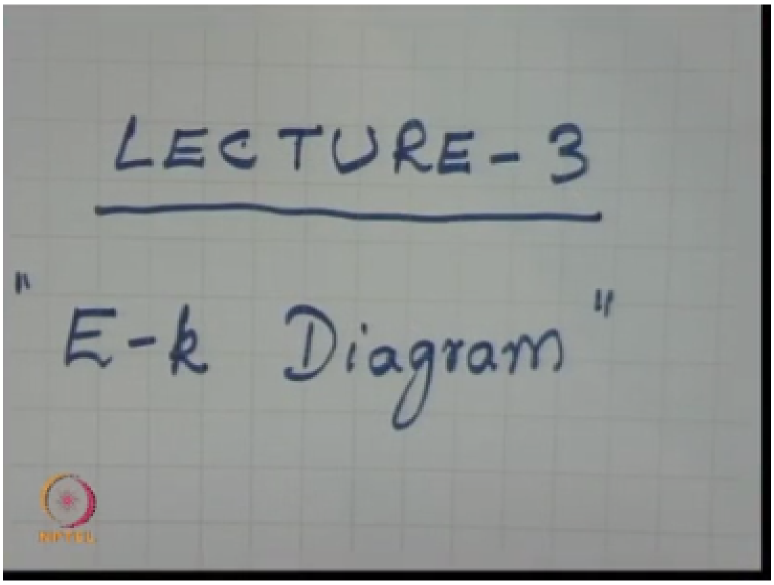

LECTURE-3

"E-k Diagram"

And therefore 2 general solids are characterized by energy bands.

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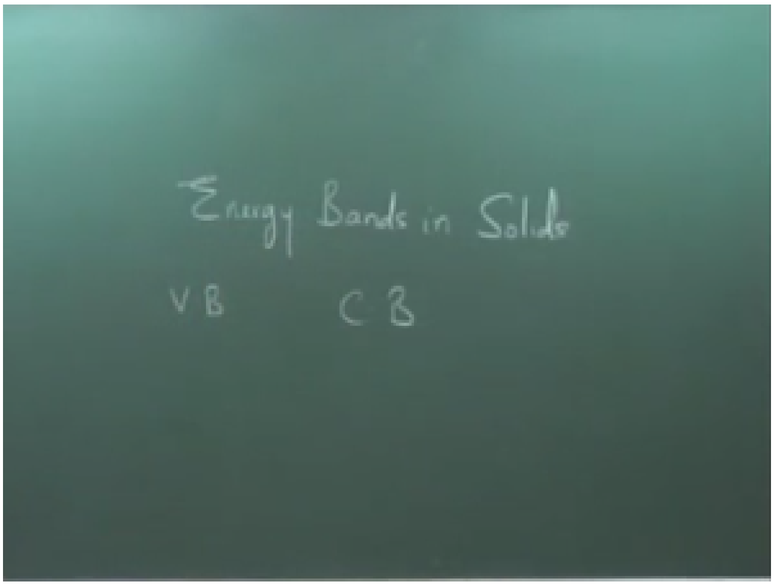

Energy Bands in Solids

VB CB

The highest band which is complete full or yearly full is called the valence band and the next band or the next higher band is the conduction band, it does not mean these are the only 2 bands there are many more bands which are below, but the electrons in those bands rarely participate in any of the electronic processes unless you use high energy exercise to knock them off.

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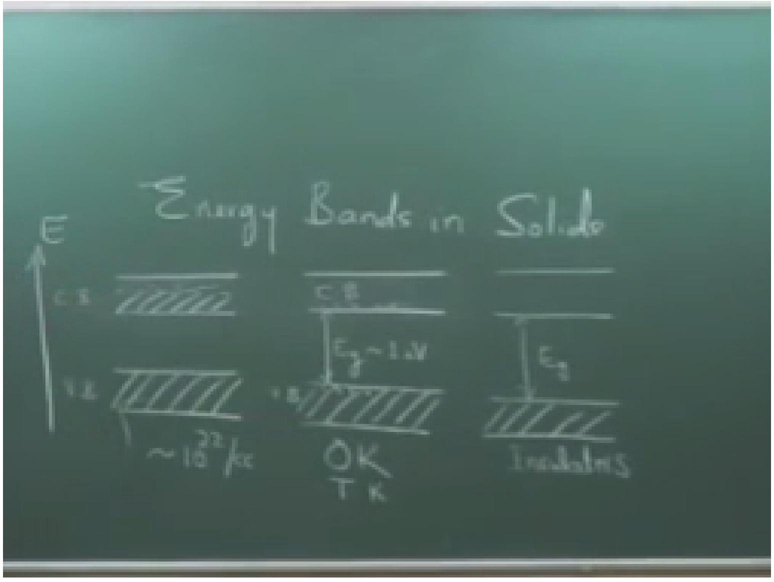

So normally the electrons which participate in optical and electronic processes are those in the valence band and conduction band. Therefore if I draw a band diagram which you have seen almost all books metals, semiconductors and insulators are basically characterized by band diagram. So let me draw the band diagram although I am cutting the bands at the same level. So this axis in all, all to the course the vertical axis will be energy.

The metals we have either a completely full valence band and almost half field conduction band and this is conduction band, this is valance band, if it is almost half field used rest of the half is empty or there are free state which are available for occupation. There are field state and free states and you have already seen the typical number of electrons is the order of 10 to the power of 22/cc which means very large number of electrons present.

And large number of free state 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 valence band overlaps and then also you have large number of electrons and large number of weekend stays in the same band.

And therefore electrons can move very easily. In the case of semiconductor at 0K valance band is completely full and the conduction band is completely empty. Typically the band gap here EG, how it out of band EG because electronics have to go up EG, is the order of 1 electron V. As I mentioned that anywhere from 0.1 electron to 3 electron volts is the band you have semiconductor.

But let us say 1 electron and any finite temperature the finite temperature T, there are electrons which go to the conduction band which lead to conductivity, electrons can there, if some electrons come here then there are free states, vacant state and electrons can start moving to the band in the presence of an applied electric field. The electrons which go here the behind holes which are nothing but vacancies in the valance band.

Holes exist only in the valence band and not in the conduction band, so vacant states in conduction band are different from the vacant states here, these are holes which are vacancy created in an otherwise field balance band. In the case of insulators the band are clear, the energy gap is very large as shown in the model in the same level but we see that these gaps are different for the 3 different material.

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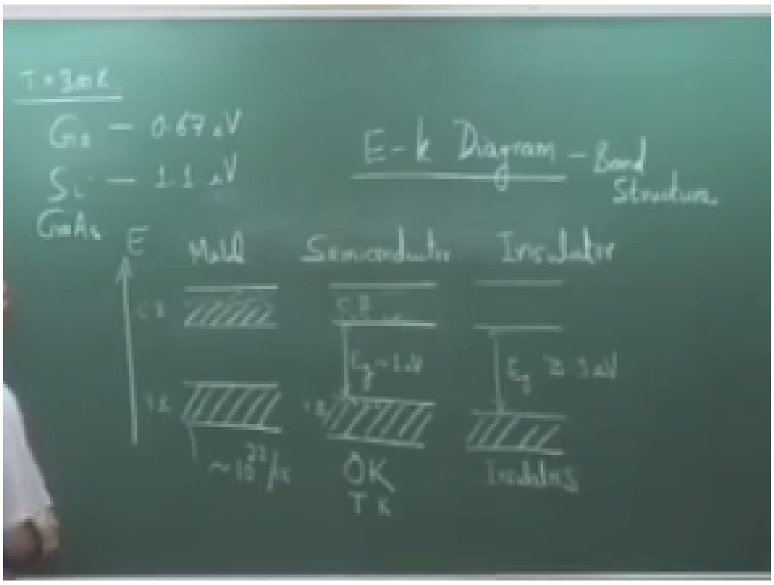

So what have drawn is energy bands in solids, so metal, semiconductor and insulator. Because the electrons in the conduction band have gone up or have made an upward transition from the valence band naturally the number of electrons present in any temperature is given by written in the gap, it not other gap larger will be the number of electrons which can make a poor transition.

And larger the gap smaller gap is there, in general when EG is greater than or a border of E electron volt 4, 5, 6 and all. Then the number of electron which can make in a poor transition becomes 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 we generally characterize metals, semiconductors, insulators in terms of this energy band.

But these energy band diagrams do not tell anything more beyond this, so to know more optical and electrical properties of a semiconductor or any material you have to go to the E-k diagram which is call the band structure E-k diagram, it is the E-k diagram which will tell you many more things. So let us discuss the E-k diagram or this is called the band structure **the band structure**.

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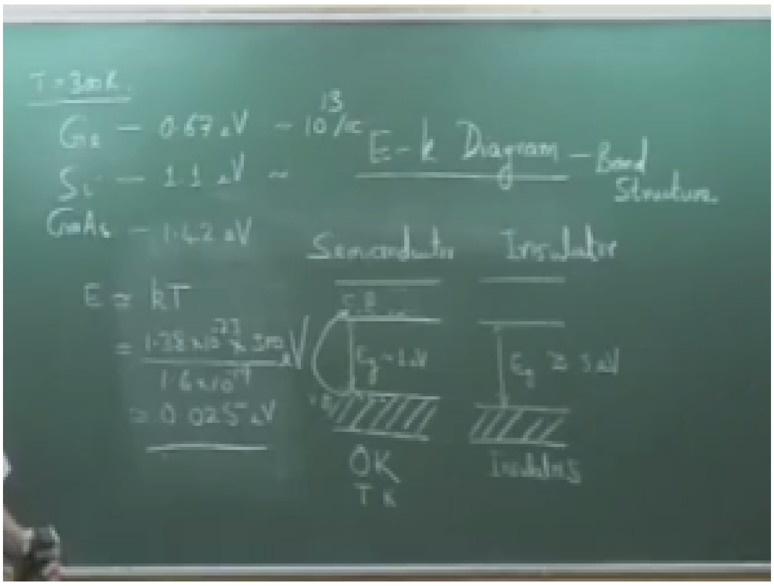

Just before I go over there you know that at room temperature let us say around at room temperate so T=300k, we have silicon, Germanium, let we see 3 semiconductors germanium, silicon, and gallium arsenide. The energy band gap is 0.67 eV for silicon it is 1.1 eV, gallium arsenide is a band gap of 1.42 eV which means if this band gap is about one electron volt then an electron which wants to make an upward transition here must have energy of the order of 1 eV or more.

But in general we know that the energy of electron average kinetic energy of electron E is of the order of kT at temperature T, where k is the both so this is 1.38*10 to the power of -23*let us say 300/1.6* 10 to the power of -19T and that is approximately 0.025 eV, we are familiar with it, or with kinetic energy of electrons, how is that when kinetic energy is or when the energy of electron is board of this.

How is it that electron is able to make an poor transition, think over this you know that at room temperature germanium has typically of the order of 10 to the power of 13 electrons/cc, silicon is not though this is intern material by intrinsic carrier concentration due to the temperature is a border of 10 to the power of 10/cc and for gallium arsenide this is the border of 10 to the power of 6/cc.

How is that so many electrons make a poor transition at room temperature at 0k semiconductor and semiconductor the valence band is full and conduction band is empty, how is it that large number of electrons exist in the conduction band at room temperature, you thought about this then we will discuss further. So let me go further to discuss the E-k diagram energy versus k.

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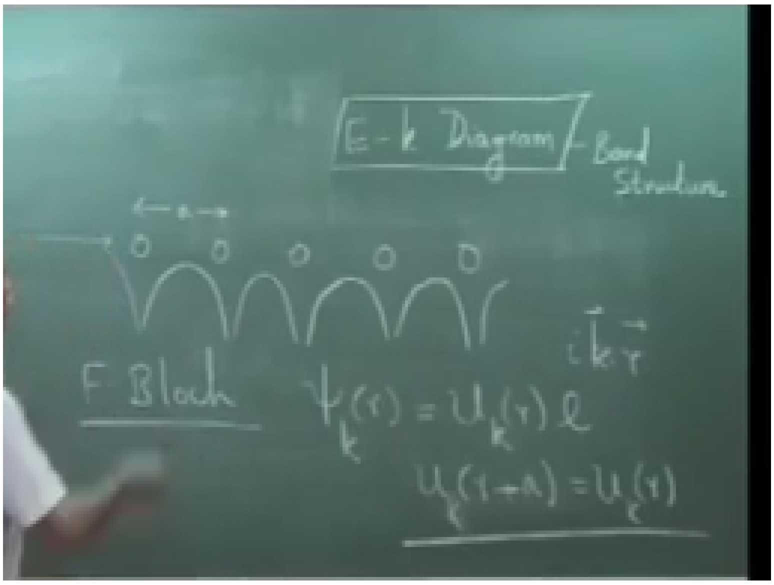

In the last class we discussed that most of the semiconductors are crystalline and in crystalline semiconductors atoms are erased periodically in lattice. The periodical arrangement if I take 1D arrangement for simplicity periodical arrangement leads to a periodical potential variation, periodical variation of potential, potential energy here, but the motion of electrons in a crystal is given by the loss of fundamentals.

If you have 1 electron, 1 proton system like 2 hydrogen atom it is very easy to solve the Schrodinger equation. But no sorry when there are large number of electrons and atoms present it is extremely complicated and difficult to solve the Schrodinger equation. But block F block I am sure you have heard of blocks, blocks observed that this 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 periodical which means the wave function should also vary periodically, we see probability of finding an electron is proportional is equal to small size that is the wave function and therefore he postulated that in such periodic medium the wave function should be of the form phy k of r=uk of r*e to the power i k dot for that is the wave function is a product of that plane way this is a plane e to the power i k dot r is the plane way.

And multiplied by a periodic function which is called the cell function uk of r is periodic, uk of r+a=uk r sometimes I write is the same k, sometimes I would have written like this, sometimes I write like this please should capital, so ik.r, so this is a periodic cell function. This is a periodic function where a is the interatomic space**.** So he postulated that wave function must be of this form.

The plane way multiplied by a periodic function. If you substitute this form of the wave function in the Schrodinger equation that is phy+2mi h power square*E-V*5=0. Then it turns out that this can be solved by several numerical and analytical techniques are several methods by which you can solve this if you substitute this form of psi in this and you can solve this and you get energy values Eigen values we see here E is energy Eigen values, V is the periodic potential.

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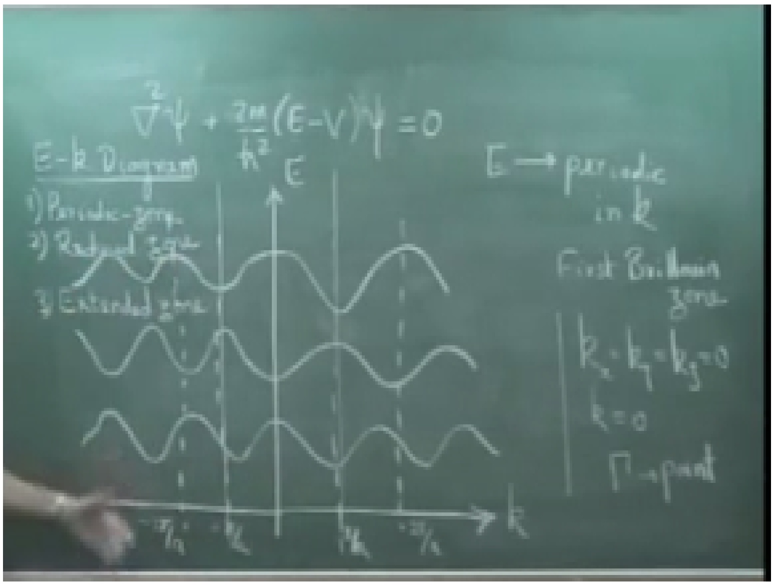

And M is the mass of the electron, and is the wave function, so you get energy Eigen values E also turns out to be periodic in which me if you plan the results of this, if you plot energy verses k, E verses k, then for each allowed energy level each allowed discrete energy level you get periodic functions. So always the vertical axis is E and this axis is k, this is E verses k which means for every given value of k.

This is K=5/a k=2phy/a, k=-phy/a and -2/a corresponding to every energy level of the single potential well you have now if periodically varying energy level. If you see the first boundary here between –phy/a and +phy/a, which is called first Brillouin zone, day was only the borders of the first brillouin zone, I will not going to the details brillouin zone wants home because this is in the reciprocal lattice some important points but what we are mainly focusing is on K=0 that is k we will see shortly that kx ky kz=0 which corresponds to a=0.

And this if you have not come across this you may go through but we are not very in this course we are not very very much Brillouin zone Gama point, X point, L point there are different various points but what I want to 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 ourself to 1 period – 5phy/a to +phy/a.

If you know the value from –phy/a-+phy/a then we know everyone because periodic and therefore in a reduced zone in the E- k diagram there are so E- k diagram there are 3 pictures and sure one of them will be the picture that you have seen. So the first one is periodic zone picture periodic zone, the second one is called the reduced zone, and the third one is called the extended zone picture.

There are 3 pictures for the E- k diagram, what I have plotted is the periodic zone, in the reduced zone picture you simply you reduce this up to the border of the first reduced zone because you know that you know beyond this. So this is the reduced zone. So normally when we see the E-k diagram we look at the reduced zone picture, these correspond to different levels.

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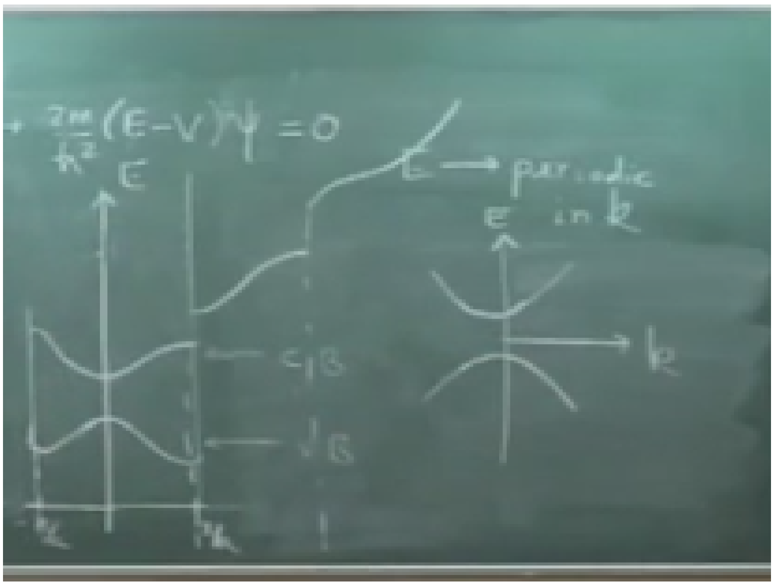

And if you see the reduced zone reduced zone picture and highest filled energy level is the valence band and the next one is the conduction band and if you look at these bands and draw the reduced zone picture then we focus only on this part of the E-k diagram, k verses E, or we focusing only on this part I will tell you in a minute. Now let we complete what is this extended zone.

In the extended zone picture if you know up to this here and then there is a PC this should would have like this, so in the extended zone picture you showed is discontinuity and why this, so you have come up to this is phy/a, this is at 2phy/a and corresponding to the next band you have it is continuity and then again going like this. So this is the extended zone picture where you show from 0 to 5 by a for 1 level, 5/a to 2phy/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 Kronig penny model, from the result of the kronig penny model you will see that there is a discontinuity and then you see the extended zone picture. But here for this course on 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 bottom, the top of the valence 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 calculate the density of states which will be our next topic. We will see that the density of states in a band is extremely large and the number of electrons are the career 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 close to the top of the valence band participate in all processes or electronic processes. Therefore it is not even you rarely meet this ends, the ends of the zone, all the practical devices almost all the practical devices utilize careers which are close to the bottom of the valence band.

And close to the top of the 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 lowest portion of the E-k diagram, the relevant portion of the E-k diagram and discuss further.

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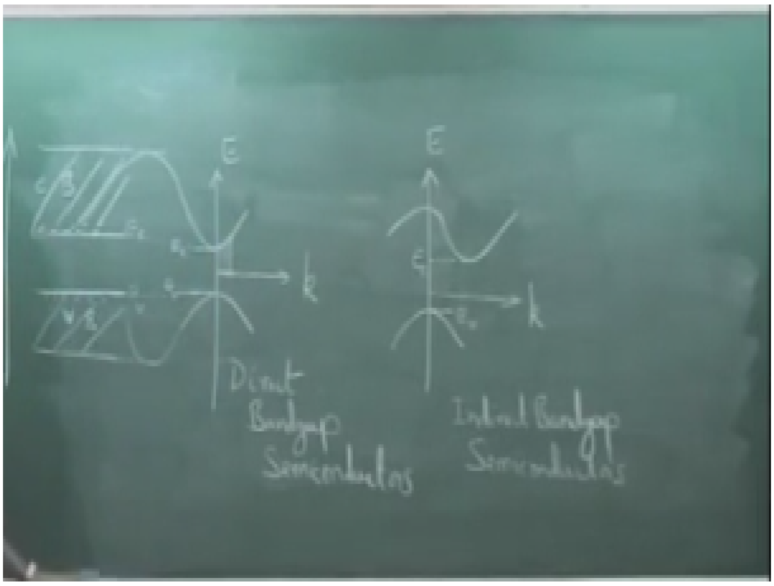

So now we have the E-k diagram when you plot the E-k diagram, so this is k, you could draw k here also, vertical axis is always E. So what is this represents, this represents for every value of k we will see shortly that the k values are discrete, for every value of k here what is the corresponding allowed energy. That is a solution of the Schrodinger equation. So what you are plotting is allowed energy values as a function k.

We will see that the k values are discrete, but the number of values are so large that you plot a continuous. So material in which there are materials in which the top o f the valence band here coincides with bottom of the conduction band and there are materials in which the top of the valence band does not coincide with the minimum of the conduction band. So materials in which of E verses k materials in which the minimum of the conduction band coincides with the top of the balance.

Coincides means occurs at the same value of k are called direct band gap symptoms, and materials in which the minima of the conduction band ec denoted by ec in and this value here is ec, the band h in the coincide does not coincide are called indirect band gap symptoms. So 2 things to note that k can take large number of values, what is this k we will see shortly again we will recall what is this k.

And corresponding to each k value there is an allowed energy value allowed energy means an allowed solution of the Schrodinger equation and we plot energy versus k and that is the E-k diagram. Also please recall that we had drawn an energy band diagram, the familiar energy band diagram where you show that ok this is the valence band and this is the conduction. So this is the conduction band and this is the valence band.

This is the bandage which is Ev and this is ec, have to clear picture that this ec is the same as of the e-k diagram share the bottom of this here ec is the same as this and the top the bandage here is the same as this and this was going up and then turning like. 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 here, but you will see that it is a E-k diagram which will tell us more about the optical and electrical properties of the material. So this is 1-1 usually the holes which are close to the top of the valence band and the electrons which are close to the bottom of the conduction band participate in all the electronic transition process.

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 will proceed little bit further to see what is this k. This k is the propagation vector of electron wave function in the propagation vector whose magnitude k is the propagation vector.

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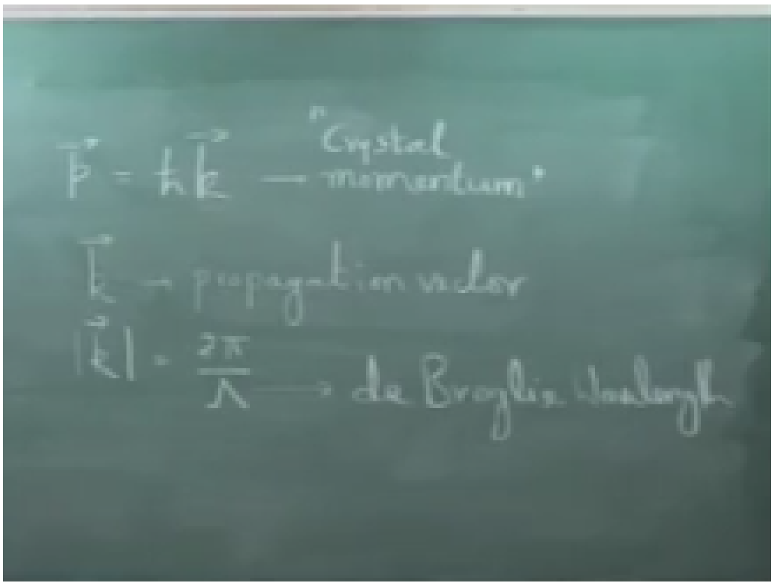

$\vec{p} = \hbar\vec{k}$ — "Crystal momentum"

$\vec{k}$ → propagation vector

$|\vec{k}| = \frac{2\pi}{\lambda}$ → de Broglie wavelength

Whose magnitude is given by 2phy/lamda where lamda is the Broglie wavelength, the 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 p. This momentum is very often called the crystal momentum

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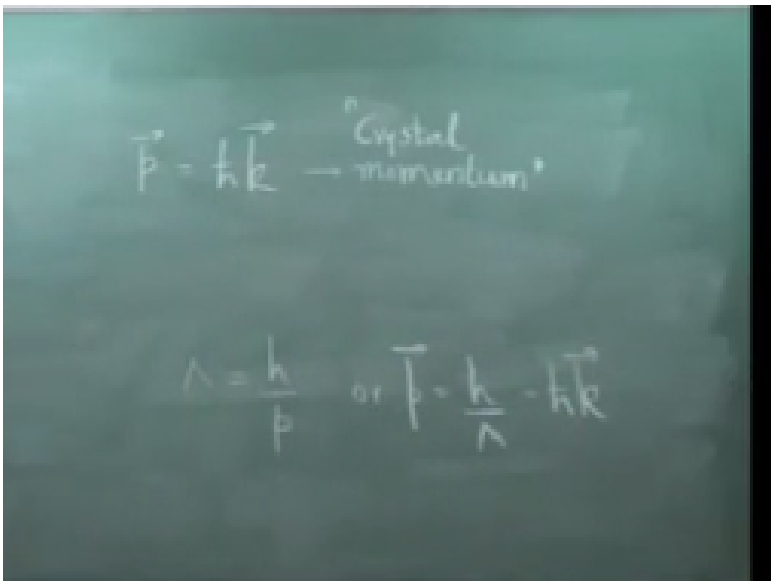

We see an important concepts here, this comes from your familiar with the Broglie wavelength lamda=h/v where h is the plants constant and p is the momentum or p=h/lamda. So if you divide and multiply by 2 phy, this is nothing but h cross k. So momentum is nothing but h cross k, ,momentum is the vector. Therefore this is h cross k. This is how you get this. Now this is call the crystal momentum.

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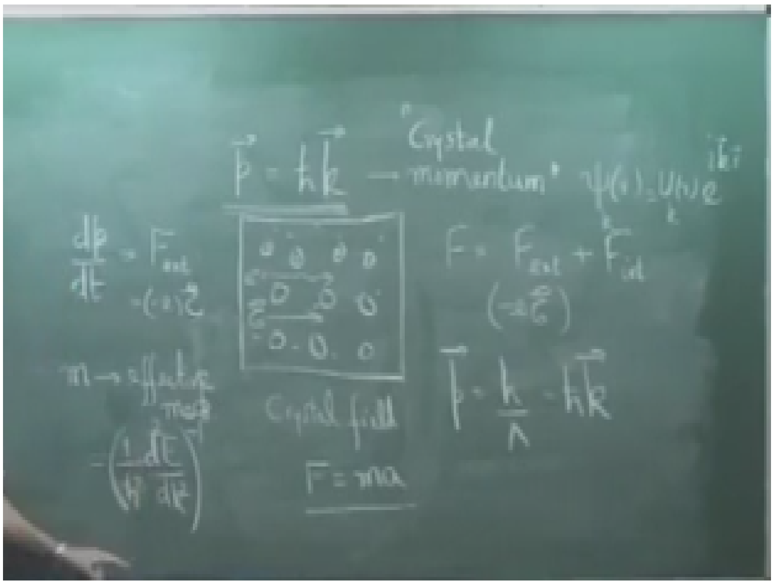

See this picture if you take a semiconductor there are large number of atoms and electrons, the ions, and electrons any electron here, any electron e is moving to this medium under the influence when there are positively charge nuclei and negatively charged electron, that is electrostatic field. So any electron which is moving through this moves under the influence of a electrostatic field which is inside the crystal. This is called a crystal field.

Electronics moving through it, it is not moving through 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 electric field so the electron start when the this is an external electric field. So you are now applied an external electric field, it is there is a internal electric filed.

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+due to F internal. Yes external is because of the applied electric field which means you know that is –e*e. This is the external filed or an applied electric field out from outside which means I say electric field e.

So the force is charged into e, -e*e, what is the internal field, it is really very complicated, if you define the momentum by this expression where this k is the same k which appear here 5k of r*uk of r8e to the power of i k.r, it is the same k which is the Broglie wavelength 2phy/lamda. If you decide that then this is call the crystal momentum which means this momentum is as if it is responding only to the external field.

And otherwise you have dp/dt what is this rate of change of momentum=F external, normally that P was the total momentum it should have been F must have been equal to dp/dt, force=rate 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 dp/dt, it is equal to F external.

This F external you know that this is very important what you know is E you do not know internal field and therefore it is as if the electron is responding to the external force as if it is a free particle you see this and then it moves with the mass which is equal to the effective mass of electron the effective mass which is defined by 1/h cross square, b square e/dk square to the power -1, I have actually skip the derivation of this.

There is a many complex derivation and there is a simple heuristic derivation both has skipped at this moment, but I would like you to appreciate is this that if I define the electron mass by this effective mass of electron it is as if this is electron which is a free electron which is directly responding to the external force which is directly responding to the when we write F=mk.

This is the mass of the particle and this is as it, this is what a free particle F=ma. So if you define an effective mass for an electron which is given by D square e by 1 over x square*D square by DK square to the power -1 then this electron inside a semiconductor can be treated as if it is a free lift moving at the influence of the field, you do not need to consider the internal forces within the semiconductor.

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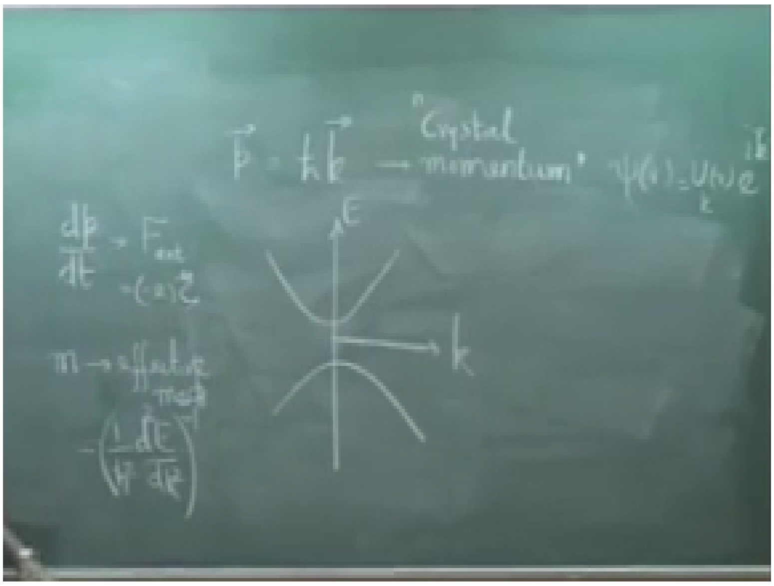

It is as if electron response directly to the external force, that is why now what you see is this is d square e by DK square where you get this from I skipped the derivation but to get D square e by DK square unit that E=k diagram, so you have the E-k diagram here. So this is E-k and the second derivative gives you D square e query by Dk square and this is the effective mass. So it is the E-k diagram which will tell you what is the effective mass.

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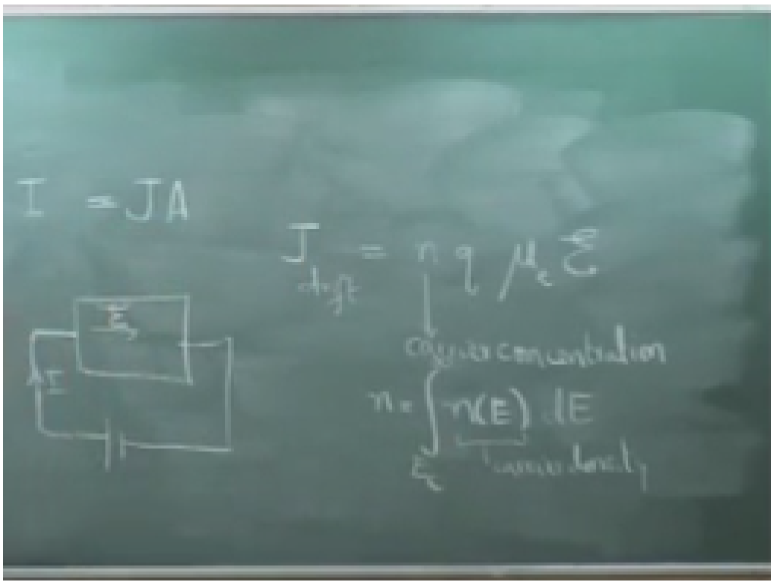

I want to give a few numbers of effective mass and why this is important why I am discussing all these, we are engineers why always details are required please see this. If you are a device engineer usually a control parameter is I, the correct I=J into a J*A, J is the current density multiplied by area. If this is your device you are applying an external field and then you want to see what is the current time.

J gives because of an applied field, so what you have is J filed=n the carrier concentration charge multiplied by the mobility e*electric field. Because of this there is an electric field here e. So the bit correct density is equal to this because we need this to know what is the current rate in this medium. So what are the things that you need to know n, career concentration. Carrier concentration in the conduction band is given by n=n of e that is at every given value of e10 is a carrier density*De.

If you are looking in the conduction band which start from Ec to E3, so this is carrier density, why all these physics for engineers that is the question, so engineers talk of current it is given by this. So this is a carrier density n, n of e that carrier density n of e please see the context of this discussion n of e=row of e*f of e, row of e is the density of states which will be our next topic density of states.

Almost every course we will come across density of states whether it is optic 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 and 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 electric charge, new e is the mobility of electrons, new e is the mobility, this mobility is given by charge e*touC/n*. This is the effective mass mobility is given by charge e or Q charge multiplied by carrier recombination time/n start where this place the effective mass.

So we need to know effective mass to know the mobility, to know the effective mass it essential to know the E-k diagram, the band structure only that will tell you what is this. So I will give you in the next class some value of mobility and effective mass in various semiconductor 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 with depends on n start.

You need to know the career concentration which depends on the density of states occupation and the probability of occupation, so to know n start you need to know that E-k diagram alright, we will see that E-k diagram is also the one which will determine the optical absorption and emission processes, radiative process and nonradiative processes that probability of occurrence is determined by the band structure is very important in optoelectronics devices. So I will stop at this point.