Semiconductor Device Modeling

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Lecture - 29
Energy Band Diagrams

In the previous lecture, we discuss the quantitative model of the energy versus wave vector relation the E–K relation for electrons in a periodic potential, so we outline 3 important features of this E–K relation based on the solution of this Schrodinger equation, the 3 features where one that the E-K relation is periodic with a periodicity = 2 pi by the interatomic distance.

So we consider a one dimensional situation where you have all the atoms located along a line in a regular fashion, the next feature was that certain energies are present for which the Schrodinger equation has no solution for real values of the wave vector K and the third feature was that for any given value of K there are multiple values of the energy E allowed for electrons in a periodic potential.

In contrast to the E-K behaviour, the E-K behaviour of free electron is very simple it is a parabola in which for any given K there is only one E or if you consider the E–K relation for electrons in a rectangular potential value then the E-K consists of a set of discrete points on a parabola for any given K there is only one value of E.

So although we did not discuss the solution of the Schrodinger equation for a periodic potential in detail we outline the important steps and showed how from these important steps the 3 features namely periodicity of the E-K relation, E being a multi valued function of K and the absence of the solution of this Schrodinger equation for certain energies for real K or the presence of forbidden energy bands these 3 features how they emerge from the solution this fact was outlined.

Then we said that since the E-K is periodic it is not necessary to show multiple periods of this relation we can show only one period and that will consist of all the required information, now this one period is called the first below in zone, now in fact since the E-K is even one may not even to show the E-K for one period one could show it for even half a period or half of the below in zone, now it is in this form that the E-K relation of real crystals.

For example, silicon and gallium arsenide are shown, so we showed the E-K diagram of silicon and gallium arsenide and we just presented the important features of this E-K diagram. Now in the lecture today we would like to discuss the utility of the E-K relation and we would like to move on to the E-X diagram and discuss how we can determine quantitatively the E-X diagram.

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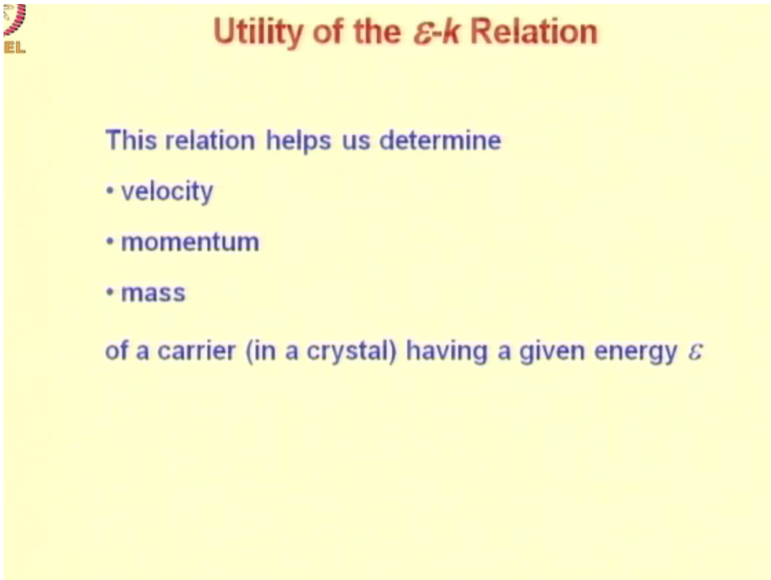

Utility of the ε-k Relation

This relation helps us determine

- velocity
- momentum
- mass

of a carrier (in a crystal) having a given energy ε

Let us begin with the utility of the E-K relation, this relation helps us determine the velocity, momentum and mass of a carrier in a crystal having a given energy E, now you might wonder that is not this determination is very simple that is the determination of the mass, energy and momentum of a carrier of a given energy. Now so far we are used to a free electron right calculating various quantities for a free electron, now for a free electron the mass does not change with energy, the mass is constant.

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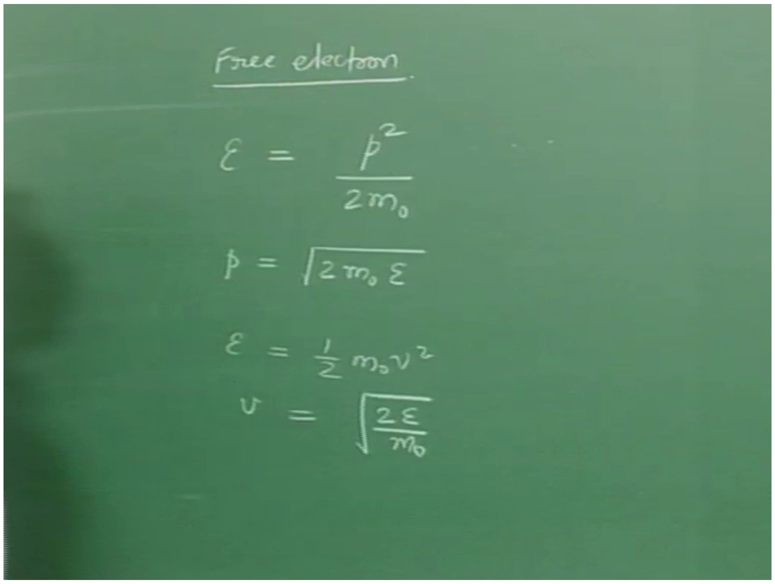

Free electron

$$E = \frac{p^2}{2m_0}$$

$$p = \sqrt{2m_0 E}$$

$$E = \frac{1}{2} m_0 v^2$$

$$v = \sqrt{\frac{2E}{m_0}}$$

For a free electron the energy momentum relation is simply energy = p square/2m0 and therefore if I want to know the momentum for a given energy I can simply use the formula p = square root of 2m0 E, if I want to know the velocity of the electron for a given energy E assuming the energy to be kinetic energy because that is when we can write E as p square/2m0 you can get the velocity as follows E equal to half of m0v square.

And therefore the velocity V is nothing but 2E/m0 under square root, now all this is fine for a free electron but for electrons in the crystal things are not so simple we will find that the effective mass or the mass of the electron depends on energy, similarly the energy versus momentum relation is more complex right, so let us look at these features.

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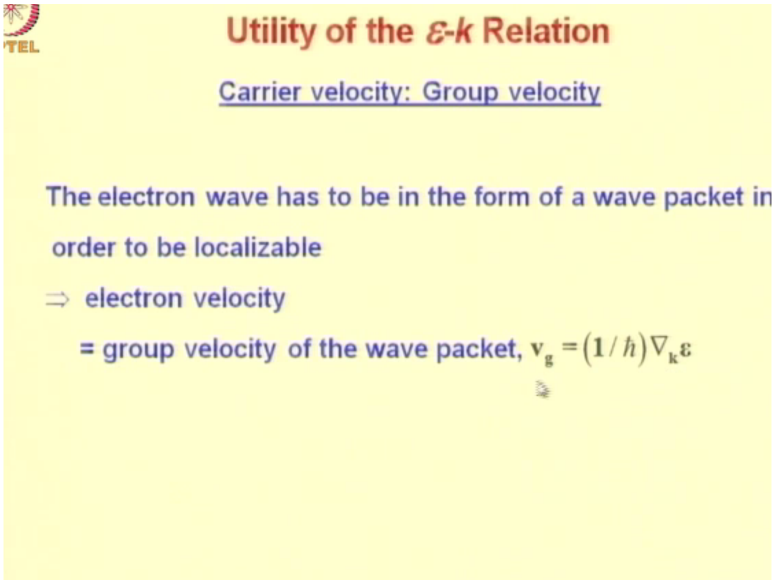

Utility of the ε-k Relation

Carrier velocity: Group velocity

The electron wave has to be in the form of a wave packet in order to be localizable

$\Rightarrow$ electron velocity

= group velocity of the wave packet, $\mathbf{v}_g = (1/\hbar)\nabla_{\mathbf{k}}\varepsilon$

Let us start with the carrier velocity okay, now the carrier velocity of, the velocity of a carrier which can mean electron or a hole so whenever I use atom electron you must always remember that you can also use the same idea for a hole, so for an electron in a crystal the velocity is the group velocity why? The electron wave has to be in the form of a wave packet in order to be localizable.

So we have pointed out that when you want to discuss the behaviour of electrons in a crystal in contrast to the situation for a free electron the electrons in crystal have to be treated quantum mechanically or electron should be regarded as a wave, now once you regarded the electron as a wave it has to be in the form of a wave packet in order to be localizable.

And therefore electron velocity is equal to the group velocity of the wave packet which is given by the formula vg = 1/h cross into the gradient of the energy E where the gradient is obtained with respect to the wave vector K okay, that is what this formula means so this is where you have to use the E-K relation, so the slope of E-K relation actually gives you the group velocity.

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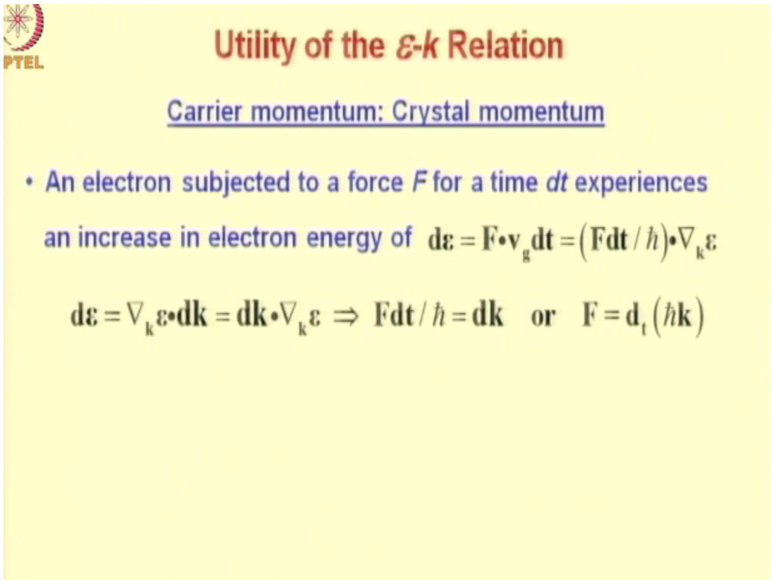

Utility of the ε-k Relation

Carrier momentum: Crystal momentum

- An electron subjected to a force *F* for a time *dt* experiences an increase in electron energy of $d\varepsilon = \mathbf{F}\bullet\mathbf{v}_g dt = (\mathbf{F}dt/\hbar)\bullet\nabla_k\varepsilon$

$$d\varepsilon = \nabla_k\varepsilon\bullet d\mathbf{k} = d\mathbf{k}\bullet\nabla_k\varepsilon \Rightarrow \mathbf{F}dt/\hbar = d\mathbf{k} \quad \text{or} \quad \mathbf{F} = d_t(\hbar\mathbf{k})$$

Let us look at the carrier momentum, the momentum of a carrier is given the name crystal momentum, now let us see what is the origin of this name how the particular momentum of a carrier that we employ in a crystal is different from the true instantaneous momentum the carrier does have a true instantaneous momentum in a crystal. However, as we will see it is not possible to determine the true instantaneous momentum easily.

And instead we use a momentum like term that we call as crystal momentum, so in electron subjected to a force F for a time dt experiences an increase in electron energy of dE = the force multiplied by the velocity this is a dot product because force and the velocity which is a group velocity are both vectors and so you have to take a dot product multiplied by dt. So force into velocity is power and then you multiplied power by time you get the energy.

Now you can write this formula as F of dt/h cross dot product of this with the gradient of the energy with respect K because just now we discussed the fact that the vg = 1/h cross time gradient of K, now we know that we could write dE as gradient of E with respect to K dot dK okay, now this is from elementary calculus.

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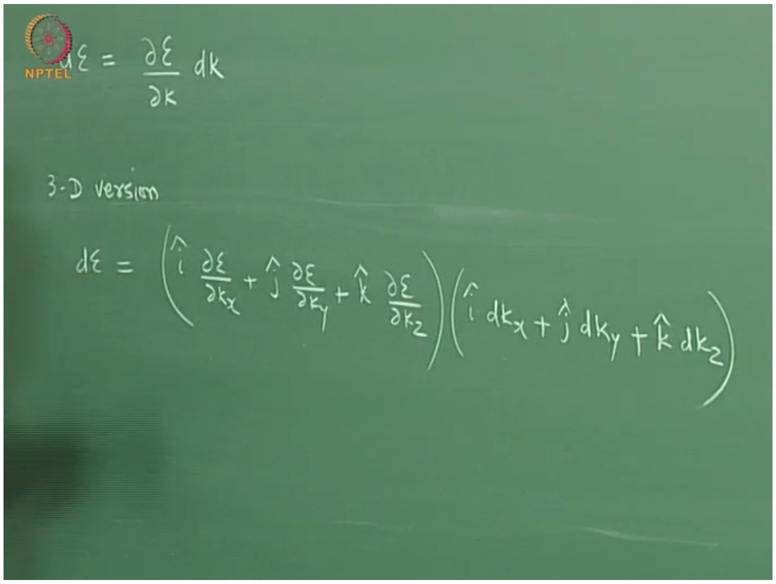

$$d\mathcal{E} = \frac{\partial \mathcal{E}}{\partial k} dk$$

3-D version

$$d\mathcal{E} = \left(\hat{i}\frac{\partial \mathcal{E}}{\partial k_x} + \hat{j}\frac{\partial \mathcal{E}}{\partial k_y} + \hat{k}\frac{\partial \mathcal{E}}{\partial k_z}\right)\left(\hat{i}\, dk_x + \hat{j}\, dk_y + \hat{k}\, dk_z\right)$$

dE = dou E/dou k into dk. Now, when you take in 3 dimension, this is written as i into dou E/dou kx+j into dou E/dou ky+k into dou E/dou kz. Now, it is important to note this k and this k are not the same this is the vector in the z direction unit vector in the z direction okay, so this multiplied by i dkx+j dky+k dkz again this k with a hat is a unit vector different from the wave vector k okay so this is how you get dE from elementary calculus.

Now that is what is written here, now you can even write the same thing as dk dot the gradient of E with respect to k, now from this relation and the relation for dE given here we get F into multiplied dt divided by h cross = dk, now this is because you compare this and this, this relation so you remove the gradient of E with respect to k form here and from here you get this term is = this term that is what is being written here.

Now, the same thing can be written as F is = dE/dt of h cross k.

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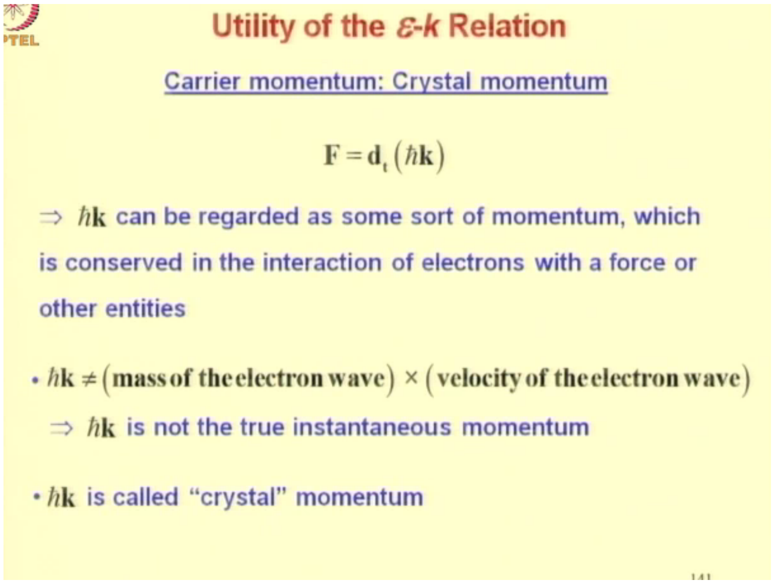

Utility of the $\mathcal{E}$-k Relation

Carrier momentum: Crystal momentum

$$\mathbf{F} = \mathbf{d}_t\left(\hbar\mathbf{k}\right)$$

$\Rightarrow$ $\hbar\mathbf{k}$ can be regarded as some sort of momentum, which is conserved in the interaction of electrons with a force or other entities

- $\hbar\mathbf{k} \neq \left(\text{mass of the electron wave}\right) \times \left(\text{velocity of the electron wave}\right)$
  $\Rightarrow$ $\hbar\mathbf{k}$ is not the true instantaneous momentum
- $\hbar\mathbf{k}$ is called “crystal” momentum

Now look at this relation F = dE by the of h cross k this relation tells you that h cross k can be regarded as some sort of momentum which is conserved in the interaction of electrons with a force or other entities now this is like a Newton's second law right relation between force and momentum which you are familiar with and this second law also implies conservation of momentum in the absence of a force.

Now the h cross k term is not = the mass of electron wave into the velocity of the electron wave which is a group velocity and therefore h cross k is not to be regarded as the true instantaneous momentum, now this is an important point although the equation F = d/dt of h cross k points towards calling h cross k or some sort of momentum it is not the true instantaneous momentum which is given by the mass into velocity.

As we will shortly see the mass of electron is not constant with energy and you have to use some sort of an effective mass why because of the presence of the periodic crystal potential or crystal forces from the atoms, therefore we give a different name to h cross k we call it as the crystal momentum.

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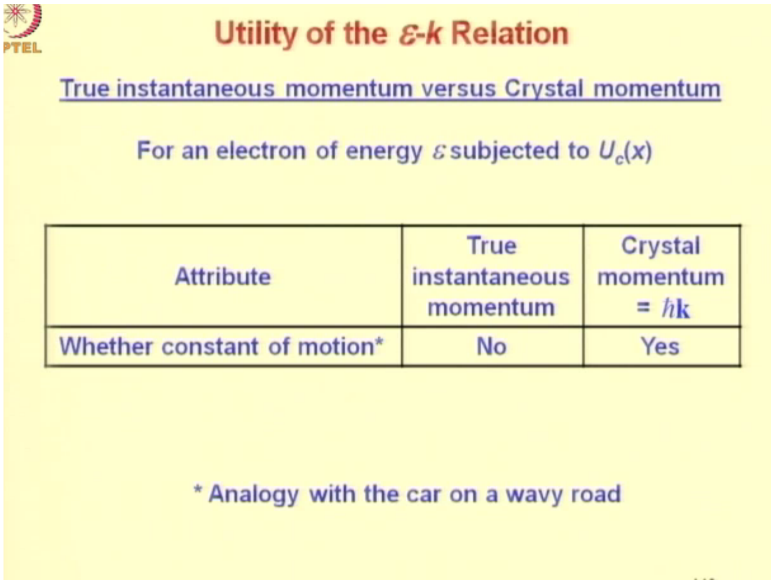

Utility of the ε-k Relation

True instantaneous momentum versus Crystal momentum

For an electron of energy ε subjected to $U_c(x)$

Attribute	True instantaneous momentum	Crystal momentum = $\hbar \mathbf{k}$
Whether constant of motion*	No	Yes

* Analogy with the car on a wavy road

Now let us distinguish between true instantaneous momentum and crystal momentum to understand the concept of crystal momentum much more clearly, for an electron of energy E is subjected to a crystal potential U c x, U c of x the difference between the true instantaneous momentum and crystal momentum = h cross k is as follows the true instantaneous momentum is not a constant of motion, whereas the crystal momentum h cross k is a constant of motion.

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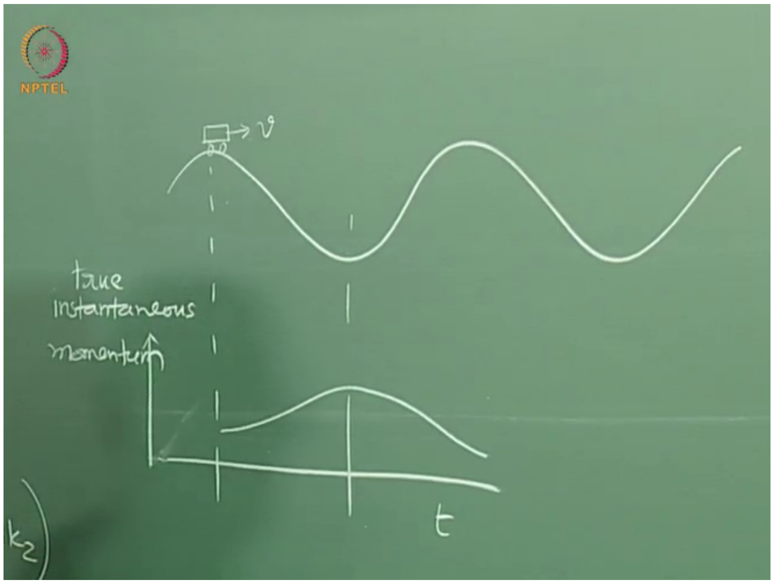

Now let us illustrate this point with an analogy of the car on a wavy road, now supposing I have a wavy road like this and there is a car moving on this okay, let us assume that when the car is at the peak here it has a velocity or speed v, let us further assume that there is no friction between the car and the road and the gravity is acting and therefore when the car moves down its velocity is going to increase in magnitude and of course changes in direction also.

Now by the time the car is here its velocity will be maximum it will be very different from this, so you see here when the car is moving on this wavy road if I were to look at its true instantaneous momentum that momentum will also be fluctuating, so if I plot as a function of time for this car so there is certain momentum when it reaches a maximum there is certain momentum here it reaches a maximum and then again it goes minimum and so on.

So you can see that if I talk about the true instantaneous momentum of this car when the gravity is acting on it because of the action of gravity and the wavy road that true instantaneous momentum is not a constant, now the picture for the electron in a crystal is similar the electron is subjected to a periodic crystal potential and therefore you cannot deal with the true instantaneous momentum because it is going to affected by the crystal potentials.

Another difference between the 2 is that the true instantaneous momentum cannot be calculated from quantum mechanics easily, whereas the crystal momentum can be easily calculated from quantum mechanics.

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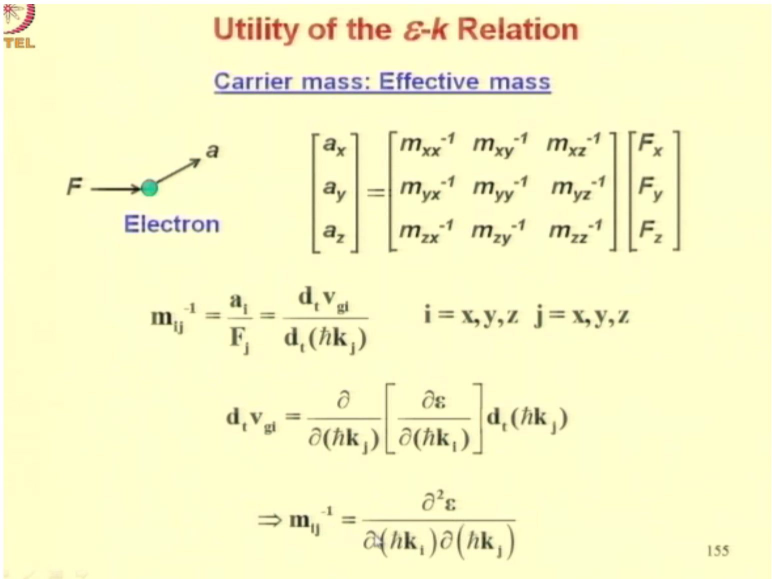

Utility of the ε-k Relation

Carrier mass: Effective mass

$$\begin{bmatrix} a_x \\ a_y \\ a_z \end{bmatrix} = \begin{bmatrix} m_{xx}^{-1} & m_{xy}^{-1} & m_{xz}^{-1} \\ m_{yx}^{-1} & m_{yy}^{-1} & m_{yz}^{-1} \\ m_{zx}^{-1} & m_{zy}^{-1} & m_{zz}^{-1} \end{bmatrix} \begin{bmatrix} F_x \\ F_y \\ F_z \end{bmatrix}$$

$$m_{ij}^{-1} = \frac{a_i}{F_j} = \frac{d_t v_{gi}}{d_t(\hbar k_j)} \qquad i = x, y, z \quad j = x, y, z$$

$$d_t v_{gi} = \frac{\partial}{\partial(\hbar k_j)} \left[\frac{\partial \varepsilon}{\partial(\hbar k_i)} \right] d_t(\hbar k_j)$$

$$\Rightarrow m_{ij}^{-1} = \frac{\partial^2 \varepsilon}{\partial(\hbar k_i)\partial(\hbar k_j)}$$

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Let us move on to the concept of carrier mass, the carrier mass in a crystal is referred to as effective mass, because you try to incorporate the effect of crystal potential on the carrier acceleration due to a force in the mass, so when you apply a force the carrier will accelerate to a different extent in a crystal as compared to a carrier in vacuum okay, now we have discussed the concept of effective mass already, now we will discuss how it can be calculated.

So the basic point is that for an electron in a crystal if the force is acting in some direction the acceleration is not in the same direction because of the presence of crystal potential, so the effective mass is actually a tensor, now this matrix representation you have come across already in the second module or the module on the qualitative discussion of carrier transport which is repeated here.

So what this matrix says is that the ex-directed acceleration can be due to Fx, Fy and Fz and each of these components will have a mass associated with it so that is how you have 3 masses okay, which contribute to every direction of acceleration and therefore you have 9 way different terms here associate with the effective mass. Now let us see how we calculate these terms so in the compact form we can write m suffix ij inverse = ai/Fj where i refers to the directions x, y and y.

And similarly, j also refers to directions x, y and z, so for example if I take this term m xx that means i and j are x and this is given by a x/Fx this is ax and this is Fx, on the other hand if you take this term m xy inverse so i is x and j is y and so this = a xy Fj. Now let us write the acceleration and force so the acceleration is given by the gradient of the velocity with respect to time, so this is d/dt of the group velocity in the i direction.

On the other hand, the force F j is the time derivative of the crystal momentum h cross k in the j direction, now V gi can be written as dou E/dou h cross ki where h cross ki is crystal momentum in the i direction. We have already defined the group velocity and shown how it is = dou E/dou of h cross k. Therefore, d/dt of V gi is nothing but dou/dou of h cross kj applied to this particular group velocity term multiplied by the time derivative of h cross kj right?

This is from elementary calculus, so you take this term and you want to get its derivative with respect to time and you take the partial derivative with respect to a particular term and then the time derivative of that term is what is multiplied here, now therefore if you substitute this term here it works out to m ij inverse = dou square/E/dou of h cross ki into dou of h cross k j, now this is how you calculate the particular term of this effective mass tensor okay.

Now, this is how the E-K relation can be used to determine the effective mass, so in general the E-K generation will be fairly complex when you look at the 3 dimensional picture.

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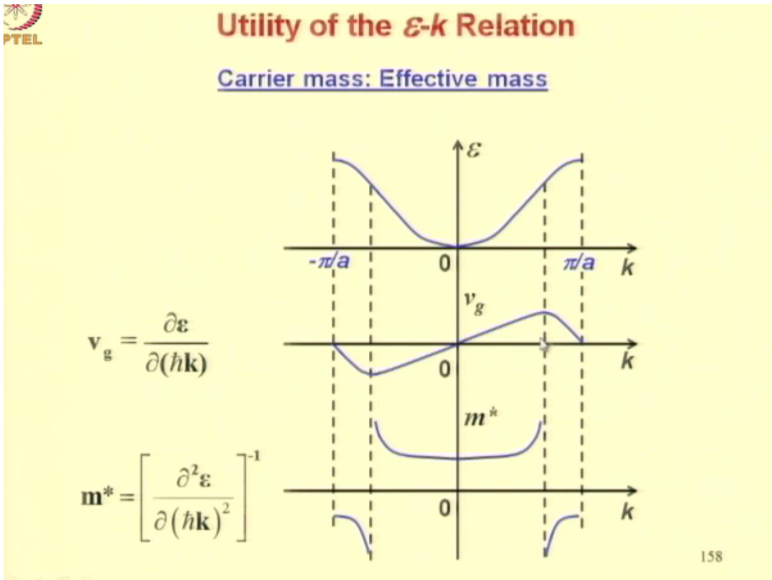

Utility of the ε-k Relation

Carrier mass: Effective mass

$$v_g = \frac{\partial \varepsilon}{\partial(\hbar \mathbf{k})}$$

$$m^* = \left[\frac{\partial^2 \varepsilon}{\partial(\hbar \mathbf{k})^2}\right]^{-1}$$

Now let us illustrate these ideas using one-dimensional situation, so for a one-dimensional case let us say this is the E-K relation as shown here in the first below in zone these are the points where the slope of this E-K relation is maximum, now the group velocity is the slope of this E-K relation and that works out to something like this, now this is interesting now what does it mean? So you find that the group velocity increases linearly with K and K represents in some form the crystal momentum because the h cross k is crystal momentum.

So, k is proportional to crystal momentum, so the velocity is increasing linearly with momentum this somewhat like and the picture of an electron in vacuum. However, as energy goes on increasing you find that at this point the velocity has reached a peak and there after even though the momentum is increasing the velocity is decreasing, now this appears counter intuitive right it is not something that you would expect, now this is something that we have to accept from the analysis of the electron in a crystal based on quantum mechanics okay.

Now what you find is even as K is increasing beyond this point the velocity is going on decreasing and goes to 0 and if you try to increase K further in fact the velocity goes negative, now that negative part can be constructed from here this part because the negative part here beyond this pi/a point, K = pi by a is same as the negative part here, because of the periodicity.

So the velocity is going negative as you increase K and then it reaches say maximum negative velocity and thereafter the velocity starts decreasing in magnitude and ultimately goes to 0 for value of K which is to 2 pi by a which is same as K = 0, so K = 2 pi by a which comes somewhere here which is same as K = 0 because of the periodicity, now what does this mean?

This means that if you try to accelerate an electron in a crystal by applying a force it is not as though the electron will move in the direction of the force all the time, we think from our experience daily experience with free particles with free electrons and so on that when you apply a force the momentum of the carrier goes on increasing continuously right, if the force is constant the momentum increases linearly the velocity increases linearly.

Whereas what we find here in the crystal from this diagram is that the velocity increases up to a point and beyond a point it starts decreasing, now this means in a crystal if you apply a force on the electron it will exhibit an oscillatory motion right, so it will move and then at some point it will change its direction and then come back because velocity becomes negative and then at some point here so the electron is moving against the force.

How can this happen? It is the effect of crystal potential and the wave nature of electron and at some point here the electron changes its direction again and it is moving to the right, so in response to a constant force with time and electron in crystal will exhibit oscillatory motion, in practice however we are not able to see such an oscillatory motion why?

Because even before the electron energy is increase to a point where this behaviour sets in where the velocity reaches its peak and comes down the electron will get scattered because of the presence of impurities and random fluctuations in the crystal structure, which will always be present in practice, so because of defects in the crystal which are always present you never observed this oscillatory motion.

So electron will get started and therefore in practice the energies of electrons would be somewhere in this region you will never go to these regions right? You cannot increase the electron energy to that reason to that magnitude okay, now what does this mean for the mass? Now the mass is given by the double derivative of E with respect to K of course with a inverse sign here, so I differentiate the velocity and then I take its inverse and then I get this picture.

So you can see here that the region where the velocity increases linearly with K is like the picture of electron a free electron in vacuum the mass of the electron is constant though it is not equal to the mass in vacuum but still it is a constant it is some effective mass whose value as to be obtained from the slope here, however has you reached this point here or here where the E-K diagram slope reaches a maximum the effective mass approaches infinity okay.

Because the velocity is peak if you take the slope of this velocity it will bE0 and 1/0 because there is an inverse operation here reciprocal so 1/0 goes to infinity and when you moved to the other side here when the velocity is decreasing with momentum you are effective mass is negative okay and it starts from a very high negative value infinite negative value and then goes on decreasing and reaches some value depending on the slope of this graph.

Now this same kind of a segment of appears on this side okay, which is related to the velocity behaviour shown here, now let us just explain in a few lines what is the reason that effective mass is changing well this is related to the fact of the changing velocity, you are applying a force and at some point the velocity beyond some point the velocity is not increasing what does it mean?

The mass has become infinite, if the mass is very large a force cannot give rise to any acceleration and so therefore it does not change a velocity now that is what is happening here, so the velocity reaching a peak and not changing in this small region amounts to infinite effective mass, so the velocity increasing at a decreasing rate here in this region is because the effective mass is going on increasing.

So your force is constant the mass is going on increasing so the amount of increase in velocity is going on decreasing, so that is how it is and very interestingly the effective mass is negative for electrons near the top of the band in fact it is this behaviour near the top of the allowed band for electrons which involves a velocity against a direction of the force and negative mass it is this feature which responsible for treating electrons close to the top of the band has positively charged carriers or holes.

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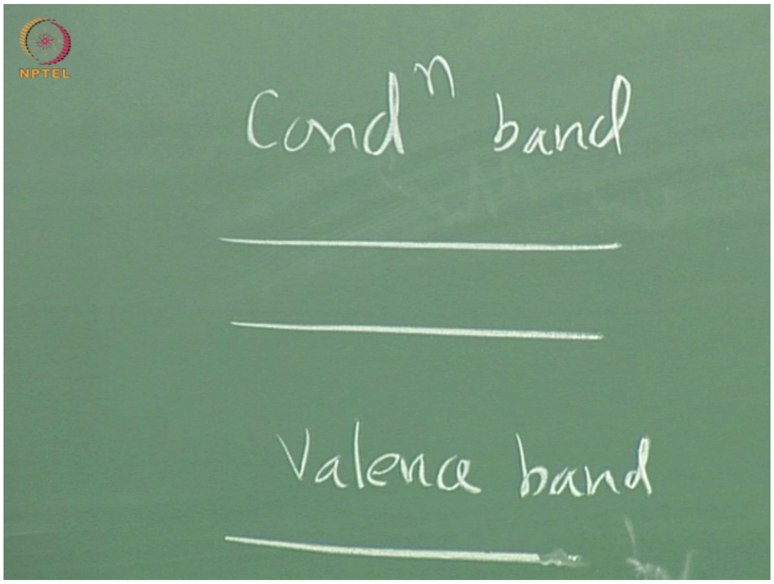

That is why electrons in the top of the allowed band in the valence band, so this is the valence band and this is the conduction band right, so while electrons near the bottom of the conduction band can be treated as equivalent to free carriers but with a different mass, the electrons at the top of the valence band will be treated in terms of a positively charged carrier right, because the electrons are moving in the direction opposite to that of the force.

And this is origin of the concept of holes you want to know more about it you can read books here we would like to move on to other aspects of band diagram which are used in practice to analyze devices.

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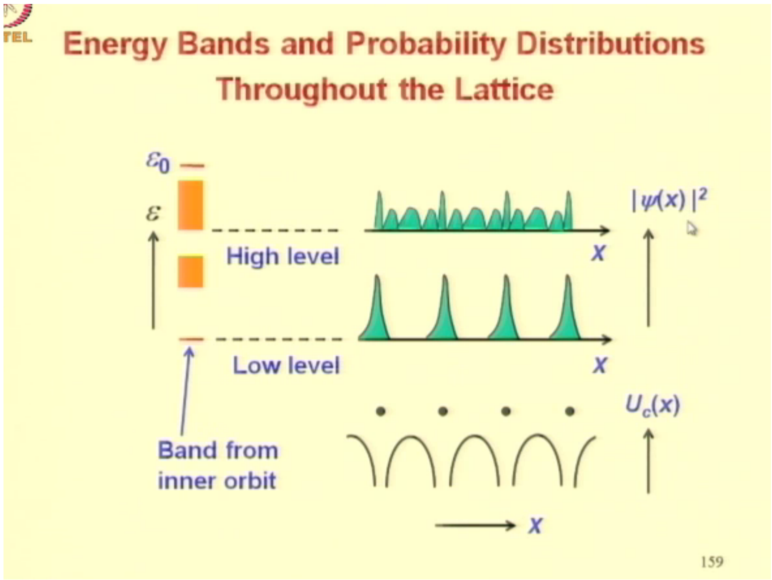

Energy Bands and Probability Distributions Throughout the Lattice

Now let us look at the probability distributions of the electrons throughout the lattice and relationship of this distribution with energy bands, so here we are plotting the wave function psi magnitude square okay, now this wave function is solved for from the Schrodinger equation, in the previous lecture we have shown some example of psi x that has been solved from somewhat realistic crystal potential right.

Now these are the kind of calculation which are represented here except that here we are plotting the square of the wave function because we want to talk about the probability, now if you take an energy level corresponding to a band from inner orbit that is this is the crystal potential and if you take an electron very close to the atom atomic core this energy level corresponds to that kind of a situation.

Now for this energy level the associated wave function give rise to this kind of probability distribution, where what you find is the distribution is reaching a peak at the location of atom and it rapidly decays to 0, so what is the meaning of this, this means the electron can be found either over here or over here or over here and so on, this means that electron is really bound to the atom localized.

On the other hand, if you take the wave function corresponding to high energy such as the one in a band which is corresponding to an electron far away from the atom then you find the square of the wave function exists all over the space and met with different amplitudes, so even here there is a greater chance of the electron coming near the atom, however there is a very good chance of electron been found elsewhere to.

And therefore the implication of this is that your electron can be moving about in the crystal, now that is why electrons in the conduction band are assumed to be freely moving about in the crystal, whereas electrons in the valence band or in other lower bands are assumed to be localized to one of the atoms in the crystal.

We shall now move on to the quantitative model of the E-X diagram that is the allowed energy levels as a function of distance.

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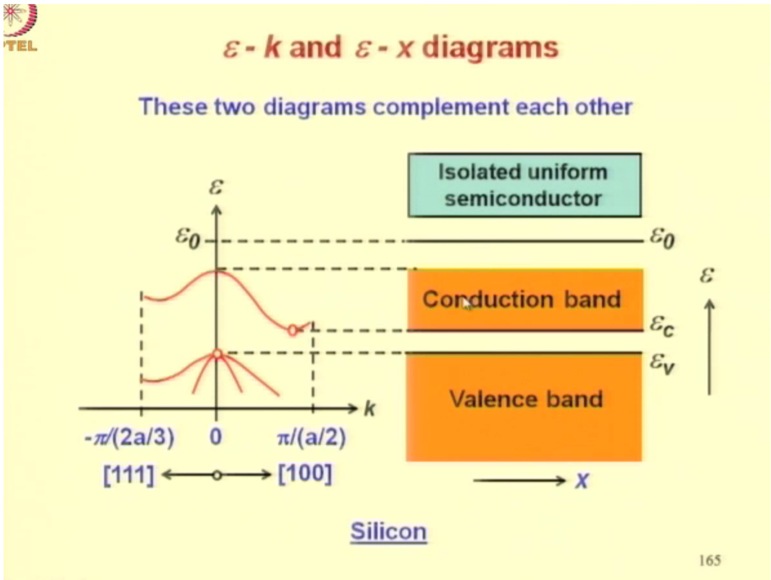

ε - k and ε - x diagrams

These two diagrams complement each other

Silicon

Now let us show how the E-X diagram arises from the E K diagram, so let us put them together because these 2 diagrams complement each other, now for example this is an E-K diagram of silicon that we had shown in previous lecture, now if you consider an isolated uniform semiconductor word isolated means that semiconductor is not subjected to any electric fields okay or any fields.

And conditions in semiconductor are uniform that is what it is meaning by uniform semiconductor, doping is uniform, composition uniform, temperature uniform and so on, now in such a case we can draw the allowed energies for electrons as a function of distance as shown in this diagram okay, so here the minimum point of the E-K diagram is the energy level corresponding to this is the presented as E C this is the conduction band.

And the maximum energy of the lower over band that is valence band is indicated as E V and these 2 levels are constant with x because the semiconductor is uniform right and there are no applied electric fields, now the top of the conduction band actually emerges from this point on the E-K diagram you also show the vacuum level E0 in the E-X diagram even this level is constant.

So what it means is the allowed energy level picture for electrons in an isolated uniform semiconductor is constant with X that is what is represented here, now we know that in practice the semiconductor will have some non-uniformity it can have P and N regions, it can have junctions the composition may change one part of the semiconductor maybe silicon, the other part maybe gallium arsenide and so on.

And then you will apply electric field in order for the device in order to make the device work.

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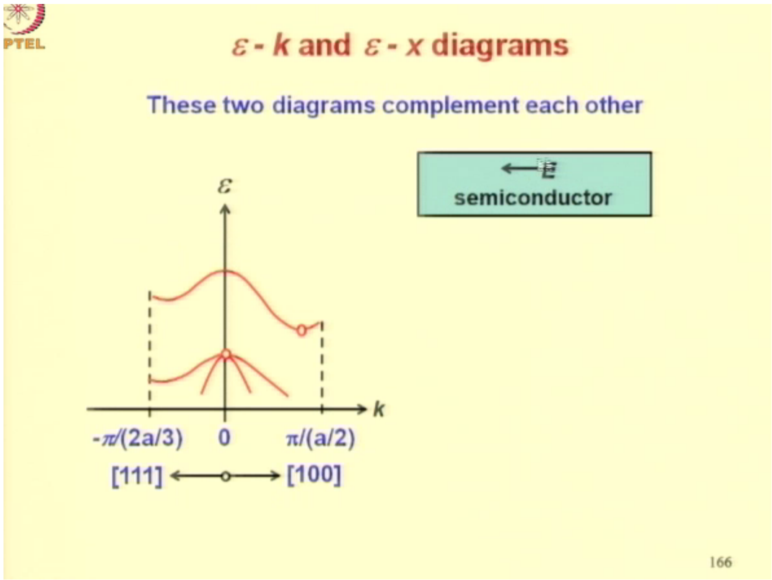

ε - k and ε - x diagrams

These two diagrams complement each other

And therefore situation is going to be something like this, so let us say this is semiconductor which is uniform in all respects except that an electric field is applied.

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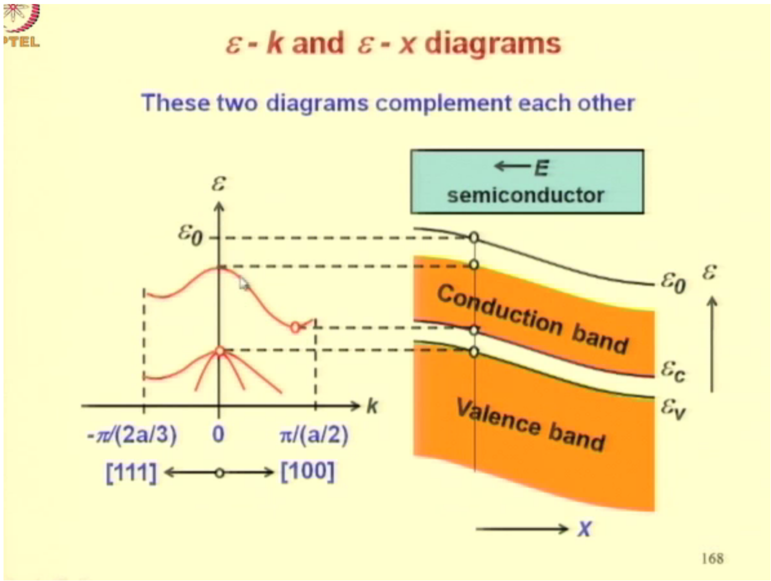

ε - k and ε - x diagrams

These two diagrams complement each other

Now in this case the bands bend are shown here, so the lines E0, E C and E V are no more constant with X, so the semiconductor at this end is more positive compared to this end because the electric field is from right to left, so at the right end your electron energies are over because this diagram shows increasing in electron energies moving upwards, so as a function of x your electron energies are decreasing right from left to right in correspondence to the direction of the electric field.

Now how do you find out the slope of the lines and so on is what we are going to discuss, now also I would like to mention here that we are not shown all the levels that are used in an energy band diagram to analyze devices, for example the diagram shown here does not indicate fermi level which is a very, very important energy level used in the analysis, now those are the levels which we are going to add on to this diagram.

And we are going to discuss how can we calculate the various features of this energy versus X diagram, now let us see the correspondence between this E-X diagram and the E-K diagram here, so the E-K diagram shown here corresponds to the energy level picture at any particular X, when you applying electric field for every X the E-K picture will be similar to this however the values of energies will change with distance.

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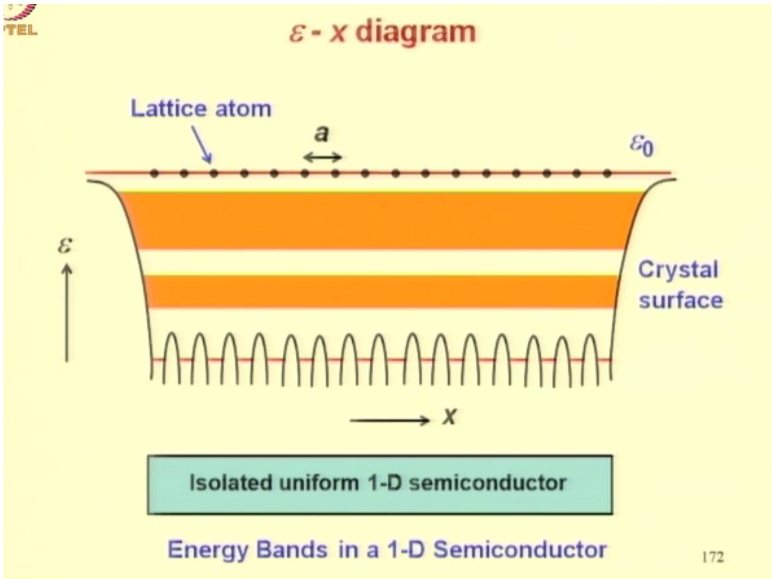

Now let us place the E-X diagram in context of the crystal potential to improve our understanding of the various bands and various energy levels okay, now this is crystal potential a very very large number of atoms here we will consider an idealized one-dimensional situation and this is crystal surface where the potential goes up to the so-called vacuum level okay, when you come out of the semiconductor here,

So the surface is here and when you come out of the semiconductor very rapidly the potential rises to the vacuum level when you go inside because of the atoms the potentials are low and it is periodic something like this, so these are the locations of the various atoms in our 1-dimensional idealized semiconductor a being the interatomic distance, so you find that the atom is located somewhere in between the 2 peaks in fact exactly in between the 2 peaks here.

Now in this crystal potential picture this is the vacuum level E0 and these are the allowed band of energies, now the orange bands are the allowed energy bands and in between you have the energy gap here, similarly this is an energy gap here, there is an energy gap here to, this line here shows that the width of the band is very, very thin, now this is true for electrons which are close to the atom, okay.

So the lower bands will all be very thin in width because electrons are tightly bound, now the potential energy of the crystal has been changed to the energy of the electrons in this diagram okay in this axis here, now this is a conduction band, there is a band gap, this is a valence band and you again have a band gap.

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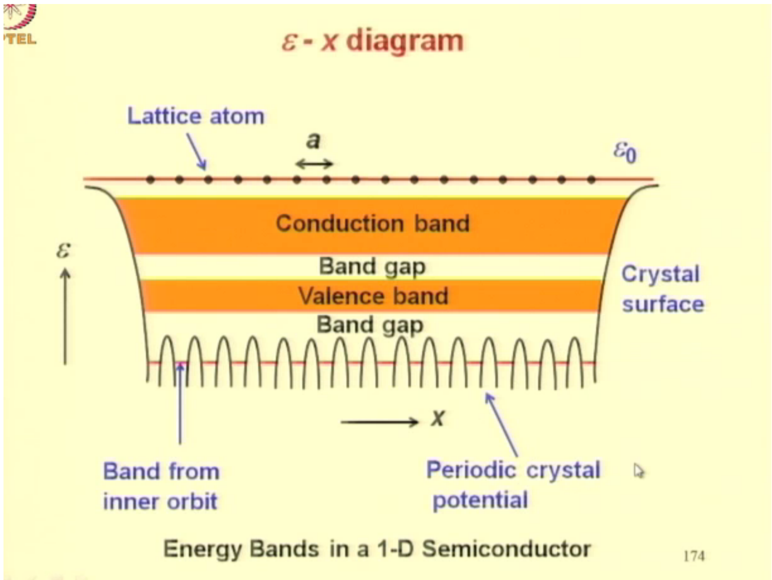
ε - x diagram



Energy Bands in a 1-D Semiconductor

This is the band from inner orbit and this is the periodic crystal potential.

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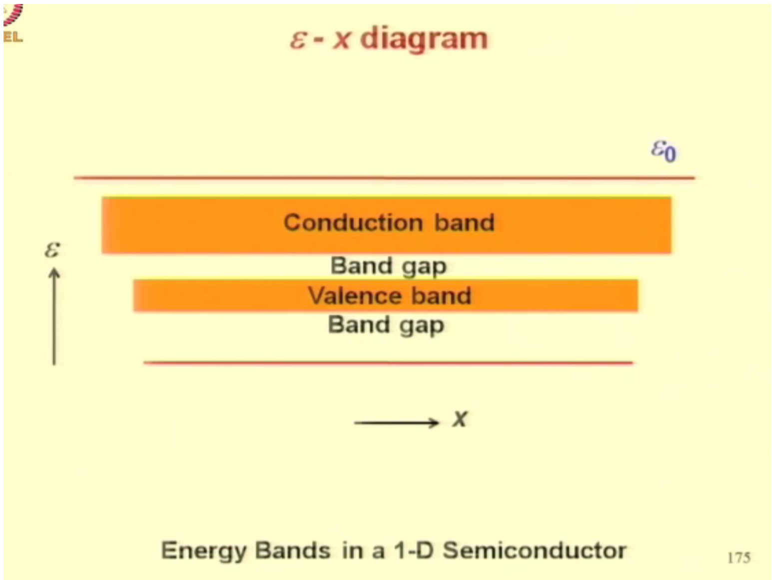

ε - x diagram

Energy Bands in a 1-D Semiconductor

Normally, we do not show all these details so we remove the crystal potential, further we do not show bands other than the conduction band and valence band and the band gap, even further we do not show the bands but we show only the levels which correspond to the bottom of the conduction band that is EC and top of the valence band that is EV and in addition the vacuum level E0.

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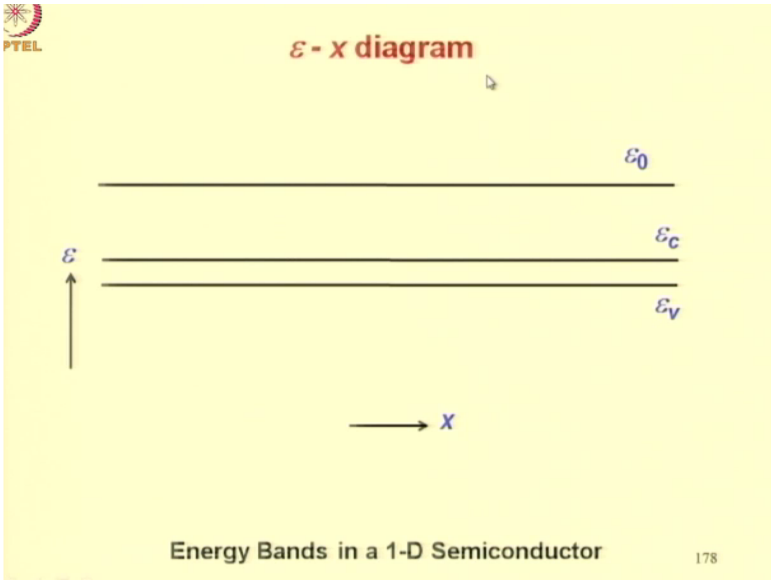

ε - x diagram

Energy Bands in a 1-D Semiconductor

So this is really the picture that we work with normally okay, however the set of slides that we should just now should clarify the meaning of these levels because when you look at them in the context of the crystal potential things become very clear.

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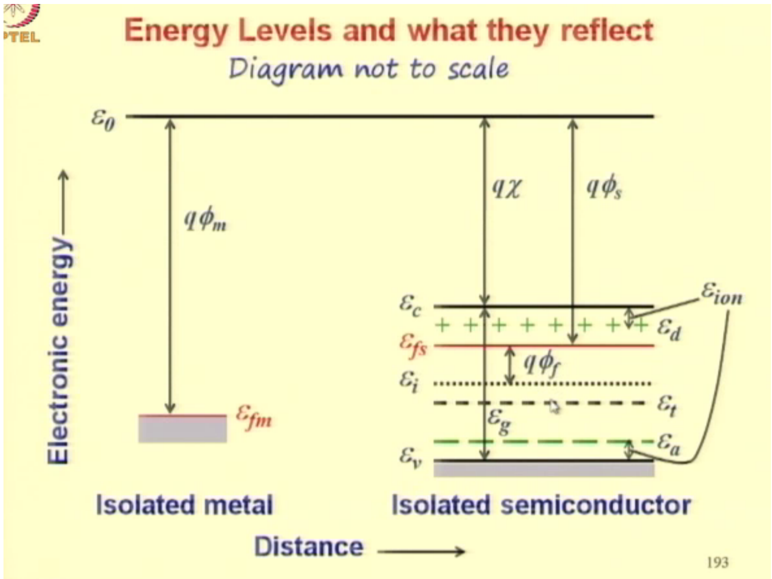

Energy Levels and what they reflect

Diagram not to scale

Let us discuss the meanings of the various energy levels, now we have come across energy band picture in the first level course, so what we are now going to do is really a review a quick review, so that we can quickly move on to discussing the methods of finding out the energy as a function of x how do you calculate okay.

The energy as a function of x and how do you use the energy band diagram to get information about electron and hole concentration, the carrier current densities and electric field and potential, so that is what we are really going to discuss, so quick review plotting electronic energy versus distance in an isolated semiconductor you show the levels EV, EC, E0 and in addition here I have added the fermi level suffix s stands for semiconductor.

So the semiconductor is isolated and we are seeing that this uniform to, therefore all these levels are just horizontal, the distance between EC and EV is called the energy gap represented as E suffix g the distance between E0 and EC is referred to as electron affinity, normally represented using the symbol chi, so chi is really the potential in dimensions and therefore q times chi is the electron affinity energy.

The difference between E0 and Ef is the work function, so phi suffixes s stands for semiconductor give you the symbol phi for work function, so phi s is potential and q times phi s is the work function in terms of energy dimensions, now compare this diagram of the semiconductor with that of an isolated metal, now here you have the fermi level alone shown because you have overlapping bands right.

So you do not have anything like a conduction band edge and valence band edge shown here, you only show the fermi level now all the electrons most of the electrons occupy levels below the fermi level, now here most of the electrons are in the valence band in a semiconductor that is what the shaded region shows shaded region here too, the difference between E0 and E f is the work function, the work function in metal is shown as phi suffix m, q times phi suffix m is the energy.

Let us locate the donor level in the semiconductor it is located close to the conduction band edge we are talking about those donors which change the resistivity that is the shallow donor's, you can have a donor level far away from the conduction band edge also but we are talking about donor's which modified the resistivity therefore the donor level is close to the conduction band edge, similarly the acceptor level which changes resistivity is shown close to the valence band edge.

Now this distance EC – Ed and Ea – EV these distances or differences are referred to as ionization energies of the impurities, because when a donor gets ionized it becomes positively charged and the amount of energy required to ionized donor is equal to this gap that is shown here that is why this is ionization energy.

Similarly, in an acceptor case ionized it accepts an electron from the valence band the energy required for this process is this difference that is why this is called ionization energy, this is a level associated with trap which can be an impurity or it could be a defect in the crystal many of the defects which affect the transient response of the semiconductor or lifetime they are near the middle of the energy gap.

That is why this trap level is shown near the middle of the energy gap, it does not mean that you have a single level in practice you may have multiple levels located in many places throughout the energy gap, now this is the intrinsic level which is very close to the middle of the energy gap the distance between the fermi level and intrinsic level is normally represented by symbol phi suffix f, f stands for fermi energy, phi f is potential and q phi f is energy.

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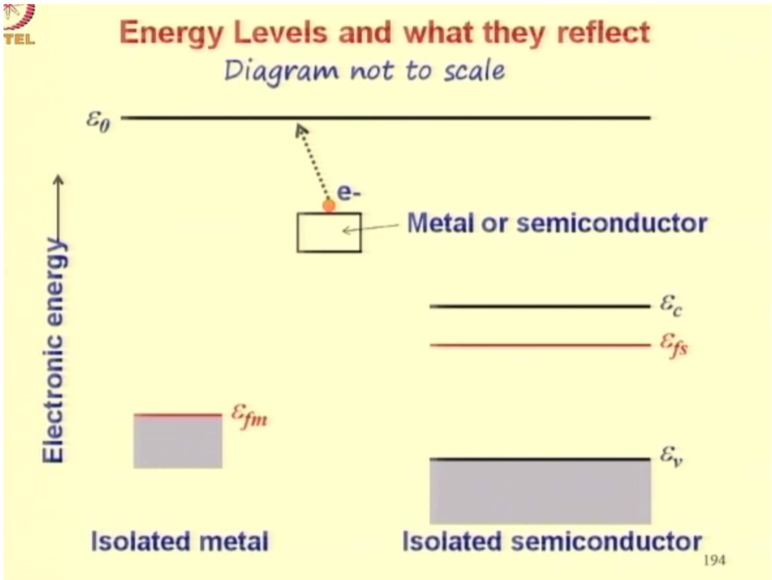

Energy Levels and what they reflect

Diagram not to scale

Now what is the vacuum level indicate the vacuum level is normally referred to as local vacuum level in the context of semiconductors,

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Local vacuum level

Local vacuum level right, the word local is important although normally this word is skipped why because it refers to an electron which is localized on the surface of the metal or semiconductor right, so it is not an electron that is removed for away from the semiconductor when you use a vacuum level in the context of an isolated atom you refer to vacuum level as energy level corresponds to an electron which is removed far away from the atom okay.

So taken into infinity whereas when you come to the context of semiconductors you talk about vacuum level as energy of an electron that is outside the volume of the metal or semiconductor but touching the surface so localized on the surface that is why we must use the word local, so energy of this electron is what is represented by E0 we will shortly see why we use a localized vacuum level right, it will reflect all the built-in potentials inside the semiconductor this point we will see later.

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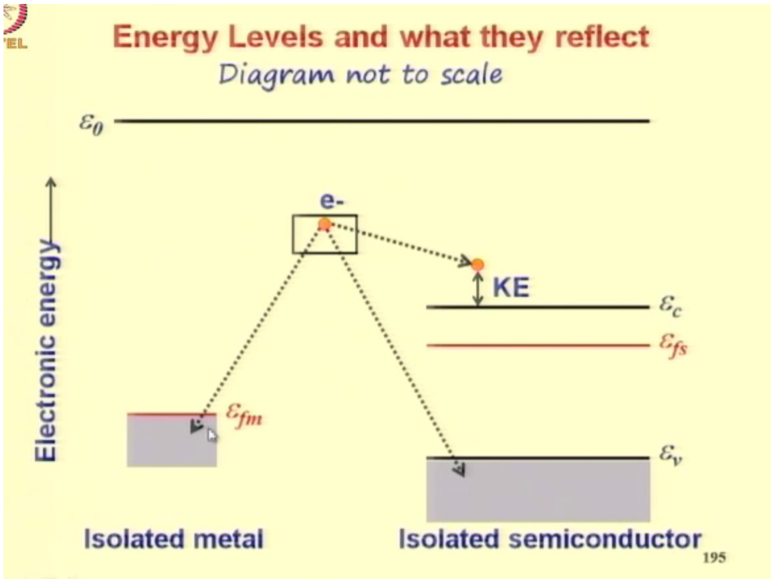

Energy Levels and what they reflect

Diagram not to scale

Now if the same electron is inside the semiconductor volume then it could be located or it can have energies any of these locations such as the conduction band, the valence band or in a metal it would lie somewhere here, the difference between the energy of the electron and EC is the kinetic energy of the electron, so EC is the potential energy of an electron a conduction electron an electron that freely moves about in the crystal that is the conduction electron.

So the energy of conduction electrons minus the energy EC which is the potential energy of conduction electron this is the kinetic energy.

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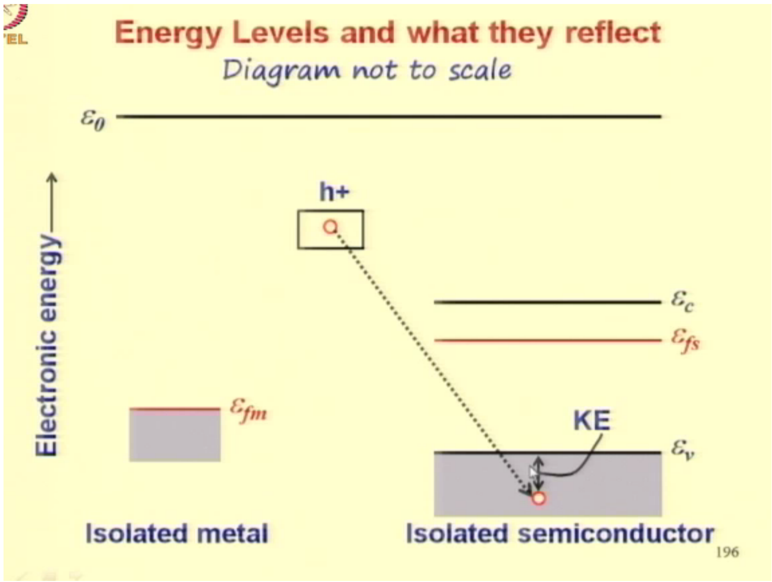

Energy Levels and what they reflect

Diagram not to scale

As a case this if you have a hole in a semiconductor you will not have a hole in metal in a semiconductor you have a hole than the EV minus the energy of the hole is the kinetic energy because EV is a potential energy of a hole.

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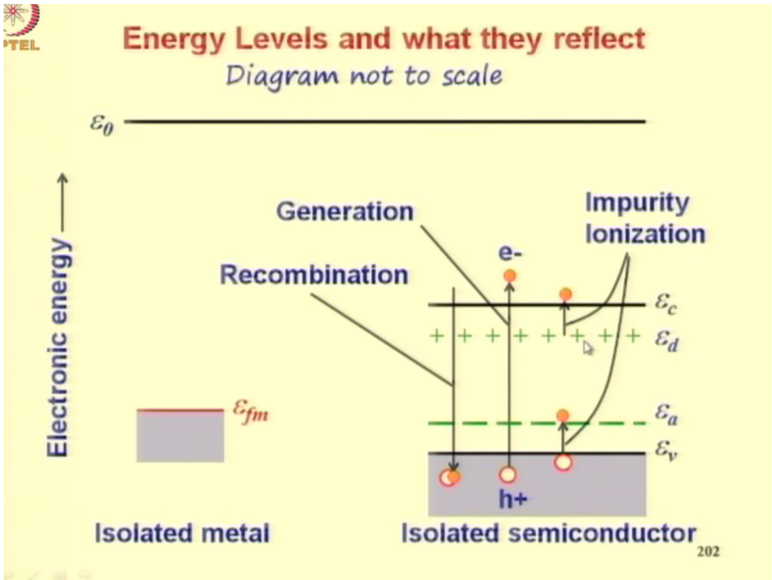

Energy Levels and what they reflect

Diagram not to scale

Now let us introduced the donor and acceptor levels and talk about a few energies in semiconductor rather few other processes on the energy band picture to see what this energy level reflect, if you want to show the generation process then this is it an electron jumping from the valence band to conduction band leaving behind a hole creation of an electron hole pair that is what the generation process.

So the electron is anywhere in the valence band and it jumps to anywhere in the conduction band, now the process that is most likely however is the one for which the energy is minimum, however in general for generation process the energy can be greater than energy gap also, the recombination is exactly its inverse an electron jumping into a hole, electron in the conduction band conduction to a hole in the valence band.

Impurity ionization an electron jumping from donor level to conduction band or an electron jumping from valence band to acceptor level right, so here a hole is created please note a hole is created here, but there is no free electron because electron is localized near the acceptor impurity, so the ionization of an acceptor impurity creates a hole which is free to move about in the crystal but the electron gets bound at the acceptor impurities side.

On the other hand the ionization of the donor impurity creates a free electron and leaves behind a positive charge that is why the positive charges shown here near a donor level now this positive charge is however not a hole because it is localized near the donor atom and so it cannot move about that is why it is not a hole it is a positive charge, similarly the acceptor levels, the acceptor level correspond to acceptor atoms its indicated as a negative sign because when a acceptor gets ionized it has a negative sign.

Now with that we have come to the end of this lecture, let us make a summary of the important points, now in this lecture we have first discussed the utility of the E-K diagram and shown how the E-K diagram can be used to estimate the effective mass, the velocity or the group velocity and the momentum or the crystal momentum of a carrier of any given energy this information is useful in analyzing the motion of electrons in a crystal electrons or holes in a crystal.

It is also useful to discuss the interaction of electrons and holes with other entities like impurities phonons, photons and so on where the momentum conservation principles can be applied, then we began a discussion of the E-X diagram okay, we showed how the E-X diagram and E-K diagram are complementary, the E-X diagram tells you the variation of the allowed energy that is the function of distance.

Whereas the E-K diagram tells you at any given location in the semiconductor what is the relation between the energy of the carrier and its momentum, so both these diagrams are very important and any of this diagram by itself does not give the complete information, then we try to understand the various levels that are used to represent an E-X diagram.

We saw what is the meaning of these levels and how some of the processes that are happening in semiconductor which has generation, recombination, impurity ionization and so on are represented on this energy band picture. In the next class we shall discuss methods of estimating these E-X diagram for various situations and various types of semiconductors and devices.