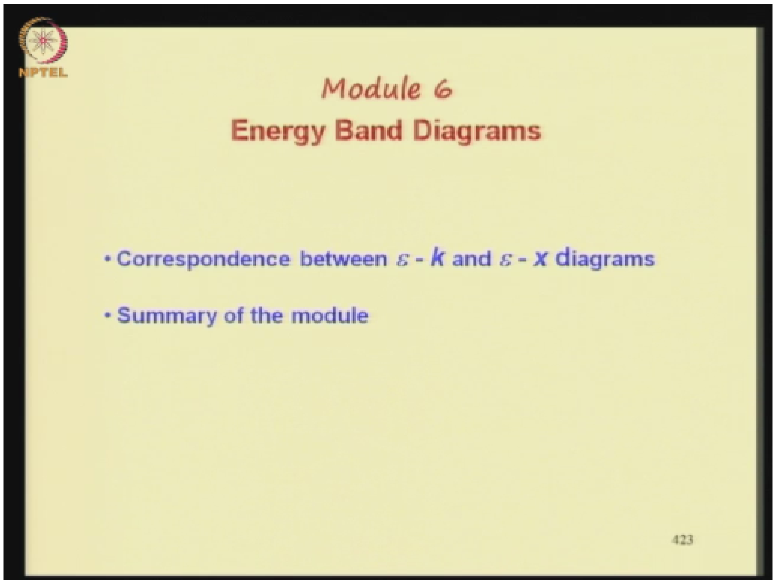
Semiconductor Device Modeling
Prof. Shreepad Karmalkar
Department of Electrical Engineering
Indian Institute of Technology – Madras

Lecture - 33
Energy Band Diagrams

In the previous lecture, we discussed the ex-diagrams of heterojunction under equilibrium. A p-n junction under high forward bias and 2 dimensional band diagrams then we also showed how the band diagram can be used as a tool for analysis of PN Junction or deriving information about full concentration, electron concentration, electron current density, hole current density, potential and electric field apart from representing a known distribution of electrons holes, JN, JP, psi and p.

In this lecture, we shall discuss the correspondence between e-k and e-x diagrams.

(Refer Slide Time: 01:01)



Module 6

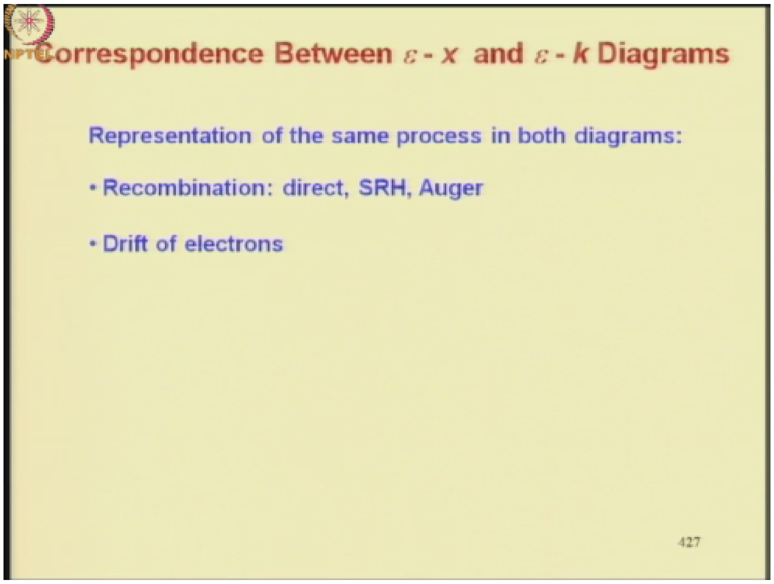
Energy Band Diagrams

- Correspondence between ε - k and ε - x diagrams
- Summary of the module

423

And then we shall summarize the important points of the entire module.

(Refer Slide Time: 01:14)



Correspondence Between ε - x and ε - k Diagrams

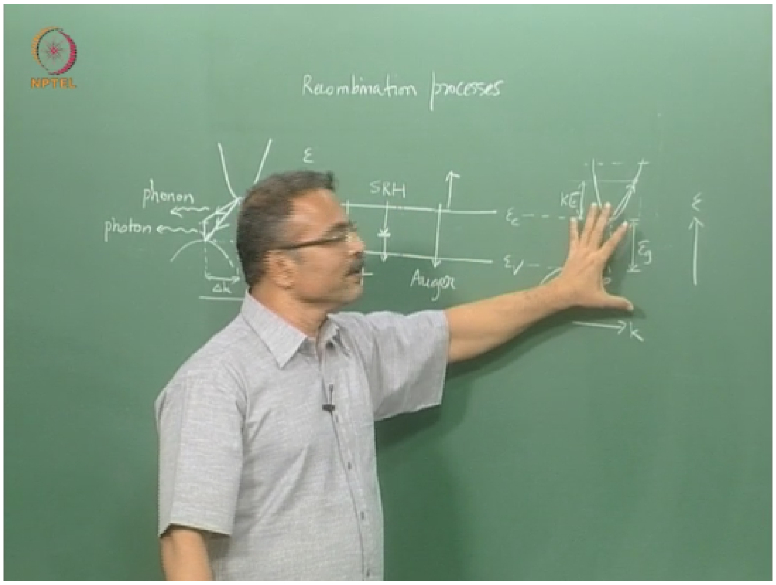
Representation of the same process in both diagrams:

- Recombination: direct, SRH, Auger
- Drift of electrons

Let us consider correspondence between e-x and e-k diagrams. Now, we shall discuss the topic by representing the same process in both diagrams the processes we shall consider would be recombination. 3 different types of recombination namely direct, SRH and Auger. I will leave it as an assignment to the student to show on the e-x and e-k diagram the corresponding generation process.

And then we shall show how drift of electrons can be represented on e-x and e-k diagrams. Let us show the recombination phenomena.

(Refer Slide Time: 02:06)



So this vertical axis is e and the horizontal axis is k. So, this is the e-k diagram. Let us show the recombination phenomena assuming a uniform semiconductor. So, this means that conduction bandage and balance bandage this will be drawn as flat lines. So, this is as a function of x. So, this is your e-k diagram and this is your e-x diagram we are considering an indirect band gap of semiconductor like silicon.

Supposing I want to show a direct recombination something like this on the e-k diagram it would look like this. This means the electron undergoes a change in energy equal to energy gap and at the same time it undergoes a change in momentum, crystal momentum represented by delta K. So, actual change in momentum, crystal momentum would be x cross delta K. Supposing I want to show SRH recombination.

So the electrons fall into a trap and then it falls into the balance band. Now how would that look? It would look something like this. So suppose this is the trap level at the same energy level. S, trap level to balance band H is a vertical transition and this is a non-vertical transition. So, in this transition electron is going a change in energy as well as crystal momentum. Therefor particle emitted as a result of this process.

So that is the particle that will take away the energy and momentum of the electron when the electron falls from here to here would be a phonon. On the other hand, if this transition there is insignificant momentum change there is only an energy change and therefore the particle which will take away this energy would be a photon. Let us show one more process that is the Auger recombination.

So, in this an electron falls from the conduction to balance band directly and its energy and momentum is taken away by let us say a free electron. You can also have a hole taking away the energy, you can draw the process on the e-k diagram in the same way as I will do for the case when the energy and momentum of the recombining electron is taken away by an electron rather than a whole.

So, in order to avoid clutter this, diagram I will draw the e-k diagram on this side and show this process on that e-k diagram. So, this process is represented by this arrow is energy and this is the wave vector. And this process is represented by an electron changing its state in the conduction band say something like this. So, this is the momentum change delta K for the recombining electron and energy change is Eg.

Now it may not be possibly to find a conduction electron whose energy and momentum relation is exactly given by this easy versus delta key. That is if I consider an electron which will take away the energy Eg the momentum of that electron may not be exactly = delta K because it all depends on the effective mass or curvature of this diagram. If I really want to know what will be the momentum of the electron that has an energy easy.

I should take this energy interval and place it here and draw a line like this and then I will get this point and this difference would be the momentum of this conduction electron which is taking away the energy and momentum of this recombine electron. So, this momentum change may be exactly be equal to this momentum change and therefore you really want to have conservation of energy and momentum. There should be another particle some phonon.

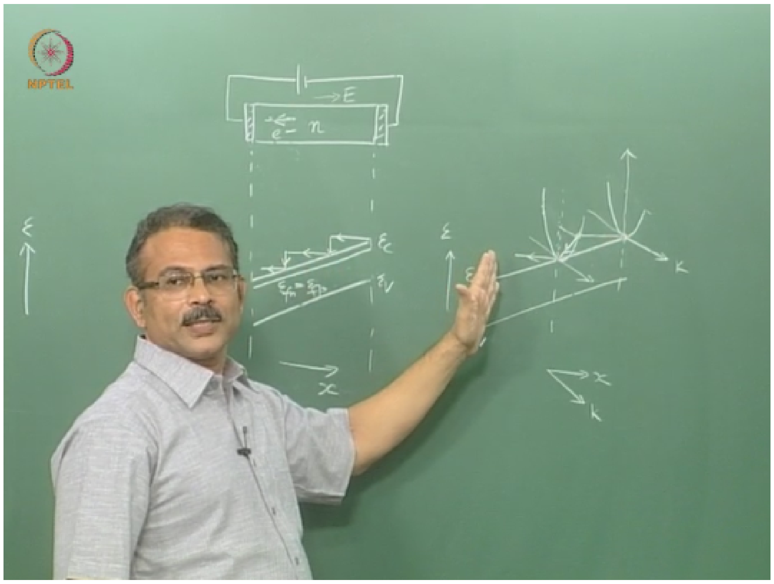
For example, which may take away the remaining energy and momentum. However, this electron will take away most of the energy and momentum therefore it has been shown using this particular transition where this energy is little less than the energy gap. So this the kinetic energy of the electron which is taking away the energy and momentum of the recombining electron. This kinetic energy has been shown a little less than Eg.

Because the momentum of this electron is not same as delta K in fact it is less than delta K therefore we should allow some third particle to take away the momentum and therefore it will have its energy also. You cannot have a particle which has only momentum and no energy. So therefore it can be a photon, it can be phonon. Now, even a photon is possible in which case it will take away the energy but it will not have any momentum.

So, that would be a transition. I take this delta K and put this delta K and put this delta K here and take the energy corresponds to the delta K I will get some energy. If that energy turns out to be less than Eg then the remaining energy can be taken away by photon. However, if the curvature of the E-K diagram is such that energy is more than the Eg then such a thing is not possible.

In other words, in that particular case material the auger recombination cannot release a photon so this is how you decide what kind of particles will be involved in recombination from drawing the recombination process in both the Ex and Ek diagram. So, Ex diagram will only give you energy changes whereas Ek diagram will give you both momentum and energy changes. Now, let us show the drift process on Ex and Ek diagrams.

(Refer Slide Time: 09:50)



So you have a semiconductor like this let us assume a uniform semiconductor to which a voltage has been applied and you want to show the drift process here. Semiconductor may be anti for p type. Let us say it is n type. Now if you show the process only on EX diagram it would look like this. So, this side is positive so you are conduction bandage and balance bandage would be something like this. We have drawn this Band diagram in one of the earlier lectures.

Uniform semiconductor a bias has been applied. This would be the so called quasi-Fermi levels. Efn = Efb because this is n type this is close to Ec but right now this Fermi level is really not important for us. So if I want now to show the motion of an electron that is drifting from the negative contact to positive contact. So, this is the direction of motion of electron. Now whatever I show for electron you can show a similar thing for holes yourself.

So, an electron will be starting from let us say here it will travel some distance and then it will encounter collision or scattering so its momentum will get randomized, velocity will get randomized. It will again start and then scatter and so on so this is the path of the electron on an EX diagram. So, between 2 collisions its energy remains constant. But its potential energy is decreasing so potential energy is being converted into kinetic energy.

So the difference between the electron and the conduction bandage indicates the kinetic energy. So, its kinetic energy is going on increasing. Its velocity is going on increasing because the electron the accelerating in response to an electric field which is there in this sample, in this direction. Now, how do you show this process on EK diagram also. Now in this case I will have to draw an EK diagram for each position x because EK diagram will vary with x.

So, how do we do that? So let me repeat this diagram here so this is your ex so this direction is x. Now, let us assume that I used this axis to show the K vector. Let us assume a simple EK relation and this axis is any way energy so if I for example draw an EK diagram at say this point it would look something like this. So, this is your k. This is your EK relation so it is being drawn in this direction so it is really perpendicular to the board.

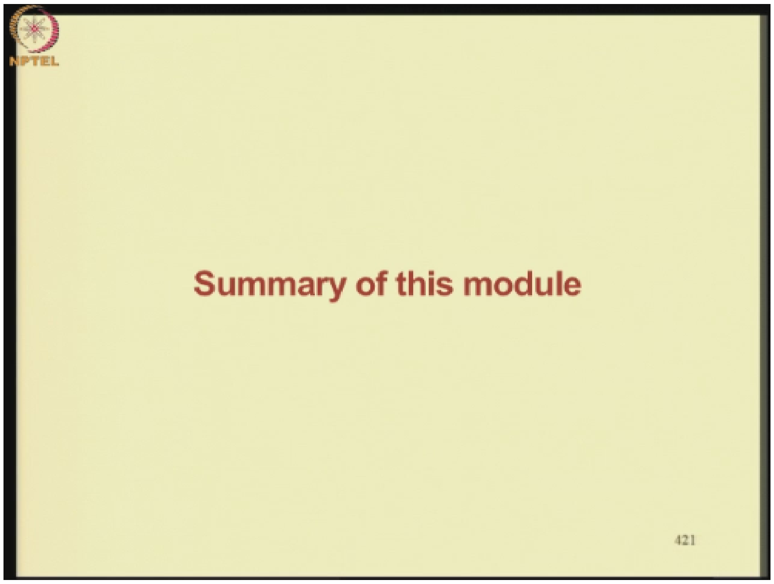
This is what you should imagine. So in the surface of the board is x direction. This k direction is perpendicular to the board and so EK is drawn like this. Now at another point if I want to draw EK here it would be the similar EK diagram I should draw here. So this is the EK relation. Now, an electron starts from here and it moves in this direction so this part when I want to show it on EK diagram also then it is moving like this.

At each point you can draw an EK diagram. So as it is gaining energy it is gaining momentum as well. So, you can see here that this difference is the momentum. This is the line corresponding to the zero momentum. This is k =0. So, this distance on this diagram represents the momentum that the electron has gained when it comes here at this x. And when it is getting scattered it is falling down.

So on the EK diagram that transition can be shown something like this. Its momentum is getting randomized it comes back to the bottom of the conduction band that is Ec. And then it starts again so I can repeat this process. So, I will have to draw another EK diagram to show the next. So, this is how the electron moves on the EK diagram when EK diagram is varying with x that is what is happening in the drift phenomena.

So, it is very important to visualize processes in both Ex and EK diagrams that gives you a lot of insight. So, in the case of recombination phenomena for example what kind of particles will be involved when electron combines with a hole? What kind of mechanism are possible depending on the material such thing can be understood from the representation of the process on both E x and EK diagrams.

(Refer Slide Time: 15:59)

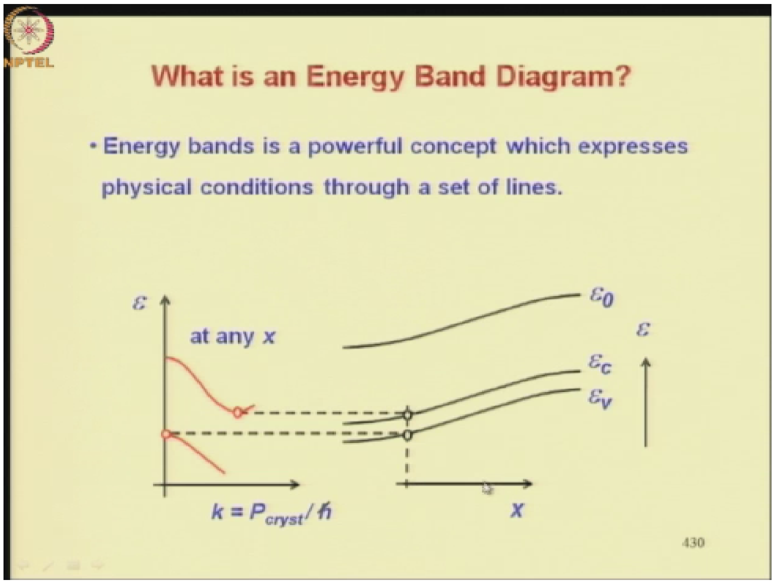


Summary of this module

421

Now let us begin a summary of the entire module. We started this module by answering the question what is an energy band diagram?

(Refer Slide Time: 16:07)



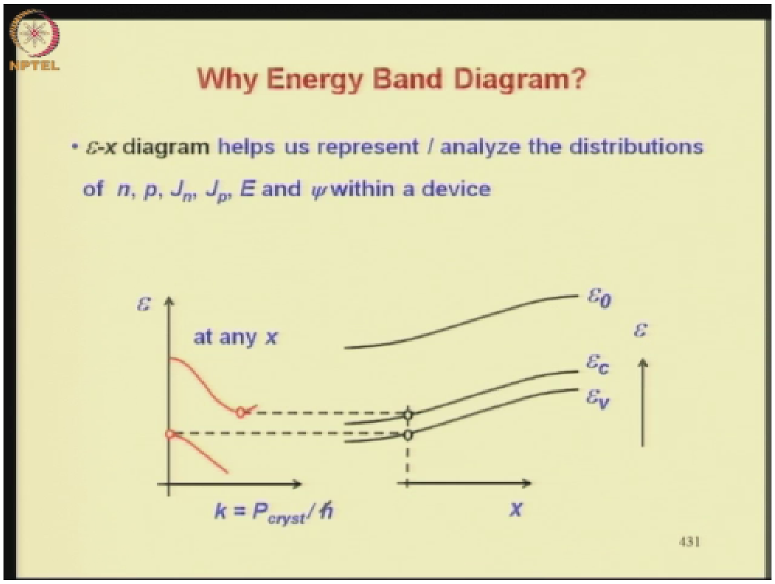
What is an Energy Band Diagram?

- Energy bands is a powerful concept which expresses physical conditions through a set of lines.

So, we said energy band is a powerful concept which expresses physical conditions through a set of lines. So, the set of lines where something like this so the diagram has 2 parts e versus x as well as versus k. Here we have shown a 1 dimensional picture essentially e versus x means e versus space. And similarly E versus k here in 3 dimensions it would mean e versus kx, ky, kz. So, there is a correspondence between the EK diagram and the EX diagram.

So if the energy levels are varying with x then the EK diagram shows you the energy momentum relation at any x. These 2 diagrams EK and Ex are complementary so together they represent in totality the information. So each part has only partial information.

(Refer Slide Time: 17:13)



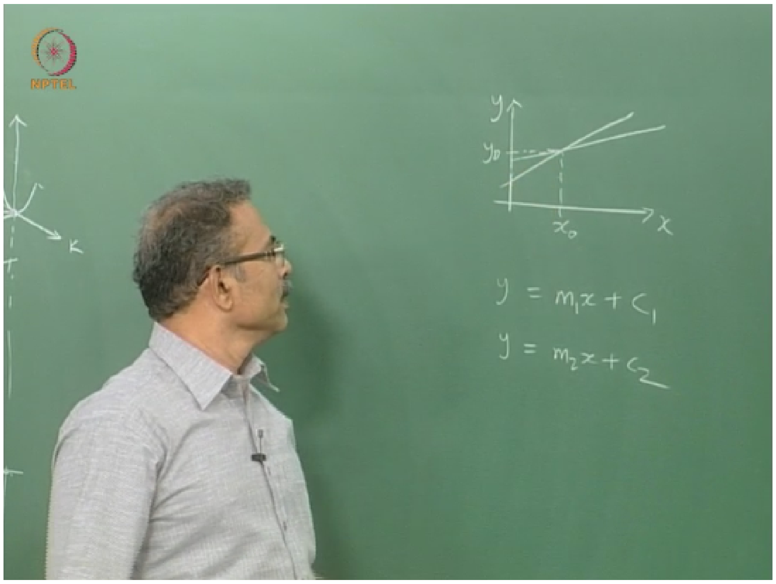
Why Energy Band Diagram?

- ε-x diagram helps us represent / analyze the distributions of n, p, J_n, J_p, E and ψ within a device

Why energy band diagram? So, we said and we in fact demonstrated that EX diagram helps us to represent or analyze to it is both a representation tool and analysis tool. So it helps us represent and analyze the distribution of n, p, Jn, Jp, E and psi within a device. So, in analogy to any graph the energy band diagram is both a representation and a problem solving tool. So you know that any graph is both a representation and a problem solving tool.

For example, let us take this equation I can use graph as a representation tool to represent this equation it would be something like this.

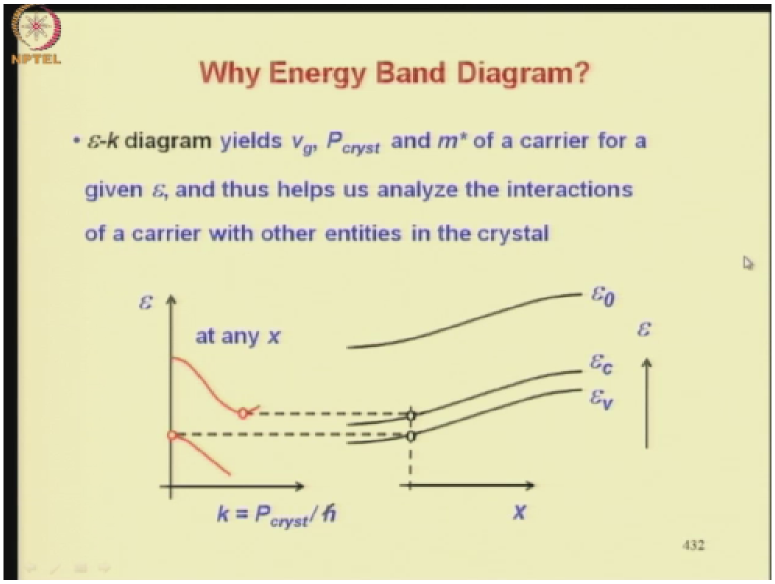
(Refer Slide Time: 17:46)



So this is y and this is x. Let me give an example where graph is used as a problem solving tool supposing I have 2 equation y = m1x+c1 and y = m2x+c2 and I want to solve this 2 equation simultaneously that is get the values of y and x which satisfies both equations. Now, you can do it solely by algebraic manipulation or you can do graphically. So what do I do I represent this line on the graph which is this one and I represent this line also on the graph.

So, may be it is something like this and then the point of intersection is actually the solution of these 2 equations. So, this x0, y0 is the solution. So this is how you have used graph as a problem solving tool. So, energy band diagram is also a graph it can be used both as a represent tool or problem solving tool.

(Refer Slide Time: 19:00)

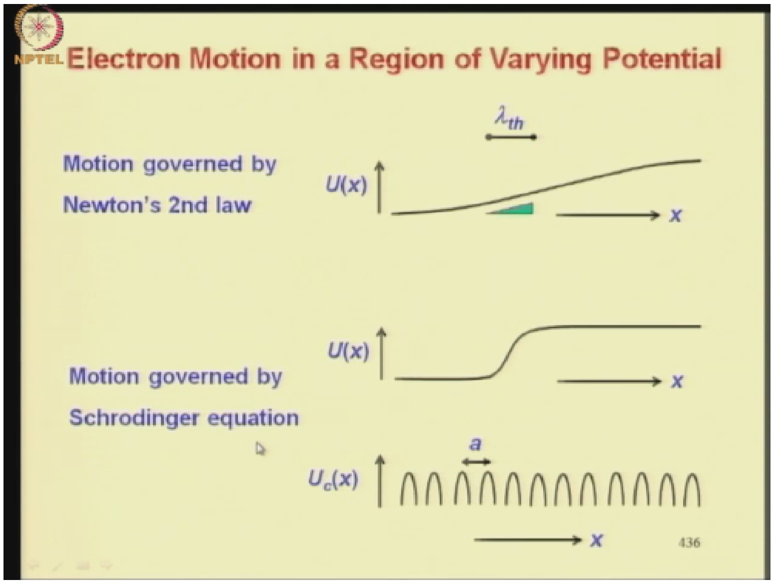


Why Energy Band Diagram?

- ε-k diagram yields v_g, P_{cryst} and m^* of a carrier for a given ε, and thus helps us analyze the interactions of a carrier with other entities in the crystal

The E-K diagram yields the group velocity, the crystal momentum and effective mass of a carrier for a given energy and this helps up analyze the interactions of a carrier with other entities in the crystal.

(Refer Slide Time: 19:17)



Electron Motion in a Region of Varying Potential

Motion governed by Newton's 2nd law

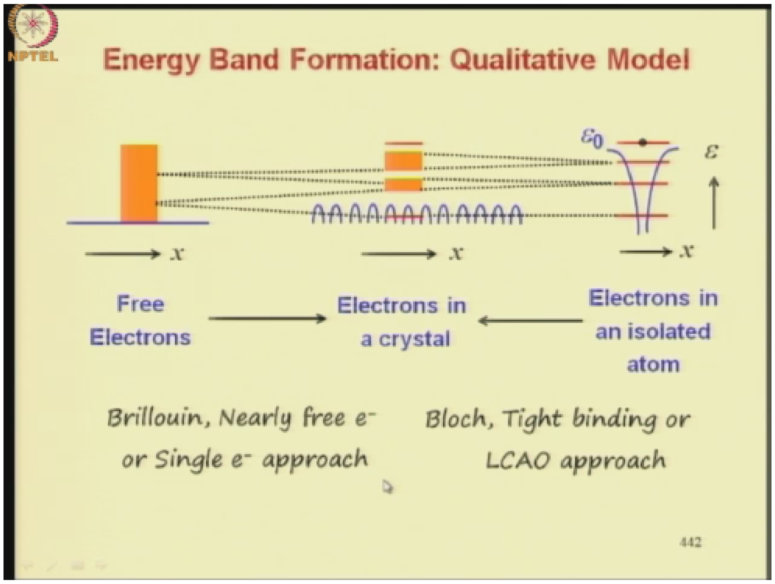
Motion governed by Schrodinger equation

Electron motion in a region of varying potential so, we said by considering different variation of the potential the following. If the potential varies slowly over a length scale of de Broglie wavelength of the electron. Thermal average de Broglie wavelength, lambda thermal. So, this is a slow variation then the motion of the electron is governed by Newton’s second law. On the other hand, if it varies rapidly over the same length scale.

So you can see the length over which the variation is occurring here is smaller than lambda thermal. So, another example of that is the crystal potential where there are rapid periodic variations in the potential if you see the length scale a, it is much less than lambda thermal, a is the distance between 2 consecutive atoms.

Then in both this cases the motion is governed by Schrodinger equation and that is why to analyze the motion of an electron in a crystal we must start from the Schrodinger equation.

(Refer Slide Time: 20:27)



Energy Band Formation: Qualitative Model

Free Electrons → Electrons in a crystal ← Electrons in an isolated atom

Brillouin, Nearly free e^- or Single e^- approach

Bloch, Tight binding or LCAO approach

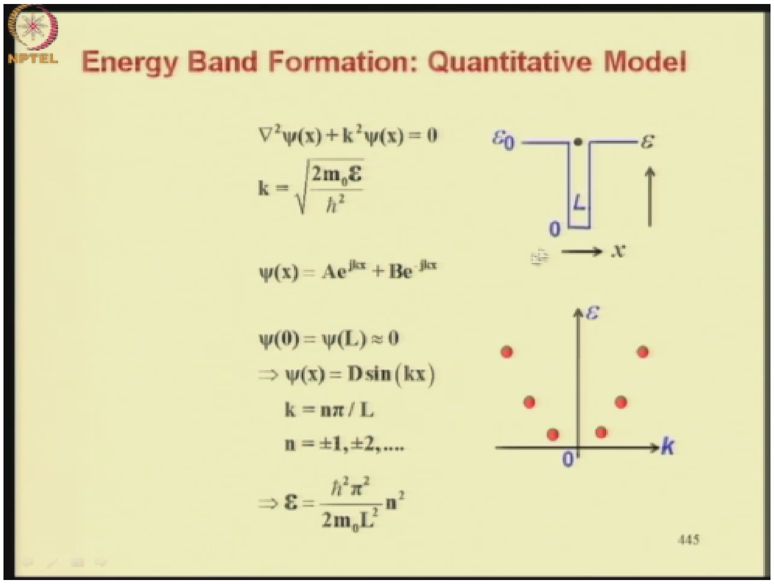
Then we discuss energy band formation. So, first we gave a qualitative model which region as follows. Electron in an isolated atom are in a potential well so this is a potential well corresponding to a single atom. And then you can put together many atoms in which case your potential variation will look something like this. So, same potential variations when you superpose for a large number of atoms placed very close to each other would look something like this.

So, for the isolated atom the energy levels will be discreet something like this where as for electron in a crystal each level spreads into a band of energies. Band of allowed energies separated by band of energies which are not allowed so forbidden energies. This splitting of an energy level or splitting of an energy level into a band can be visualized as consequence of Pauli Exclusion Principle in which or according to which no 2 electrons in a system can have the same energy.

So when you put a large number of atoms together, all the electrons cannot have the same energy which they had when the atoms were isolated. So therefore they have developed different energies and since there are so many electrons their energies are very close to each other and so the allowed energies becomes a band. This approach of developing the allowed energy bands from discreet levels of isolated atoms is referred to as the bloch, tight binding or Linear combination of atomic orbitals approach.

You can have an alternate approach in which you develop, the development of forbidden energy bands rather than allowed energy bands from the picture of free electrons in which all the energies are allowed for the free electrons. So from a continuous band of allowed energies you are developing forbidden bands. This approach is referred to as Brillouin, nearly free electron or single electron approach.

(Refer Slide Time: 22:58)



Energy Band Formation: Quantitative Model

$$\nabla^2\psi(x) + k^2\psi(x) = 0$$

$$k = \sqrt{\frac{2m_0\mathcal{E}}{\hbar^2}}$$

$$\psi(x) = Ae^{jkx} + Be^{-jkx}$$

$$\psi(0) = \psi(L) \approx 0$$

$$\Rightarrow \psi(x) = D\sin(kx)$$

$$k = n\pi / L$$

$$n = \pm1, \pm2, ...$$

$$\Rightarrow \mathcal{E} = \frac{\hbar^2\pi^2}{2m_0L^2}n^2$$

Then we considered a quantitative modal of energy band formation. So simplify calculations and analysis we approximated the actual potential picture. So for an isolated atom we assume that the potential well is rectangular of width L and then we showed that if you solve the energies for the electrons from Schrodinger equation you get this kind of EK relation. So, the equations used were as follows.

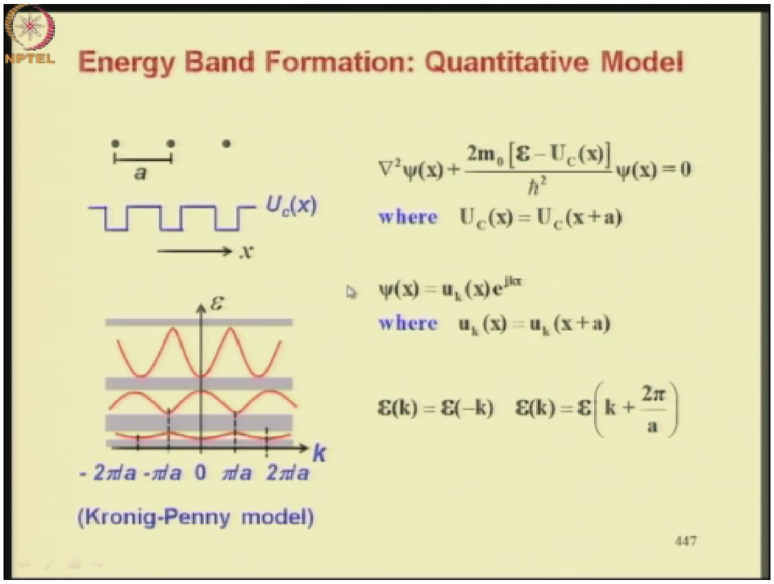
So, this is a Schrodinger equation which depends only on the space we have removed the time dependent time part because this is how we solved the Schrodinger equation. Where this k is related to the electronic energy the solution of this equation is as shown here consists of a combination of 2 complex exponentials. And if you impose a boundary condition corresponding to a rectangular well.

So this is actually Schrodinger equation written for a constant potential region. And that constant potential has been assumed to be zero and the fact that at the boundary x =0 and x = L. The potential energy goes to infinity here it is show to be going to E0. In practice this E0 this vertical height is very, very large so we can assume it to be approximately infinity in which case the wave function goes to 0 at both x = 0 and x = L.

So, that is why we assume the boundary conditions to be wave function going to approximately zero, assuming an infinite potential well. Putting this boundary conditions on this equation the solution is a sine or cosine function and the k here therefore becomes discretized according to this formula where n = =/- 1, 2 and so on. Now the same information has been represented graphically here.

So, these are different values of k and if you put these values of k in this formula you get this relation between e and other parameters of the situation. So, these are the energies. So discretization of k which is a consequence of the boundary condition that wave function goes to zero at both these ends.

(Refer Slide Time: 25:57)



Energy Band Formation: Quantitative Model

$$\nabla^2\psi(x)+\frac{2m_0\left[\mathcal{E}-U_C(x)\right]}{\hbar^2}\psi(x)=0$$

where $U_C(x)=U_C(x+a)$

$$\psi(x)=u_k(x)e^{jkx}$$

where $u_k(x)=u_k(x+a)$

$$\mathcal{E}(k)=\mathcal{E}(-k)\quad \mathcal{E}(k)=\mathcal{E}\left(k+\frac{2\pi}{a}\right)$$

(Kronig-Penny model)

447

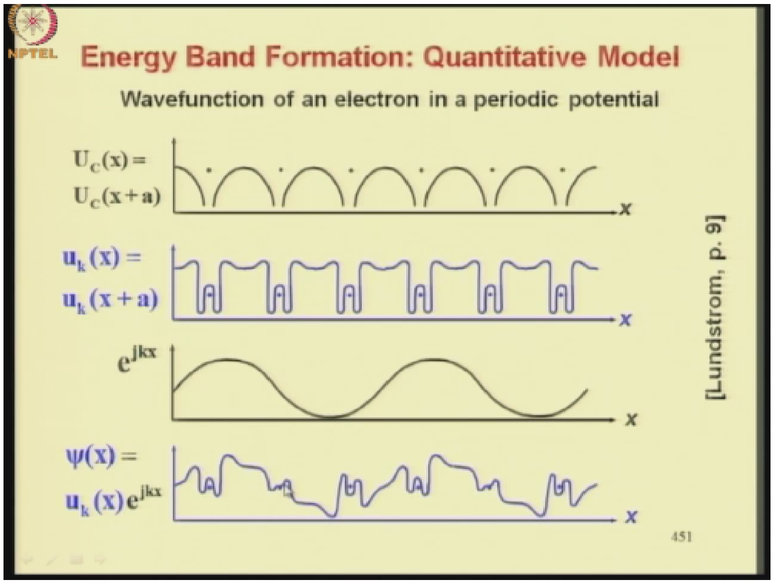
We adopted a similar approach for a periodic potential and in this case we showed that the EK relation is considerably more complex then what we showed here. The differences being instead of allowed energies discreet energies you have allowed bands. Secondly, the EK relation is periodic. Here it is a point here EK relation is periodic with a period = 2 pi/a and third for every value of k you have many values of energy.

So the EK relation is a multivalued function of k. Whereas here for any given value of k you have only one energy. Now, these kind of features where a consequence of the Schrodinger equation of this particular situation so Schrodinger equation is written in this form where Uc is the crystal potential. Again for quantitative modeling we assume rectangular kind of shape for the periodic potential.

So that the analysis become simple so U c x is periodic with a period = a, which is the interatomic distance. So we consider a 1 dimensional crystal where all atoms are arranged in 1 dimension only. According to Bloch's theorem for this kind of Schrodinger equation the solution psi x is of the form Ukx into e to the power j, k, x. So, the e power jkx type of solution for constant potential gets modulated by a Bloch's function UkX where this function has the same periodicity as the crystal potential.

The consequence of this kind of situation is that the EK relation is even. So E of k = E of –k. We argued why this should be so and further E of k is periodic. With period 2 pi/a so both these are consequences of this kind of a solution of the Schrodinger equation for period crystal potential.

(Refer Slide Time: 28:13)



Energy Band Formation: Quantitative Model

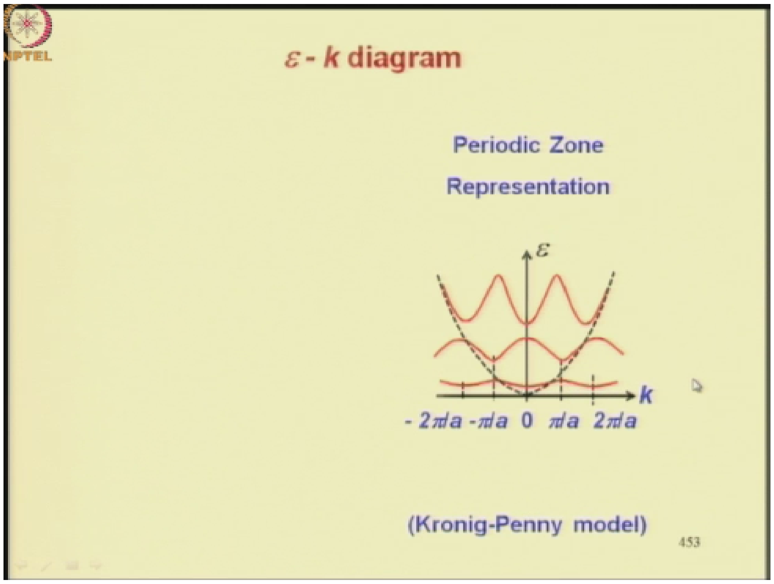
Wavefunction of an electron in a periodic potential

[Lundstrom, p. 9]

We gave an example of a wave function for a periodic crystal potential how it looks? So, in this example, Ucx was show something like this and the Bloch's way had this kind of a shape this is just to give you a feel for how the wave function looks like for period crystal potential and this is the exponential the complex exponential we can take as real or imaginary part. And the wave function is obtained by multiplying this e power jkx with the modulating function Uk of x.

So these are functions when you multiply these 2 you get a function like this. So you see the wave function of an electron in a periodic crystal potential is fairly complex.

(Refer Slide Time: 29:06)



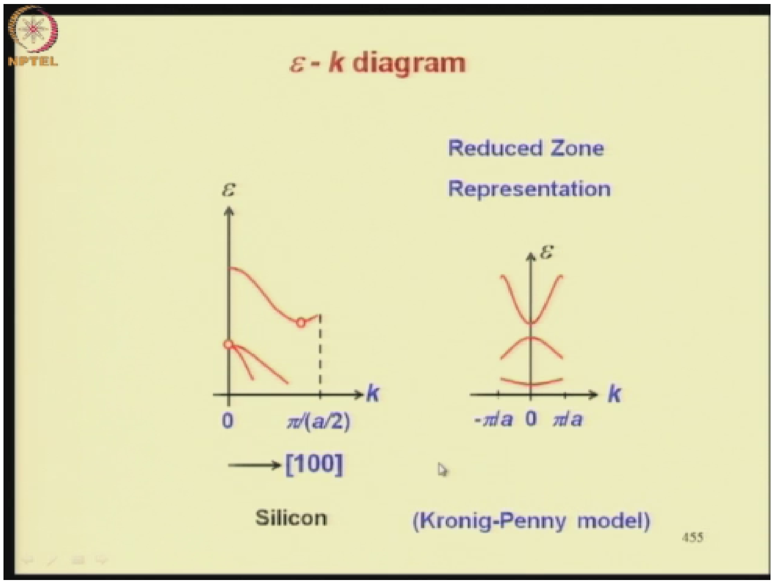
ε - k diagram

Periodic Zone Representation

(Kronig-Penny model)

Then we discussed features of E-k diagram. This form of representation of E-k diagram is referred to as period zone representation. So you see that the E-k relation is being shown for several periods even though it is periodic and you can probably show that information only in one of the periods and then the same thing will apply to other periods.

(Refer Slide Time: 29:35)



ε - k diagram

Reduced Zone Representation

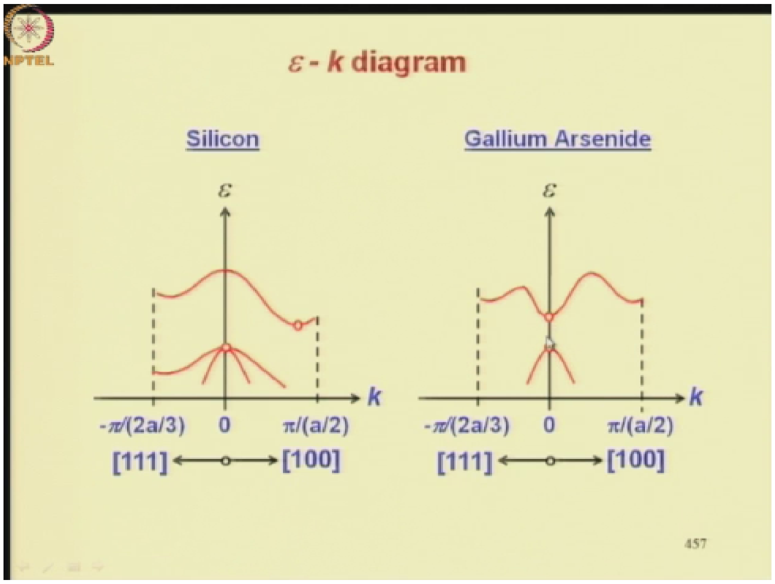
Silicon

(Kronig-Penny model)

That is why you come up with the reduced zone representation where you show just one period from -pi a to+pi/a further if here also the function is even you can even restrict the information to just zero to pi/a because the same thing reflected on the region 0 to -pi/a. So, in fact this is the kind of thing that is used to show E-k diagrams of real semiconductors which are more complex.

For example, here for silicon in the 100 direction the E-k diagram looks something like this the bottom of the conduction band and top of the balance band are not at the same value of K. In contrast to the situation in the Kronig-Penny model or the simple 1 dimensional case with rectangular potentials. You can use the other half to represent the E-k relation in another direction. So this way you can make a compact representation of a lot of information on the same graph.

(Refer Slide Time: 30:41)



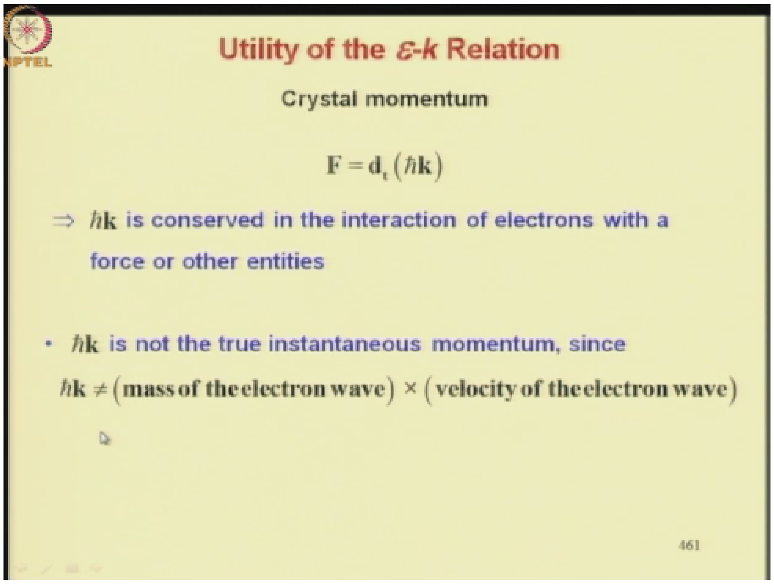
ε - k diagram

So, in fact that I what is done. So another crystal axis is 111, so the E-k diagram in that direction is shown on this side evidently this is different from this. So, for example you can see that the difference between the bottom of the conduction band and top of the balance band which is the energy gap on 111 side is more than that on the 100 side. So, you will find the E-k diagram for silicon to be shown mostly on the 100 side.

Or you will find in the analysis this particular part of the diagram being shown often because it is the smallest energy gap that is of interest. For Gallium Arsenide the E-k diagram is different from silicon in that the bottom of the conduction band is right above the top of the balance band. So, there is direct band gap semiconductor whereas here an electron jumping from conduction to balance band will undergo a change in energy as well as momentum.

And therefore more likely transition is that electron jumps into an intermediate level first and then jumps into a balance band. So, it makes an indirect transition that is more likely therefore this is called an indirect band gap semiconductor. Here however the electron in the conduction band can jump directly into the balance band.

(Refer Slide Time: 32:15)



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

Crystal momentum

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

⇒ $\hbar\mathbf{k}$ is conserved in the interaction of electrons with a force or other entities

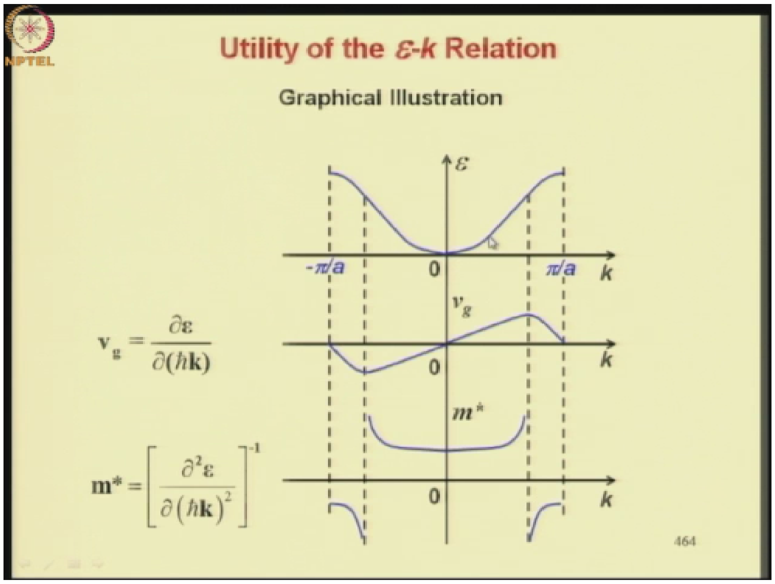
- $\hbar\mathbf{k}$ is not the true instantaneous momentum, since

$$\hbar\mathbf{k} \neq \left(\text{mass of the electron wave}\right) \times \left(\text{velocity of the electron wave}\right)$$

The utility of E-k relation we pointed out that the E-k relation can be used to get crystal momentum because the force on electron in a crystal is equal to the time derivative of the product h cross K. So, this implies hk is conserved in the interaction of electron with a force or other entities and that is the reason why it is called a momentum namely the crystal momentum. However, it is not the true instantaneous momentum.

Since the true instantaneous momentum is mass of the electron multiplied by velocity of the electron. But we have shown that h cross k is not of this form. Therefor it should not be regarded as true instantaneous momentum.

(Refer Slide Time: 33:01)



Utility of the ε-k Relation

Graphical Illustration

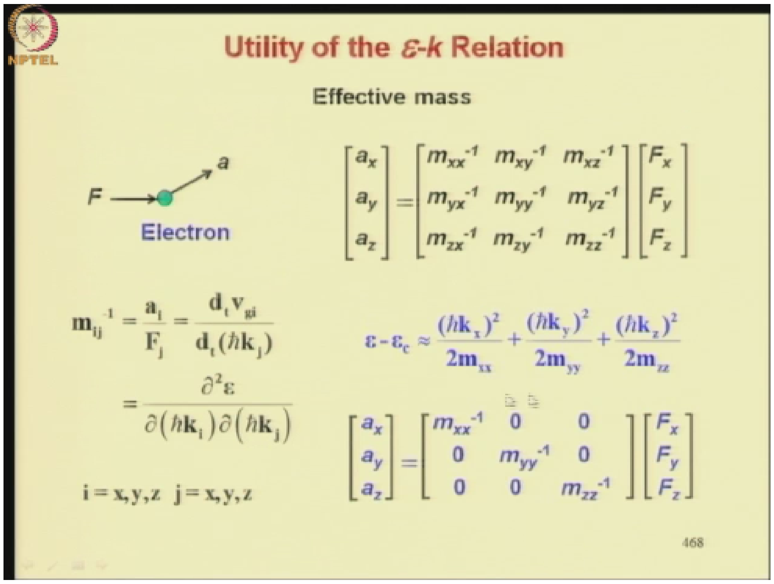
$$v_g = \frac{\partial \varepsilon}{\partial(\hbar \mathbf{k})}$$

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

You can use the E-k relation to derive quantities such as if I differentiate the E-k relation then I can get the group velocity. So this is a typical E-k relation and it give you a group velocity something like this. We showed what is the meaning of this kind of a variation of the group velocity. If you double differentiate the E-k relation and take a reciprocal you get the effective mass. So for this E-k relation your effective mass picture is something as shown here.

So, if I restrict myself to a small region around this point here then this E-k relation will be approximately a parabola and therefore its double derivative will be constant and that is the origin of, the use of a constant effective mass in many cases so long as the energy of the electron does not become very high, kinetic energy of the electron does not become very high. So, for this point the kinetic energy is zero and its kinetic energy as it increases it moves up, electron moves up on this E-k diagram.

(Refer Slide Time: 34:11)



Utility of the ε-k Relation

Effective mass

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

$$\mathbf{m}_{ij}^{-1} = \frac{\mathbf{a}_i}{\mathbf{F}_j} = \frac{d_t \mathbf{v}_{gi}}{d_t(\hbar \mathbf{k}_j)} = \frac{\partial^2 \varepsilon}{\partial(\hbar \mathbf{k}_i)\partial(\hbar \mathbf{k}_j)}$$

$$\mathrm{i} = \mathrm{x,y,z} \quad \mathrm{j} = \mathrm{x,y,z}$$

$$\varepsilon - \varepsilon_c \approx \frac{(\hbar \mathbf{k}_x)^2}{2\mathbf{m}_{xx}} + \frac{(\hbar \mathbf{k}_y)^2}{2\mathbf{m}_{yy}} + \frac{(\hbar \mathbf{k}_z)^2}{2\mathbf{m}_{zz}}$$

$$\begin{bmatrix} a_x \\ a_y \\ a_z \end{bmatrix} = \begin{bmatrix} m_{xx}^{-1} & 0 & 0 \\ 0 & m_{yy}^{-1} & 0 \\ 0 & 0 & m_{zz}^{-1} \end{bmatrix} \begin{bmatrix} F_x \\ F_y \\ F_z \end{bmatrix}$$

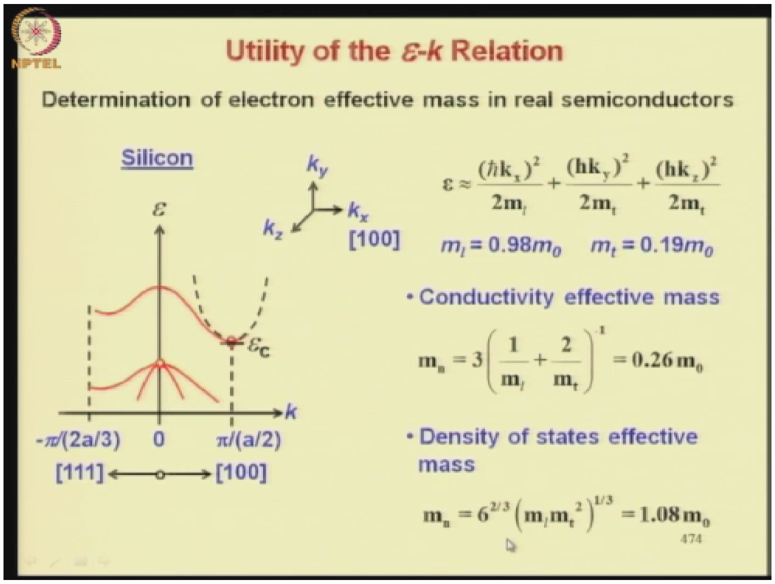
Now the effective mass is actually a tensor because in a crystal the acceleration experienced by the electron is not in the same line as the force so the acceleration and force are non-collinear. So, therefore you have this kind of relation between acceleration and force and you get a matrix representation of effective mass. You can determine each element of matrix using a formula like this so if I want mij where i and j can be x, y, z.

So mij reciprocal of this is equal to acceleration by the force. The acceleration is in the i direction and this acceleration in i direction is response to a force in j direction. Then you can write this as d/dt of Vgi/dt of h cross k in the j direction. Because acceleration is time derivative of the group velocity and force is time derivative of the crystal momentum and then simplifying this formula result in a formula.

Like this dou square e/dou of h cross ki into dou of h cross kj that is the reciprocal effective mass, mij. Now very often we assume that the E-k relation is paraboloid in 3 dimensions. It is parabolic in one dimension and in such a case what happens is you have only the diagonal terms of the effective mass matrix mxx, myy and mzz other terms become 0. This can be easily seen by applying this formula for this kind of a situation.

So, apply this formula for this parabolic relation and you will end up getting this fact.

(Refer Slide Time: 36:08)



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

Determination of electron effective mass in real semiconductors

$$\varepsilon \approx \frac{(\hbar k_x)^2}{2m_l} + \frac{(hk_y)^2}{2m_t} + \frac{(hk_z)^2}{2m_t}$$

$m_l = 0.98m_0$ $m_t = 0.19m_0$

- Conductivity effective mass

$$m_n = 3\left(\frac{1}{m_l} + \frac{2}{m_t}\right)^{-1} = 0.26\,m_0$$

- Density of states effective mass

$$m_n = 6^{2/3}\left(m_l m_t^2\right)^{1/3} = 1.08\,m_0$$

In real semiconductors how are the effective masses determined, real semiconductors are 3 dimensional. So you have kx, ky, and kz all 3 dimensions to be considered. For the case of silicon, the 100 direction is very important because the energy gap corresponds to the energy gap of the E-k relation in this direction. Let us assume that kx is 100 and if you represent the E-k relation of the electron in the conduction band.

As a paraboloid assuming the bottom of the conduction band to be origin here. So, this point is origin so therefore the left hand side becomes simple it is simply e. The effective mass term coming here is referred to as longitudinal because it is in the direction of principle axis 100, kx. Ky and Kz are transversed to this axis therefore the effective mass terms coming here are represented by the symbol mt. So, this is transverse, so transfers to this.

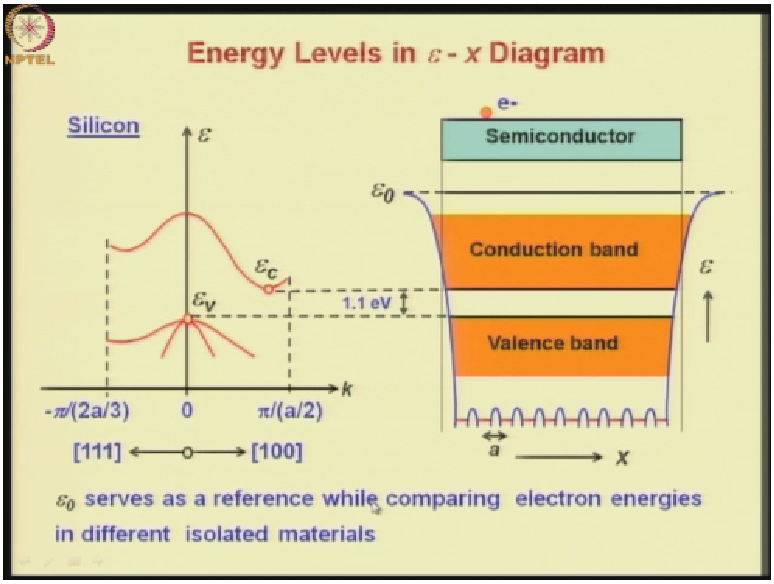
Where kx is assumed to be the principle 100 direction. Now, we have put the same mt for both these terms ky and kz terms because it turns out that the shape of parabolic for silicon is such that the curvature in ky and kz directions are identical. It turns out that ml is 0.98 times the mass of electrons in vacuum and mt is 0.19 mass of electron in vacuum and from this ml and mt you can determine effective masses for different situations.

2 situations are conductivity and density of states. So a conductive effect mass is obtained by averaging the conductivity in x, y and z directions. And the result of this is an equation mn = 3

times 1/ml+2/mt reciprocal. So, this is kind of a harmonic mean of ml, mt in the other 2 directions. That is why the factor 2. So, this value turns out to be 0.26 m 0 if you substitute these values of ml and mt.

Using the same values of ml and mt in the case of density of states however the effective mass is different 1.08-time m 0 because the detailed derivation shows that the averaging is of a geometric kind, there is a geometric mean. ml into mt square whole thing raise to 1/3 with of course a factor coming here.

(Refer Slide Time: 39:02)



Energy Levels in ε - x Diagram

ε_0 serves as a reference while comparing electron energies in different isolated materials

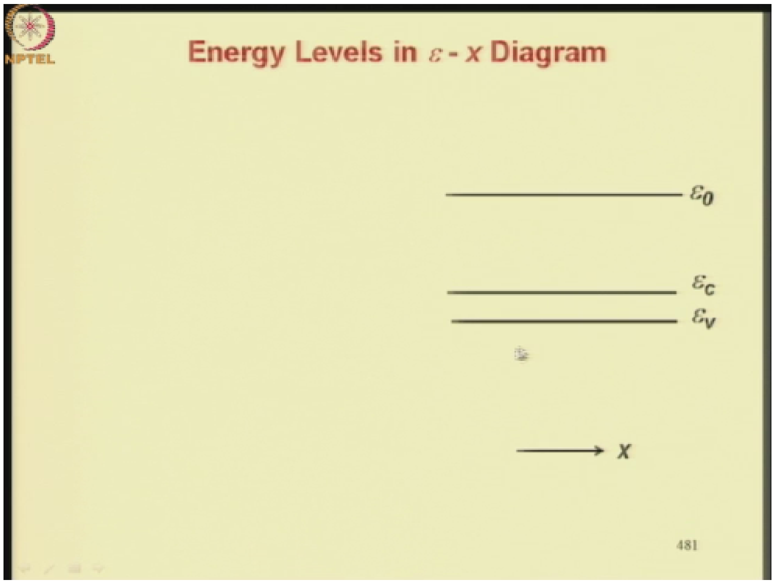
For the case of Gallium Arsenide similar approach gives you the conductivity and density of states effective mass. The reason in this case ml and mt are both identical and = 0.067 m0. So, you see if you compare it with silicon the effective mass of electron in Gallium Arsenide is much smaller. So electron feels much lighter in presence of Gallium Arsenide crystal potential as compared to silicon crystal potential.

And that is why the mobility of electron in Gallium Arsenide is very high if you apply force because the mass is small the electron gains a high acceleration or high drift velocity in Gallium Arsenide as compared to silicon. Various energy levels in the E-x diagram from E-k diagram we moved on to E-x diagram so the energy levels can be shown to emerge from the E-k diagram. The 2 energy levels which emerge from the E-k diagrams are Ec and Ev bottom of the conduction band and top of the valence band.

A variation of Ec and Ev as a function of x enables you to get the picture of the E-k relation throughout the volume of the device. So, Ec and Ev as a function of x reflects the special variation of the E-k relation. You get the level E0 from the crystal potential which is responsible for the conduction and valence bands. So E0 versus x reflects the special variation of electrostatic potential psi or electrostatic field E of the drift diffusion modal.

So, this is because the energy E0 corresponds to the energy of an electron touching the semiconductor from outside or from vacuum and you can easily show that as you move this electron over the surface it will experience psi or e of this semiconductor. Now, E0 serves as a reference while comparing electron energies in different isolated materials. So E0 really is very, very important.

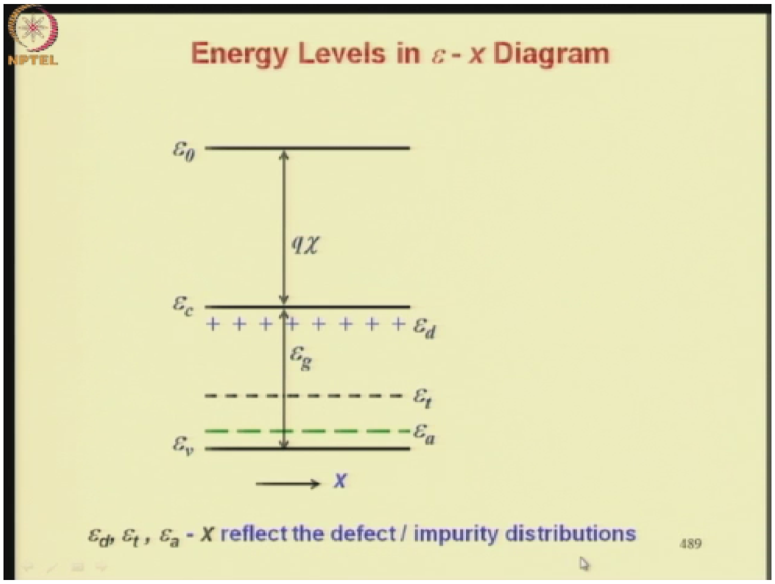
(Refer Slide Time: 41:17)



Energy Levels in ε - x Diagram

In practice we do not show the conduction and valence bands and crystal potentials. We got the energy valence band diagram that is the EX diagram will become very complex. We just extract the levels E0, Ec and Ev and show their variations with respect to x.

(Refer Slide Time: 41:31)



Energy Levels in ε - x Diagram

ε_d, ε_t , ε_a - x reflect the defect / impurity distributions

So the E0 variation is obtained from the drift efficient modal formula. So, here the relation between E0 and psi is E0/q = constant -psi or gradient of E0/q is E. You can locate Ec below E0/value qx where this electron affinity is obtained from the E-k diagram and crystal potential. So, chi can be a function of x if the crystal potential is varying with x as it happens in a hetero-structure or compositionally graded structure.

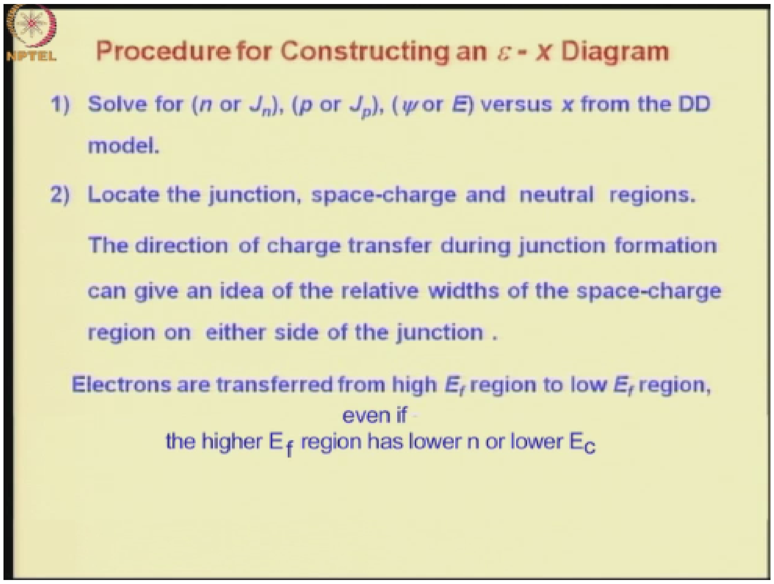
Similarly, easier the function of x, can also obtained from E-k diagram and doping profile. We have shown that the energy gap is a function of doping and for heavy doping the energy gap decreases. So, if the doping varies in a semiconductor the function of x for example the energy gap can change as the function of x. Energy gap can also change if the composition is varying as a function of x.

So, from this energy gap you can locate the Ev below Ec. You can locate the quasi Fermi level for electrons below Ec using this formula. Another relation that is related to variation of the quasi Fermi level is this equation of the drift deficient modal where in the electron current density is represented in a compact form in terms of the gradient of the quasi Fermi level. So both drift and diffusion are compressed in this one term.

One can similarly locate Efp from Ev using this formula. You also have a formula for gradient of Efp in analogy for the formula for gradient of Efn. So, Efn and Efp as a function of x reflects the distributions of n, p or Jn, Jp of the drift diffusion modal. So, this 2 formula show the relation of Efn, Efp with concentrations where these 2 formula for gradient of Efn and gradient of Efp show the relation between the variation of Efn and Efp with current density Jn and Jp.

You can also locate the quasi formula for electrons and holes with reference to Ei using these formula. You can locate within the energy gap the energy levels corresponding to impurities or defects. So, Ed, Et and Ea as a function of X reflect the defect or impurity distributions.

(Refer Slide Time: 44:29)



Procedure for Constructing an ε - x Diagram

1) Solve for (n or J_n), (p or J_p), (ψ or E) versus x from the DD model.
2) Locate the junction, space-charge and neutral regions.

The direction of charge transfer during junction formation can give an idea of the relative widths of the space-charge region on either side of the junction .

Electrons are transferred from high E_f region to low E_f region,
even if
the higher E_f region has lower n or lower E_C

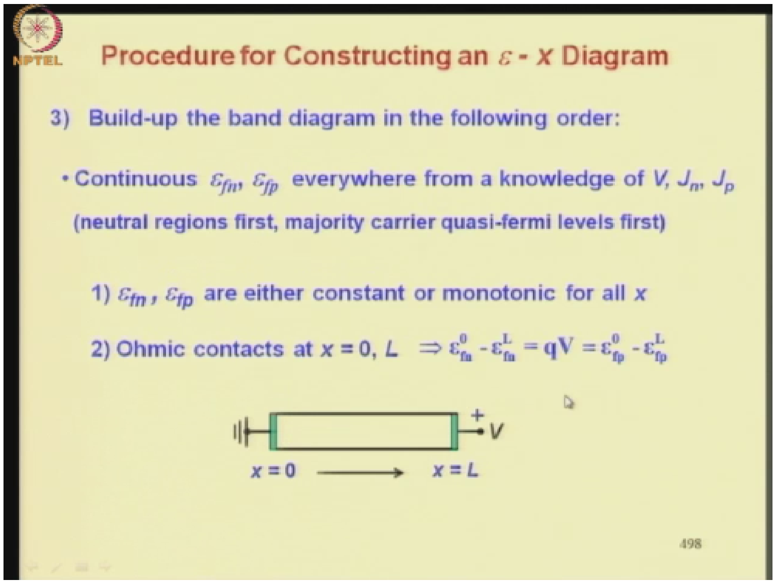
We outline a procedure for constructing an E-x diagram. This procedure is very, very important if you follow this procedure properly then you can draw an E-x diagram for even a very complex situation where composition, doping and so on are changing with distance in a device and a voltage has been applied in a very easy manner. So, the first step is to solve for n or Jn, p or Jp and psi or E versus x from the drift diffusion modal.

So, this is the first step. So, here we are looking at E-x diagram as representation tool for conditions in the semiconductor. So, these are the drift diffusion modal equations from which you get this information. In the next step you draw the device physically and locate the junction space charge and neutral regions. An important point the direction of the charge transfer during the junction formation can give an idea of the relative widths of the space-charge regions on either side of the junction.

So, when you are drawing the energy band diagram e as a function of x you would like to know what is the width of the space charge region on either side of the junction at least the relative values or relative qualitatively the relative magnitudes. So, this information is obtained from the direction of charge transfer and how does the charge transfer occur? Electrons are transferred from high Ef region to low Ef region.

So you draw the band diagram with the 2 materials separated and see the relative values of Ef.

(Refer Slide Time: 46:15)



Procedure for Constructing an ε - x Diagram

3) Build-up the band diagram in the following order:

- Continuous ε_{fn}, ε_{fp} everywhere from a knowledge of V, J_n, J_p (neutral regions first, majority carrier quasi-fermi levels first)

  1) ε_{fn}, ε_{fp} are either constant or monotonic for all x

  2) Ohmic contacts at $x = 0$, L $\Rightarrow \varepsilon_{fn}^{0} - \varepsilon_{fn}^{L} = qV = \varepsilon_{fp}^{0} - \varepsilon_{fp}^{L}$

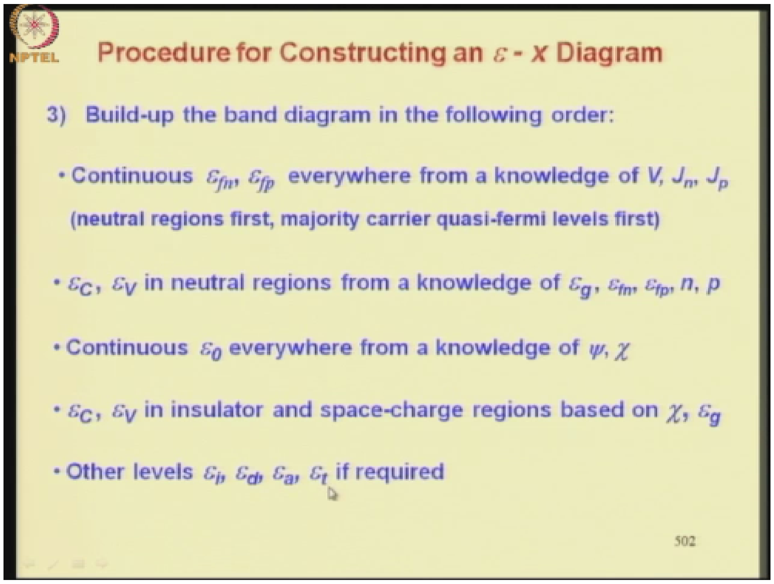
498

After that you can build up the band diagram in the following order. So, first draw continuous Efn and Efp everywhere from a knowledge of applied voltage and current density. In this first draw the quasi formula in neutral region and first draw the majority carrier quasi-fermi levels and then the minority carrier quasi-fermi levels. The reason why you start from Efn and Efp is being Efn and Efp are either constant or monotonic for all x.

We have given reason for this. Reason why Efn and Efp is continuous is because any abrupt change in Efn and Efp would mean infinite currents which are not possible physically. Second important reason for using Efn and Efp is that the variation Efn and Efp are directly related to the applied voltage when the device contacts are ohmic. So, if you have ohmic contact at x =0 and L then Efn 0 -Efn L is q times V. Efp 0 - Efp L is also q times V.

So, the total variation of the quasi fermi levels in the device would be equal to the applied voltage provide the contacts are ohmic. It does not matter what kind of a complicated material structure this region has.

(Refer Slide Time: 47:41)



Procedure for Constructing an ε - x Diagram

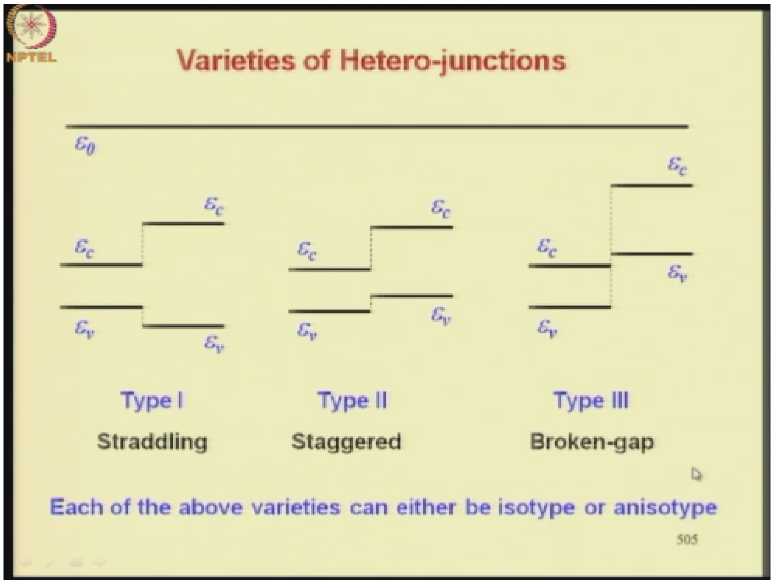
3) Build-up the band diagram in the following order:

- Continuous ε_{fn}, ε_{fp} everywhere from a knowledge of V, J_n, J_p (neutral regions first, majority carrier quasi-fermi levels first)
- ε_C, ε_V in neutral regions from a knowledge of ε_g, ε_{fn}, ε_{fp}, n, p
- Continuous ε_0 everywhere from a knowledge of ψ, χ
- ε_C, ε_V in insulator and space-charge regions based on χ, ε_g
- Other levels ε_i, ε_d, ε_a, ε_t if required

The next step would be to draw Ec and Ev in neutral regions from a knowledge of energy gap Efn and Efp and n and p. Then sketch E0 as a continuous line everywhere from a knowledge of electrostatic potential and chi. So, note that we have assumed that we have used the drift diffusion modal to solve for n p and psi before we start drawing the band diagram. Now why not E0 be continuous.

Because any abrupt change in E0 means an infinite electric field at that point which is none physical. Next step would be to sketch Ec and Ev in insulator and space charge regions based on electron affinity and energy gap. Finally, one can sketch other levels like EI, Ed, Ea, Et if required.

(Refer Slide Time: 48:28)



Varieties of Hetero-junctions

Type I Straddling

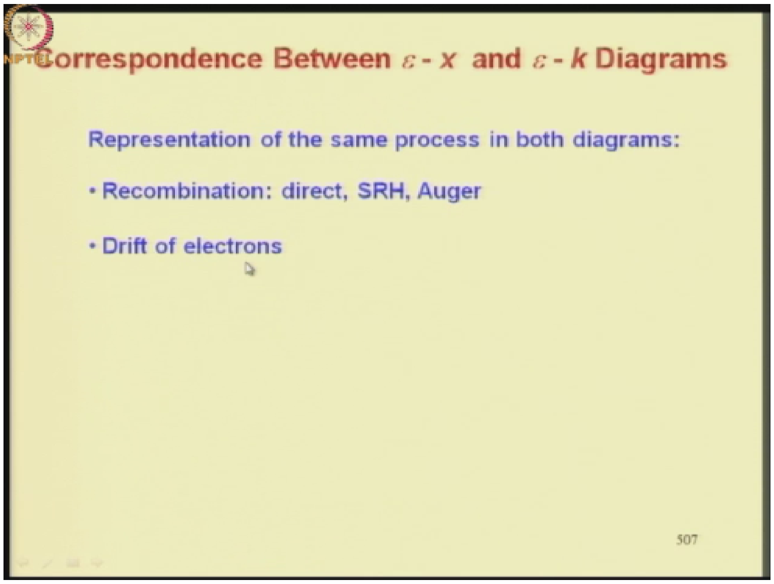
Type II Staggered

Type III Broken-gap

Each of the above varieties can either be isotype or anisotype

We explained various varies of hetero-junctions Type 1, Type 2 and Type 3 depending on how the conduction and valence band edges are located for the wider band gap material with reference to the lower band gap material. Now, each of the above varieties or types can be either isotypes or anisotype. Isotypes means both sides are p or n type. An isotypes means one side polarity is opposite to the other side polarity.

(Refer Slide Time: 49:04)



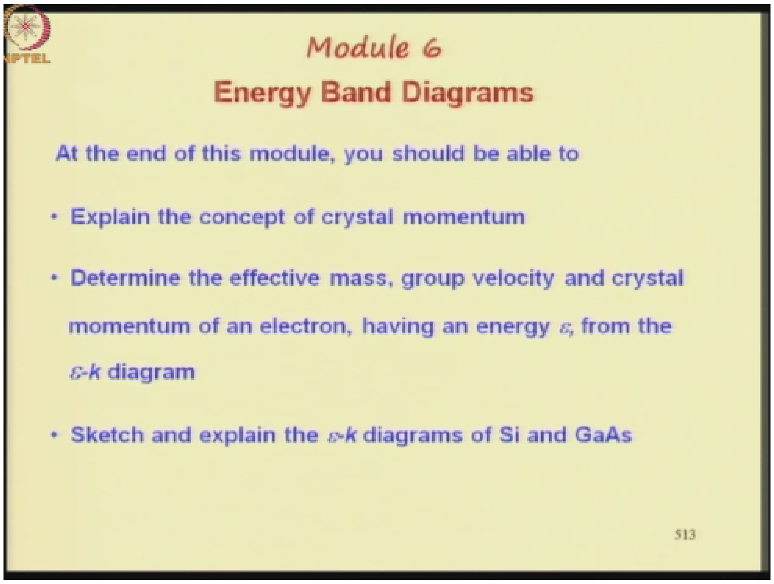
Correspondence Between ε - x and ε - k Diagrams

Representation of the same process in both diagrams:

- Recombination: direct, SRH, Auger
- Drift of electrons

Finally, we discussed the correspondence between E-x and E-k diagrams. We did so by representing the same process in both diagrams, namely direct recombination, SRH recombination, Auger recombination and drift of electrons. So, these are the diagrams. So direct recombination, SRH recombination, Auger recombination show on this. So here this is direct and this is SRH and here this is process is Auger. Similarly, this is the method of representing drift on EK diagram.

(Refer Slide Time: 49:51)



Module 6

Energy Band Diagrams

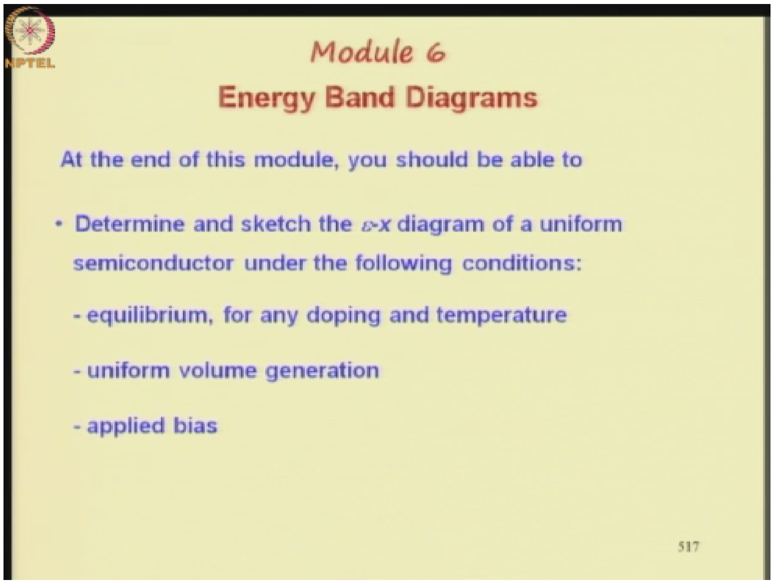
At the end of this module, you should be able to

- Explain the concept of crystal momentum
- Determine the effective mass, group velocity and crystal momentum of an electron, having an energy ε, from the ε-k diagram
- Sketch and explain the ε-k diagrams of Si and GaAs

Let us recapitulate in a minute the various learning outcomes so we hope that after going through all this discussion you are able to explain how the wave nature of electrons restricts the allowed energy e of electrons subjected to a periodic potential to certain energy bands. We are able to outline the features methods of determination and utilities of EK and EX diagrams of a semiconductor.

So you are also able to point out the correspondence between these 2 diagrams. Explain the concept of crystal momentum. Determine the effective mass, group velocity, and crystal momentum of an electron having an energy e from the E-k diagram. Sketch and explain the E-k diagrams of silicon and Gallium arsenide.

(Refer Slide Time: 50:42)



Module 6

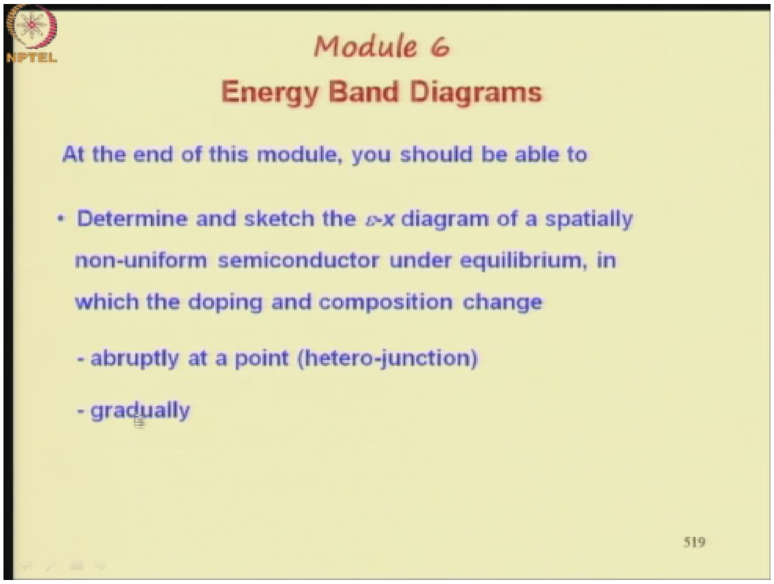
Energy Band Diagrams

At the end of this module, you should be able to

- Determine and sketch the $\mathcal{E}$-x diagram of a uniform semiconductor under the following conditions:
  - equilibrium, for any doping and temperature
  - uniform volume generation
  - applied bias

You should be able to determine and sketch the E-x diagram of a uniform semiconductor under the following conditions, equilibrium for any doping and temperature, uniform volume generation and applied bias.

(Refer Slide Time: 50:54)



Module 6

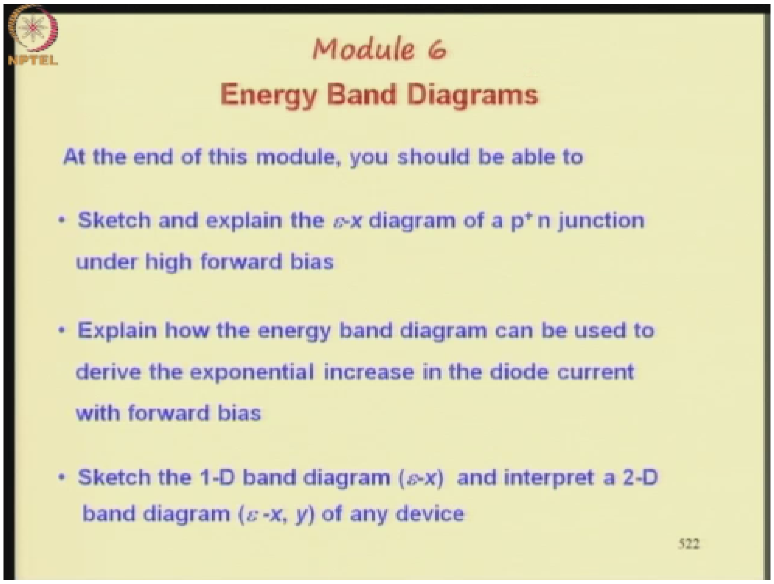
Energy Band Diagrams

At the end of this module, you should be able to

- Determine and sketch the $\mathcal{E}$-x diagram of a spatially non-uniform semiconductor under equilibrium, in which the doping and composition change
  - abruptly at a point (hetero-junction)
  - gradually

You should be able to determine and sketch the E-x diagram of a specially none uniform semiconductor under equilibrium in which the doping and composition change abruptly at a point and gradually.

(Refer Slide Time: 51:09)



Module 6

Energy Band Diagrams

At the end of this module, you should be able to

- Sketch and explain the ε-x diagram of a p^+n junction under high forward bias
- Explain how the energy band diagram can be used to derive the exponential increase in the diode current with forward bias
- Sketch the 1-D band diagram (ε-x) and interpret a 2-D band diagram (ε-x, y) of any device

You should be able to sketch and explain the EX diagram of ap+n junction under high forward bias. Explain how the energy valence diagram can be used to derive the exponential increase in the diode current with forward bias. And finally sketch the 1-dimensional band diagram and interpret a 2 dimensional band diagram of any device with that we have come to the end of this module. We will start a fresh module in the next lecture.