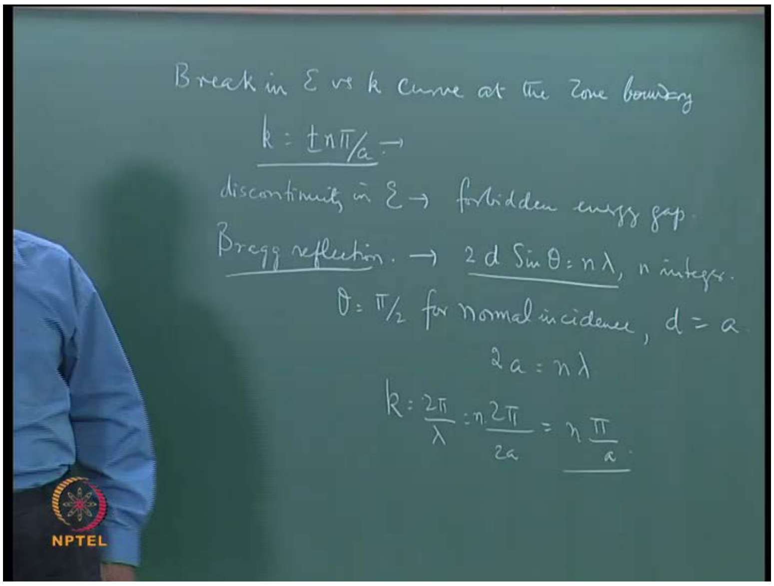
Condensed Matter Physics
Prof. G. Rangarajan
Department of Physics
Indian Institute of Technology, Madars

Lecture - 35
Electron Dynamic in a Periodic Solid

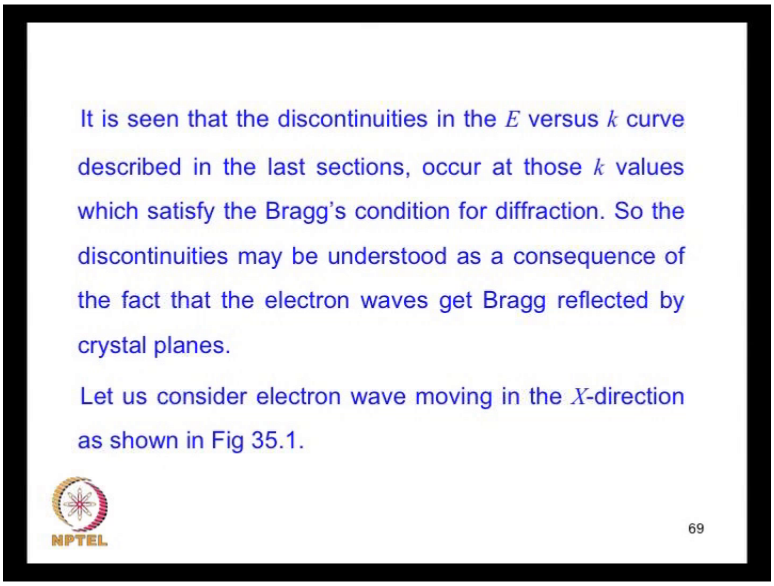
There are some very interesting consequence to the what we saw yesterday to the formation of energy bands in crystals. In particular we will discuss a particularly interesting feature of this propagation of electron waves in the crystal lattice.

(Refer Slide Time: 00:42)



There is a break in the e verses k curve at his own boundary corresponding to k equal to plus minus phi by a. These give you a discontinuity in e which corresponds to a forbidden energy gap, the existence of these forbidden zones may be interpreted as being due to Bragg reflection of the electron waves in by the crystallographic planes.

(Refer Slide Time: 01:50)



Now, what happens is these values of k at which these discontinuities occur maybe shown to liven side with the condition for Bragg reflection or Bragg diffraction, in order to understand this.

(Refer Slide Time: 02:17)

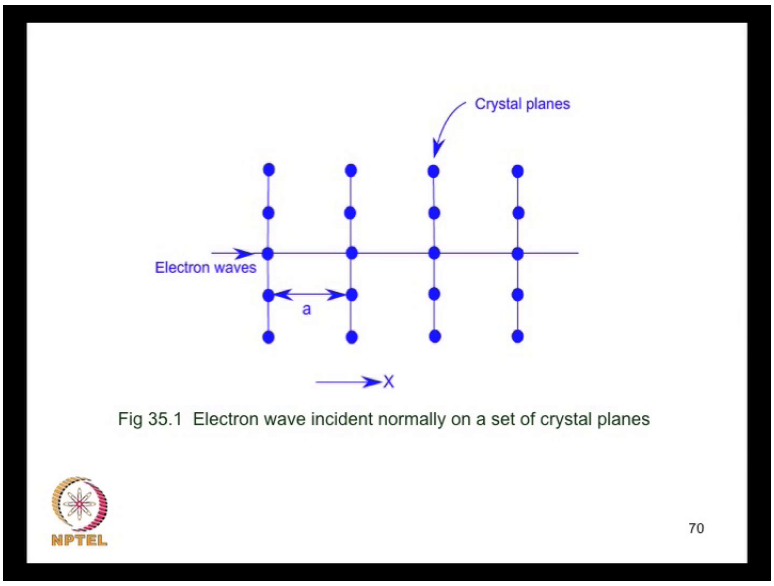
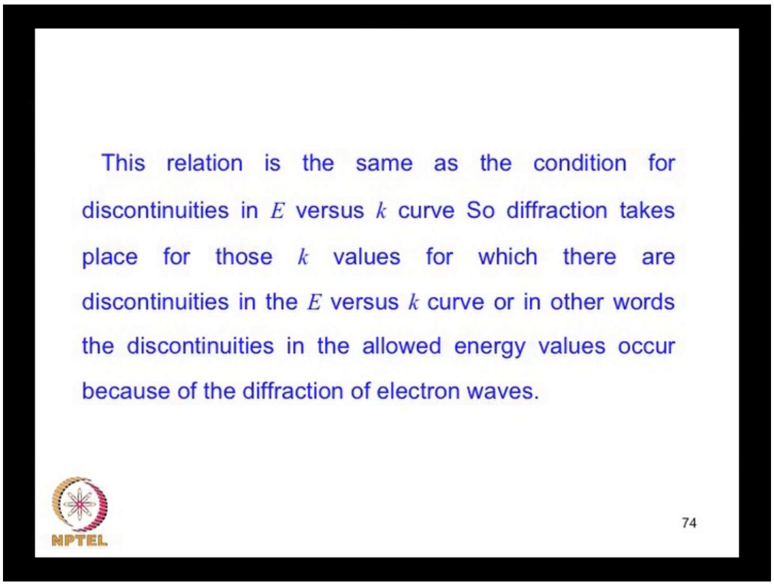


Fig 35.1 Electron wave incident normally on a set of crystal planes

Let us consider an electron wave moving in the x-direction as shown in figure. This electron waves are incident normally incident on the set of crystal plans, and according to the Bragg's law defection occur the Bragg condition is well known corresponds to two d sin theta equal to n lambda n, where n is an integer the electron waves are incident normally. Therefore, this is the condition for diffraction same as that for x-rays here d is the inter planner spacing theta is the angle between the incident. And the diffracted lambda is the wave length of the electron wave n is the order of diffraction inter planning spacing is d for normal incidents theta is 90, and d equal to a the spacing between principal planes. Therefore, this condition becomes 2 a equals to lambda or k which is 2 phi by lambda is 2 phi by 3 a into n or n into phi by a. So, this is the same as this here really this is n phi by a and we are talking about the reduce zone in which n is 1.

(Refer Slide Time: 04:24)



So, the two conditions are identical therefore, the conditions for Bragg reflection of the electron waves by the crystal planes is identical to the condition corresponding to the discontinuities at the zone boundary, which corresponds to the forbidden gaps. So, this is very interesting concept that electron waves behave in exactly the same way of x-rays, but are reflected at the zone boundary, therefore it also follows that the motion of the electron inside of solid, where there is a periodic potential due to the ion course in the crystal lattice the motion of the electron is restricted. And this restriction can be understood by looking at the e versus k curve which is shown in figure.

(Refer Slide Time: 05:29)

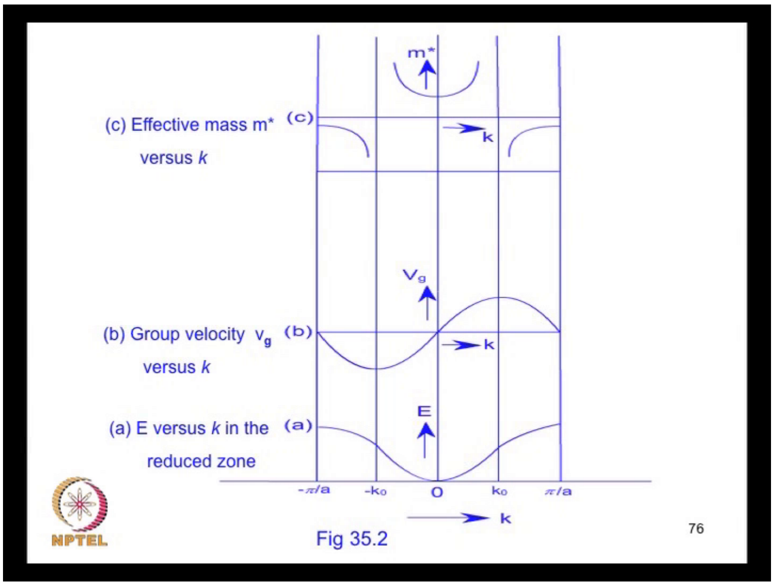
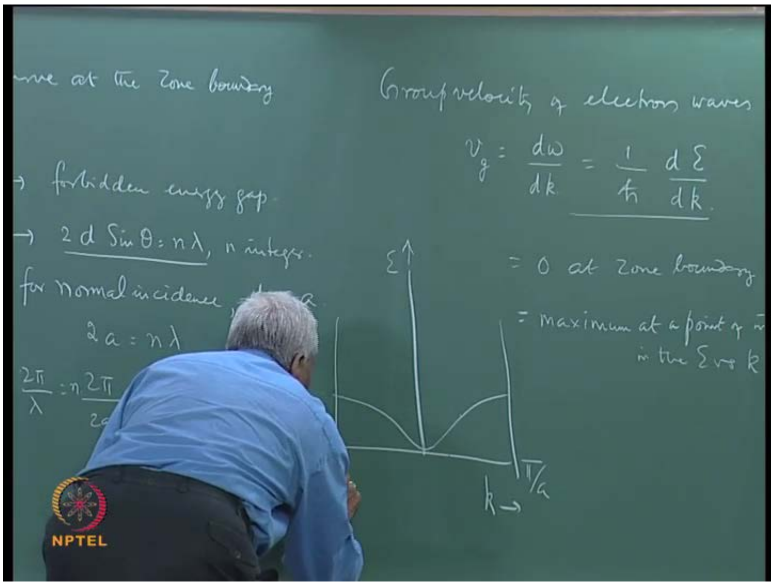


Fig 35.2

The bottom most well here in order to understand the motion of the electron, we considered the group velocity of the electron waves.

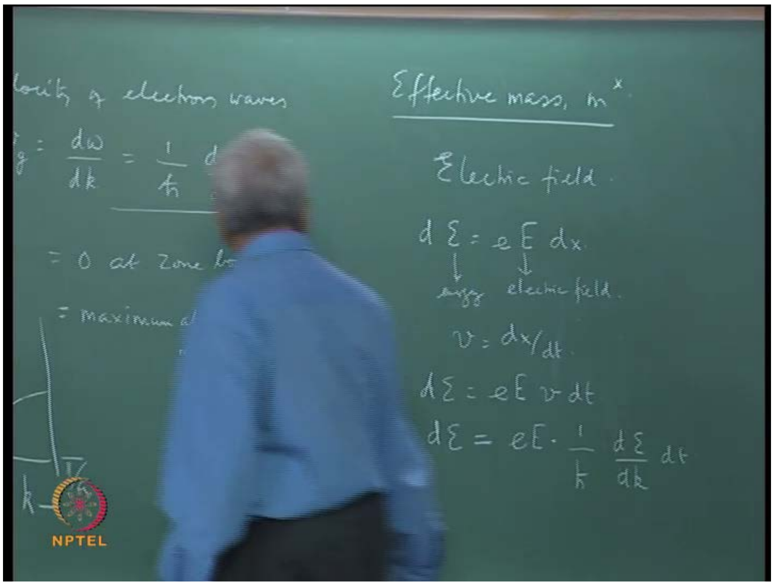
(Refer Slide Time: 05:38)



This is vg is d omega by dk, this is the standard definition of the group velocity. And since we know e is h cross omega we can also write this as. So, you can see there is a close connection between the group velocity and the slope of the e versus k curve at any point in the zone boundary in particular at the zone boundary the group velocity since the e versus k curve becomes this slope is 0.

So, this is 0 at zone boundary were Bragg reflection occurs actually we can see . So, these are the zone boundaries. So, you can see that the velocity the group velocity is a maximum at a point of inflection in the e versus k curve that corresponds to this point. So, this slope is negative above this and actually it start from zero here at the center of the zone and then increases is positive and increases, and reaches a maximum value at this point have inflection and then starts decreasing this slope is negative till the slope becomes actually zero. So, this phenomena of the curvature of the e versus k curve can be understood by introducing.

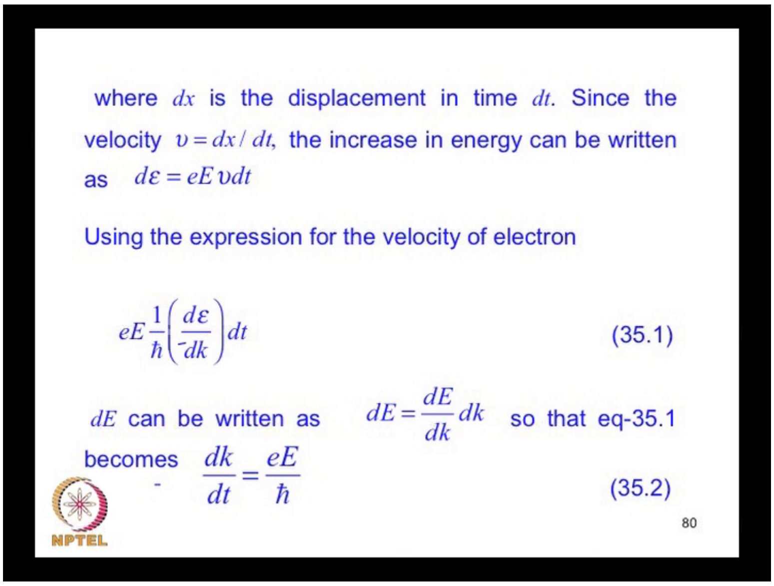
(Refer Slide Time: 08:24)



The concept of what is known as effective mass usually denoted as m star so. We will assign a effective mass to the electron which reflects the influence of the periodic potential, and emotion of the electron in order to understand the concept affair effective mass let us consider an external field electric field. So, we have the energy increment in an applied electric field is e e d x this is the field this is the energy.

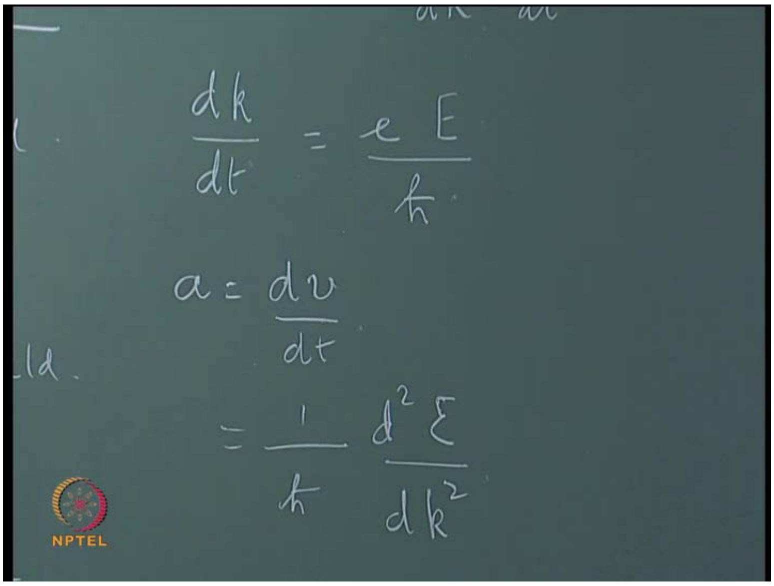
So, the external field act on the electron and causes a display spent d x in d t in interval of time d t and the velocity is just d x by d t. So, using this we can right d e as e e v d t. And the since we have d e and we also want to write d e as starting with this the velocity is given by this. So, we can write substitute here the particle velocity of the electron is the same as the group velocity of the electron waves. So, we can borrow this expression and write 1 by h cross d e by d k into d t.

(Refer Slide Time: 10:57)



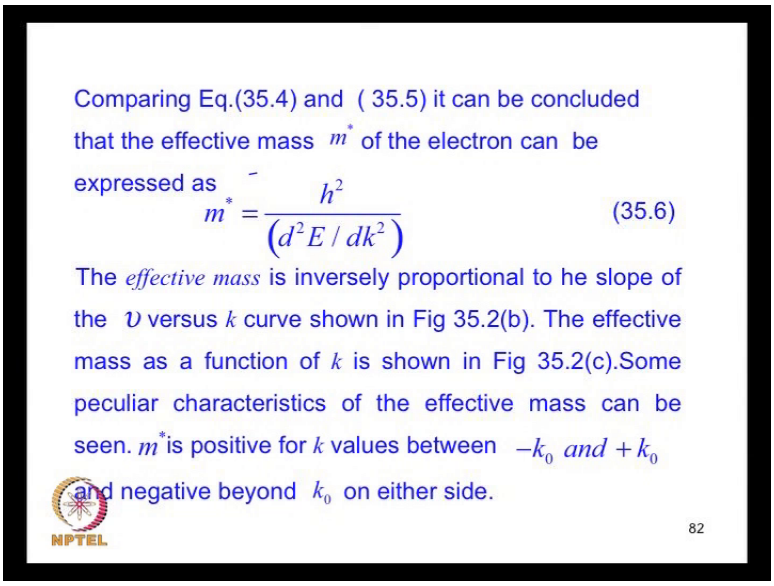
Now, d e can be written as d e by d k into d k by d t therefore, I can write d k by d t by going from this. So, I have d e by d k which can be written as therefore, I get e e with the electric field by h cross. So, since I have d k by d t, what is d k by d t d k by d t is nothing but the acceleration because k is related to the momentum.

(Refer Slide Time: 11:55)



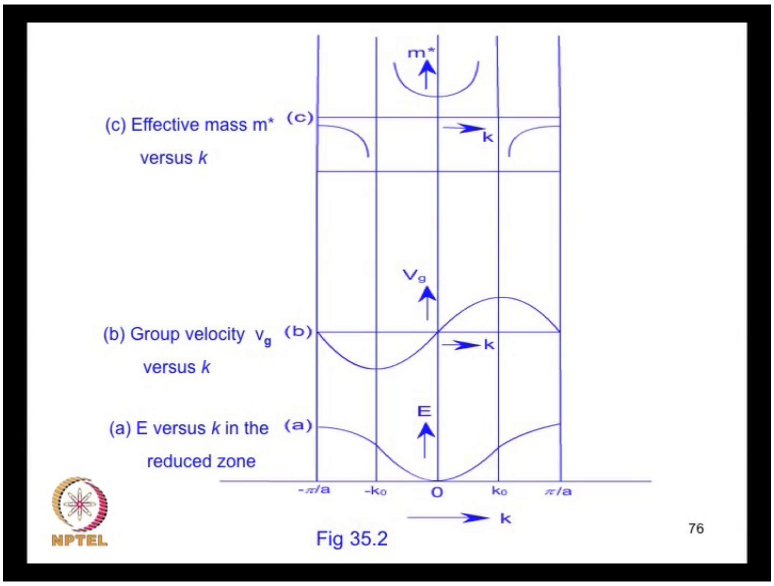
So, a is d v by d t which can be written as one by h cross this square e by d k square times d e. So, you can see that the acceleration of the electron is related to the curvature the second derivative of the energy with respect to k, and usually the acceleration is e e by m which we will denote as m star, because it therefore need to identify this as the effective mass. So, I have expression finally, for the effective mass.

(Refer Slide Time: 13:03)



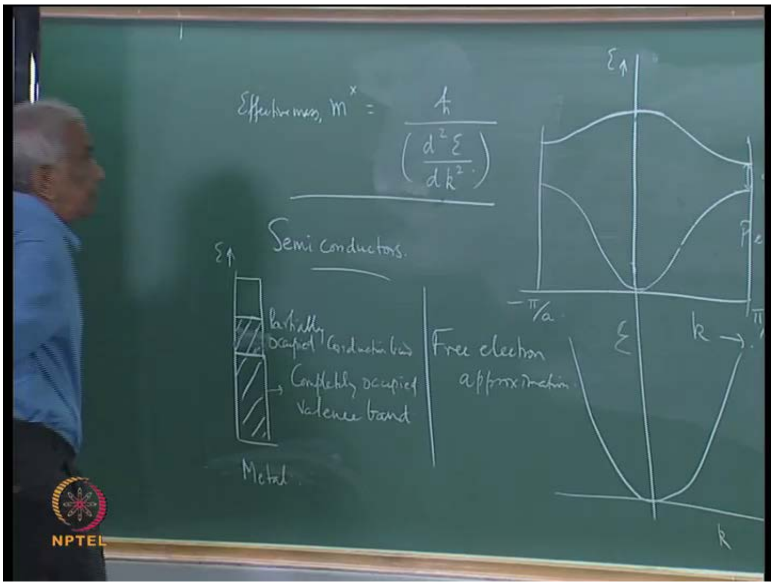
So, we see that the man star the effective mass is inversely proportional to the second derivative of the e versus k curve.

(Refer Slide Time: 13:24)



So, the effective mass is also shown in the figure, which also depict along with the e versus k curve the variation of the group velocity as well as that of the effective mass m star. So, they concept of effective mass is therefore, closely related to the second derivative of the e versus k curve. So, the effective mass is positive for k values which lie from 0. And the maximum value on either side minus k naught and plus k naught well k naught corresponds to the wave vector corresponding to the point of inflection were the group velocity is the maximum beyond k naught m star becomes negative on either side. So, the lower. Portion the lower half of the energy band, you have positive m star values and the upper half has negative m star values will it reaches this zone boundary we reached the zone boundary where m star is actually 0.

(Refer Slide Time: 14:47)

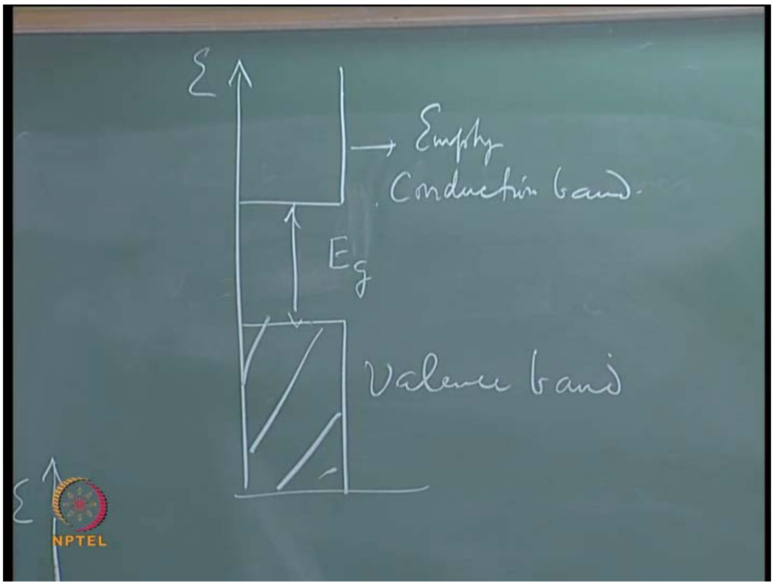


So, you have the important concept of effective mass which flows from the concept of the fact that the e versus k curve has breaks discontinuities at this one boundary. So, have and so on. So, this is the gap unlike the free electron approximation which predicts a simple parabolic variation without any breakup this is free-electron approximation this is a periodic potential electron in a periodic potential inside this solid. So, this periodic potential creates a discontinuity in the e versus k curve at this zone boundary and correspondingly, there are very many there are interesting deviations from this discontinuous parabolic variations.

And these interesting deviations are associated with the fact that the effective mass of the electron under the influence of the periodic potential is such that it goes from zero to a maximum value in the lower half of the energy band. And then from the maximum value, it becomes it goes to 0 corresponding to a negative group velocity. And then it even gets there is Bragg reflection, therefore the electron actually gets reflected at the zone boundary.

So, these are some very important and interesting consequences of the formation of energy bands and crystals which we will use. Now, when we start discussing semiconductors we already discussed how materials can be classified has metals insulators and semiconductors based on the nature of the band. For example, in a metal the highest occupied band is here and then this as a partially occupied or half occupied this is there is a gap. So, partially occupied conduction band, and this is completely occupied valence band. So, because of this partial occupation this is the picture for a metal whereas, in the case of an insulators, it is different.

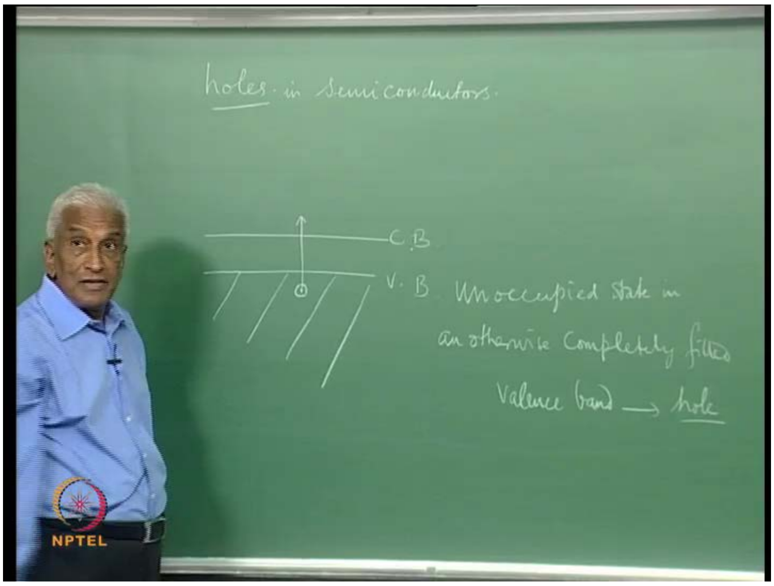
(Refer Slide Time: 18:39)



So, you have a completely occupied valence band, and the forbidden gap in the energy value, and then a completely empty conduction band with a large energy gap because this energy gap is very large the carriers, which are completely occupied the state's inside the valence band are unable to cross or overcome this barrier. And get into the conduction band therefore, conduction is not possible and this is the behavior of an insulators and then be talked about a semiconductor in which this picture is the same, but the energy gap is much smaller. And because the energy gap is smaller thermal activation excitation of carriers from the valence band into the conduction band is possible and when the valence band an electron leaves the valence band, then it leaves behind what is known as a hole this is another important concept by which comes from the energy band theory.

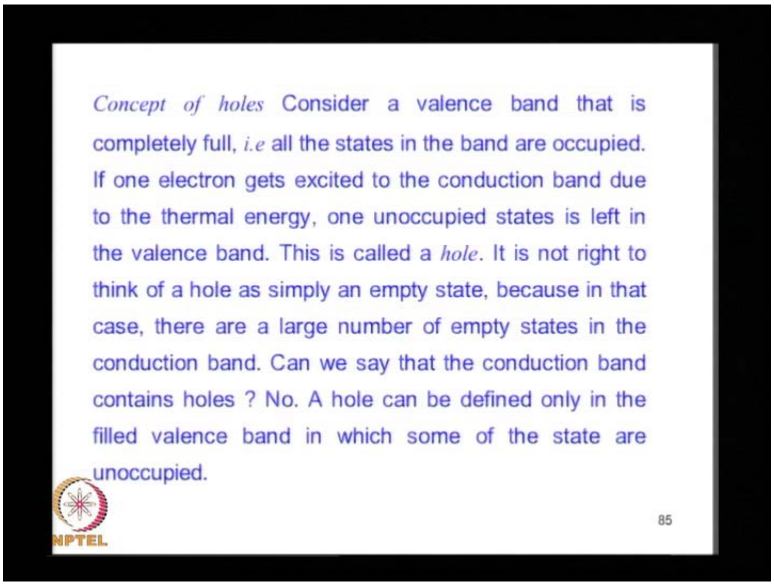
So, there is a hole here and this electron gets excited across when this energy gap is small. So, this hole goes across this energy gap into an empty state in the conduction band the electron moves in the conduction of band and the hole moves in the valence band. So, in a semiconductor conduction by electrons un holes in a semiconductor.

(Refer Slide Time: 21:16)



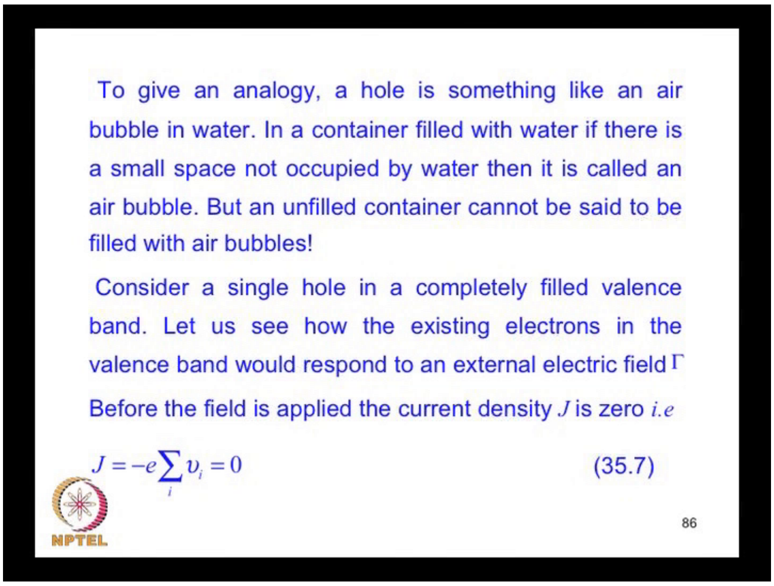
So, these are some of the important features, which arise as a consequence of the periodic potential. We next consider the concept of holes in semiconductors for this let us consider valence band a valence band is here, and this is the conduction band. Let us consider a state here in the valence band which is completely filled it is full.

(Refer Slide Time: 21:47)



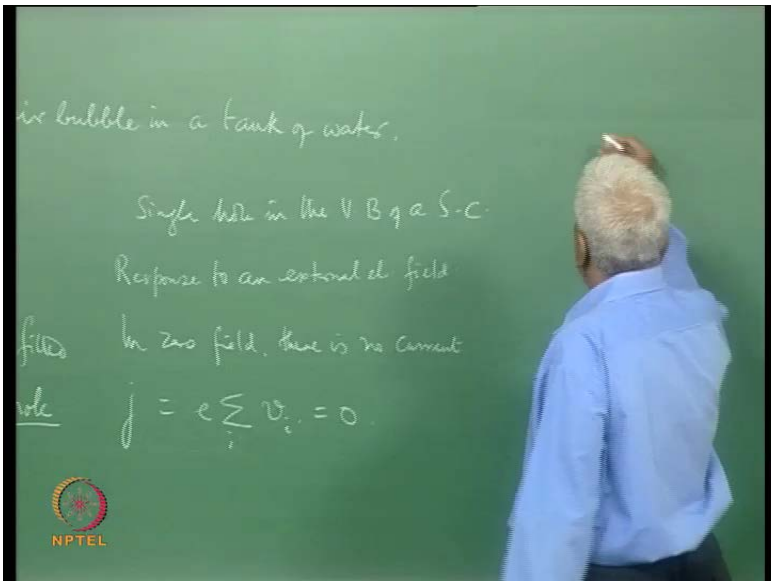
But let us consider one state here as being one from which an electron which occupy is this gets excited thermally into the conduction band leaving a vacancy here an unoccupied state. Now, this is unoccupied state in and otherwise completely filled valence band this is called a hole. Now we should not regard the hole as simply an empty state if this is. So, in the conduction band there are a lot of empty state that does not mean that there are lot of holes in the conduction band a hole is defined only in a filled valence band.

(Refer Slide Time: 23:22)



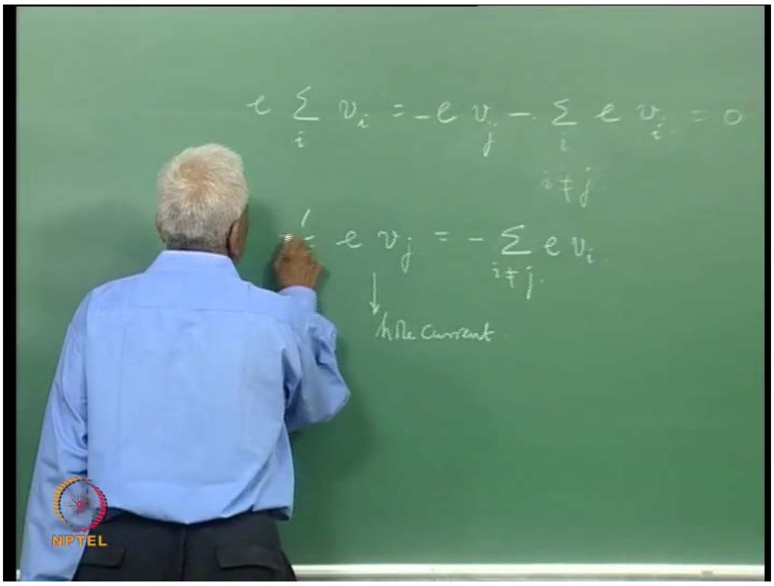
In which some the states are not occupied to give were an analogy is an air bubble in a tank of water.

(Refer Slide Time: 23:32)



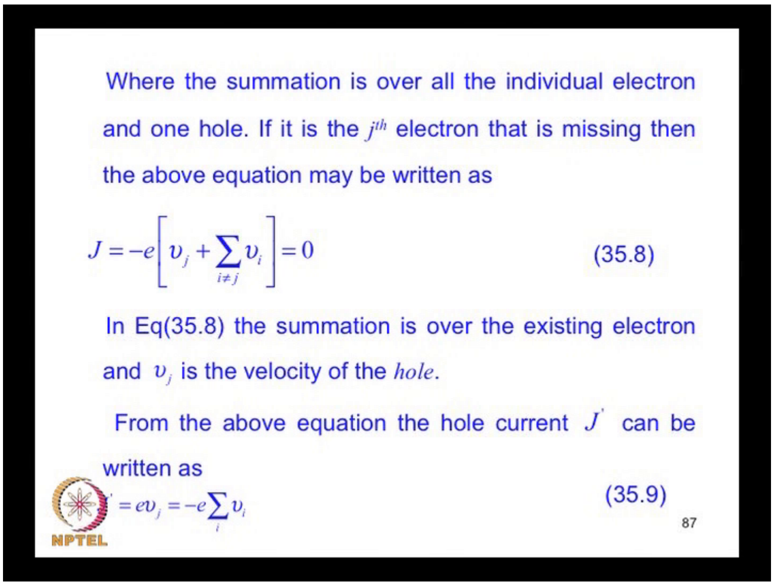
Suppose if this tank is filled with water and there is a small space which is not occupied by water then the air will fill their. and we will have an air bubble, but that does not mean that a container which is completely empty cannot be said to be filled with the air bubbles it is filled with air. So, consider a single hole let us consider a single hole in the valence band of the semiconductor. Now if this hole is to respond to an electric field how it will it respond response to an external an electric field now if this field is zero in zero field we know that there is no current we know their lives the current. In other words the current density which is e sigma vi that is the j this is zero over all the i’s. Now let us right these i over all the states which are there.

(Refer Slide Time: 25:44)



Now, we can write the summation e sigma i e i as e let us put an negative sign because these is we are considering the current due to the electrons. So, that can be written as. E b e plus sigma e v j over j where j not equal to i, and we can write or let us say i i not equal to j.

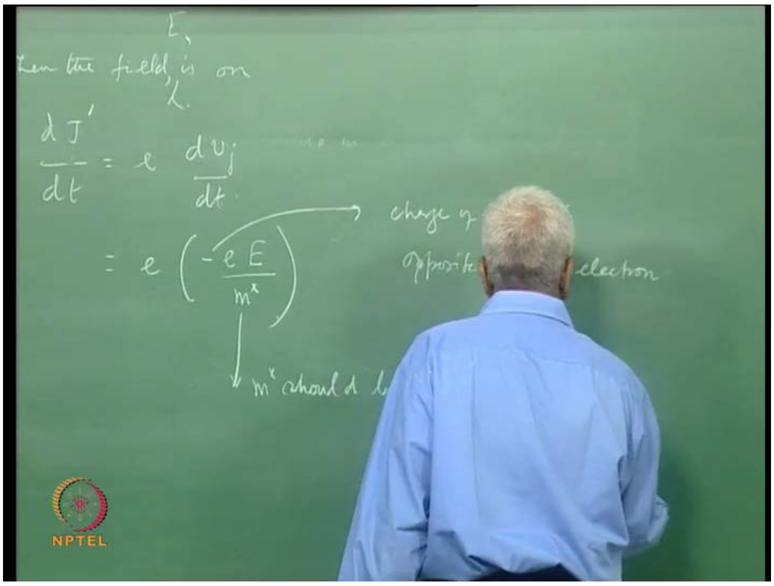
(Refer Slide Time: 26:32)



That is we are taking a state j a out at these totality of state's I, and that is kept outside the summation and then all the rest of them where the i does not include j. They are connected consider in the sum now this is this total is 0 in other words be can write e v j that is minus e or sigma e e i i not equal to j.

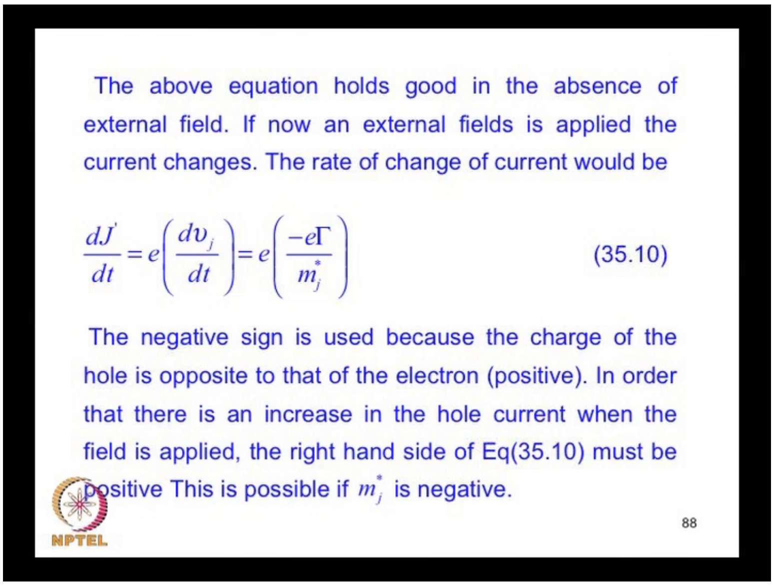
So, this can be return as the hole current this is same as the current due to all the electron in which the unoccupied state is not consider and the total current density is consider. So, this is the hole current. Now if we have an external field then the way the current density changes with time dependence on the time derivative off this. So, this k prime the current density.

(Refer Slide Time: 28:26)



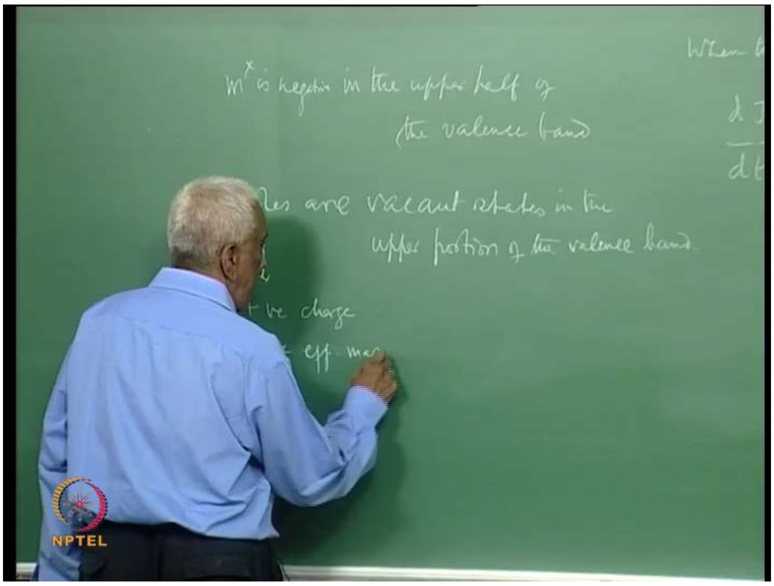
Let me right it has a capital the way the hole current changes, then there is when the field is on.

(Refer Slide Time: 28:39)



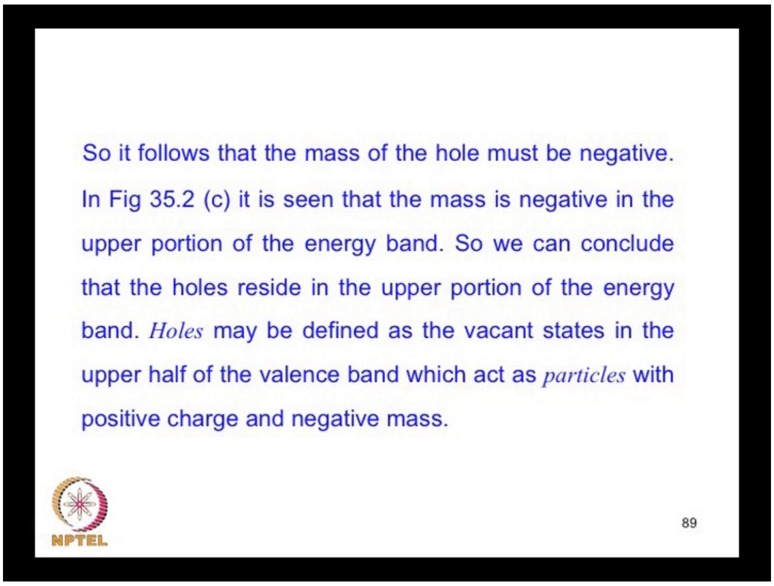
That can be written from here as e d v j by d t prime and that is e time minus e by m star where e is the electric field a put a negative sign, because it is a hole which has a charge which is opposite of that of the negative sign. Because of charge of hole is opposite to that of electron. Now if we want an increase in the hole current as a result of the it field being switched on then; that means, m star should be negative for all hole current to increase. In the presence of e, and if we consider the effective mass m star should be negative where is the m star negative here a we come across such as a situation we can see that in figure 352, we have plotted.

(Refer Slide Time: 30:44)



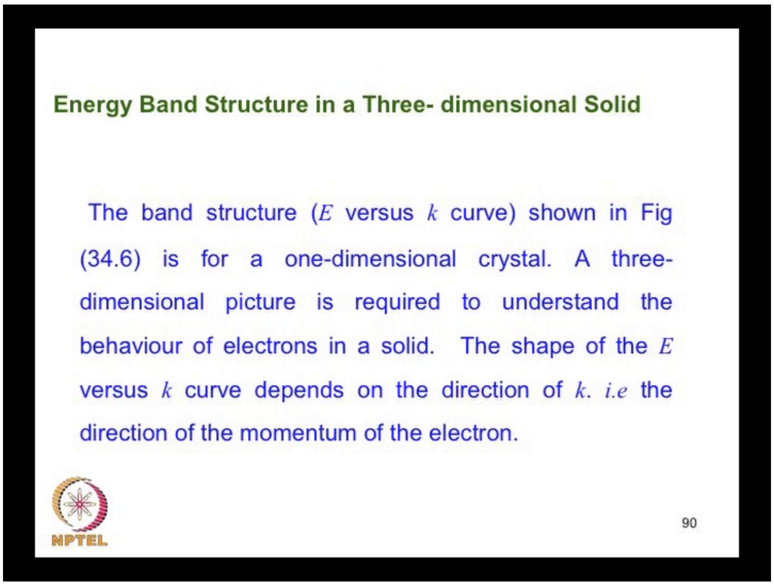
The effective mass versus k, and we find that the m star is negative in the upper half of the valence band the holes resides in the upper portion of the energy band the valence band.

(Refer Slide Time: 31:04)



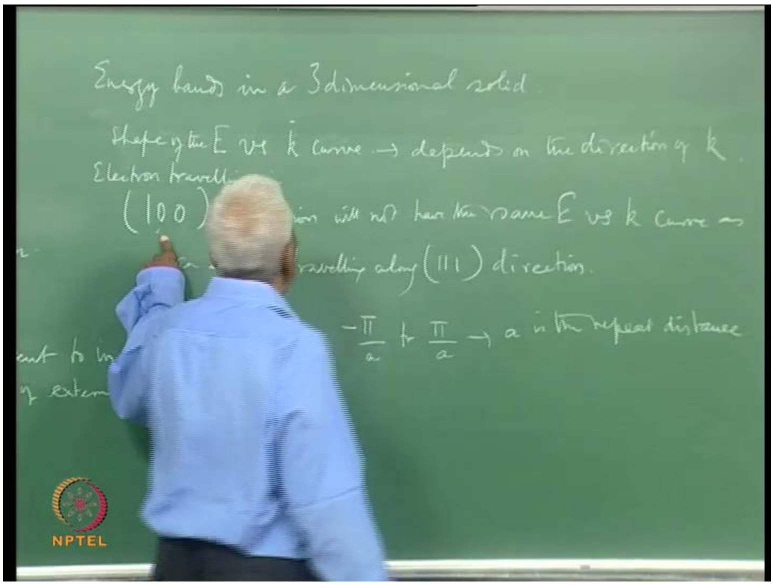
So, holes are thus defined as vacant states in the upper portion of the valance band where the effective mass is negative. So, they have a positive charge positive charge, and negative mass they have a charge opposite in sign to that of the electron and negative effective mass these are the two characteristics of course.

(Refer Slide Time: 32:05)



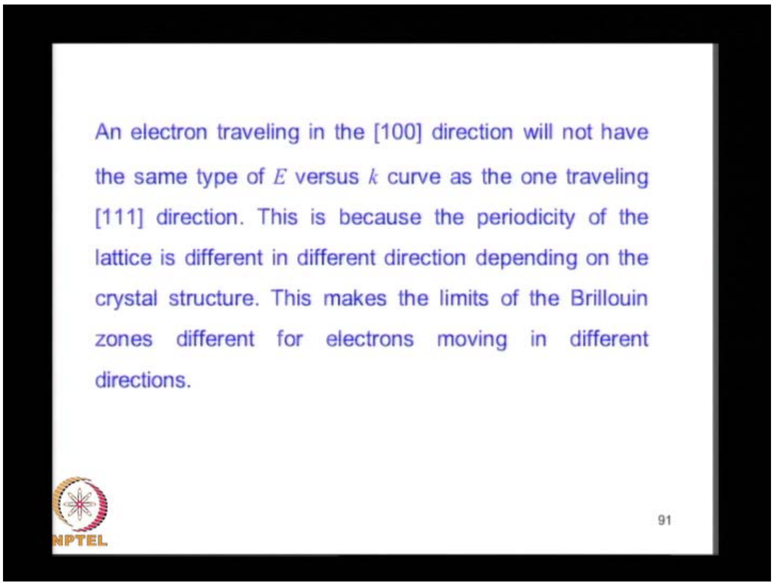
Next we wished to talk about we have been considering energy band structure.

(Refer Slide Time: 32:18)



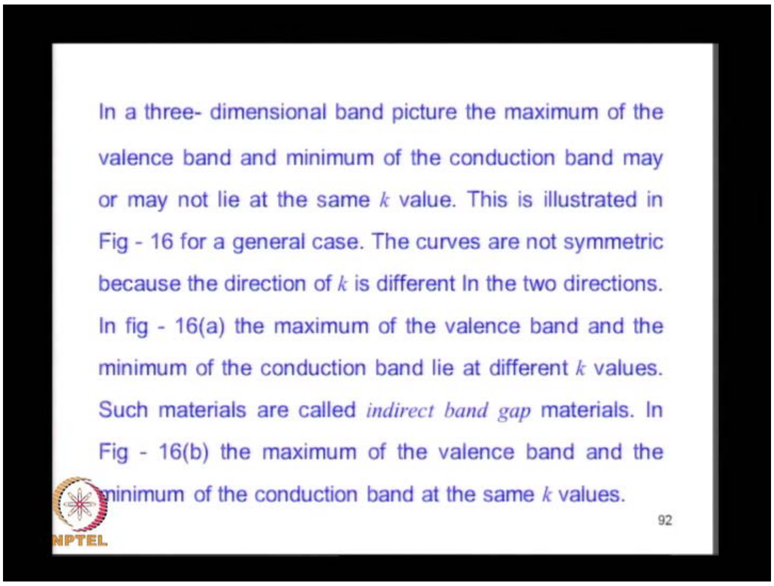
In one dimension oppose energy bands in a three in a three-dimensional solid this is because if we have the shape of the e versus k curve depends on the direction of k, so in the three-dimensional solid suppose, we have electron traveling in 100 directions. So, it will not have in this direction electron traveling in 100 direction will not have the same e versus k curve as an electron traveling along 111 say that is because the lattice constants the lattice repeat distance. And the Brillivan zone extents from minus phi by a to plus phi by a where a is repeated distance. Since the repeat distance changes depending on whether it is 100 or 111 correspondingly the e versus k curve will also be different.

(Refer Slide Time: 34:39)



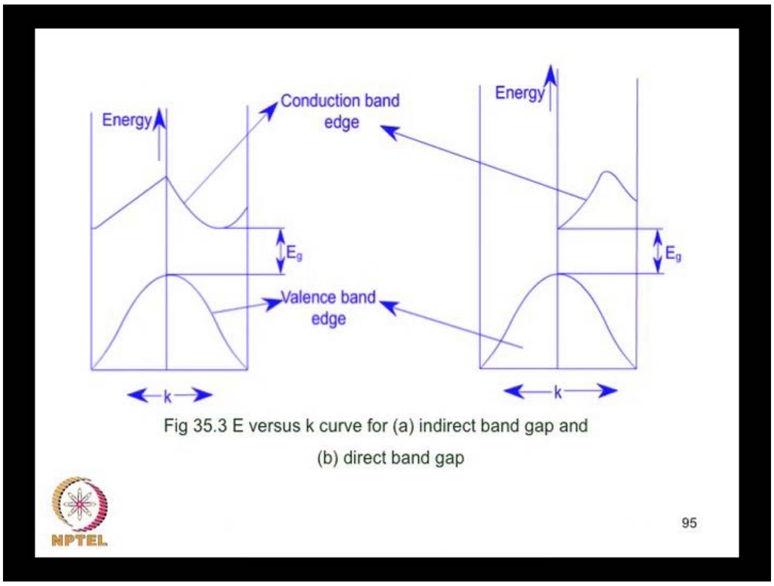
So, the limit of the Brillivan zone are different for electrons moving in different directions.

(Refer Slide Time: 35:09)



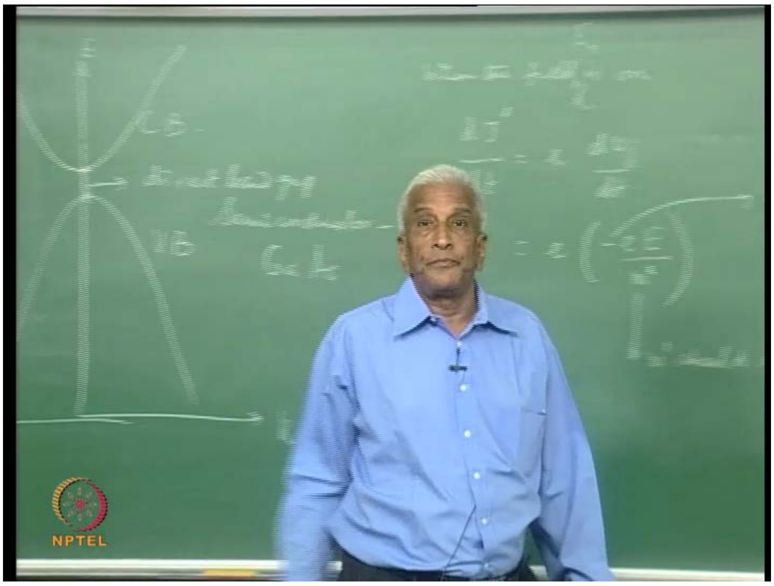
So, the maxima and minima in the e versus k curve may not go inside their may or may not lay at the same k value in different directions.

(Refer Slide Time: 35:46)



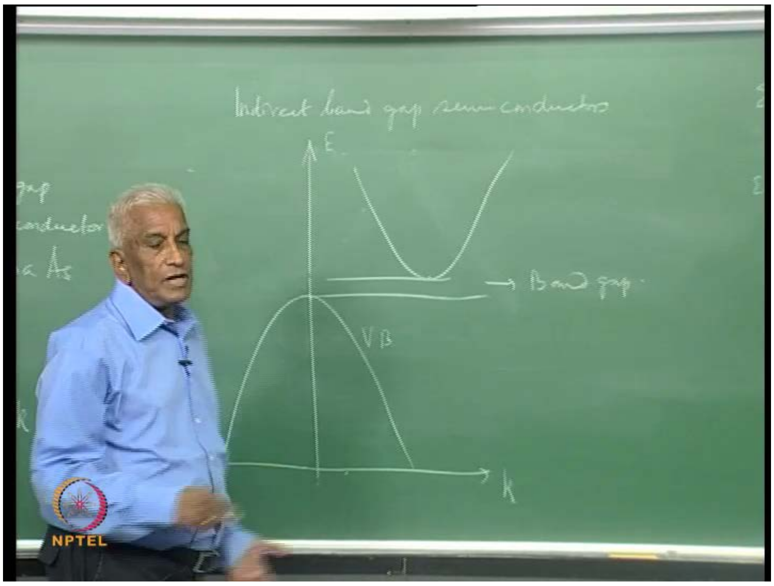
So, what is the consequence of this the consequence that this is shown in figure where, the energy versus k curve is shown for the valence band edge and the conduction band.

(Refer Slide Time: 36:01)



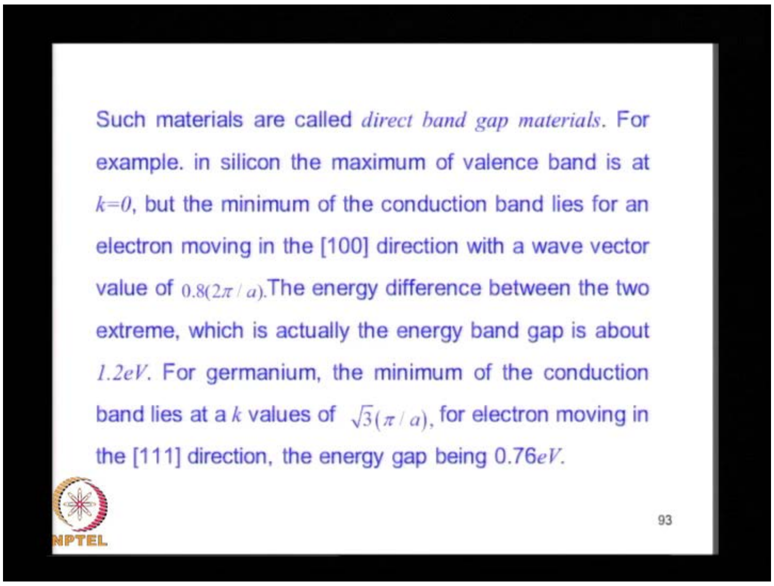
Suppose. So, I have the this is conduction band this is valence band here the maximum valence band lay’s at the same k value as the minimum in the conduction band. So, this known as a direct band gap semi conductance any kind he founded gallium arsenide has such a band structure on the other hand. If you consider materials like silicon they do not have such a band structure Silicon.

(Refer Slide Time: 37:06)



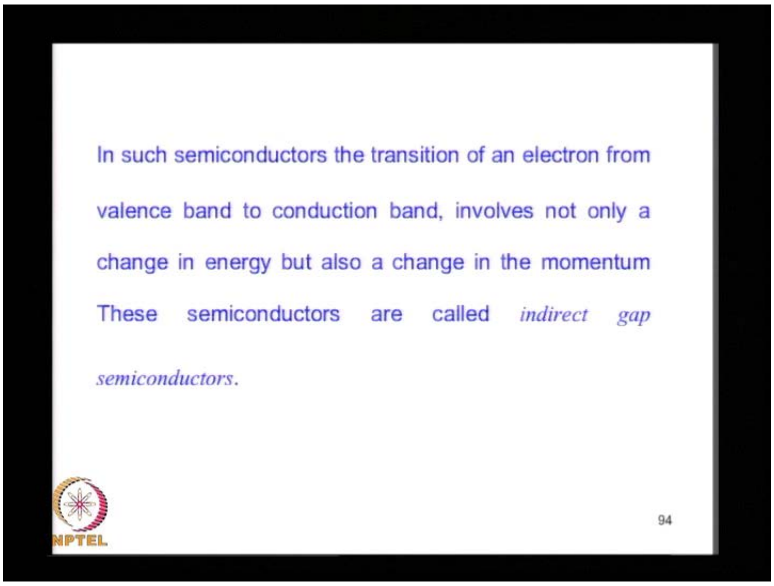
For example, for germanium or indirect band gap semiconductors what does it mean? This means that the e versus k curve will be such that there is a maximum in the valence band this is the valence band and the minimum in the conduction band is situated somewhere else. So, we have this, and this is the band gap in the indirect band gap the maximum of the valence band.

(Refer Slide Time: 38:11)



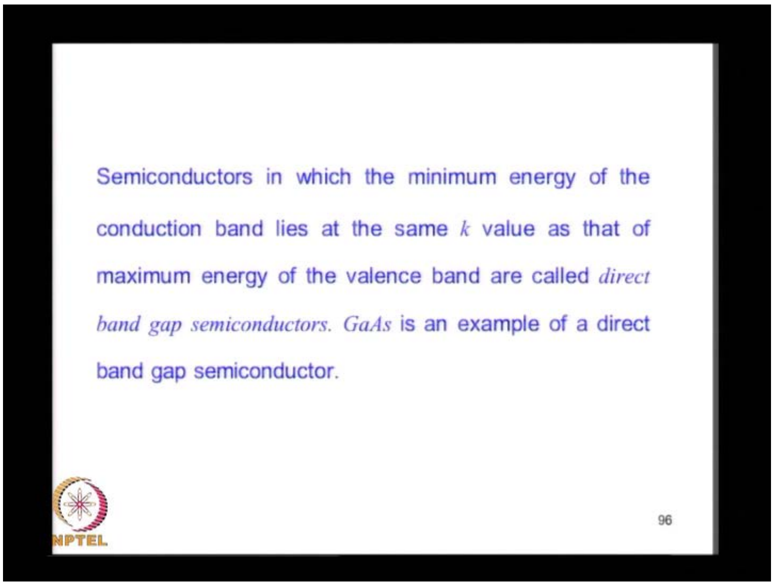
And the minimum of the conduction band do not occur at the same k value. So, the minimum of the conduction band will be in a different k value, and we will have to consider this energy difference between these two extreme, which use your a band gap of something like 1.2 e v for silicon, because there is a change in the k value corresponding to the there is a change in the momentum.

(Refer Slide Time: 38:51)



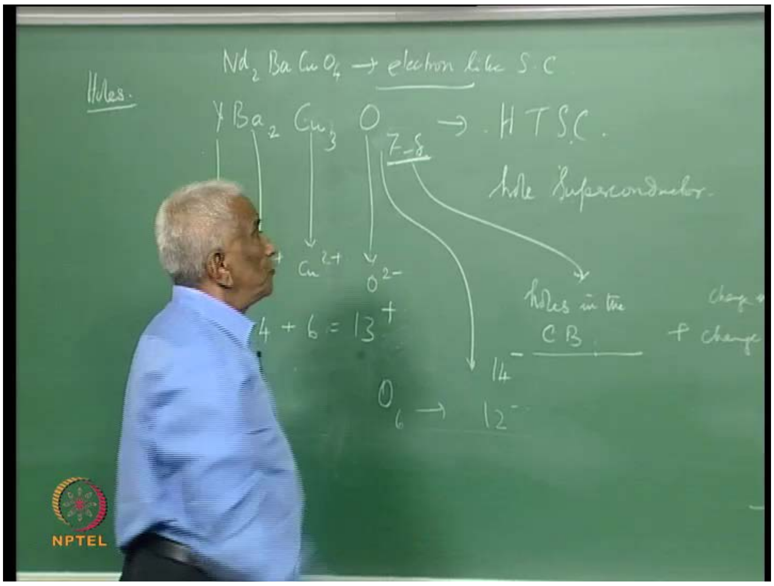
And therefore, the kinetic energy. So, that has to be added. So, there is also not only a change in energy a transition from the valence band into the conduction band involves a change in the energy equal to the energy gap, this gap plus a change in momentum corresponding to a change in wave vector from here to here.

(Refer Slide Time: 39:31)



So, such semiconductors are known as indirect band gap semiconductors direct band gap semiconductors are as special interest now having considered holes.

(Refer Slide Time: 39:43)



We can briefly rework back to what we discuss in connection with a high temperature superconductor you may recall that we have a high-temperature superconductors, such as y B a 2 C u 3 o 6.9, that is a high temperature superconductor, which we call the hole superconductor. We can now understand why this called like this considering the valence of this victims is three plus various is two plus copper is also two plus and oxygen is minus. So, if you consider the charge balance we have three plus four two into two plus three into two which is six which is 13 that is plus and o.

if I have o seven for example, suppose I have seven then o seven will give me fourteen minus. So, for charge balance you require exactly, if it is o six for example, this is twelve where, but we have positive ion case is 13 plus. So, the charge balance require that this should be more than six point five actually this becomes you reduce it by a small amount to delta from the strike cemetery of seven. We get the behavior of high temperature superconductor, and this is because this charge balances affected living if you holes in the conduction band and that is the reason for superconductivity. So, that is why we call this a hole superconductor were as the medium was called as an electron like apartment again for the same reason. So, this is the reason for the nomenclature and it is hole conduction in a pairing a hole, which is possible for superconductivity in the high-temperature superconductor hip we now pass on to a discussion of semiconductors.