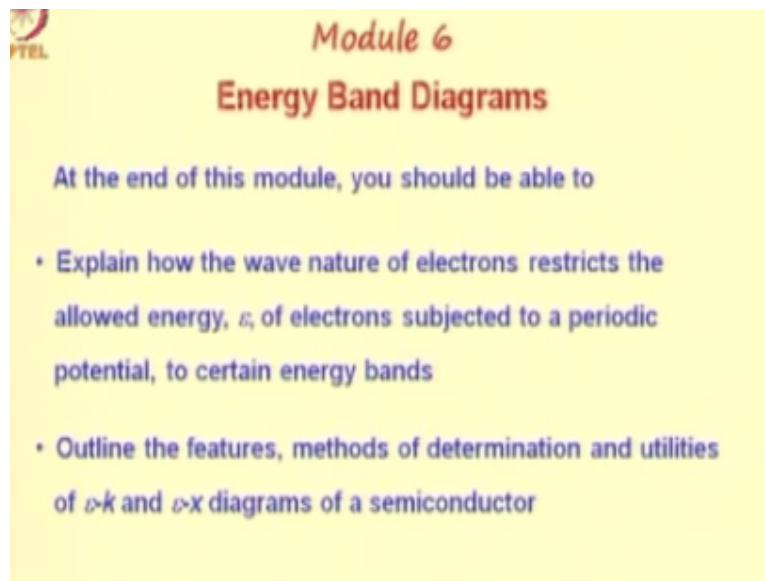


Semiconductor Device Modeling
Prof. Shreepad Karmalkar
Department of Electrical Engineering
Indian Institute of Technology – Madras

Lecture – 27
Energy band diagrams

Now, in this lecture, we start a new module on energy band diagrams. This is a very important topic in device modelling, so we will discuss this in detail.

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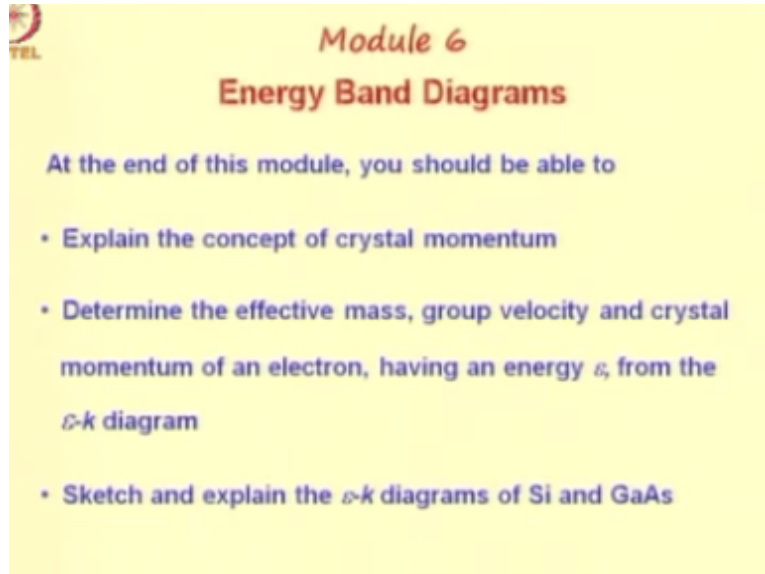
Module 6
Energy Band Diagrams

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

- Explain how the wave nature of electrons restricts the allowed energy, ϵ , of electrons subjected to a periodic potential, to certain energy bands
- Outline the features, methods of determination and utilities of ϵ - k and ϵ - x diagrams of a semiconductor

At the end of this module, you should be 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. You should be able to outline the features, methods of determination and utilities of E_k and E_x diagrams of a semiconductor.

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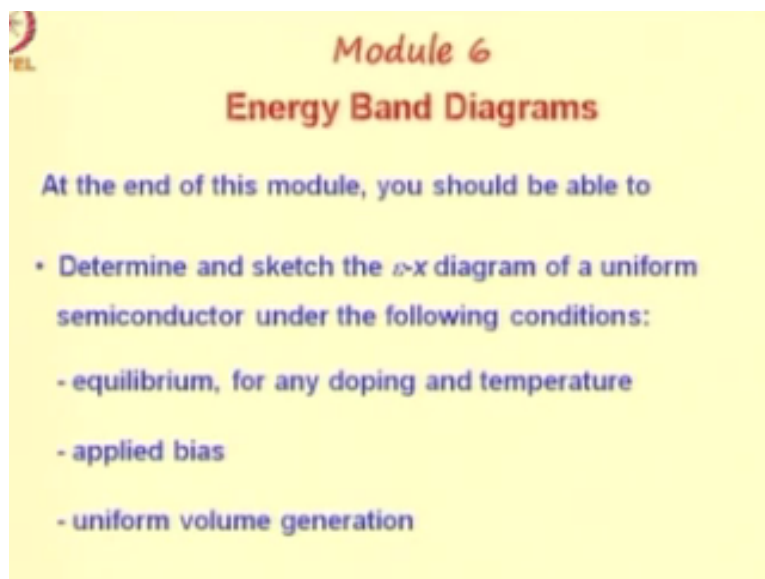
Module 6
Energy Band Diagrams

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

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 E from the E_k diagram. Sketch and Explain the E_k diagrams of silicon and Gallium arsenide.

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Module 6
Energy Band Diagrams

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

- Determine and sketch the ϵ - x diagram of a uniform semiconductor under the following conditions:
 - equilibrium, for any doping and temperature
 - applied bias
 - uniform volume generation

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 applied bias and uniform volume generation.

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Module 6
Energy Band Diagrams

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

- Determine and sketch the ϕ - 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 ϕ - x diagram of a spatially non uniform semiconductor under equilibrium, in which the doping and the composition change abruptly at a point as in a hetero junction and when the doping and composition change gradually.

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Module 6
Energy Band Diagrams

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

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

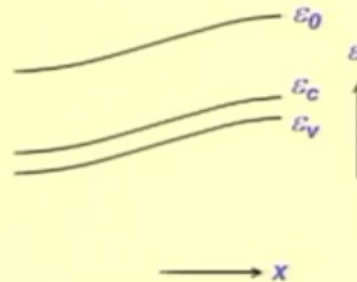
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You should be able to explain how the energy band diagram can be used to derive the Exponential increase in the diode current with forward bias. Sketch and explain the ϕ - x diagram of a p^+n junction under high forward bias and finally you should be able to sketch the 1-dimensional band diagram that is the ϕ - x diagram and interpret a 2 dimensional band diagram that is E as a function of x, y of any device.

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What is an Energy Band Diagram?

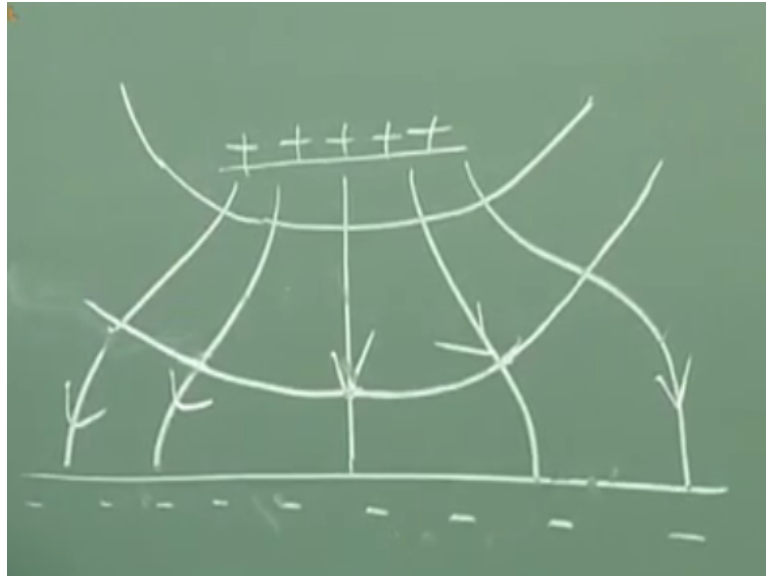
- Like the field lines of force and equi-potential lines, energy bands is a powerful concept which expresses physical conditions through a set of lines.



So, you see, we want to really develop the ability to draw and interpret band diagrams under a variety of conditions that is the goal of this module. Now, let us start with what is an energy band diagram. In the first level course on solid state devices, you have already drawn energy band diagrams for pn junction, bipolar transistor and mass effect, so whatever those like. Here is an Example, where we show E_0 as a line and in parallel with it lines E_c and E_v .

So, in this diagram the x represents the distance and the y axis is the energy. Now, you know that there can be many other lines in the band diagram such as fermi level, donor level and so on. We shall come to those lines in a moment, here we are only giving an Example of an energy band diagram and we want to appreciate what this line mean? So, like the field lines of force and equipotential lines, energy bands are a powerful concept which expresses physical conditions through a set of lines.

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So, you have already come across lines of force; equipotential lines, right. For Example, let us look at a parallel plate condition like this, where you have a small electrode here, say positively charged, so here you have positive charge and you have negative charge on this and if you were asked to draw the field lines, they would look something like this, right. These are field lines of force.

One could also draw equipotential lines here; they would be perpendicular to the field lines at any point, so you have already come across these lines. For example, this is an equipotential line; here is another equipotential line, right and so on. So, these lines indicate physical conditions within the device, so for Example if you look at this line, it tells you if I were to place a test positive charge here, and which direction would it move?

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What is an Energy Band Diagram?

- Like the field lines of force and equi-potential lines, energy bands is a powerful concept which expresses physical conditions through a set of lines.
- $E-k$ and $E-x$ band diagrams complement each other.

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It would move in this direction. On the other hand, if I place a charge here, it would move in this direction, okay and so on. So, like lines are used in this case to represent physical conditions, energy bands also consist of a set of lines, which express physical conditions. So, for example here as you know, E_c is the edge of the conduction band, so electrons which are in this band of energies participate in conduction that is why it is called as conduction band

And similarly E_v is the top edges of the valence band, now I could look at the condition at any x in the device, let us say at this x . Now, the slope of this line indicates the electric field conditions within the device, you would recall this from the first level course. You could draw another set of lines giving more information about the behaviour of electrons in a crystal. Now, this is called an E_k diagram.

So, as against an E_x diagram, where you plot allowed energies for electrons as a function of spatial distance. In this diagram, at any x such as this x , you are plotting the allowed energies as a function of what is called the momentum of the electron in the crystal. Now, this momentum is called the crystal momentum. The crystal momentum is very different from the instantaneous true momentum of an electron, which is the momentum as we understand it, right. So, we will discuss this aspect in detail later.

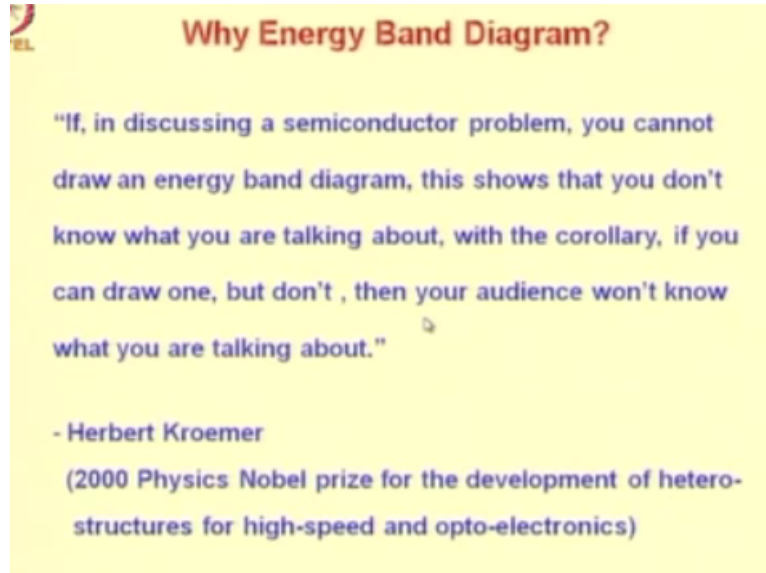
Right now, we only want to show, what the different types of lines that are indicated are; that are used in the energy band diagrams. So, at any x , E versus K could look something like this, so this represents the energy as a function of crystal momentum. Here, the minimum of this E_k line corresponds to the conduction band edge and the maximum of the E_k line over here corresponds to the valence band edge.

So, this is the behaviour of electrons in valence band, what is the energy of the electron in the valence band as a function of momentum and this line represents the energy as a function of crystal momentum in conduction band okay. So, the top of this line here corresponds to the top of the conduction band. So, we are going to discuss this aspect in more detail, right now we are presenting the set of lines, which are used energy band diagram to represent physical conditions.

The E_k and E_x band diagrams complement each other, so you need to understand both these diagrams; the E_k and the E_x diagram, right to really derive information about energies and

momentum and velocity and so on of electrons in a crystal. Now, why energy band diagram? We want to build up a motivation for understanding the energy band diagram, right, so we need to know why? We need to answer the why question.

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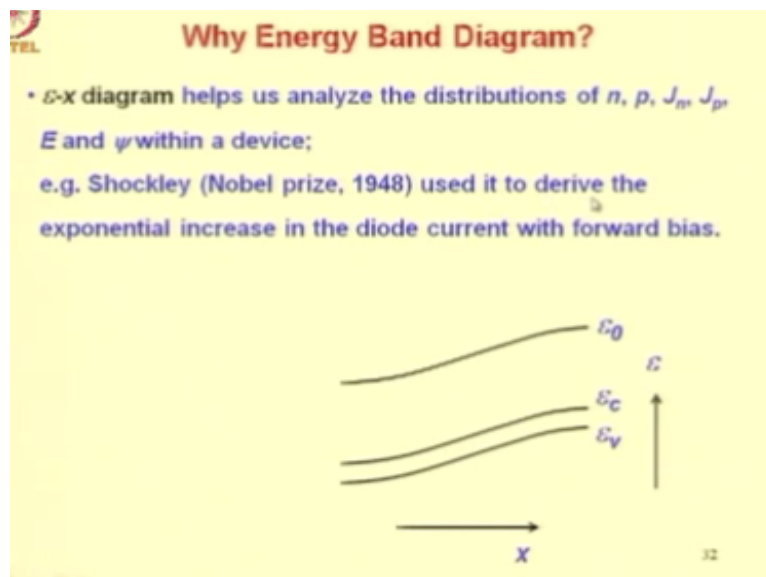
Why Energy Band Diagram?

"If, in discussing a semiconductor problem, you cannot draw an energy band diagram, this shows that you don't know what you are talking about, with the corollary, if you can draw one, but don't, then your audience won't know what you are talking about."

- Herbert Kroemer
(2000 Physics Nobel prize for the development of hetero-structures for high-speed and opto-electronics)

This is what Herbert Kroemer, who got Noble prize in 2000, for the development of hetero structure for high speed and optoelectronic applications, said about energy band diagram. If in discussing a semiconductor problem, you cannot draw an energy band diagram; this shows that you do not know what you are talking about. With the corollary, if you can draw one but do not, then your audience would not know what you are talking about.

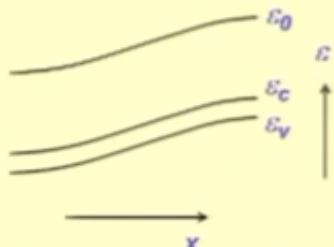
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Why Energy Band Diagram?

- \mathcal{E} - x diagram helps us analyze the distributions of n , p , J_n , J_p , E and ψ within a device;

e.g. Shockley (Nobel prize, 1948) used it to derive the exponential increase in the diode current with forward bias.



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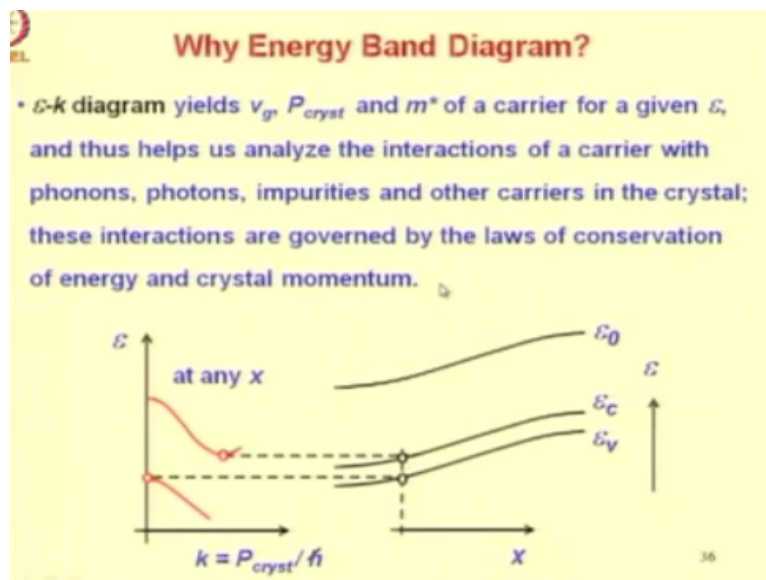
So, the energy band diagram of a semiconductor device is really very very important to understand the device operation and also to communicate your understanding of device

operation to others. Let us look at E_x and E_k diagrams separately, the E_x diagram such as the one drawn here, helps us analyse the distributions of electrons, holes, electron current density, hole current density, electric field and ψ within a device.

You recall that in earlier modules, we have said that we can understand everything about device, if you know n , p , J_n , J_p , E and ψ , as a function of space and time within a device. So, the energy band diagram really reflects the variations of these quantities, okay. Now, I must mention here that not all lines are indicated here and therefore just from these 3 lines, you would not be able to figure out all these quantities, okay.

So, we will look at this point in more detail later. Now, for example, Shockley, who win a Noble prize in 1948, used the E_x diagram to derive the exponential increase in the diode current with forward bias. So, this is an example to show how an important aspect of diode operation was analysed and concluded based on energy band diagram.

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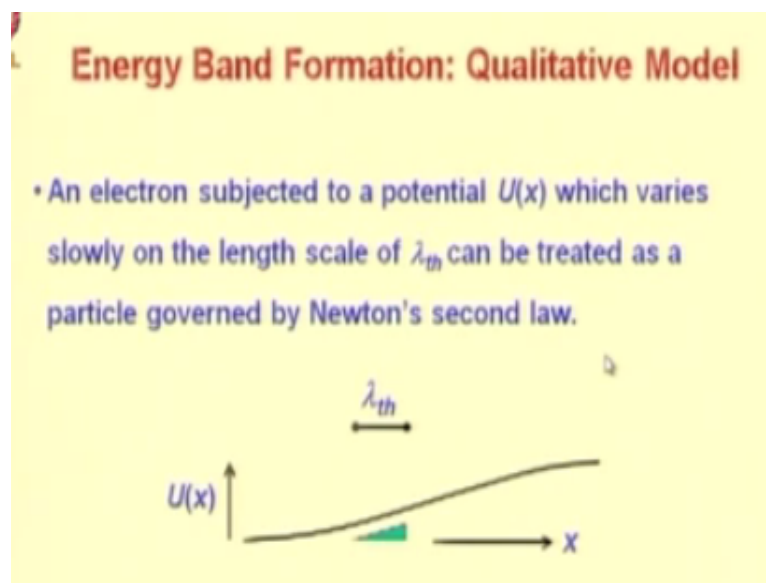
The E_k diagram, now what does this give you, now the E_k diagram gives you the group velocity, the crystal momentum and effective mass of a carrier, which can be hole or an electron for a given energy E . Now, the electron velocity in a crystal is a group velocity the electron momentum of interest in a crystal is a crystal momentum and the electron mass of interest in a crystal is an effective mass, okay.

And from the knowledge of these quantities, the E_k diagram helps us analyse the interactions of a carrier with the phonons, photons, impurities and other carriers in the crystal. These

interactions are governed by the laws of conservation of energy and momentum namely the crystal momentum. Now, so we have understood, what do we mean by energy band diagram? What kind of lines we are talking about?

Though, we did not mention about all the lines that are used in energy band diagram so far. In the first level course, you would have come across these lines, however when we discuss further, we will assume that you are not aware of energy band diagram much and now we want to develop the concept of energy band diagram from first principles, that is what we are going to do now.

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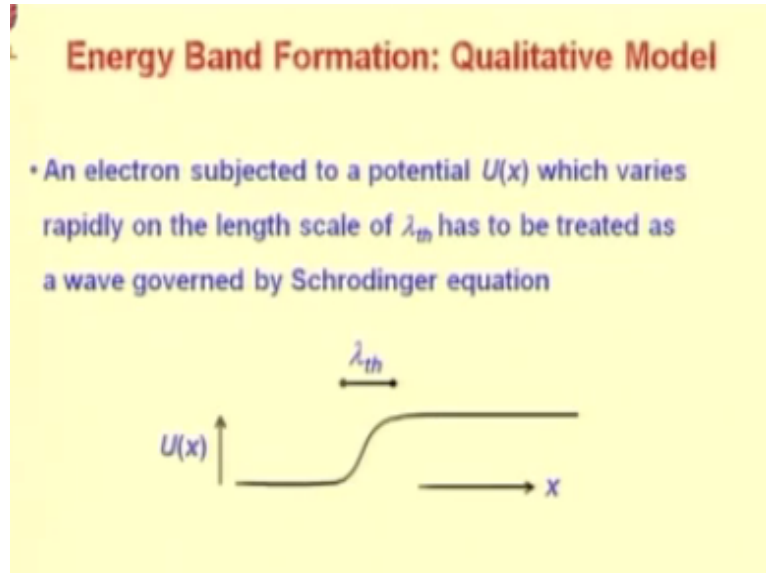


Let us start with the qualitative model, we have discussed this point that any model should first be developed qualitatively, okay and qualitative model should only follow after qualitative understanding, which involves logical reasoning without the use of any integrate equations. Now, we know that an electron subjected to a potential Ux , which varies slowly on the length scale of thermal average wavelength of an electron in a crystal.

So, here is an example of a slowly varying potential as a function of distance. Let us assume that this length represents the lambda thermal, the thermal average (()) (14:08) the wavelength of electron. The slowly varying potential would mean that over this length scale the variation is small, now this triangle indicates the amount of variation the height of the triangle; it indicates the amount of variation over the lambda thermal.

Now, this is really very small, therefore this is a slowly varying potential as a function of distance. Now, if an electron is subjected to such a potential variation, then it can be treated as a particle governed by Newton's second law.

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Now, as against this, an electron subject to potential $U(x)$, which varies rapidly on the length scale of λ_{th} has to be treated as a wave governed by Schrodinger's equation. Now, this is an example of a rapidly varying potential over the λ_{th} length scale. So, here you cannot treat electron as a particle owing Newton's laws. For instance, if an electron is coming from this side and hitting this barrier, classical mechanics would say that the electron would just rebound, right.

Whereas, quantum mechanics would give you a nonzero chance of finding an electron on the other side of the barrier depending on the width of the barrier and the height of the barrier, right. So, this is the important difference between behaviour based on wave properties and Schrodinger equation, rather than behaviour based on particle nature and Newton's laws. So, rapidly varying potentials, you have to use Schrodinger equation to treat the electron as a wave.

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Energy Band Formation: Qualitative Model

- An electron subjected to a crystal potential $U_c(x)$ which varies periodically on a length scale of $a \ll \lambda_{th}$ has to be treated as a wave governed by Schrodinger equation

The diagram illustrates a periodic potential $U_c(x)$ along the x -axis. The potential is represented by a series of regular, periodic peaks. The distance between two adjacent peaks is labeled a . The thermal wavelength is labeled λ_{th} , and it is shown to be significantly larger than a , indicating that the potential varies rapidly compared to the electron's thermal wavelength.

Now, let us come to a crystal, which is what is of interest to us, so an electron subjected to a crystal potential $U_c(x)$, which varies periodically on a length scale of A much less than λ_{th} , where A is an interatomic distance, so this is a 1-dimensional crystal in a real crystal which is 3-dimensional, A normally represents the lattice constant. So, this A is much less than λ_{th} .

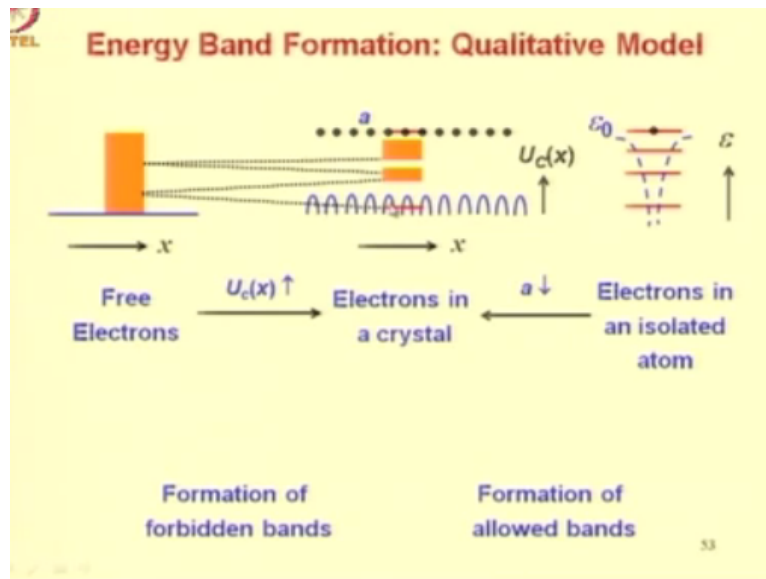
Now the way the diagram is drawn here, A appears to be less than λ_{th} but is not necessarily much less than λ_{th} . So, the diagram is not to scale, if you really made the A very small then the diagram would not be clear. Now, in this case also the electron has to be treated as a wave governed by Schrodinger equation. So, if you want to understand the behaviour of electrons in a crystal, you have to start from Schrodinger equation and not Newton's laws.

Now, I would like you to recapitulate from the earlier modules, what the crystal potential represents? So, you have a regular arrangement of atoms, each atom has a positively charged core which gives rise to this kind of a potential variation. So, a series of positively charged cores of atoms regularly arranged give rise to this potential, right periodic potential. However, there are other electrons apart from the electron that you are concentrating on.

And the effect of all the other electrons is also absorbed in this periodic potential by making an adjustment in its value, right. So, the crystal potential includes the periodic potential due to the positively charged ionic cores of all atoms adjusted to accommodate the potential of all

the electrons other than the electron that you are focussing on, right. So, this is an important point, one must there in mind.

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So, in such a case, we need to use Schrodinger equation to develop the behaviour of the electron. Now, let us see how do we develop the behaviour of electrons in a crystal. One approach is to start from electrons in an isolated atom, so in an isolated atom, your potential variation, electronic potential variation would look something like this. We have discussed this point in sufficient detail in earlier modules.

So, this is the single atom, okay location of the single atom and this is the potential due to the atom. The maximum value of the potential here is referred to as the reference potential and we call it as E_0 , also referred to as vacuum level and as you move close to the electron, the potential goes to minus infinity, okay. Now, a quantum mechanics tells us that electron in any such potential well have only discrete energies allowed, right.

The electrons can only occupy discrete energies. Now, this you already know from the many courses that you have done in physics, chemistry and may be even the solid state devices at a fundamental level, that when the electron is in a potential well, only discrete energies are allowed. Let us move on to electrons in a crystal and build up this picture from the picture of an electron in an isolated atom.

Now, the crystal is obtained by bringing in a large number of such atoms close to each other and in a regular arrangement. Now, this is what is shown here, so here are a larger number of

atoms regularly arranged, the inter atomic distance being A , so you can regard this isolated atom as a limiting case in which this A has become infinite, okay. On the other hand, you can build up a crystal by bringing together isolated atoms so that is what is indicated here.

So, as you progressively decrease inter atomic distance between various atoms, then you end up with a crystal like this from an isolated atom or a set of isolated atoms. Now how do you built up the picture here from this? Now, when you come to electrons in a crystal each allowed energy level of isolated atom spreads into a band and the energy levels which correspond to electron away from the atom spread into a wider band than the energy level which correspond to electrons, which are very close to the atom, okay.

The band width is small, now how do you explain this spreading of a level into a band which is what is shown here; well this can be readily done by applying the Pauli Exclusion Principle, okay. In an earlier module, we have explained that all of quantum mechanics related to the behaviour of solids can be explain the quantum mechanical phenomena related to solids can be explained based on just 2 things that are Schrodinger equation and Pauli Exclusion Principle.

So, when you apply Pauli exclusion principle here to electrons in a crystal, no 2 electrons can have the same energy state and therefore the electrons corresponding to all these atoms, which are very large in number in a practical crystal should all be different from each other therefore a single energy level spreads into a number of levels, right, but which are all closely spaced and therefore this appears like a band.

So, the formation of the band from a single level of an isolated atom the formation of a band of energies, allowed energies in a crystal, form an energy level in an isolated atom can be explained based on Pauli Exclusion Principle, which requires that electrons in any system cannot all have the same energy state and therefore same energy. Thus, the formation of allowed bands from an isolated atom is what we have discussed just now, okay.

So, the approach we have taken develops the allowed bands from the isolated from energy levels in an isolated atom. In contrast, you can have an alternate approach, you start from free electrons, now free electrons have a constant potential subjected to them, okay. While

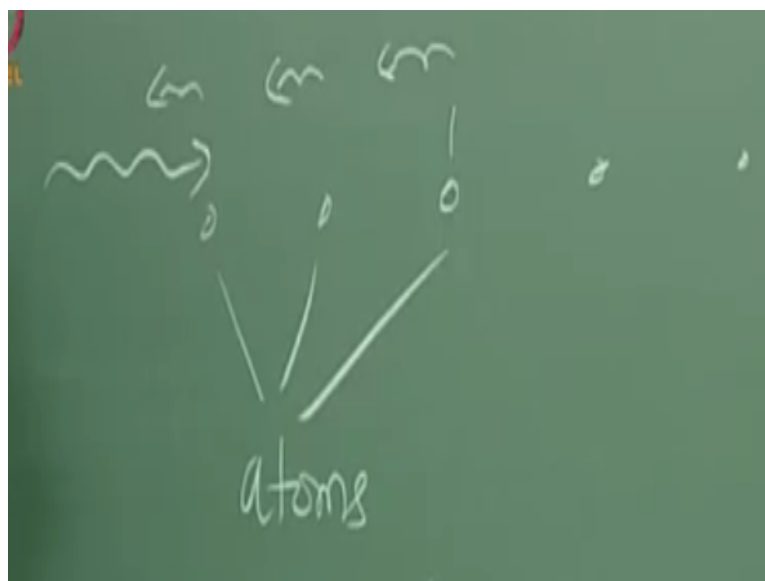
electron in an isolated atom is subjected to potential well, so these electrons are in a potential well, free electrons are in a region of constant potential.

Now, we know that for free electrons, a continuous band of energy is allowed, in contrast to electrons in a potential well which can only occupy discrete energy levels. Suppose, we subject these free electrons to a periodic potential, $U(x)$, now the constant potential can be viewed as a limiting case of $U(x)$ becoming 0. So, this periodic potential as its height becomes 0, it becomes the constant potential, okay.

And therefore, the movement from free electrons to electrons in a crystal can be seen as a case of increasing the periodic crystal potential from 0 to a finite magnitude that is what is seen here. Now, once you have the periodic potential here, then you get what are called forbidden band, certain energy levels are not allowed. So, while for a free electron all energies are allowed for electrons in a crystal, certain bands of energies are not allowed.

Now, how do we come to the conclusion that any crystal certain energy bands will be forbidden for electrons. Now, this can be understood from the wave nature of electrons as follows. When an electron is subjected to a periodic potential, the electron wave gets reflected from each of these atomic locations by the periodic potential. Now, the incident wave and the reflected wave from each of the atoms sum together can destructively interfere with each other for certain wave lengths, okay.

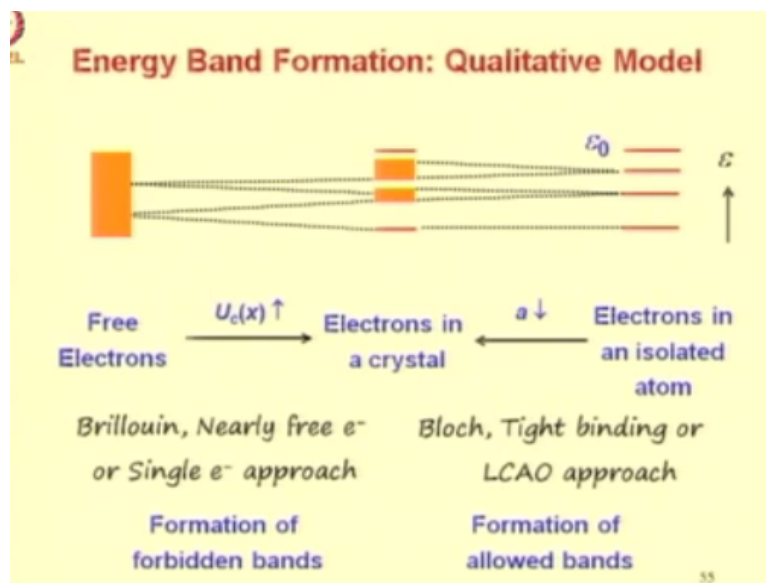
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So, it is something like this, so you have these atoms and you have an incident electron wave and you have a reflected wave from each of this like this. Now, this reflected wave and the incident wave can destructively interfere with each other and therefore they will cancel each other, in other words, for certain wave lengths, no electron wave can exist because of the presence of these multiple atoms and the periodic potential associated with these, which will reflect the electron wave, right from the location of these atoms.

Normally, this is refer to as blurred reflection, okay. Now, when the reflected an instant wave interfere destructively, the wave cannot exist. For all such wave lengths for which the wave cannot exist, okay, the energy associated with the wave is therefore is not allowed. So, one find out those wave lengths which will depend on the interatomic distance of the crystal and find out the energies corresponding to those wavelengths and those energies therefore will not be allowed as electrons with those energies cannot exist in the crystal.

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And that is how you get forbidden bands of energies. So, this is the simplified diagram representing the formation of allowed bands from allowed energy levels in isolated atom or formation of forbidden bands from a continuous band of allowed energies of free electrons, okay. Now, these 2 methods; that is formation of forbidden bands and formation of allowed bands are referred to as follows.

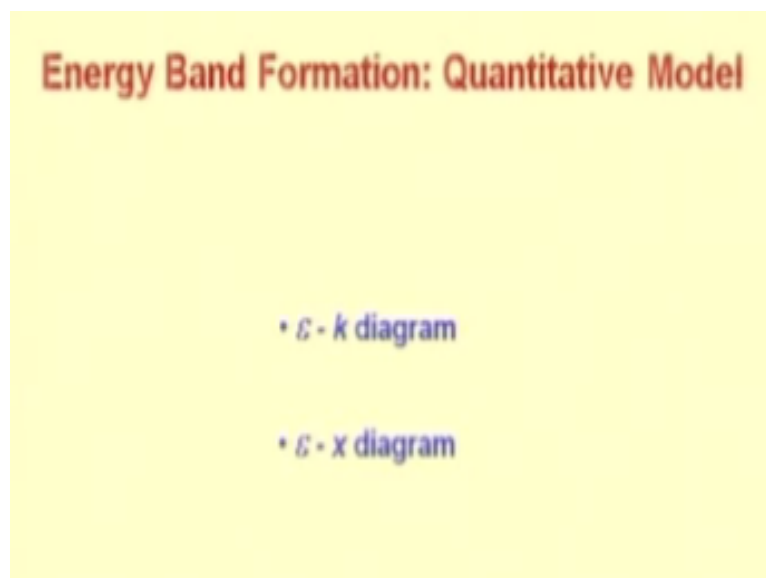
So the formation of forbidden bands from the picture of a free electron the continuous energy levels of a free electron is referred to as Brillouin, nearly free electron or single electron approach. On the other hand, the formation of allowed bands from energy levels of an

isolated atom is referred to as the Bloch, tight binding or LCAO approach, where LCAO stands for linear combination of atomic orbitals, okay.

The wave functions of individual atoms are referred to as atomic orbitals and linear combination, so you superpose these wave functions to get the picture of a crystal, okay where you have a number of atoms. So, consider the wave functions of every atom associated with every atom and you superpose them, and then you get the picture for a crystal. So, this approach is referred to as LCAO approach.

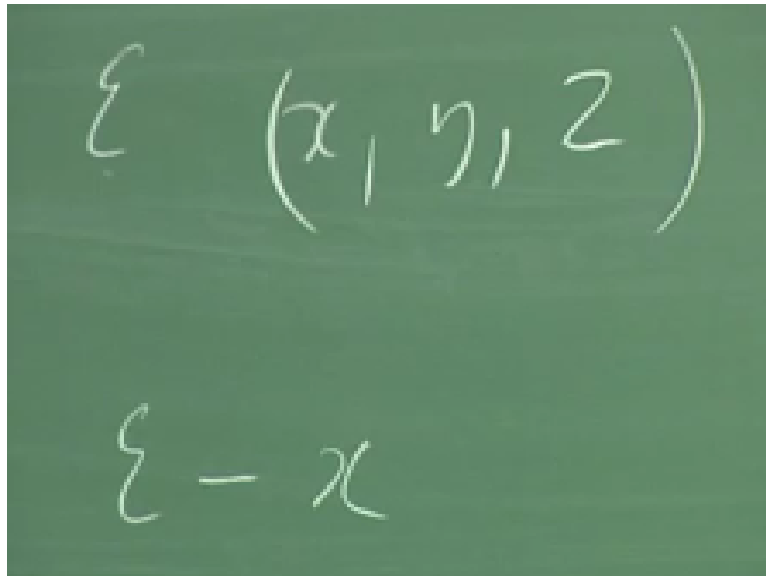
So, Bloch is the name of a scientist and so is Brillouin; the scientist Brillouin proposed the formation of forbidden bands from picture of a free electron and the scientist Bloch proposed the formation of allowed bands from allowed levels of an isolated atom. So, both these approaches can be used and they have their own advantages.

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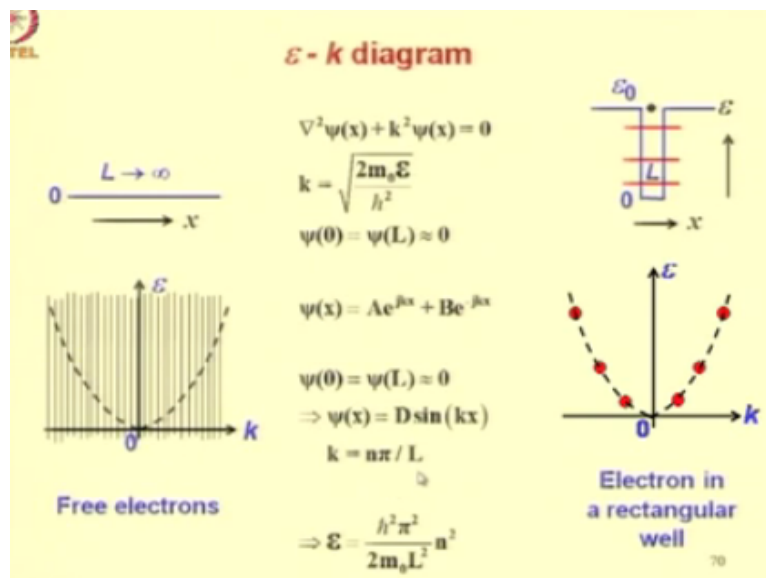
Let us now come to a quantitative model of energy band formation, after a qualitative model, we discussed the quantitative model. Now, in this we will consider 2 separate types of band diagrams namely; the allowed energy bands as a function of distance that is called the Ex diagram, when you consider one-dimension right.

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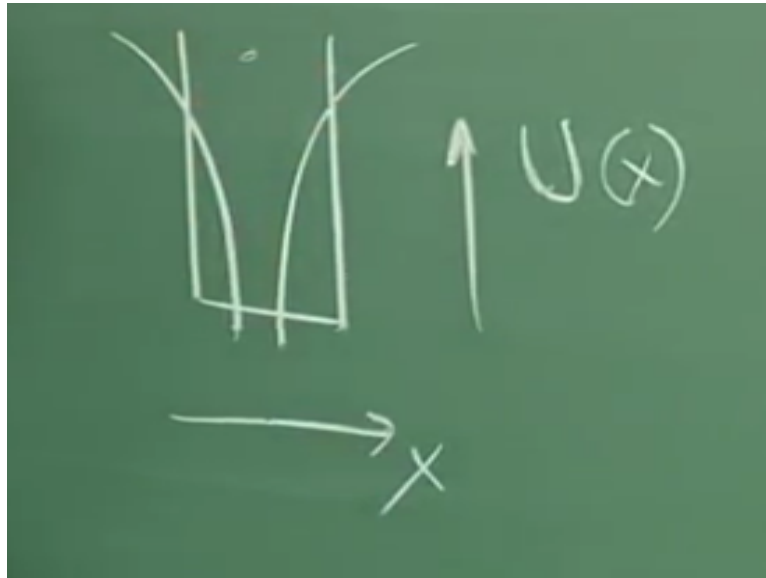
So, E_x, y, z so allowed energies as a function of space; spatial variation of allowed energies, right. This is the one type of band diagram. Normally, we call it and abbreviate it as just E_x diagram because most cases we consider the diagram in one dimension and the other diagram is the E_k diagram, okay. The allowed energies as a function of the wave vector, the k ; the symbol k stands for wave vector and from the wave vector; one can get the momentum of electron in crystal.

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The appropriate momentum that is called the crystal momentum, which we will discuss in detail shortly. Let us start with the E_k diagram, how do you develop the E_k diagram? Consider an electron in a rectangular well, for an Example, because we are considering the quantitative model, we have simplified the actual potential picture of electron in an isolated atom; the actual picture is something like this, right.

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We have drawn U , a potential in electron; electronic potential as a function of distance, it looks like this. Now, the mathematics of solving the Schrodinger equation for this kind of potential is little more complex than that if I approximate this by a rectangular potential well and so since we want to keep our mathematics simple, we are going to use a rectangular potential well to represent the picture in an isolated atom.

Now, this well has a height E_0 , so the bottom of the well is potential 0 and the height is E_0 , will assume that this height is fairly large, and so that you can approximate this well to be an infinite well and the width of this is well is L . Now, how will you find allowed energy levels? You will solve a Schrodinger equation, so Schrodinger equation comes out in this form, because the potential energy U is 0.

The simple form of the equation is; $\nabla^2 \psi + k^2 \psi = 0$, where k^2 is related to the energy E , potential U is 0, so only the energy E of the electron enters into this picture. So, the $k = \sqrt{2mE}$, where m is the electron mass into the energy of electron divided by h^2 , where h is the Planck's constant. Also, whenever we are solving an equation, you need to construct the boundary conditions apart from the equation.

So, the boundary conditions here are that the wave function ψ is approximately 0 at both $x = 0$ and $x = L$, that is the wave function goes to 0 at this end as well as this end. Now, we are saying approximately 0, because the height of this well is not really infinite, it is large but not

infinite, okay, that is why the approximate sign here. When it is infinite, it will be exactly 0, okay. So this equation has to be solved subjected to this boundary condition.

And this boundary condition is very very important because as we will see, it is the boundary condition, which says that the wave function should go to 0 at the 2 ends of the well, which gives rise to quantisation of energy and momentum. So, the wave function solution for the simple differential equation is $\psi(x) = A \cdot e^{jkx} + B \cdot e^{-jkx}$, okay; this simple second order differential equation.

One can easily see by substitution that if you have an exponential with the complex Exponent then when you double differentiate okay, you will get the form of $\psi(x)$ and the forms of $\Delta^2 \psi(x)$ to be similar but opposite in sign, so that you know you will get the sum of these to be 0. The complex exponent can be either positive or negative, since you have 2 boundary conditions, you have 2 coefficients here.

Now, you can get A and B from the boundary conditions and the result will be that $\psi(x)$ is given by a constant $D \cdot \sin(kx)$, where kx is coming in the exponent here, okay and the k is related to the energy of the electron as given in this formula, okay and this k is coming here in the coefficient of the wave function in this Schrodinger equation. Now, the boundary conditions $\psi = 0$ and ψ at 0 and ψ at $L = 0$ will be satisfied, if the k here is the integral multiple of π/L .

Now, this can be easily understood, right, from all the courses that you have done, so I do not need to spend time in explaining this fact. Now, this is where the quantisation of energy is coming about, so only certain values of k are allowed, these are integer multiples of π/L , note that though the wave function satisfies the boundary conditions with $n = 0$; $n = 0$ is not a solution, this is because for $n = 0$, k is 0 and the energy is also 0, which means that $n = 0$ corresponds to a stationary electron, which is physically not acceptable for our problem.

Now, this is the quantisation aspect coming in as a solution of Schrodinger equation, okay and this is what is going to give you the quantisation of energy because the k the so called wave vector is related to the energy E by this formula, so if k is quantised, the E also is going to be quantised. So, the quantisation of k is what is represented here, let us say this is the k axis and this represents the 0 value corresponding to $n = 0$.

So, n can be 0, -1, -2, -3, and so on the negative side and positive side; 1, 2, 3, 4 and so on, right. So, that is what we mean when you say n is an integer, so that is why we have shown discrete points of k on both positive as well as negative side of k. Now, putting these value of k here in this equation, we can get an expression for E as a function of k and that would be $E = \frac{h^2 k^2}{2m_0 L^2} n^2$, where they already use the value of k, okay.

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$$E = \frac{h^2 k^2}{2m_0 L^2}$$

$$p = \hbar k$$

If you want to write the Ek relation, well it is just the inverse of this, with the square root sign removed. Let me write that on the board, so $E = \frac{h^2 k^2}{2m_0 L^2}$, that would be the Ek relation and this you substitute for k, so this $k = \frac{n\pi}{L}$. So, the allowed energies E given by this equation are represented here, okay for different values of n. Now, since E as a function of k is a parabola.

That parabola is what is indicated here with the dotted line and the discrete points of this parabola, which are obtained by intersection of these vertical lines showing the discrete values of k given by his formula, okay, represent the allowed energy states of the electron. These are the allowed energies, the points of intersection, so this formula when plotted on a graph would look like this set of points, okay shown here by red dots.

So, I removed the lines to clear the figure to indicate the discrete values of energy and momentum, which are allowed for electron in a rectangular potential well. So, this is the Ek diagram, okay of electron in a rectangular potential well, where this k represents the wave

vector or it can be used to represent the momentum. So $\hbar \mathbf{k}$; quantity $\hbar \mathbf{k}$ is like the momentum of the electron \mathbf{p} .

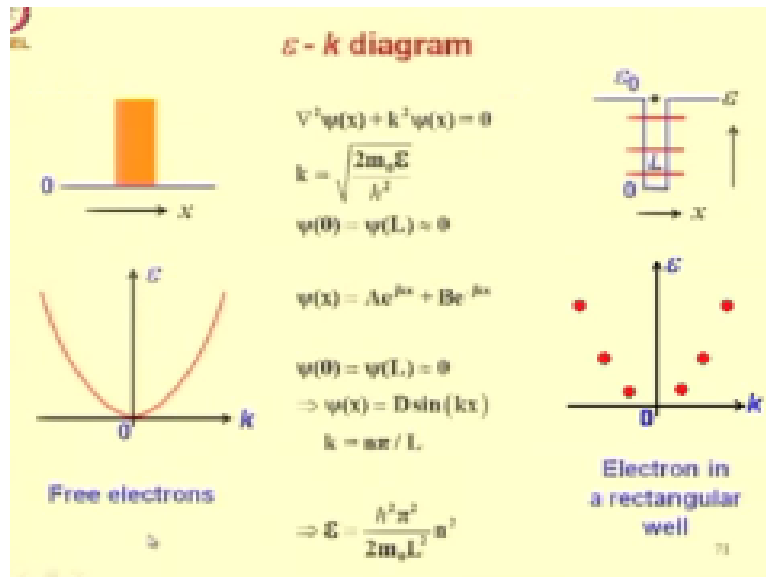
And therefore this can be regarded as energy momentum relationship, okay. You can easily check that $\hbar \mathbf{k}$ has a dimension of momentum. Now, if you want to understand this picture physically, what it means is the electron is moving in this well, in this 1-dimension with some velocity and it is bouncing off the walls, right. So, the speed of the electron remains the same as it is oscillating and bouncing off from the walls, right.

And the energy and momentum associated with this, is what is indicated here. So, if the electron has a high energy, it would be moving rather fast and bouncing off more frequently from the walls, right and for the lower energy this would happen slowly. Now, let us look at the picture of free electrons, now this picture can be regarded as corresponding to the picture of an electron in a potential well of width L going to infinity, okay.

When L tends to infinity, the picture is that of a free electron. Now, let us see what happens to these formulae, when you put L tending to infinity, so clearly as L becomes larger and larger, your k values which are allowed start coming closer and closer because π/L becomes smaller and smaller, okay. Now, this is indicated here that a large number of k values, which are allowed will appear on the k line.

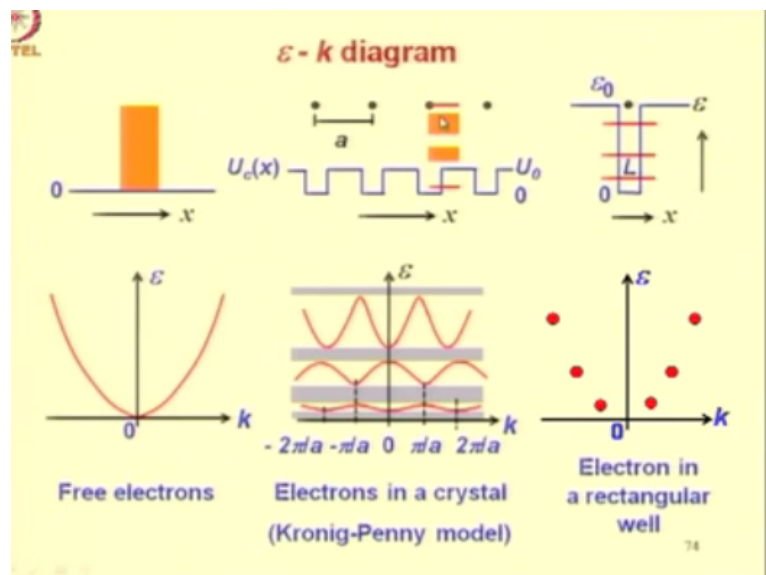
And the distance between these k values will start coming closer and closer as L becomes large and in the limit L tends to infinity, it will become a continuous line, okay. Whereas, here the k was discrete, when L was non infinite or finite. Now, again you put the relation between energy and momentum, the parabolic relation, this is this line and the points on this line which are intersecting with these vertical lines tell you all the allowed energies.

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And in the limiting case of L tend to infinity is entire line would be allowed, right and that is what is shown here. So, E_k diagram, the E_k relation becomes a continuous line for a free electron as L tends to infinity, this picture can be obtained from, this picture of discrete points. This point all start getting very close to each other and they become a continuous line and therefore allowed energies also start coming very close to each other and become an allowed band.

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Now, this is; what is shown here. Now, we shall just introduce the picture for electrons in a crystal and stop this lecture and we will develop the picture in the next class. So, let me introduce a picture of electrons in a crystal, so in a crystal you have a periodic potential that is approximated here by this rectangular $U(x)$ line, this is called; the symbol for this is $U_c(x)$, the crystal potential, it is an approximation of the crystal potential.

Now, here we will assume that the maximum value is U_0 and the minimum here is 0, the inter atomic distance is a , now if you solve a Schrodinger equation for such a periodic potential, then we will find this kind of an interesting E_k behaviour, here you have forbidden energy bands as shown by these shaded lines. This should not be surprising because you did come across forbidden energy regions here.

However, you have allowed energy bands rather than levels, okay. So this entire band of energies is allowed and within the band, their behaviour of energy verses momentum is periodic, okay. So, these are the features of this E_k diagram, so E as a function of k is periodic then there are certain bands of energies which are not allowed and certain bands of energy which are allowed.

So, you have alternatively located allowed and forbidden energy bands and another important thing is for any given k , you have multiple values of energies allowed, whereas if you see here for Example, for any k , there is a single value of energy, right. For given value of energy, of course, there are 2 values of k ; one in the positive side, other in the negative side, right. But for any given k , there is only one energy, same if true for the free electron.

For any given k , there is only one energy, but if you come here for any given k , there are multiple energies allowed okay. So, periodicity of p verses k , E being a multiple function of k , multivalued function of k and Existence of alternatively located allowed and forbidden energy bands. These are the features of the E_k diagram in a crystal, which we shall develop in the next class.

This model is referred to as Kronig Penny model after the scientist, who proposed the above solution for E_k diagram, okay and the location which define the periodicity of E_k are related to the inter atomic distance a , that is given here, okay. So, we will develop these features in the next class. Now, before we close we just show the allowed and forbidden energy bands existing alternatively here.

So, this is an allowed band, which is very thin followed by a forbidden band, now below this you have a forbidden band, now this is an allowed band followed by forbidden band here, then allowed band and so on. Let us make a summary of important points of this lecture. So,

we have pointed out that like the field lines of force and equipotential lines, energy band diagrams also consist of a few lines which represent very vividly and in a best possible manner the various physical conditions in a device.

It is a very important diagram used in the analysis of devices, so the 2 types of band diagrams are the E_x diagram, where you plot allowed energy levels or energy bands of electrons in a crystal as a function of distance and the E_k diagram, where you plot at any location in the crystal at any x , for example the allowed energy as a function of the crystal momentum of the electrons.

So, normally the crystal momentum is represented in terms of the wave vector k and therefore this is called the E_k diagram. The E_x diagram helps us to analyse the electron and hole distribution; the electron and hole current density distribution and electric field and potential distributions in the device as a function of space and time. On the other hand, the E_k diagram helps you to derive the velocity, mass and momentum of the electron, which are referred to as group velocity, effective mass and crystal momentum.

Now, this information is important because the interaction of electrons with other carriers, impurities, phonons, photons etc, are governed by the laws of conservation of energy and crystal momentum. So, one can study the behaviour of these interactions based on the E_k diagram. We developed a qualitative model for the energy band formation. 2 approaches were discussed; one approach called the Brillouin approach the nearly free electron approach or the single electron approach.

It consists of developing the allowed band picture of electrons from the picture of a free electron. For a free electron, the entire band of energies varying continuously is allowed, moment you introduce a periodic potential and subject the electron to this periodic potential, then certain bands of energies become forbidden. So, the formation of forbidden bands is what is the; characteristic of Brillouin, single electron or nearly free electron approach.

The formation of forbidden bands was explained based on Bragg reflection of the electron wave from the various atomic locations in a crystal and destructive interference of the reflected waves and the instant waves, okay. So, certain wavelengths are not allowed for

electrons, they do not exist in a crystal and the allowed and the energies corresponding to this wavelengths also cannot exist and that is how you talk about formation of forbidden bands.

On the other hand, another approach called the Bloch tight binding or linear combination of atomic orbitals approach; here you develop the picture of electron in a crystal from the picture of electron in an isolated atom. So, in an isolated atom, you have discrete allowed energies for electrons. Now, when you bring together a number of atoms to form a crystal, we apply the Pauli Exclusion Principle to this system which says that, no 2 electrons can have the same energy.

And therefore the electrons of all the various atom should have different energies. In this manner, a discrete energy level of electrons in an isolated atom spreads into or splits into a number of levels for electrons in a crystal consisting of many atoms and since this levels are very close to each other because the number of atoms is very large, we refer to this group of closely spaced energy levels as a continuous band of allowed energies.

So, formation of allowed bands is the characteristic this Bloch tight binding or LCAO approach. After developing the allowed or forbidden band picture for electrons in a crystal in a qualitative manner we then went on to discuss quantitative model for the energy band picture. The quantitative model can be split into 2 parts; a model for the E_k diagram and the model for the E_x diagram.

Now, we began with the model for the E_k diagram in which we first develop the E_k picture for electron in a rectangular potential well based on the Schrodinger equation and we showed how application of the boundary condition on the wave functions solution results in formation of discrete allowed k vectors for the electrons and therefore the state allowed energies.

And the E_k relation is parabolic but only certain case are allowed and therefore only certain E is get allowed, so the E_k diagram of an electron in an isolated atom or electron in a rectangular potential well is a set of discrete points all falling on a parabola, which talks about the parabolic relationship between E and k . Next, we showed that the limiting case of this rectangular potential well is the free electron picture.

Where if you assume the width of the rectangular potential well to go to infinity, you get the picture of a free electron where all the various points on the EK diagram move very close to each other and become a continuous line and therefore a continuous parabola for E as a function of k is the picture of electrons in constant potential or free electrons. Then finally we introduced the picture of electron in a periodic potential.

And we said that we will develop this picture in detail in the next class and this picture was that the E versus k relation for electrons in a periodic potential is periodic in k is multivalued for a given k , so you have many energies for the same k and you have an alternate arrangement of forbidden and allowed band of energies. So, we shall continue in the next class from this point onwards.