Semiconductor Devices and Circuits
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Lecture- 05
Solids: Kronig-Penny Model - Continued

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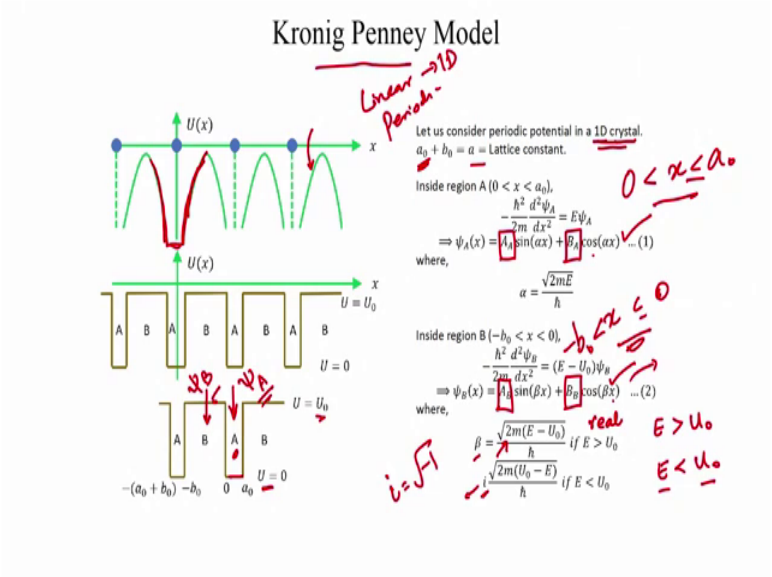

Kronig Penney Model

Linear → 1D Periodic

Let us consider periodic potential in a 1D crystal.

$a_0 + b_0 = a =$ Lattice constant.

Inside region A $(0 < x < a_0)$, $0 < x \leq a_0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_A}{dx^2} = E\psi_A$$

$$\Rightarrow \psi_A(x) = \boxed{A_A}\sin(\alpha x) + \boxed{B_A}\cos(\alpha x) \quad \dots(1)$$

where,

$$\alpha = \frac{\sqrt{2mE}}{\hbar}$$

Inside region B $(-b_0 < x < 0)$, $-b_0 < x \leq 0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_B}{dx^2} = (E - U_0)\psi_B$$

$$\Rightarrow \psi_B(x) = \boxed{A_B}\sin(\beta x) + \boxed{B_B}\cos(\beta x) \quad \dots(2)$$

where,

real

$$\beta = \frac{\sqrt{2m(E - U_0)}}{\hbar} \text{ if } E > U_0$$

$$i\frac{\sqrt{2m(U_0 - E)}}{\hbar} \text{ if } E < U_0$$

$E > U_0$

$E < U_0$

$i = \sqrt{-1}$

So, now in order to make the definitions of these wave functions psi of A and psi of B much more specific, we need to identify these four coefficients. What are A of A; B of A; A of B; and B of B? So, the moment we identify these four coefficients, we can clearly identify psi of A and psi of B. And how do we identify these four coefficients? We need four boundary conditions. So, what are these boundary conditions?

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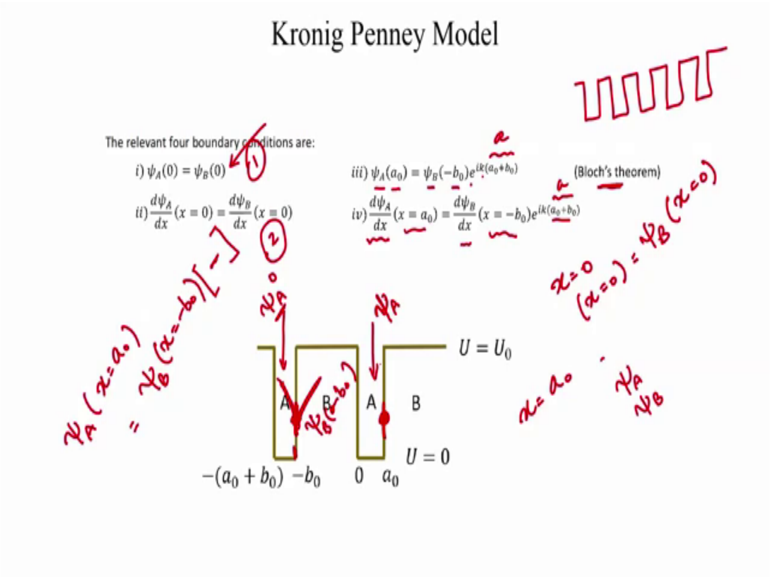

Kronig Penney Model

The relevant four boundary conditions are:

i) $\psi_A(0) = \psi_B(0)$

ii) $\frac{d\psi_A}{dx}(x = 0) = \frac{d\psi_B}{dx}(x = 0)$

iii) $\psi_A(a_0) = \psi_B(-b_0)e^{ik(a_0+b_0)}$ (Bloch's theorem)

iv) $\frac{d\psi_A}{dx}(x = a_0) = \frac{d\psi_B}{dx}(x = -b_0)e^{ik(a_0+b_0)}$

So, you might be familiar with two of these boundary conditions. The first boundary condition is that of the continuity of the wave function. So, since if you look at point x equal to 0, at x equal to 0, the wave function psi of A, the amplitude of the wave function psi of A, at x equal to 0; must have the same values the amplitude of the wave function psi of B, at x equal to 0. So, these two amplitudes should be the same. And, therefore psi B at x equal to 0 must be equal to psi of A at x equal to 0, so that is the first boundary condition.

The second boundary condition is that not only is the wave function continuous, but the derivatives of the wave functions, but all also be continuous ok. So, therefore d psi of A by d x, and d psi of B by d x at x equal to 0, must have the same value ok, so that is the second boundary condition. Now, the next two boundary conditions may not be may not be very familiar ok. And the arise from something called as Bloch's theorem, and which is applied when you have a periodic arrangement or a periodic potential profile. So, when you have an infinitely periodic potential profile, they can use something called as Bloch's theorem.

And what does Bloch's theorem? Now, since these two regions that is A and A here ok, are essentially twins nature does not make any that is not distinguish between, where these coordinates occur. In other words, see this choice of the origin is completely arbitrary, we chose this we define this origin to be here. And, we therefore defined psi of

A to exist here, and psi of B to exist here. But if he just translate this entire potential profile by one period, which is by one lattice constant. This potential well would exist here. And therefore that potential well would then start having this wave function psi of A ok.

So, therefore the wave function in this potential well must be related to the wave function in this potential well. And the wave function here is psi of A. And this relation is brought out by Bloch's theorem. So, what Bloch's theorem tells us is let us take the wave function the value of the wave function at this point at x equal to a naught. So, let us look at this point x equal to a naught. Now, this edge and this edge are twins. And therefore the values of the wave function at this point, and the value of the wave function of this box, at this point must have the same amplitude.

So, let us let say to make this clear. Let us call this as psi A, and let us call that as say some psi A naught. So, what Bloch's theorem tells us is that psi of A at x equal to a naught that is at this location is related to the value of the wave function, psi A naught at x equal to minus b naught at this location, at this right side boundary by a certain multiplication factor ok. And that multiplication factor is e to the power i k a; where a is your lattice constant; and k is a coefficient that represents the wave, and wave vector ok.

Now, it is not necessary for us to define this new wave function psi A naught, because the value of psi A naught at x equal to minus b naught is exactly the same as the value of psi of B at x equal to minus b naught, because of the continuity of the wave functions in this edge. And therefore, we can replace psi A naught at x equal to minus b naught; by psi B at x equal to minus b naught.

And, therefore the Bloch's theorem says it provides the relation between the wave function here; and the wave function here. And it says that psi A at a naught is equal to psi B at minus b naught into e to the power i k a naught plus b naught, which is the lattice constant. And this relation also holds true for the derivatives, d psi A by d x at x equal to a naught is equal to d psi B by d x at x equal to minus b naught into e to the power i k a. And, now using these 4 boundary conditions, we can we can now solve for psi A and psi B and obtain a wave function that is much more accurate. And then we can go ahead and start calculating energies. And all the other attributes of the wave particle that exists in this periodic potential well.

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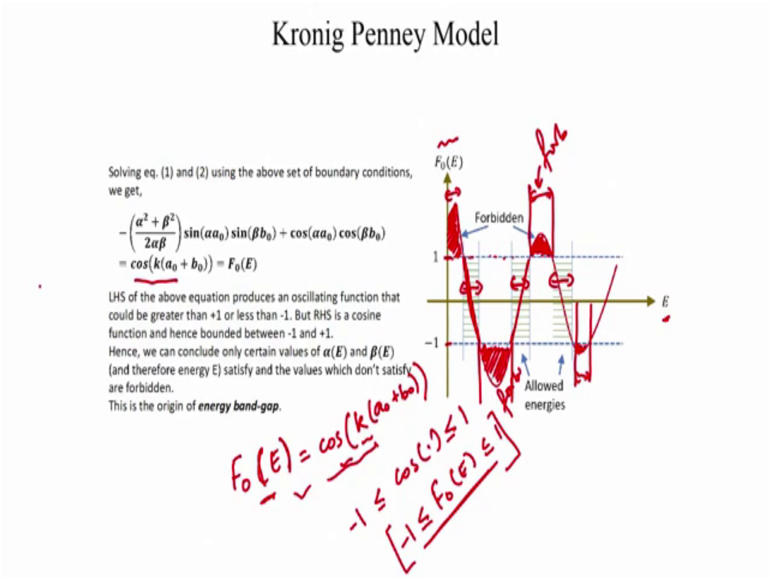

Kronig Penney Model

Solving eq. (1) and (2) using the above set of boundary conditions, we get,

$$-\left(\frac{\alpha^2+\beta^2}{2\alpha\beta}\right)\sin(\alpha a_0)\sin(\beta b_0)+\cos(\alpha a_0)\cos(\beta b_0)$$
$$=\underbrace{cos}\big(k(a_0+b_0)\big)=F_0(E)$$

LHS of the above equation produces an oscillating function that could be greater than +1 or less than -1. But RHS is a cosine function and hence bounded between -1 and +1.

Hence, we can conclude only certain values of $\alpha(E)$ and $\beta(E)$ (and therefore energy E) satisfy and the values which don't satisfy are forbidden.

This is the origin of ***energy band-gap***.

$F_0(E) = \cos(k(a_0+b_0))$

$-1 \le \cos(\cdot) \le 1$

$\boxed{-1 \le F_0(E) \le 1}$

Now, upon solving these linear equations, and after calculating these coefficients, we will end up with the relation of this sort ok. I have not shown you the details here, but we will end up with the relation of this particular form. So, you have a large term here, and this term comprises of terms like alpha; beta; a naught; and b naught. Now, alpha and beta are both functions of energy.

So, if you go back here, we see that alpha is a function of energy, and beta as a function of energy. So, alpha and beta are functions of energy; a naught is the width of the potential well; b naught is the width of the potential barrier. And, therefore this entire term in brackets is a pure function of energy, which is denoted by this function F naught of E. So, we will define a function F naught of E, which is basically this expression here and it is a, it is a function of energy. And, now that function has to be equal to this particular term here, so we have F naught of E being equal to cosine k a, which is a naught plus b naught, where k is the wave vector. So, we have this particular relation.

So, we first so what does this tell, so let us first sketch F naught of E versus energy. So, we have here a plot of F naught of E versus energy E. And that curve would look like there is a red curve here ok, to trace this particular path. But then the nature imposes a limit on F naught of E, and what is that limit, it says that F naught of E must be equal to this cosine of k a naught plus b naught. And, therefore since a cosine function cannot be greater than 1 or less than minus 1. F naught of E is also bound by these limits, it cannot be greater than 1 or less than minus 1, so this is the limit imposed by nature.

So, nature says that the electrons in this linear arrangement of atoms must obey this condition that F naught of E must be less than 1 less than or equal to 1, and must be greater than or equal to minus 1. And, therefore this purely mathematical function is now bound by these 2 bounds ok, so it says here is the bound by the bound of 1, and here is minus 1. And, therefore nature allows the electrons to only exist take up values of F not of E, which are these values, which are inside these bounds.

And all these places, where F naught of E exceeds 1 or goes below minus 1 are all forbidden ok. So, the electrons cannot take up values of F naught of E of this kind. Or in other words; if you look at the energy axis the electrons are forbidden, from taking these particular energies, because, these particular energies permit F naught of E to go above or below plus 1 or minus 1 respectively. So, these energies are all forbidden. And the electrons are only allowed to take these energies, where F naught of E stays within these bounds ok. So, we see that from a very simple mathematical relation, we see the enforcement of the discretization or the presence of energy gaps occurring in a, in a linear arrangement of atoms.

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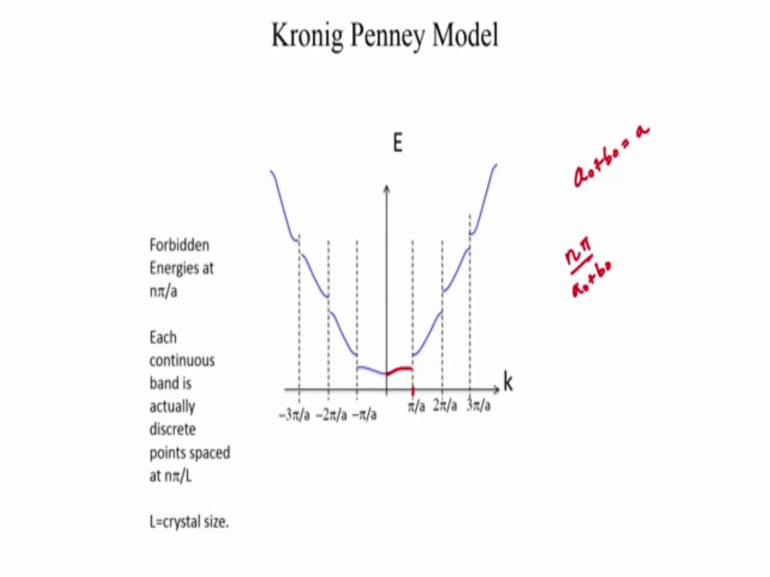

Kronig Penney Model

Forbidden Energies at nπ/a

Each continuous band is actually discrete points spaced at nπ/L

L=crystal size.

$a_0+b_0=a$

$\frac{2\pi}{a_0+b_0}$

So, if we were to now plot E versus k ok, so we saw that F of E is equal to cosine k a naught plus b naught, and a naught plus b naught is equal to a. And if you were to plot this plot of E versus K, we would end up with a plot looking like this ok. So, here these little blue curves are all a very finely spaced energies, it's almost continuous energies ok. And the electrons are only allowed to occupy these energies. And these little S shaped stitches, if I may use the term are the energy levels the electron is allowed to occupy. So, then electron is allowed to occupy these energy levels, the electron is allowed to occupy these energy levels and so on.

But, at these boundaries when k takes a value of an integer times pi by the lattice constant, at those boundaries, you find that there is a sudden jump in energy, there is a discontinuity. So, the electron can take all these values, but then beyond this it has to jump into the next set. So, you see these discontinuities that keep occurring at these points, and this is the presence of an energy gap or the location of an energy gap, now and these are the forbidden energies.

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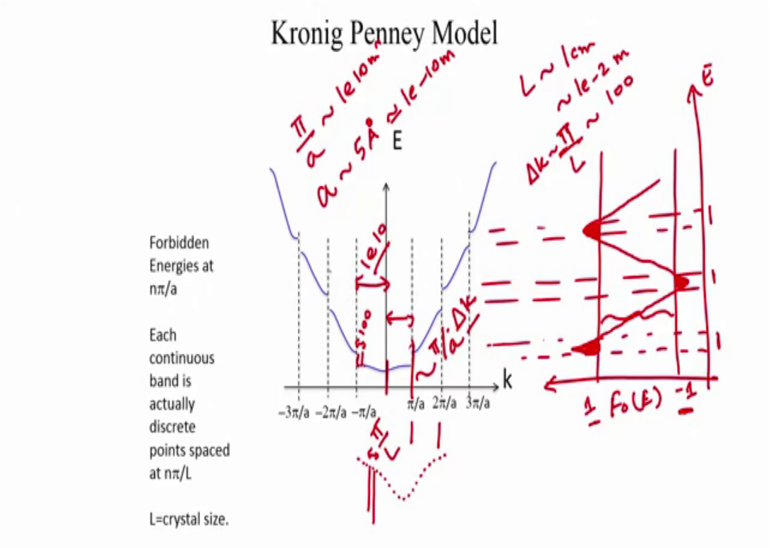

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So, if you want to imagine this better, let us also plot energy versus F naught of E, the plot of energy versus F naught of E. So, let us plot let us plot it sideways F naught of E versus energy. So, we are looking at the same plot that we discussed here, but we just plotting it sideways. And let us just draw little dotted lines corresponding to these jumps and energy. And here once again let us place our bounds of plus 1 and minus 1. So, we find that the places, where these jumps occur are the exact same spots, where F naught of E crossed these bounds etcetera.

So, we found that F naught E, F naught of E was taking all sorts of values, and nature permitted F naught of E to only exist in within these bounds imposed by minus 1 n 1. And it is at these energy points or these energy levels that F naught is E crossed these bounds. And, therefore nature does not permit the electrons to take up those energy levels. And, therefore you see these gaps occurring at these points in K, which is an integer times pi by a, so that is the first aspect that comes out from this discussion.

The second detail is that if you look at one of these blue curves ok, they appear to be very continuous, because, I have drawn it in a very continuous manner. But, in fact they are composed of very tiny points or tiny energy values that the electrons could take up ok. And what are these tiny values, these tiny values are the discreteness that came about, because of the larger box the electrons were occupying.

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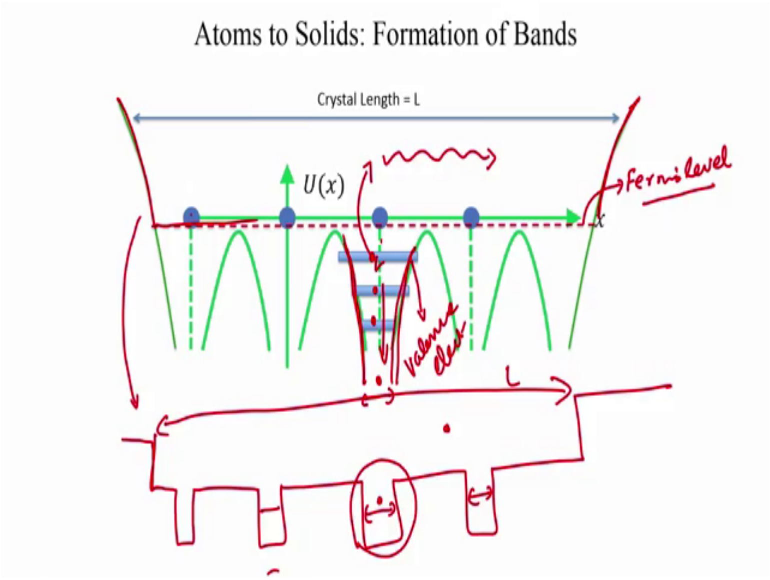

Atoms to Solids: Formation of Bands

So, let us go back to our discussion here. So, we saw that the electrons were seeing two potential wells. So, the electrons that were still held by the atom were seeing this potential well given by a Kronig Penny model, but the electrons that had escaped the clutches of the atom, and that were free to roam about in the crystal, were seeing the potential well imposed by these bounds of the crystal.

So, it is as though you have so let us let us just draw it a little cleaner. So, this was a Kronig's penny model. If it take all this and transfer in to your rectangular potential profiles, it is as though, you have this to be your potential profile. So, this is the length of the entire 1 d crystal, and these are your little potential wells because of the different atoms. And, therefore the electrons here, experience this potential well, and the electrons there are sitting in a much wider box. And what happens, when the boxes the length of the box increases, we saw the distance or the def the difference between the energy levels, drops down significantly, and that is exactly what this is indicative off.

Therefore, if you think of the difference in k ok, so the difference in k here is the order of pi by a ok, so that is your delta K, for the electrons sitting in the inside in the clutch of the atoms. But, if you look at these finely spaced k points, so what does the order of this K, it is the order of pi by L, where L is the size of your crystal or the size of this periodic arrangement. So, if you were to take a crystal, where L is about 1 centimetre, so which is about 1 e minus 2 meters, then 1 by L or pi by L ok, so the delta k because of these points is of the order of a 100 ok. So, you can imagine that the distance between these two is about say 100.

And what is the distance between these two points? It is the order of pi by a and a is basically a lattice spacing in the crystal, which is say let us say 5 angstroms, so, the order of 1 e minus 10 meters. And therefore, pi by a so the order of 1 e 10 ok, so meter inverse. And, therefore while this is all 100, we are talking about 1 e 10 here, so that is what the order of 1 e 10. So, therefore these points are about 1 e 8 times more closely spaced as compared to these jumps here. And, therefore it appears like as though it is a continuous distribution of or continuous line or continuous bunch of states that the electrons could occupy. So, this is the second point to denote.

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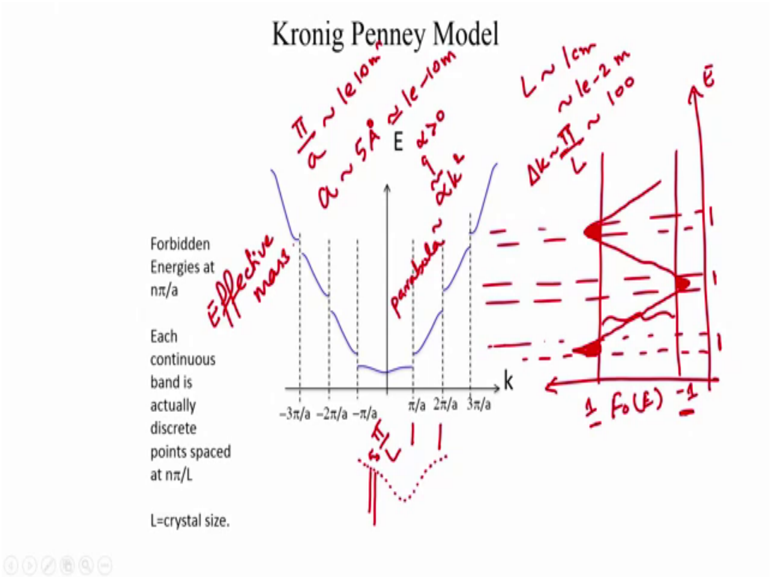

Kronig Penney Model

Forbidden Energies at nπ/a

Each continuous band is actually discrete points spaced at nπ/L

L=crystal size.

The third point denote is that you will see that these E k stitches that, we defined have got a little gentle S shaped nature, they are all looking like little S ok. In other words more mathematically this lower end here could be described by a parabola, which is of the form alpha k square, where alpha is greater than 0. So, of course there could be a constant here, and there could be constant there, but let us not worry about that I am just describing the general nature.

And this nature this region here the top of this S is another parabola, which is the order of say minus beta k square, where beta is greater than 0, and therefore you have a negative sign outside. And the reason for these this kind of a relation will become very apparent, when we go further down, and discuss the concept of something called as the effective mass of an electron in a crystal.

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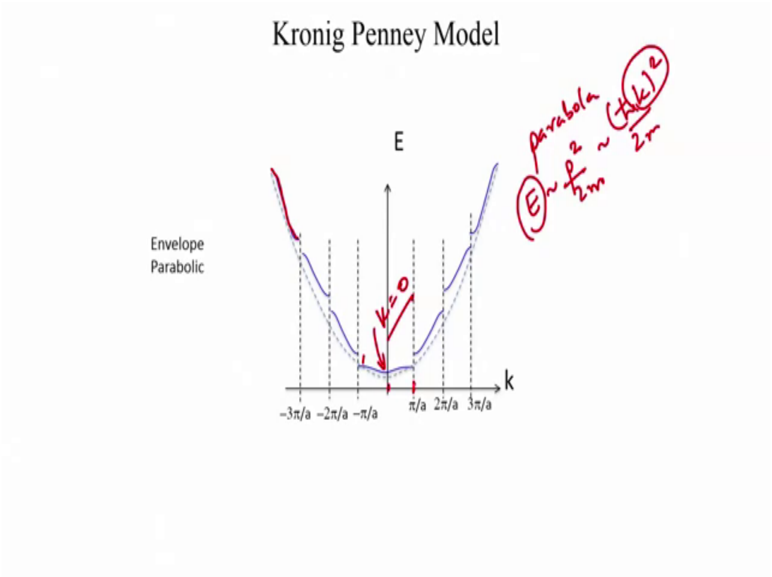

Kronig Penney Model

Envelope
Parabolic

$E \sim \frac{p^2}{2m} \sim \frac{(\hbar k)^2}{2m}$

Now, moving to the very last the other two points or the not the last, but there are two other aspects that we need to discuss. So, moving on, we find that these are the states the electrons could occupy, and there are these little discontinuous jumps. But, then the general envelope or the general trend of this plot is in itself a parabola ok.

And do we expect that? The answer is yes, because if you were to head towards classical mechanics, you will find that your energy is nothing but your P square by 2 m and P, which is the momentum is h bar k and h bar k square h bar k whole square by 2 m provides a parabolic relation between E and k. And, therefore you will find that the envelope is a parabola. So, as we head towards classical mechanics, these discrete the discreteness of all this would disappear and we would effectively have an E k relation that looks like this envelope shown here.

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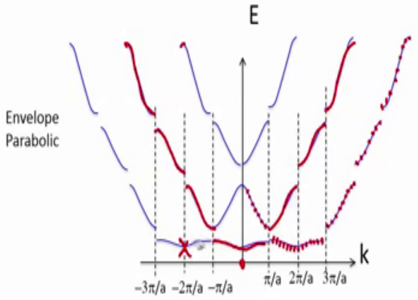
Kronig Penney Model



Now, let us continue this discussion. Now, the E k diagram that is shown here by these blue curves; to draw this E k diagram, we arbitrarily defined the origin, we said k equal to 0 is at this point. But, that need not be the case, nature does not distinguish between say this point in K, and that point in K. And, therefore if you were to draw the same E k diagram here, it we could draw another, we could draw a similar kind of a picture, but just translated along the k axis. So, for example, this is the E k diagram that, we just studied ok, so that is the picture that we studied.

So, you can see you can see that the origin was chosen here, but we might as well draw an E k diagram here, which is again got the same kind of an energy profile ok. So, you can see the little stitches just translated by this period. And once again, you could also draw an E k diagram here and so on, and you could fill up the entire k space by drawing such E k diagrams. And when we do that you can see this general bands of energy beginning to appear.

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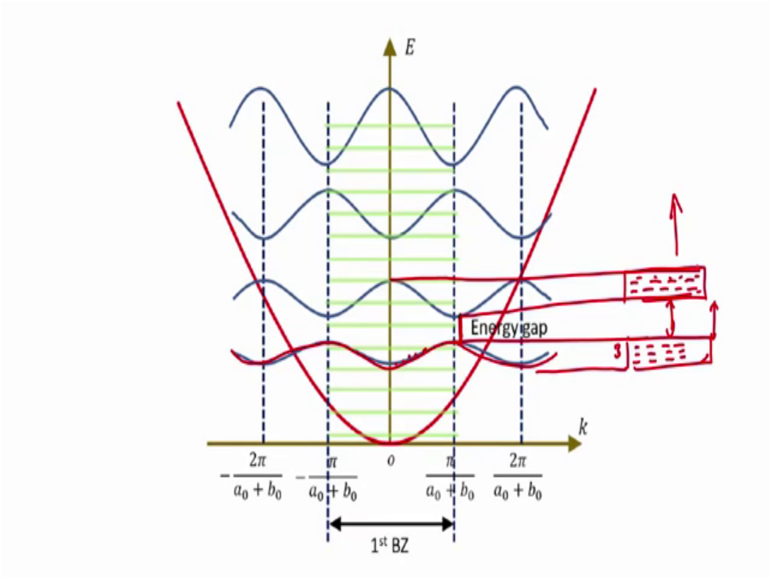

So, let us do that completely, and you will find that, you have these little bands of energy ok. So, if you were to, if you were to take this apart here, and draw this as a band, you will find that there is an energy band here, which the electrons are allowed to occupy. And this these energy bands are now composed of very finely spaced energy levels ok. And, we already saw that the spacing here is all of the order of you know it depends on this 1 by L.

So, they are very finely spaced energy levels. And then you have a gap, you have a discreet gap, because nature does not allow the electrons to take up those energies. And then you have another band, you have another band that is formed, which is also composed of discrete energy levels and so on. So, therefore this Kronig Penny model shows us the formation of energy bands in a more mathematical or quantitative sense. And, we got here by simply solving Schrodinger's equation for our simplified model, where in we simplified the potential profile to the rectangular potential profile.

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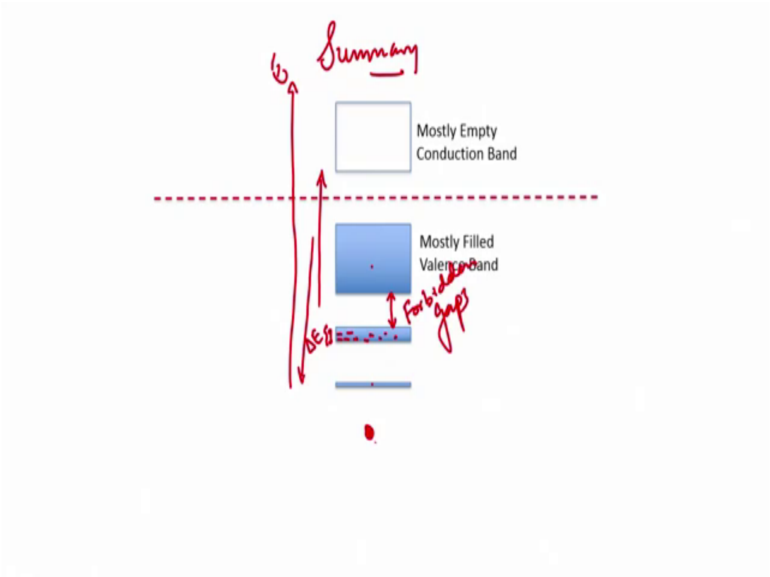

So, just to summarize everything we have looked at, I think this picture is quite important ok. So, all our discussion so far has told us that, when we bring arranged atoms closer and form, start forming, constructing, solids, wherein the atoms begin to feel each other, then we find that the electrons are permitted to occupy bands of energy. So, you have these different bands that are composed of finely spaced energy levels, and these bands are themselves separated by large forbidden energy gaps ok.

So, as we move up, so what we have here is the energy axis as the y-axis. So, as we move down in these energies, we encounter electrons that are occupying these different energy levels, and that are more tightly held by the nucleus of the atom. And as we move up an energies, we encounter the electrons present in the outer shells, and those electrons are less tightly held by the nucleus.

Now, of interest to us in this course are two kinds of energy bands ok. Of course, all energy bands are important I mean without that, you would not have an atom. But, as far as this course is concerned, we are interested in 2 kinds of energy balance, and those energy bands are described by these 2 Blogs that I have shown here. So, there would be a point in this energy profile that, you will have an energy band, which has got energy levels, which are big and these energy levels are basically solutions to Schrodinger's equation. And, you will find that this band of energy is mostly filled with electrons. When you say a band is mostly filled it implies that electrons are occupying these energy levels or these electrons have taken up solute those solutions prescribed, where Schrodinger's equation that corresponds to these energy states.

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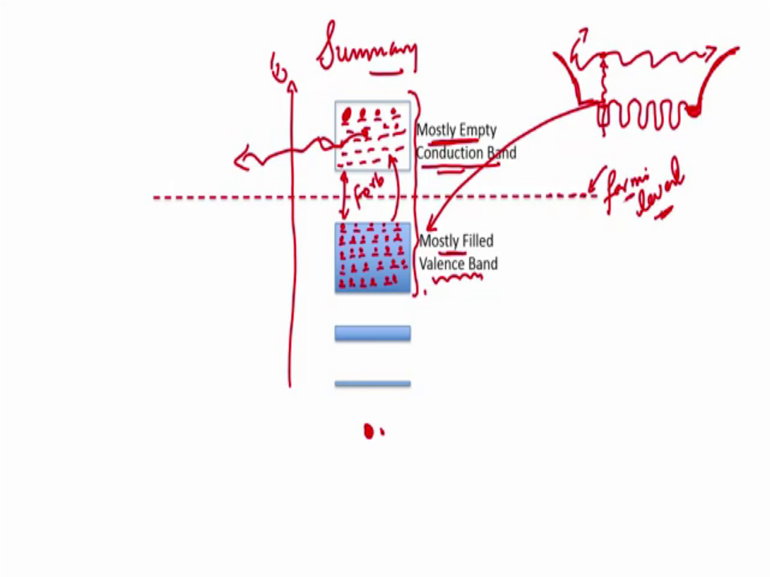

So, these energy levels are mostly filled with electrons. And just above that band would be a forbidden gap; and further above that band, you will encounter, another band of finally spaced energy levels, but which is mostly empty, which is mostly empty, which implies that there are solutions that the electron could take up. But, there has been no electron or very few electrons that have actually taken up those solutions, and are having an energy level as defined by the energy levels in this band ok.

So, you have this mostly filled band, and you have this mostly empty band. And this mostly filled band, typically corresponds to the outermost shell of the electron outermost shell of the atom,. And therefore this is something called as the valence band. And these energy levels ok, correspond to the larger potential well, which we saw in our Kronig's penny model. And these energy levels are something called as the conduction band, and they are mostly empty. So, it requires the electron sitting in a valence band, which still held by the nucleus by the clutch of the atom, but is very weakly held by the nucleus ok.

So, you consider an electron there, which corresponds to the electron in the valence band. The moment this electron would receive some energy, it would climb up, and across this energy gap; and it would enter something called as this conduction band. And it enters the conduction band, it essentially sits in a much larger potential well. And, therefore in this much larger potential well, the electron is free to move about in the crystal.

And therefore, the electrons in the conduction band are free to move about in the crystal. And therefore the word conduction, which means the electrons now being charged carriers are free to move about, and they become carriers or they become entities, and lead to charge transport, and therefore currents in a crystal. And this red line here is our fermi level. Now the fermi level could lie anywhere, but just for the sake of definition, just for the sake of connecting you at the previous picture I have located this fermi level. And we will define the fermi level much more carefully further down the road.

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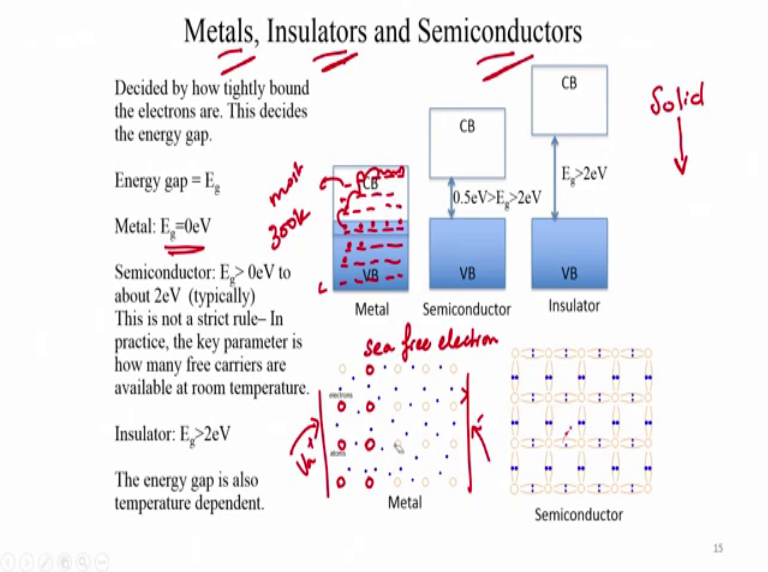

Metals, Insulators and Semiconductors

Decided by how tightly bound the electrons are. This decides the energy gap.

Energy gap = E_g

Metal: E_g=0eV

Semiconductor: E_g> 0eV to about 2eV (typically)
This is not a strict rule– In practice, the key parameter is how many free carriers are available at room temperature.

Insulator: E_g>2eV

The energy gap is also temperature dependent.

So, now we are in a good, we are in good shape to describe the difference between metals, insulators, and semiconductors. So, we are slowly heading and making our way from the general study of solids towards understanding three kinds of solids that are of great use for us. And these classifications are based on the conductivity of the solid as to how much, how easily they can conduct electric current ok, and they are called as metals, insulators, and semiconductors.

Now, metals in the case of metals the conduction band that is the mostly empty states overlaps with the valence band, which is the mostly filled states. So, essentially what the electron sees is a continuous distribution of energy levels. There is no energy gap or in other words the energy gap is 0 ok, so there is no energy gap. And, therefore these states are mostly filled, but it requires the electron to just acquire a very small amount of energy before it enters the conduction band, and begins to move about in the crystal.

So, it is only at 0 kelvin that it is quite like it is that it is it is possible that, we find no electrons in the conduction band. But, with any once the temperature starts increasing above 0 kelvin, and particularly at temperatures, which are close to the room temperature, which is say about 300 kelvin. It is very, very easy for the electron to enter these higher energy levels, and occupy states in the conduction band. And, therefore these electrons ok, as shown here this is the picture of metal, as seen from the point of view the lattice.

So, these are the different atoms that form this periodic arrangement in the metal. And these are the electrons in the metal. And these electrons are free to move about, because they can easily escape the clutch of the atom and enter the conduction band. And therefore, the metal can be said to have a sea of free electrons. And there and therefore these free electrons would respond quite actively, and in large numbers to any applied voltage difference. And therefore the metal would have extremely good conductivity because of these free electrons.

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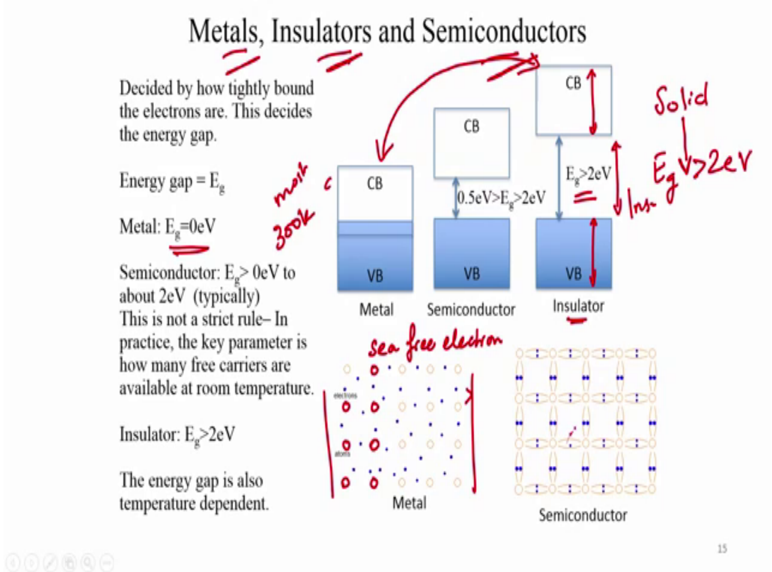

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Insulator: E_g>2eV

The energy gap is also temperature dependent.

So, now let us head towards the other end of the spectrum, which is basically your insulators, so these are insulators. Now, what is an insulator? In case of an insulator, you have the valence band states, and you have the conduction band states. And these two bands are separated by a very large band gap ok. The forbidden gap is very, very large. And for the sake of a quick estimate, we have defined the energy gap to be greater than 2 electron volt. But, this does not mean that nature is imposed a strict limit of 2 electron volts. Nature does not classify these materials say for example a semiconductor, and insulator by noticing as to whether the energy gap is greater or less than 2 electron volts. In other words, nature is not sitting there saying that ok, this material has got an energy gap with 2.1 electron volts. So, let me call this as an insulator.

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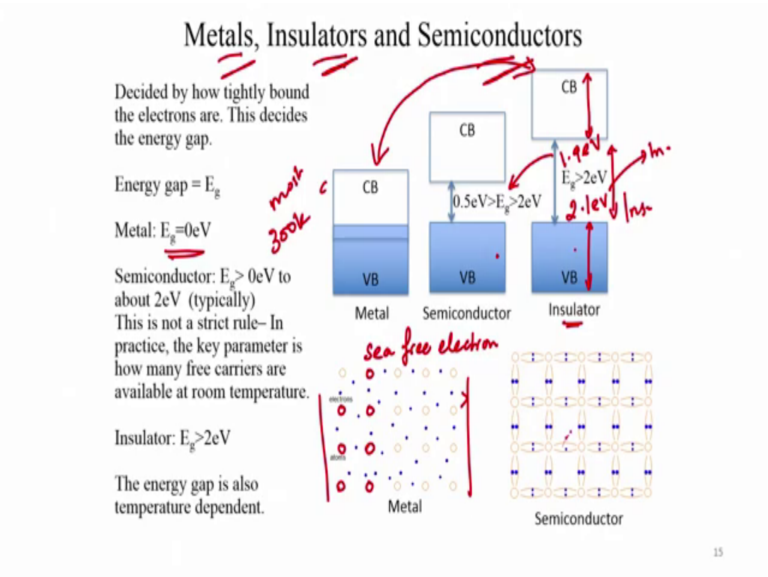

Metals, Insulators and Semiconductors

Decided by how tightly bound the electrons are. This decides the energy gap.

Energy gap = E_g

Metal: E_g=0eV

Semiconductor: E_g> 0eV to about 2eV (typically)
This is not a strict rule– In practice, the key parameter is how many free carriers are available at room temperature.

Insulator: E_g>2eV

The energy gap is also temperature dependent.

Whereas, this material has got an energy gap of 1.9 electron volts, so therefore let me classified as a semiconductor, no, that is not the case. Now, the purpose of these numbers ok, so you can see that it is quite a vague the difference between an insulator, and a semiconductor is quite vague. Both of them have an energy gap, both of them have conduction band, and valence bands described like this. The only difference is the values that we have assigned.

And what I am telling you is that these are not strict values. For example, you could have, you could have a semiconductor having an energy gap, which is slightly greater than 2 electron volts, in fact these are called as wide band gap semiconductors. So, what tells a what provides this classification of as to what is a semiconductor, and what is an insulator ok. Now, the answer has got to do with that conductivity at room temperature ok.

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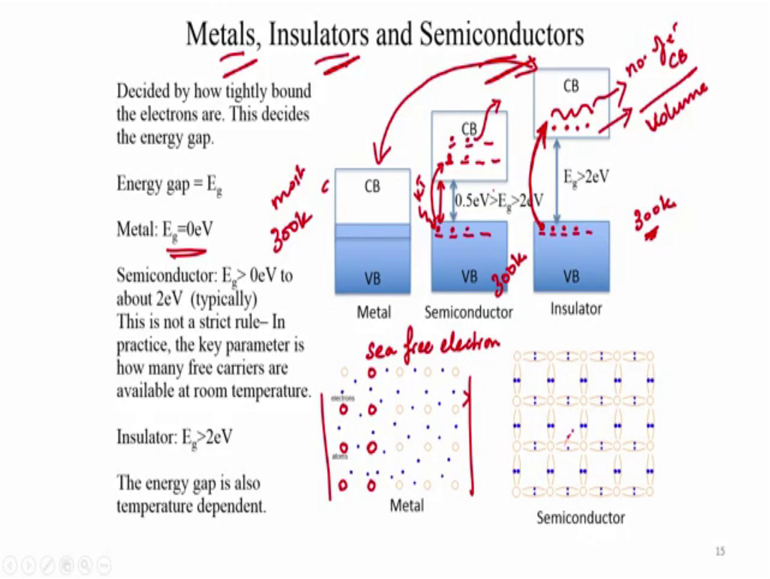

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And let me explain that a little clearer; let me explain that a little more clearly. So, let us take an insulator. In the case of an insulator, you have some electrons sitting in the valence band. Now, at room temperature, which is 300 Kelvin, these electrons would acquire some amount of energy, and they would now jump to the conduction band. Now, in the case of an insulator, this gap is so large that at 300 Kelvin, it is very unlikely that the electrons would get a get the energy required to jump across the gap.

And, therefore at 300 Kelvin while it is possible for us to find a few electrons this count statistically speaking is not very large. So, one way to look at the electron concentration in the conduction band, which is the number of electrons sitting in the conduction band per unit volume of the material. If one were to look at this particular estimate, we will find that this number is quite low. And, therefore the conductivity or the current carrying capacity of these carriers in the in this material that we call as an insulator is very low, and the measurable current is extremely low, and therefore we classify this as an insulator.

But, in the case of a semiconductor, the band gap is much smaller; there does exist a band gap, but it is much smaller. And, therefore the electron sitting at 300 kelvin has a good possibility of acquiring the thermal energy and getting excited to head into the conduction band. And at room temperature it is possible that, we find a large enough number of electrons in the conduction band that, we can now have a measurable estimate of the conductivity or the current. So, it is this aspect that defines and distinguishes a semiconductor from an insulator.

And, therefore in a semiconductor, we will see that the electrons do participate in all your bonding. So, for example here we have shown something, which is equivalent to silicon lattice. And you do have electrons participating in bonding, so these are your valence electrons that are being shared, and that are participating in bonding. But, upon receiving some amount of energy say thermal energy, it is possible for the electron to escape the clutch of this atom clutch of the nuclei, and enter into the crystal, and begin to conduct through the crystal. And this electron, which escapes from this clutch leaves behind a vacancy ok and that we vacancy is something called as a hole.