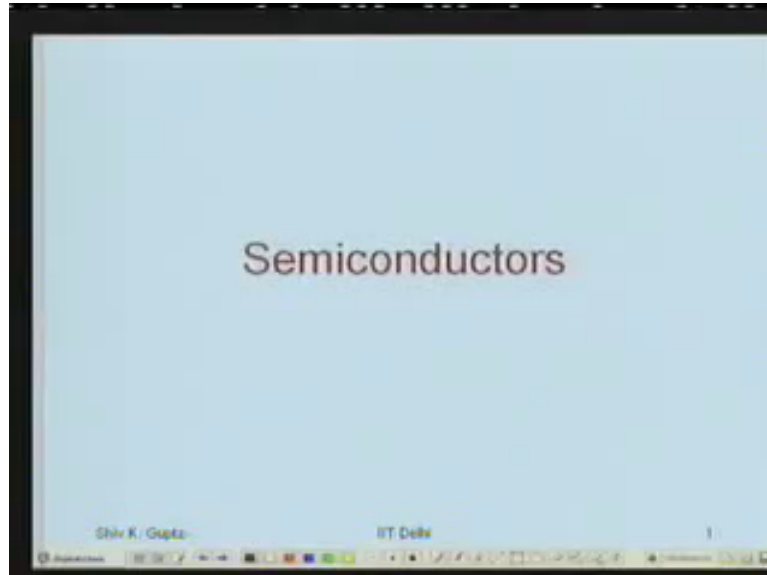


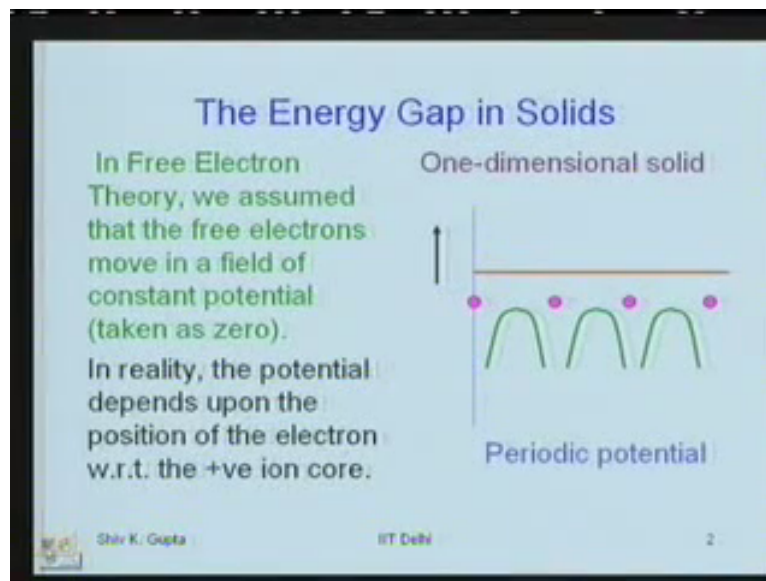
Material Science
Professor S. K. Gupta
Department of Applied Mechanics
Indian Institute of Technology Delhi
Lecture No 37
Superconductors (Contd.)

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Alright we had been looking at some of the materials which can conduct electricity and their engineering applications though we are going to look at materials which are provided as the present-day computers, the chips the integrated circuits and it all started sometime in 1948 before which we had bulky vacuum tubes working as a diodes and triodes, the 1st transistor came in 1948 and ever since we have not looked back and every few months you find a new technology in this area. This is a very important class of materials from that point of view because all your work on the automation, artificial intelligence involves circuitry, digital memory and all kind of things are being worked with this kind of materials and therefore they are important for us to look at and as I said while introducing these materials with further electrical properties.

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We start with a free electron theory and that theory we assumed that there are free electrons such as the outermost electrons in the solid provided by each atom and they all move in a field, electric field for a constant potential which is a uniform potential throughout the volume of the solid and we take it that to be 0. So that the all the energy of the electron we are talking about is only the kinetic energy. In reality as I told you that is only an assumption the situation is not like that, what happens is in here I am showing you one-dimensional solid having positive ion core of the nucleus here 2nd one, 3rd one, 4th one so all along this length solid exist, the electrons which are in the outermost orbit they are more attracted towards the center of the nucleus here, here, here and here the potential energy is very low in these locations but at the intermediate position between the 2 nuclei where it is neither in the attraction of this or nor in the attraction of that potential energy have.

In other words what it produces in a solid is a periodic potential like this which is very small highly negative means attractive near the nucleus and as we go away from here it increases and we have taken the average to be somewhere here 0 in the free electron theory but in reality this is the situation and it depends of course as you can see in the space the position of the positive ion core or the nucleus where it is and therefore get a periodic potential field in a solid, crystalline solid three-dimensional solids are there I have just shown it with the help of one-dimensional and, it can be extrapolated to 2nd and the 3rd dimension.

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2. Diffraction of electrons

$$\rightarrow n\lambda = 2d \sin \theta$$

In one-dimensional solid $\theta = 90^\circ$

$$\frac{n\lambda = 2d}{\lambda = \frac{2d}{n}}$$

The wave number $k = \pm \frac{2\pi n}{2d} = \pm \frac{n\pi}{d}$

Diagram: A horizontal line with vertical tick marks representing lattice planes, with a distance 'd' between two planes.

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2nd thing in free electron theory very said electrons are travelling with all wavelengths they are treated as dual characteristics of way as well as particle and De Broglie wavelength you worked out could be of any value, however we have studied in a crystalline solid certain wavelengths which are in the same order of magnitude as the spacing between the atoms they get diffracted, a certain value of those wavelength not all values of wavelength and that is given by the Bragg law which is $n\lambda = 2d \sin \theta$ where you recall we said n is the order of diffraction, λ is the wavelength, d is the interplanar spacing and θ is the diffraction angle, the Bragg angle.

In one-dimensional solid electrons are travelling only in one direction say if I have taken the direction like this this electron can travel only in this direction this and if I would read these as crystallographic planes here what is the Bragg angle? θ is 90 degrees, if θ is 90 degrees I substituted here $\sin \theta$ becomes one and I get the condition $n\lambda = 2d$ and therefore I get $\lambda = \frac{2d}{n}$ where n is an integer which is called the order of diffraction. Wave number k which is $\frac{2\pi}{\lambda}$ I put the plus minus sign will be equal to $\pm \frac{2\pi}{\lambda} = \pm \frac{2\pi n}{2d} = \pm \frac{n\pi}{d}$ again n is only an integer. In another words at $k = \pm \frac{n\pi}{d}$ if the electron has that wavelength it will be diffracted, what happens if the electrons is getting diffracted?

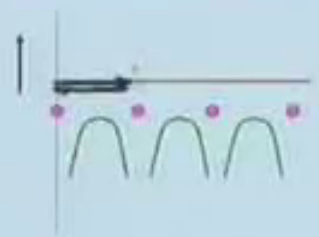
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The Energy Gap in Solids

In Free Electron Theory, we assumed that the free electrons move in a field of constant potential (taken as zero).

In reality, the potential depends upon the position of the electron w.r.t. the +ve ion core.

One-dimensional solid



Periodic potential

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2. Diffraction of electrons

$\rightarrow n\lambda = 2d \sin \theta$

In one-dimensional solid $\theta = 90^\circ$

$n\lambda = 2d$ $\lambda = \frac{2d}{n}$

The wave number $k = \pm \frac{2\pi n}{2d}$

$= \pm \frac{\pi n}{d}$



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Electrons is trying to travel let us say starting from here goes in the direction gets diffracted here starts travelling in the opposite direction gets diffracted that means it is travelling to and fro between 2 planes or in other words it becomes stationary it is not travelling the three-dimensional solid, it is getting localised when this deflection condition is satisfied the electrons are no more travelling I consider them as travelling waves, they are no more travelling they are getting stationary, they are getting localised near the 2 nuclei.

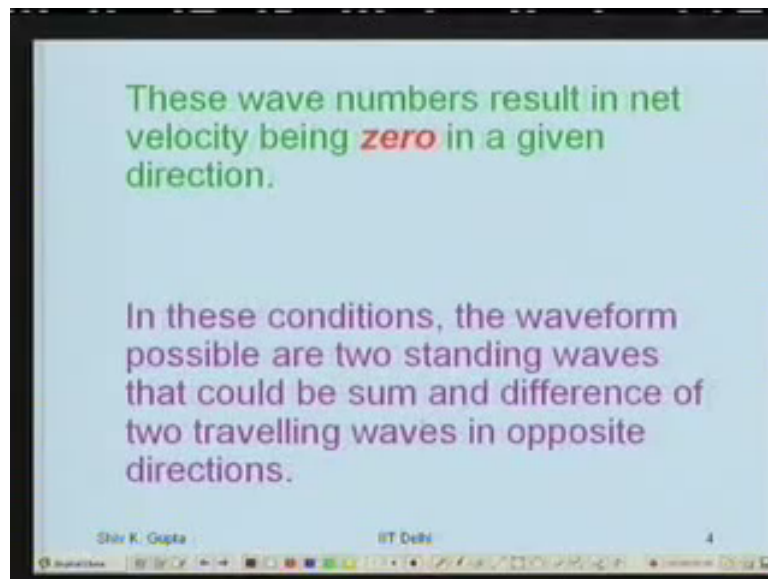
Student: (())(8:33) specific lambda?

Prof: Specific lambda not all at any other lambda it will be travelling.

Student: So other electron may have different member which will be travelling?

Prof: Yes I am not denying that but when the wavelength is equal to this it becomes stationary, when the wave number is plus minus $n\pi/d$ electrons are going to become stationary and they should be represented by stationary or the standing waves rather than the travelling waves, so that is what we have come across that is what the meaning of this diffraction taking place of the electrons alright that is different from what we treat it in the free electron theory, okay.

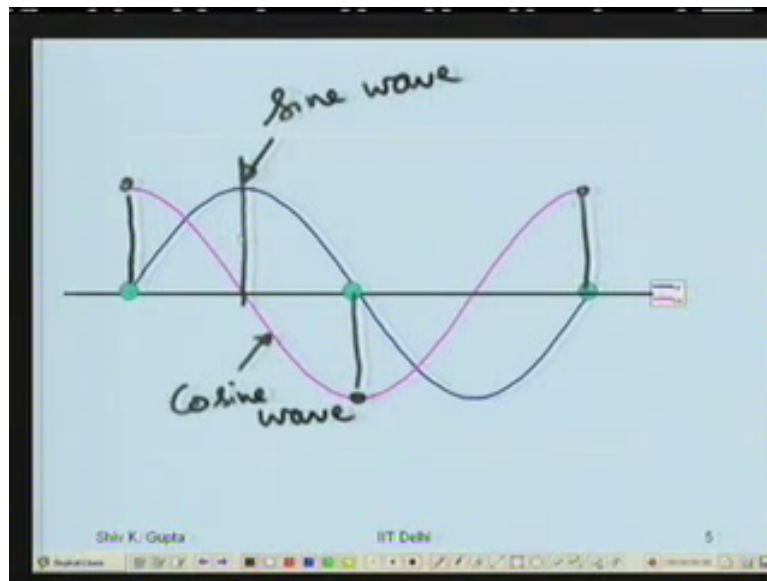
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These therefore result in the net or average velocity of the electron being 0 because it is not travelling and in these conditions as I already said it should be standing wave possibilities are there 2 waves forms which are can provide me a standing waves one could be sine wave other could be cosine wave that means the amplitude for one is maximum on the nucleus and in the other case it is minimum on the nucleus 0 on the nucleus. Once we consider these electrons which are the travelling waves provided by the solution of the Schrodinger equation and this solution is not one solution you know that there are number of travelling waves which are present all these are the electrons outermost electrons.

Some of the 2 travelling waves can provide one standing wave similarly the difference of the 2 travelling wave and provide one standing wave and if these both of the solutions, both travelling waves are solution of Schrodinger equation their sum and difference will also be the solution of Schrodinger equation that is the characteristics of all differential equations. So therefore these are also the solutions possible waves or possible arrangement for the electrons they can be treated like these standing waves and these as I said 2 possibilities one is sum other is the difference.

(Refer Slide Time: 11:38)



Well this is what I show it here this one at the nucleus it is 0 and in between the 2 nuclei it is the maximum is the sine wave, the maximum at the nucleus, the positive sign minus sign while this is the cosine wave. This is the representation of the electrons which is at the wavelength which is getting diffracted, it is for that electrons which is getting diffracted the wavelength is plus minus or the k wave number is plus minus $n\pi$ by d is for those electrons this is the situation. Now the probability of locating the electron we already said that is given by the square of the amplitude.

The one which is sine wave the probability of the location lies somewhere in the middle of the tool the maximum probability and the one which is the cosine wave maximum probability lies on the nucleus only, okay it is here is found there. In other words the one electron which is represented by the sine wave is localised between the 2 nuclei and that is the one if you look at the potential, periodic potential function has a maximum potential energy and the one which is presented by the cosine wave is localised on the nucleus and here its potential energy is lowest.

Student: (())(13:48)

Student: What decides whether an electron will have a cosine wave or sine wave (())(13:56).

Prof: What is represented by?

Student: How we can decide that this electron will be represented by the sine wave...

Prof: No I have not said that which electron is been...what is the possibility, once it is produced the sine wave this is the same wavelength and the cosine wave that the same wavelength and this is the wavelength which will be getting diffracted.

Student: Is it possible that network exist at the nucleus the maximum probability I feel is (ψ^2) (14:25).

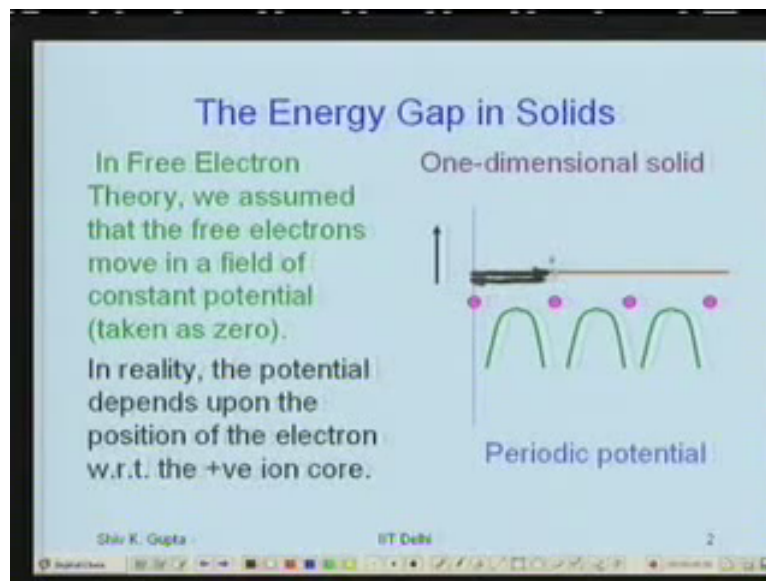
Prof: At the nucleus you what I mean in the three-dimensional solid, size of the nucleus is very small as compared to the size of the solid localised there means it is right on the orbit of their it is not going in the space outermost electrons you consider to be free electrons, free electron gas which is pervading the all three-dimensional volume everywhere it is not only the orbit around the nucleus.

Student: Which means if there is supposed just one atom then around that in whatever orbit that is what (ψ^2) (14:56) and...

Prof: Yes but now we are referring to the solid we are not referring to one single atom please mind it, we are referring to the solid, solid has 10^{23} to the power if you have a small 1 centimetre cube (ψ^2) (15:11) dimensional solid it may have 10^{23} or more atoms in it so many nuclei and they are spaced the size of the nucleus is smaller than the distance between 2 of them much smaller than that rest of the space where the electrons are there localised near on the nucleus means it is on that orbit right and somewhere in between is taken away from the means... not in the attractive field of the nucleus it is away from there.

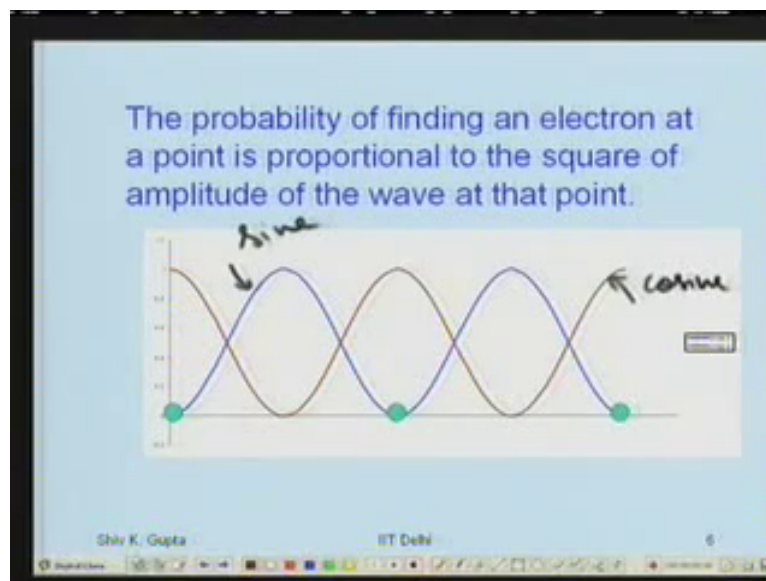
When it is in between the 2 nuclei it is not in the attractive field of that all those orbits anyway it is somewhere in between right that means it is like more free electron as compared to the one which is onto the nucleus, the one onto the nucleus is not like a free electron, the one between the 2 is like a free electron it is not being pulled by any one of them that much try to understand that because when I say the potential energy is more attractive for this one is not so attractive for this one, is that clear? What is the meaning of this wavelength and the amplitude of this wave and location of the electron in the solid? I am not talking about the free atom please, things are different in free atom and free atom does not cause diffraction does not provide me the free electrons is only when they are in the solid they provide me free electrons also the outermost electrons. Alright so this is what is going to happen, so probability is this maximum location the sine wave and if it is cosine wave location is this and there is going to be difference in the potential energy of the 2.

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What I am trying to say is if it is localised here its potential energy somewhere down and it is localised here potential energy is here, so there is a difference in the potential energy of the 2, okay that is the meaning of it.

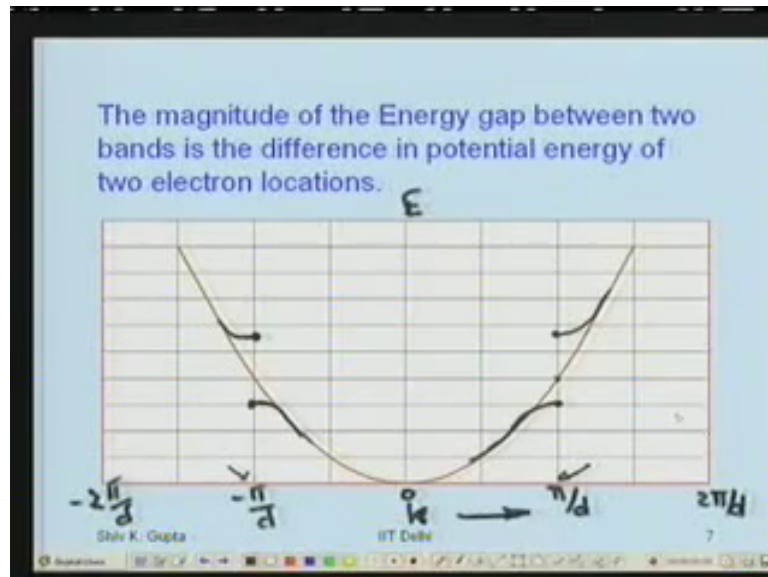
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Here I have shown the probability which is the square of the amplitude and therefore square of the negative number also becomes positive so there is no negative here that is a 0 in the probability and the probability is 1 here maximum and that is for the cosine wave this is the one and this is the sine wave. Cosine wave is localised at the nuclei and it is sine wave and which is in between the 2 and that is what I describe in words earlier that is we have to take

the square of the amplitude of the sine wave the cosine wave which are representing these 2 electrons which are in this state particularly which is getting diffracted.

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Alright this is my energy versus k curve wave number let us say my wave number is 0 here let us say it is π/d here, $2\pi/d$ there similarly minus π/d here and minus $2\pi/d$ here. When it comes to the π/d this is the electron which is going to get diffracted and is stationary it is not travelling and its potential energy is small, what happens with total energy? Kinetic energy plus potential energy, potential energy is very high negative value will be smaller, so this curve actually whenever it comes here starts to deviate like this, similarly here but for the same wavelength wave number there is another electron which has a higher potential energy, its kinetic energy will be or the total energy will be more than this it will be somewhere here and that is the one it will go on like this. So I find at this value π/d or minus π/d 2 energies of the electron and it is not a continuous function anymore I get a break.

Student: Why it is $(())(20:55)$...

Prof: I treat it in a free electron theory potential energy to be 0 and what I plotted was a kinetic energy as a total energy. Now when my electron is getting diffracted at the value π/d and it is getting localised either on the nucleus which is a cosine wave or addition between the 2 nuclei it is the sine wave. Potential energy of the cosine wave is very low and potential energy of the sine wave is very high that is what the 2 states I have demonstrated here because total energy is the kinetic energy plus the potential energy this is less than that and

that is more than that. This is the kinetic energy which is taken as total energy when the potential energy was taken to be 0 which is not the case now.

So the E versus k gets curve gets modified with similarities appearing at π/d by π/d alright, so E versus k curve though I have said that they are quantized state in this and I treated the different energy between the 2 quantum states is very small so I treated that to be a continuous function. That stays I am considering that will be like this but I know that there are quantized states but at the wave number equal to π/d this electron is getting to get diffracted continuously repeatedly and therefore not going to travel in the solid anymore is going to become stationery and when it becomes stationery it has 2 locations one on the nucleus one taken away from the nucleus and one is that is the cosine wave as the sine wave. Potential energy of the cosine wave is smaller total energy become smaller, potential energy at the sine wave is higher so total energy becomes higher okay so that is potential energy is no more 0 and that is how these curve gets modify which singularities being produced at regular intervals of π/d , $2\pi/d$, $3\pi/d$ and so on and so forth alright.

(Refer Slide Time: 23:29)

Effective mass of an electron near the critical condition, $m^* < 0$

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

$$= \frac{h^2 k^2}{8\pi^2 m}$$

$$\frac{h}{p} = \lambda$$

$$k = \frac{2\pi}{\lambda}$$

$$= \frac{2\pi p}{h}$$

$$p = \frac{h k}{2\pi}$$

Graph showing Energy (E) versus wave vector (k). The curve is a parabola that starts with a positive slope, reaches an inflection point where the slope is zero, and then continues with a negative slope. The inflection point is labeled 'Inflection'.

Now what is the meaning of this...what is happening if you look it carefully this is a parabola right up to the inflection point the slope is increasing and after the inflection point the slope of the curve start to decrease I am talking about E versus k curve and that is the breakpoint and this is the inflection point from beyond the inflection point the curve has a negative slope while here it has a positive slope and that means though kinetic energy is increasing for the electron but it is...travelling becoming slower slow and ultimately it is stationery that is depicted in common man's language as the effective mass of the electron beyond the

inflection point is becoming negative, what is the meaning of that this is what I wanted to tell you it is mass of electron if you talk about the mass content of anything is not going to become 0 or negative for that matter it can be small but a positive number.

Energy we wrote as what? Kinetic energy can be written as p^2 by $2m$ and we have written h upon p as λ so or in other words let us put this in terms of k , k we said is 2π by λ and it would be 2π divided by h into p and so p can be written as h times k divided by 2π so I substitute it there what I get is $h^2 k^2$ upon $4\pi^2$ into 2 is $8\pi^2$ into m , mass is the electron, k is the wave number, h is a constant, so h^2 upon $8\pi^2$ is a constant here right alright.

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Effective mass of an electron near the critical condition, $m^* < 0$

$$E = \frac{h^2 k^2}{8 \pi^2 m}$$

$$\frac{\partial E}{\partial k} = \frac{h^2}{8 \pi^2} \frac{2k}{m}$$

$$\frac{\partial^2 E}{\partial k^2} = \frac{h^2}{4 \pi^2} \frac{1}{m^*}$$

$$m^* = \frac{h^2}{4 \pi^2} \left(\frac{1}{\frac{\partial^2 E}{\partial k^2}} \right)$$

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Alright that is what we wrote is...right. Let us differentiate this with respect to k I talked about the slope of this E versus k curve being positive up to the reflection point and negative beyond the inflection point. dE by dk is h^2 upon $8\pi^2$ is a constant $2k$ by m alright then I differentiate it 2nd time d^2E by dk^2 is equal to well 2 will come there so h^2 upon $4\pi^2$ divided by m this if I call the effective mass of the electron then I can say m^* is equal to h^2 upon $4\pi^2$.

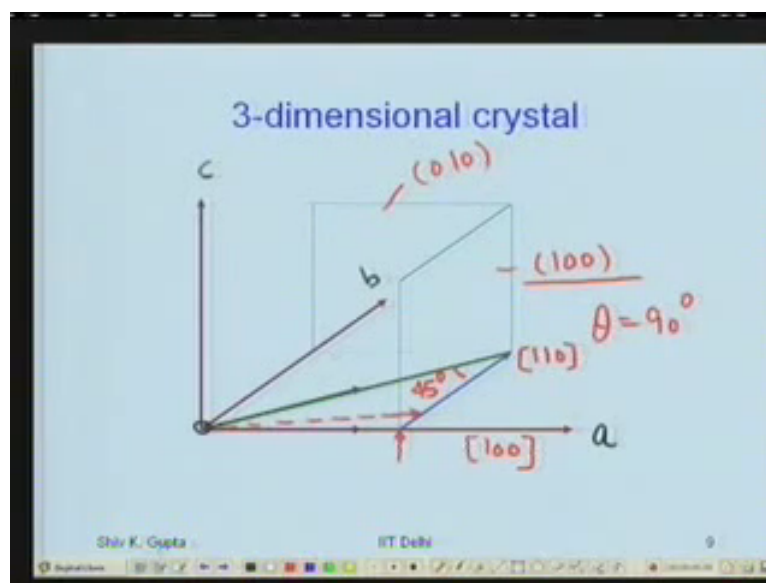
Student: Should not it be ideally valid with $(\frac{\partial^2 E}{\partial k^2})$ (28:09) till $(\frac{\partial^2 E}{\partial k^2})$ (28:13)

Prof: Yeah.

Student: So E is what exactly proportion to k^2 .

Prof: That is what I am trying to tell you the meaning of effective mass, I am trying to explain you the meaning of effective mass in terms of my classical theory which have used okay, so the m^* is $\frac{\hbar^2}{4\pi^2} \frac{1}{\Delta^2 E} \frac{d^2 E}{dk^2}$. This $\Delta^2 E$ by Δk^2 up to the inflection point is positive and $\Delta^2 E$ by Δk^2 beyond this is negative that is why the number becomes negative because $\hbar$ positive π is positive that number becomes negative beyond the inflection point that is why we call the effective mass is becoming less than 0 alright why I was saying this you must understand why I am talking about the effective mass because I am trying to related to the classical theory okay.

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Alright the next problem is instead of one-dimensional and I have 3 dimensions solid usually. Let us say I talk about this as an axis this is my b axis this as my c axis that is my origin here and this is the one okay let us put this as 1 0 0 plane and this one as 0 1 0 plane, is this clear? Alright now when an electron is travelling in the 1 0 0 direction which is this it is getting diffracted between these planes we have worked that out situation alright so we will look into that and then if the electron is not travelling on 1 0 0 direction it tries to miss it here theta is going to be 90 degree as compared to the plane 1 0 0 alright what I am trying to say is I am considering the deflection from a 1 0 0 setup planes let me simplify the problem for you.

Considering the diffraction from 1 0 0 setup planes electrons travelling in the 1 0 0 direction theta is 90 degrees. If it travels in a direction different from 1 0 0 let us say it is travelling in this direction what is the theta? Less than 90 degrees and it goes on like this still it goes into this corner which is the direction 1 1 0 and what is the angle there 45 it is a cube I am talking about the cubic material angle is 45 degrees, so from theta equal to 90 I can go to theta equal

to 45 and the angle changes in this electrons is still travelling in the plane made by a and b axis okay it can travel in 3 dimensions anywhere but at this position you would notice that it also makes an angle of 45 degrees with the 0 1 0 plane.

Something which is getting diffracted at 45 degrees from 1 0 0 plane will also get diffracted from 0 1 0 plane, is that clear? Now if the angle further reduces to 45 degrees it begins to make an angle greater than 45 degrees with 0 1 0 the situation of diffraction which you are here considered here from 90 to 45 will be there from 45 to 90 for 0 1 0 this kind of thing happen in 3 dimensions also to keep repeating like this and the effect of that result of this will become clear when I say the next step.

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Diffraction from (100)

Electron travelling in [100] $\theta = 90^\circ$
 $\sin \theta = 1$
 $n \lambda = 2d$
 $k = \pm \frac{n 2\pi}{2d} = \pm \frac{n\pi}{d}$

Electron travelling in [110] $\theta = 45^\circ$
 $\sin \theta = \frac{1}{\sqrt{2}}$
 $n \lambda = \frac{2d}{\sqrt{2}} = \sqrt{2}d$
 $k = \pm \frac{2\pi n}{\sqrt{2}d} = \pm \frac{\sqrt{2} n \pi}{d}$

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Alright when the electron is travelling in 1 0 0 direction theta is equal to 90 degrees and sin theta is 1 and n lambda is equal to 2d. When the electron is travelling in 1 1 0 direction theta is equal to 45 degree I am still talking about 1 0 0 and sin theta is one upon under root 2 and n lambda is equal to 2d divided by under root 2 is equal to under root 2 of d. This one gives me the wave numbers for diffraction conditions plus minus 2 pi by 2 d is equal to plus minus pi by d and this one gives me plus minus 2 pi by under root 2 of d or lambda for n equal to 1 sorry so then it should be n somewhere here so it would be under root 2d into n so that becomes plus minus under root 2 n pi by d.

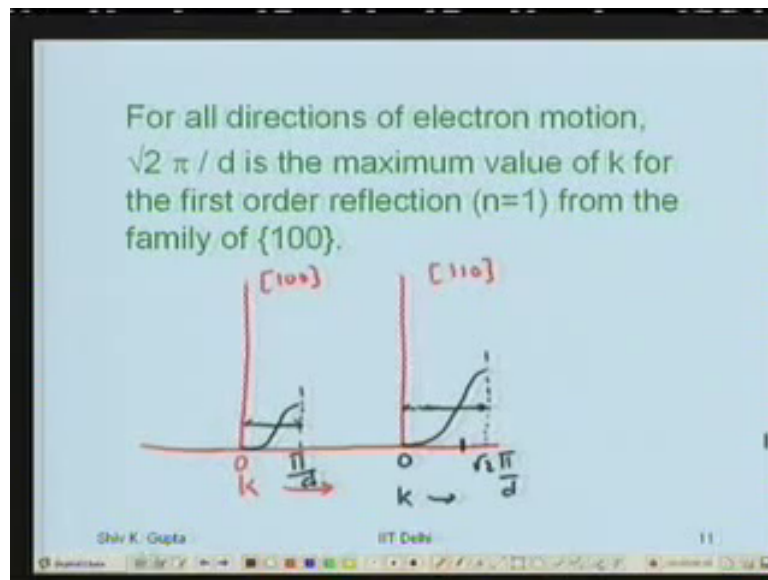
Why I have talked about this 1 0 0 direction and 1 1 0 directions people have worked out for what are the possible directions in three-dimensional space and they have found out that that is the condition for smallest condition for wave number and this largest value of the wave

number in between different directions all the wave number will come which will be getting diffracted, so that is the minimum and that is the maximum. They are in between the situations are they are going to be directions in which these wave numbers will be getting diffracted in some direction or the other.

Student: Beyond the value (π/d) (35:29)

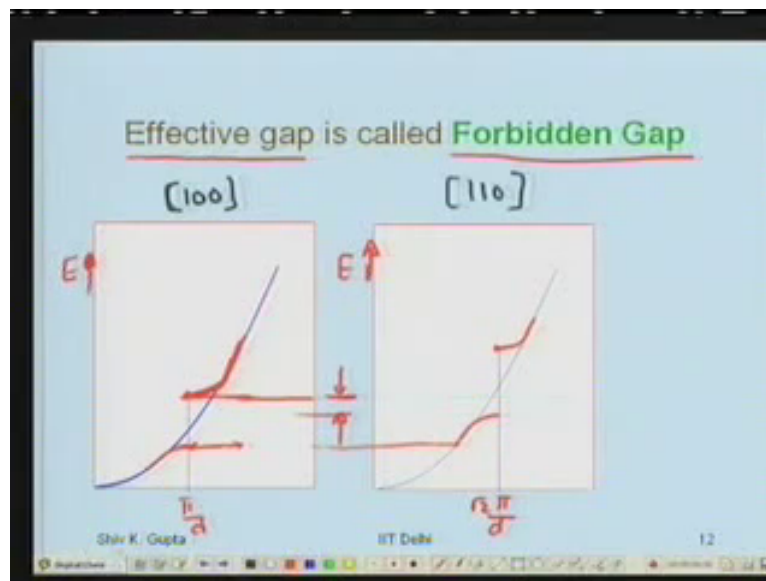
Prof: I am talking about this plus minus sign n will be one integral coming so between this I am considering n let us say equal to 1 then with π by d and under root 2π by d is the condition minimum and the maximum okay I am not proving that but I am just using that result.

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For all direction of electron motion that is what I said it has been worked out under root 2π by d is the maximum value of k for the 1st order reflection where n is equal to 1 from the family of 1 0 0 planes okay we consider only 1 0 0 planes first. What does it mean let us say this is k and I show only the positive side let us not worry about the negative side alright and then if I consider for the 1 1 0 this is for the 1 0 0 direction and for the direction 1 1 0 this happens at under root 2π by d . See this is going to be this distance here on this axis is more than this distance here you can see that on the wave number this is π by d this is 1.414 times of that is π by d is here for this let us say between this and this there will be other directions where there will be diffraction of this kind of condition will be taking place alright that is the meaning of what we have worked out.

(Refer Slide Time: 38:31)



Alright now I just want to talk about something what is the gap of energy between the 2 electron states one the cosine wave other the sine wave the one which is getting diffracted alright this is for the 1 0 0 direction that is where the 1 1 0 direction minimum and the maximum which I am considering okay. Now look at that the electrons when it reaches the value of this energy it is no more travelling in the 1 0 0 direction, however with this energy it can still continue travel if it changes its direction towards 1 1 0 but when it comes to this value of energy it is not able to travel and it is not able to travel even in the 1 0 0 direction because in 1 0 0 direction anything that can travel is now should have this energy should go to sine wave which is in between the 2 nuclei and is almost free to travel with a slight more (())(40:50) can travel there right.

So that is the one therefore this is the one in this energy level can still travel but however when it comes to this energy level it cannot travel anymore because it is not able to travel at 1 0 0 which is the lowest and it is not able to travel in 1 1 0 which is the highest and then in 1 1 0 direction it can travel only when it is required this energy however in 1 0 0 it can travel it acquires this much energy so electron has to change its direction it can still travel but effectively there is an energy range between this and this where even if the electron is the energy neither in 1 0 0 nor in 1 1 0 nor in between any direction it can travel that is what is the effective band gap, energy gap.

Energy gap which was created between the 2 electron states which are localised states stationary waves one on the nucleus, one in between the 2 nuclei these are the 2 states. The one in between the 2 nuclei is not in the attractive field of any one of them little more (())

(42:04) can travel the one which is localised on the nucleus cannot travel and that is what I am trying to show here that is happening in 1 0 0 direction this is what is happening in 1 1 0 direction but the one which is not able to travel in 1 0 0 direction with in change in direction can continue to travel, however when it comes to this level of energy it certainly cannot travel either in 1 0 0 or in 1 1 0 or in between anywhere other direction. Similarly when it increases the energy to further value which goes to the 1 0 0 is the lower value, lowest value it can travel but in 1 1 0 direction it can travel only if it requires that energy not otherwise, however in the three-dimensional solids electron cannot travel if it requires this energy and electron will not be able to travel till it requires that energy this is what is called the forbidden energy region which I call the forbidden gap.

Student: The forbidden gap will decrease with n ?

Prof: With...?

Student: n the value n , $(\frac{2\pi}{d})$ 2π by d and $\sqrt{2}\pi$ by d gap should decrease.

Prof: When it goes from 2π by d from under $\sqrt{2}\pi$ by d to 2π by d next stage?

Student: Yes.

Prof: Well I am not very sure about that I have not tried to look into it, why should it decrease?

Student: because this overlap currently it is like 1 and 1.4 $(\frac{2\pi}{d})$ 2π by d so it is just 0.6 region where it will not exist but if you go like upward it will be 2.8 and 3 so that is overlap region will increase.

Prof: No the gap will also increase if that is the case it remains I thing more or less the same and probably does not change. Let me look into it and before I answer that.

Student: So in this forbidden gap there are electrons will not travel in any direction?

Prof: Yes it cannot in this with electron with these energy values cannot travel in any direction, just cannot travel because it is stationery it is getting diffracted if you travel okay. So that is the one which is not going to travel at all and that is what is called the effective gap though the gap is more in 1 0 0 direction it is in 1 1 0 direction but because of the 2 positions overlapping conditions there are certain energy level not allowed in 1 0 0 but allowed in other directions therefore there is an effective band gap there could be a solid effective band gap is

0 there could be a solid effective band gap is 0 there could be a solid effective band gap is large there could be a solid effective band gap is small and it is this what is going to characterise is a conductor not a conductor, insulator or is it going to be a semiconductor.

Student: (())(45:20) value of d.

Prof: d, why should it depend on d?

Student: Where else would it depend on?

Student: Different material has different spacing...

Prof: Energy, it depends upon this energy depends upon k wave number and why should it depend upon the spacing of the between the atoms.

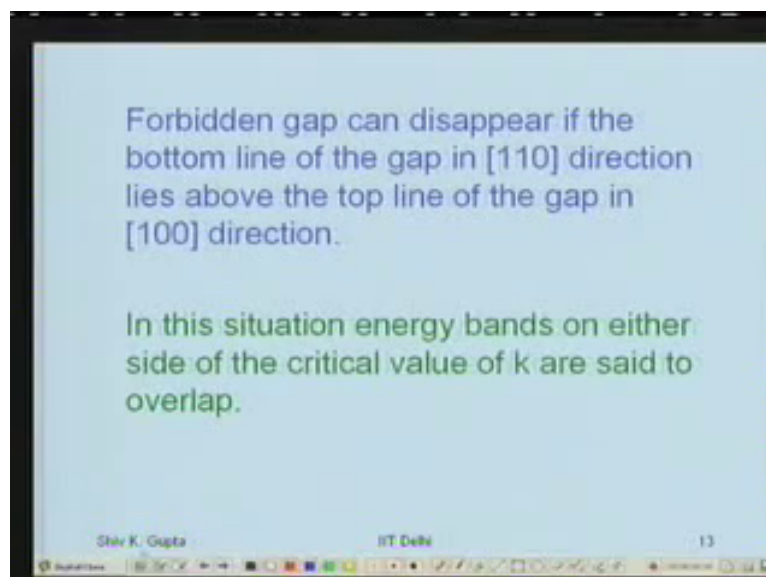
Student: Wavelength will depend upon that.

Prof: Wavelength will depend upon that yes wavelength will depend upon that.

Student: k is (())(45:53) depend on d.

Prof: Yes but between them there are different energy levels available to electrons to travel okay.

(Refer Slide Time: 46:15)



That is what I was trying to say forbidden gap can disappear if the bottom one of the gap in 1 1 0 direction lies above the top line of the gap in the 1 0 0 direction. I showed you its line below but now if it lies above then it will there will be no gap and in that situation energy

band on either side of the critical value of k are set to overlap. That means when there is an overlap electron has to merely change its direction of motion that means it change its momentum and it will keep travelling it will keep conducting, okay. That is the meaning of it even if it reaches a situation of diffraction in 1 0 0 direction it will keep travelling by changing its direction. Change of direction means change of momentum of the electron, is this clear?

Alright, now what I want to know is between the situation, one situation where the electron is unable to travel it is getting diffracted another one where it is going to get diffracted in between all the wave number is or in between these 2 wave number is all the energy values it should be able to acquire and it should be able to travel, the singularities are provided only at these 2 wave number is right between these 2 wave numbers how many energy states I have and how many electrons can be there in that energy range that is what we want to look at.

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Handwritten notes on a screen showing the derivation of the number of states and electrons in a 1D solid. The notes include the wave number $k = \pm \frac{n\pi}{dL}$, the condition for diffraction $md = L$, and the resulting number of states m and electrons $2m$. The notes also mention "m no of atoms per unit volume" and "2m electrons per unit volume".

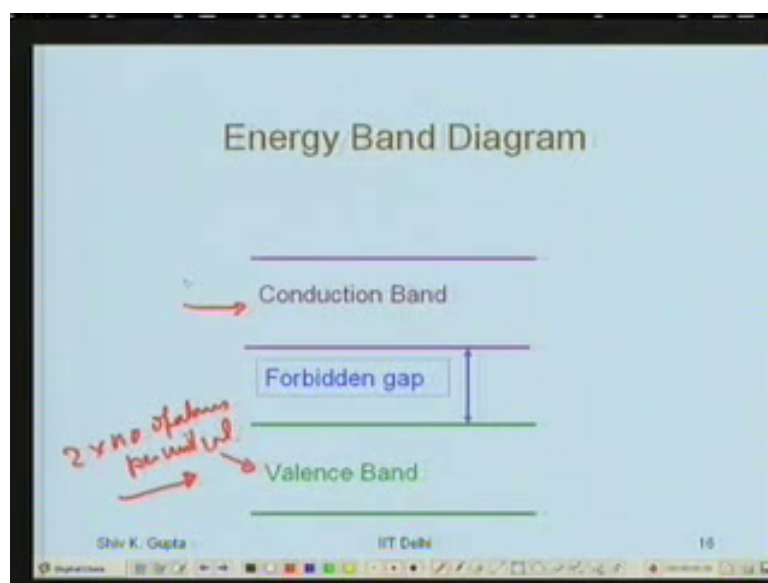
You recall that we said the wave numbers can be plus minus $n\pi$ by d which I call $n\pi$ by l okay let me put it instead of d , plus minus and π by l , l is the dimensions of the solid okay I am treating a very crude treatment between these 2 levels of diffraction, if I consider a unidimensional solid with spacing between the 2 nuclei as d and their m such positions m into d is my length of the solid, m is an integer. I am avoiding the m effects to start with here that is what I said I am making a very crude calculation, so when I put this allowed values of wave numbers are $n\pi$ by $m d$, n is an integer and m is an integer alright started from 0 n equal to 1, n equal to 2, n equal to 3 you can keep on and when shall it stop travelling, when shall I reach the band gap? When k becomes...?

Student: (0)(50:26) pi by d.

Prof: k becomes π by d , the 1st diffraction taking place at π by d in 1 0 0 direction at that position n shall be equal to m . Well n is the number of quantum states and m is the number of nuclei in the solid, so how many energy states do I have between k equal to 0 and k equal to π by d . Similarly you can go on from n plus 1 to $2n$ where you should have the next one, next diffraction taking place at $2n$ start from n plus 1 go to up to n , it will you will find that it will be $2m$ and it will be starting from m plus 1 because 1st band has taken this 2nd one will start go from n plus 1 go up to $2m$ sorry this is not there this will be m only in the denominator, start with n plus 1 goes to $2n$ and it will be the condition will be $2n$ is equal to $2m$ meaning thereby I have between n plus 1 and $2n$ states in the 2nd bands, in the 1st band I have up to 1 to n , 2nd one from n plus 1 to $2n$, 3rd one I have $2n$ plus 1 to $3n$ and so on and so forth.

So how many energy states I have in each band before a gap arrives m I have m states and each state can have how many electrons? 2 plus k minus k so that is $2n$ electrons, so if a solid has m number of atoms per unit volume I am extrapolating it to three-dimensions one band can have $2m$ electrons per unit volume, is it clear? So each band before the gap I have $2m$ electrons next $2m$ electrons, $2m$ electrons and m is the number of atoms per unit volume number of nuclei per unit volume, so that is the density of states which we have within a band and the number of electrons within that band.

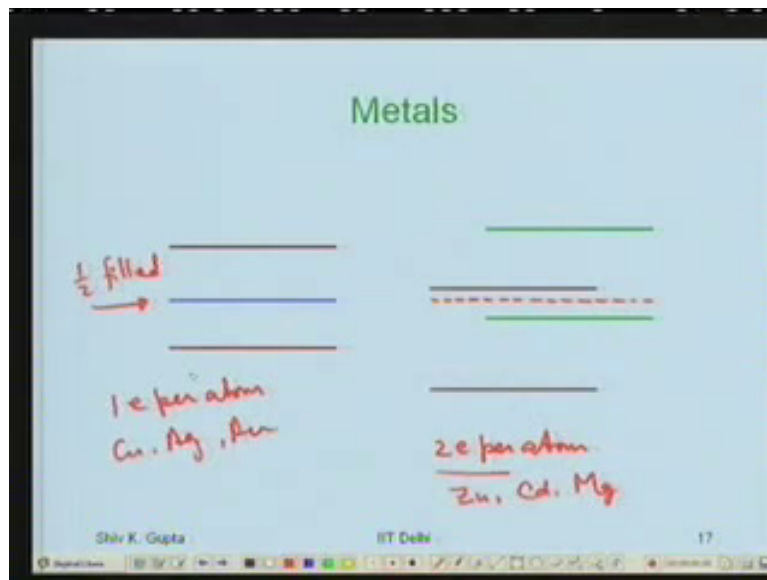
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Now I represent this in terms of only the energy level not the wave numbers, the same thing and here I show you one band then band gap and then the 2nd band alright I am talking about the outermost electrons if I have... If I have outermost electron only one outermost orbit only one electron per atom which is gone into the free electron (())(54:34) that is the one electron I am considering, one band is the one which shall have those electrons and it will be half filled...

It shall be half filled that such a band is called the valence band then we have a forbidden gap the energy cannot be acquired by the electrons in the outermost orbit then it is called the next band which is available is called the conduction band well as I said this can acquire twice the number of atoms per unit volume or in a solid you can say twice the number of atoms, number of electrons which can go into the valence band, same number can go into the conduction band, same will go in the band after that and so on and so forth. The one which has a electrons outermost electrons I call the valence band and the band above that I call the conduction band and in between the energy gap it is called the forbidden gap. Just a minute I will not take much time.

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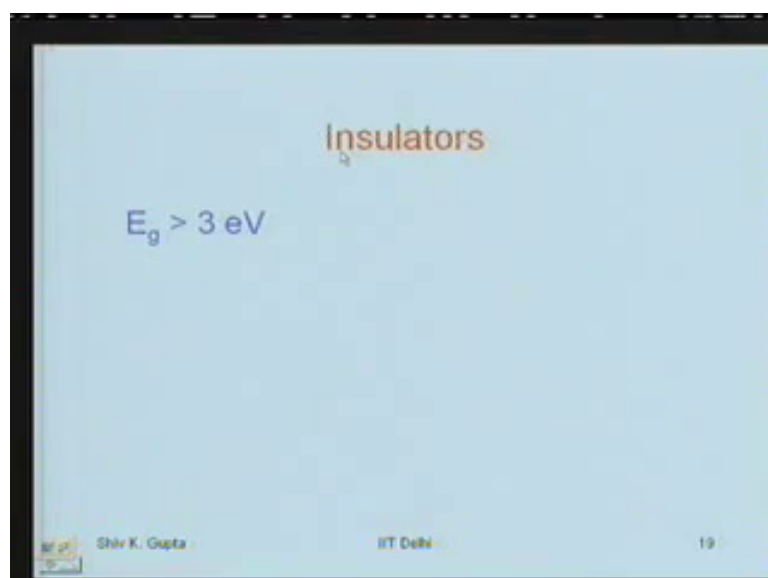
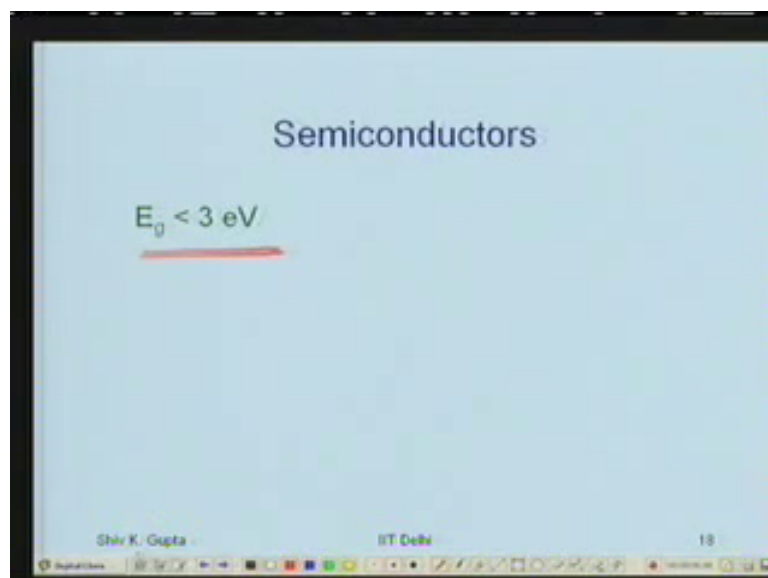


Well when metals particularly group 1 where only one electron per atom I have the valence band which is half filled, exactly half filled now you can understand why it is half filled and that all the energy level above that are available and empty that is the (())(56:22) level and these electrons can get excited by applying field and they can go to higher energy levels because they are free empty, those levels are not occupied and electron can get excited and can

conduct. When the valence is 2 means there are 2 electrons per atom like zinc, magnesium et cetera.

We will find that the valence band and the conduction band overlap though if it is purely the valence band it will be completely full but because conduction band begins here even the valence band is not full and the electrons here also find a few free states while these electrons in the conduction band find lot of free electron states they conduct but conductivity is not very good because they have to change the direction, to go from this state to that state they have to change the direction momentum has to be changed okay, so therefore the conductivity is not very good for these metals like zinc, cadmium, magnesium et cetera while here you have copper, silver, gold you have a very good conductivity.

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Well when the band gap becomes less is less than 3 electron volts, band gap was not a problem in metals it is called a semiconducting material and when it is greater than 3 electron volts we call it insulator. We shall look at the semiconductors in the next class.