

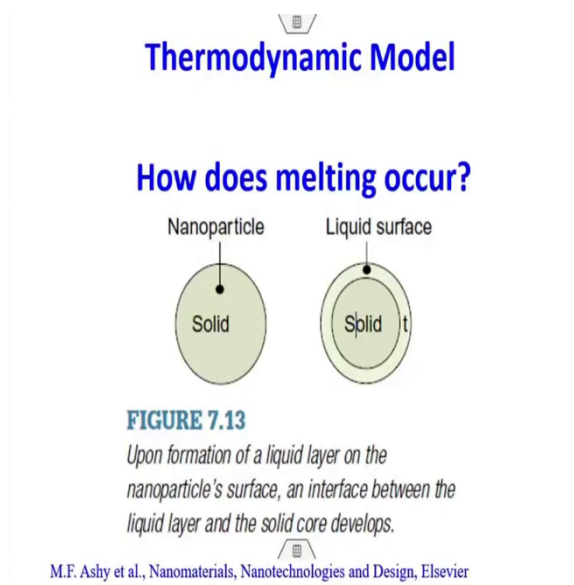
Nanomaterials and their Properties
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Lecture - 23
Electrical Property of Nanomaterials

Students, we are going to start the lecture number 23 and this will be on a new topic that is on Electrical Properties. So, the last lecture we completed our discussion on the topic called thermal properties of nanomaterials. As you know thermal properties are very important for the nanomaterials because of varieties applications on which for which nanomaterials are used. Now, the question is whatever we have discussed let us first do a recap.

Thermal properties of nanomaterials have been discussed in the light of following two topics. One the melting temperature of nanoparticles or nanomaterials, how the size dependency of melting temperature affects the uses of this materials and then we have discussed about thermal transport; that means, how the heat transport happens in a nanomaterial.

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So, for the sake of completeness for the in case of melting temperature we have started with the thermodynamic model of a spherical particle which is been melting down. So, in this

process the liquid layer a thin liquid layer forms on the surface of the solid and then this liquid layer moves slowly inside the solid particle and that is how actually melting happens.

So, at any instant of time an interface between the liquid layer and the solid core develops and based on that we developed a model and showed how the melting temperature can be related with the of the nanoparticle related with the bulk.

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Thermodynamic Model

$$\Delta G^{\text{total}} = \frac{L(T_m - T)}{T_m} \cdot V_L + A_L V_L + A_{SL} Y_{SL} - A_S Y_S$$

$$\Delta G^{\text{total}} = \frac{L(T_m - T)}{T_m} \cdot V_L + 4\pi r^2 Y_L + 4\pi(r-t) Y_{SL} - 4\pi r^2 Y_S$$

$$\frac{\Delta G^{\text{total}}}{4\pi} = \frac{L(T_m - T)}{T_m} \cdot V_L + r^2 Y_L + (r-t) Y_{SL} - r^2 Y_S$$

Assignment

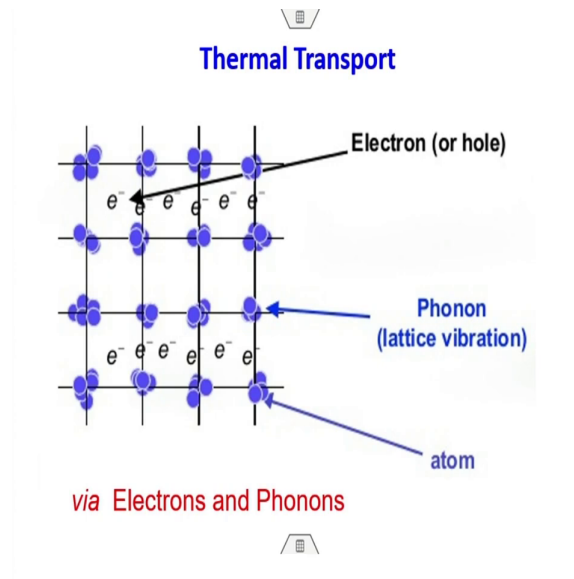
$$\frac{\partial (\Delta G^{\text{total}})}{\partial t} = \frac{L(T_m - T)}{T_m} \cdot 4\pi(r^2 - t^2) + r^2 (Y_L - Y_S) + (r-t) Y_{SL}$$

$$= \frac{L(T_m - T)}{T_m} \cdot 4\pi(r^2 - 2rt) + (2t - 2r) Y_{SL}$$

$$= \frac{L(T_m - T)}{T_m} \cdot 4\pi r(n-t) + 2(n-t) Y_{SL}$$

And this is how the model have been developed. Looking at different kinds of surface energies and the bulk thermodynamical parameter like bulk Gibbs free energy change.

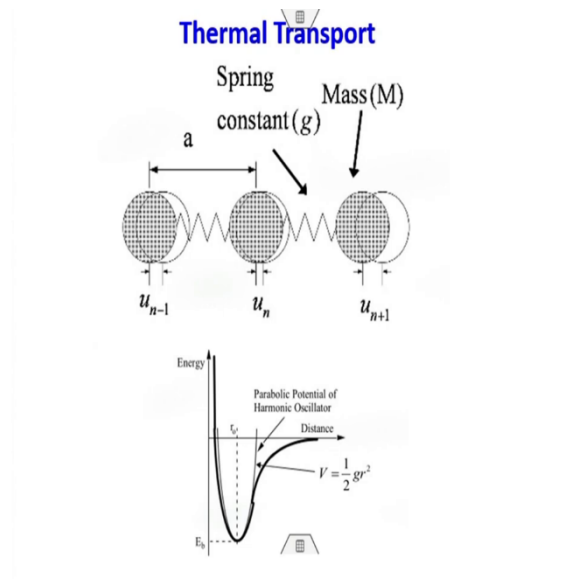
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Then we looked into some of a thermal transport things like you know in a crystalline material thermal transport happens by electrons and phonons. Electrons are easy to understand. If you energize electrons they will move and depending in the type of bonding electrons movement will be fast or slow or rather will happen or not happen. Like in case of metals electrons are freely available they are not bound to any particular species.

So these metals actually this electrons actually are not delocalized. So, they act as a electron gas. So, therefore, they can move easily, but in case of non metals like ceramics and polymers especially ceramics and many of the carbon based materials you have very less free electron appilables. So, therefore, the transport happens by the phonons are nothing but travelling waves due to movement of the or the atoms from its mean position during heating up.

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So, phonons are nothing but lattice vibrations we have discussed a lot about that, and because of these concepts that at the bonding between the atoms can be thought of like a spring attached to the among the atoms. So, therefore, as soon as you heat it up the atoms actually move from a secular position to both the sides, and because of these, the push and pull of the atomic species or the bonds can happen.

That mean, the spring attached to the atom can be pushed or pulled during this to and fro motion from the not to and fro motion, but because of the motion of the atom from its mean position. Let this can lead to change of or create a stationary wave call a travelling wave and that is what is known as is the phonon.

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Thermal Transport

Interatomic Bonding

Energy

Distance

Parabolic Potential of Harmonic Oscillator

E_0

r_0

$V = \frac{1}{2}gr^2$

Equation of motion with the nearest neighbor interaction

$$m \frac{d^2 x_n}{dt^2} = g(x_{n+1} + x_{n-1} - 2x_n)$$

Solution

$$x_n = x_0 \exp(-i\omega t) \exp(inKa)$$

1-D Array of Spring & Mass System

Spring constant, g

Mass, m

Equilibrium Position

Deformed Position

x_{n+1} , x_n , x_{n-1}

And we can do a simple maths by develop a phonon you know equations and find a solution and then we can get a phonon dispersion map and then discuss about how these movement of the phonons can affect. But, you know in nanomaterials both the electrons and the phonons can get confined or quantum confined because of the size effect. And we have discussed a bit of that in the last lecture, we are going to discuss again quite a bit of it today's lecture also.

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Development of electronic properties as a function of cluster size

antibonding

bonding

Conduction band

Valence band

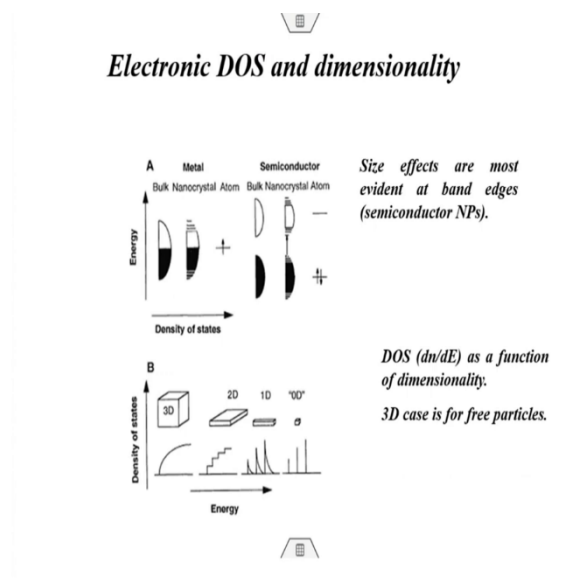
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Each band has a width that reflects the interaction between atoms, with a bandgap between the conduction and the valence bands that reflects the original separation of the bonding and antibonding states.

So, therefore, these quantum confinements is basically way important. To understand that what we did we discussed first the simple atomic structure or the bonding structure of the materials. And you know electrons participate in the bonding the antibonding orbitals normally lead to formation of conduction bands and bonding on metal leads to formation of the valence band.

And each band has a width that reflects the interaction between the atoms with the particular band gap between the conduction and the valence bands. This reflects original separation of the bonding and the anti bonding steps. In case of metals there is no band gap the both the valence and the conduction band overlap.

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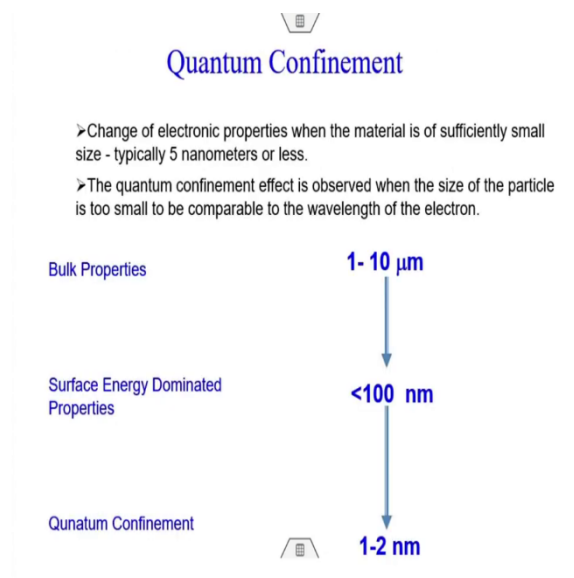
So, therefore, electrons are free to move, but in case of semiconductors and insulators there is a definite band gap in case of semiconductor the band gap can be easily crossed by the electrons by providing of thermal energies or by doping, but insulators it is not possible. So, therefore, these electrons now can actually depending on the nano material dimensions electrons can undergo what is known as a the quantum confinements.

What is that actually? Well, this is nothing but discretization of the bands. In case of bulk nano metals the conduction and the balance bands they not only do overlap, but also the bands actually are continuous ok. But, in case of nanocrystalline materials the bands actually

they will be divided and become discrete; that means, with each specific band we will have separate layers of energy levels. And therefore, electrons cannot stay at any energy level they want and depending on the dimensionality, this can change 0, 1D or 2D it can change.

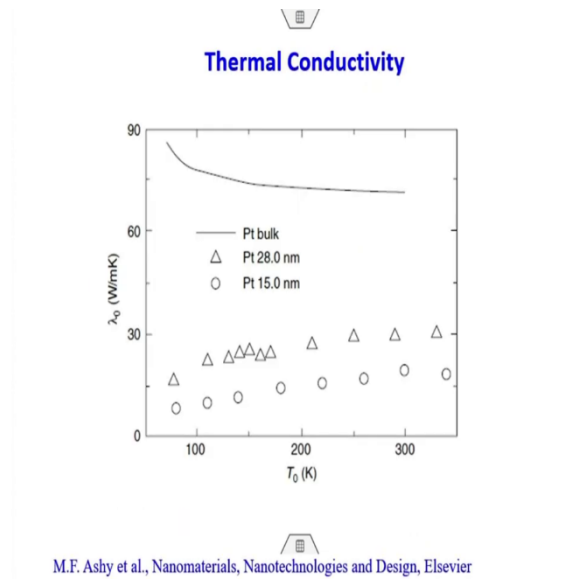
Semiconductor same thing can happen whether it is a valence or the conduction band both of them can actually undergo such a kind of discretizations. Therefore, the density of states can be plot as a function of energy as its shown in the bottom of a picture, but 3D it is a continuous curve for 2D there is a step functions for 1D and 0D its becomes very sharp or discrete actually.

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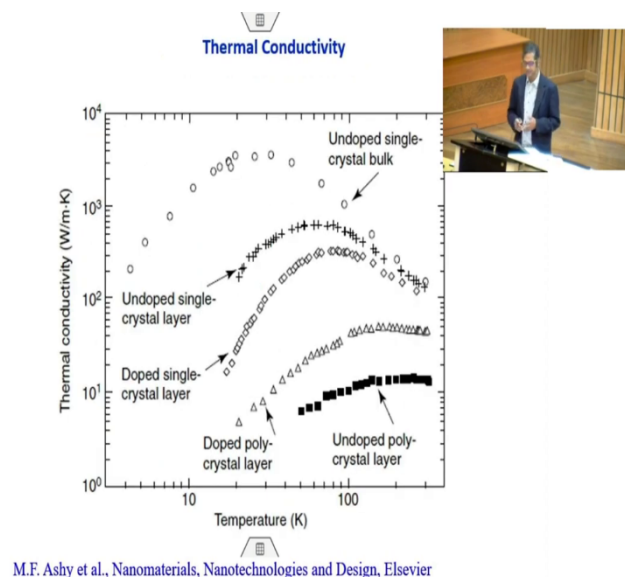
So, that is the difference and quantum confinements is normally observed in very small size particles like about 22 nanometers preferably, but now it can be seen to be happening in particles with less than 5 nanometers.

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And then we discussed about some of the effects of 2D quantum 2D term nanomaterials that is thin films. So, thin films the conductivity decreases substantially its compared to bulk, it is just for the platinum.

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Or this is for the silicon or the single layer double layer thermal conductivity do gets affected significantly.

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Electrical Conductivity



Now, let us talk about electrical conductivity. I know there is some overlap between electrical conductivity and thermal conductivity. Thermal conductivity is decided by both electrons and phonons. Electrical conductivity is only decided by the electron and the whole movements ok. The phonons do not participate in the thermal conductivity at all.

So, now the question is this. You know as you have seen the electrical you know electronic contributions of the in case of nano materials have been discussed and the conduction electrons are delocalized in case of metals; that means, electron can fully move from in all dimensions.

As they travel their paths electrons are primarily scattered by the various you know kind of mechanisms such as phonons impurities, interfaces. So, therefore, electron movement resembles like a random walk process right. So, however, two distinct things are very important ok. So, one which is very important is the quantum effect.

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Electrical Conductivity

① Quantum Effect
Quantum Confinement

② Classical Effect.
Mean free path \approx size of system.

3D - nanomaterials
Scattering of e^- due to
large no. of grain boundaries
↓
↓ Electrical Conductivity

So, electrical conductivity is significantly affected by two distinct aspects. One the quantum effect. What is that we will discuss in a moment. Second one is what is known as a classical effect. Quantum effect is already discussed. What is that? Well, due to electron confinement happens because of the size effect right.

That means, energy bands are normally displaced replaced by the discrete energy states leading to case where conduction materials can behave like a semiconductor or insulator yes that is what happens because of discretion of the energy bands then electrons can no longer stay at all energy levels.

So, therefore, the band gap develops and depending on the type of band gaps semiconductor or the insulating properties can come in that is what is basically quantum effect. So, this is nothing but quantum confinement right. And what is classical effect? Well, in the classical effect the mean free path of the inelastic scattering becomes comparable with the size of the system and this can lead to reduction in the scattering events.

That means, if you reduce the grain size or the crystallite size of the material and then this size become comparable with the mean free path of the inelastic scattering events. Then scattering will be substantially reduced and conductivity can be increased. So, this is to

something relate with mean free path comparable to size of the system right that is what will happen.

So, we have to discussed the electrical conductivity considering these two aspects this is the main two aspects this is what we should discuss right you have to understand that these were the two things we will discuss in terms of this. Now, in 3D nano material where the all the three spatial dimensions are more than 100 nanometer. In case of 3D 3D nano material what happens all the three spatial dimensions are above the nano metric range that is more than 100 nanometers.

So therefore, these effects will not make any significant issue on the electrical conductivity right and that way you can ignore even these effects at all. So however, bulk nano crystalline materials exhibit high grain boundary to volume ratio and this can lead to increase electrical electron scattering.

And as a consequence nano size grain or 3D nano materials can so, decrease electrical conductivity. So, because this is basically because of the scattering effect, scattering of electrons ok due to large number of grain boundaries. This can lead to decrease of electrical conductivity right but what happens 2D nano materials?

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Quantum Confinement

- This is very similar to the famous particle-in-a-box scenario and can be understood by examining the Heisenberg Uncertainty Principle.
- The Uncertainty Principle states that the more precisely one knows the position of a particle, the more uncertainty in its momentum (and vice versa).
- Therefore, the more spatially confined and localized a particle becomes, the broader the range of its momentum/energy.
- This is manifested as an increase in the average energy of electrons in the conduction band = increased energy level spacing = larger bandgap
- The bandgap of a spherical quantum dot is increased from its bulk value by a factor of $1/R^2$, where R is the particle radius.*

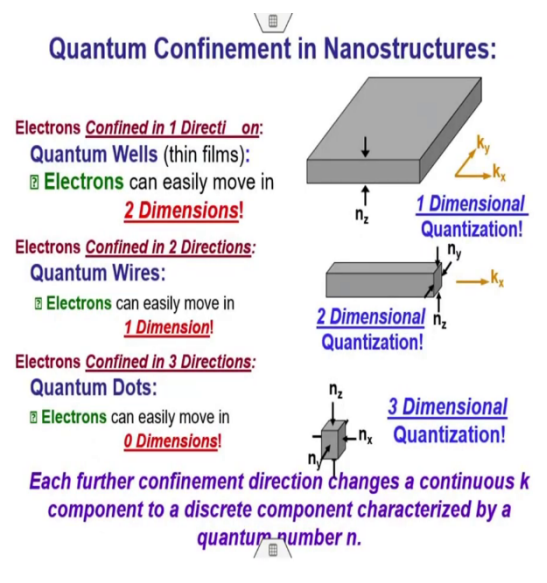
- Based upon single particle solutions of the schrodinger wave equation
- valid for $R <$ the exciton bohr radius.



So, before we discuss about that let us talk about what is this quantum confinement again and we will discuss in both in physical and mathematical terms together ok. This is very similar problem as we discussed in last class in a particle in box situation that is what we are going to bring it ok. And therefore, because of this situation Heisenberg uncertainty principle can be applied and it can lead to more spatially confined.

Remember this word spatially confined and localized electronic bands and therefore, because of that broader range of momentum energy of electrons is possible. And this can be manifested in terms of average energy of electrons in the conduction band is equal to increase energy level spacing or rather larger band gaps correct.

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So, that is what is the effect we see and now in case of 2, 1 and 0 dimension nanomaterials in case of two nanomaterial 0 dimension nanomaterials like in thin films the electronic motion is confined in the thickness directions. It is free in the plane of the thin film like x and y directions, but in case of 1D nanomaterials like a quantum wires nanowires on a tubes electronic motion is quantized in two directions.

Only in one direction like z directions electronic motion is free ok, but in the other two directions electron motions are confined. In case of 3D as I quantum dots ok the electrons can

easily move in no direction whereas, 0 dimension ok. So, therefore, in case of quantum dots you have a three dimensional quantization happen.

In case of quantum wires or two or 1 dimensional material you have 2 dimensional quantization happens and incase of quantum wires like in thin films you have 1 dimensional quantization can happens. And you know this confinement direction charge changes a continuous k component to a discrete components characterized by quantum number n ok.

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The 1d (infinite) Potential Well ("particle in a box")

- We want to solve the **Schrödinger Equation** for:

$$x < 0, V \rightarrow \infty; 0 < x < L, V = 0; x > L, V \rightarrow \infty$$

$$\Rightarrow -[\hbar^2/(2m_0)](d^2 \psi/dx^2) = E\psi$$
- Let us apply Boundary Conditions:

$$\psi = 0 \text{ at } x = 0 \text{ \& } x = L \text{ (} V \rightarrow \infty \text{ there)}$$
- Energies are quantized:

$$E_n = (\hbar n \pi)^2 / (2m_0 L^2), \quad n = 1, 2, 3$$
- Wave functions are given by

$$\psi_n(x) = (2/L)^{1/2} \sin(n\pi x/L) \text{ (a standing wave!)}$$

Qualitative Effects of Quantum Confinement:
Energies are quantized & ψ changes from a traveling wave to a standing wave.

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How it is happens let us do that. Well, that is can be treated in a simply looking at 1 dimensional case 1D potential well like particle in a box. So, what does it mean? So, it means that you have a particle inside a box. The particle is $x=0$ to $x=L$ and then you have particle sitting here like this with the mass m right that is what it is. So, what will happen to the energy levels of that particle that is what is important right and the particle is basically electron here.

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The 1d (infinite) Potential Well ("particle in a box")

$$E\psi = \hbar\omega\psi = j\hbar\frac{\partial\psi}{\partial t} \quad \hbar = \frac{h}{2\pi}$$

$$-j\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x)$$

B.C.s
 At $x=0$ $\psi=0$
 $k_n L = n\pi$
 $\psi(0) = 0$
 $x=L$ $\psi=0$
 $\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$
 $E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$

$V(x)=0$ $0 < x < L$
 $E\psi_n = -\frac{\hbar^2}{2m}\frac{\partial^2\psi_n}{\partial x^2}$
 $\frac{d^2\psi_n}{dx^2} + k_n^2\psi_n = 0$
 $k_n = \frac{2n\pi}{L}$
 $\psi(x) = A \sin k_n x + B \cos k_n x$
 $= C_1 e^{jk_n x} + C_2 e^{-jk_n x}$

So, let us do that. Say you know in order to treat such a kind of things we should first solve the as you seen here first you need to solve the Schrodinger equations. What is Schrodinger equation is? We know that Schrodinger equation is like this. $E\psi = \hbar\omega^2\Psi = j\hbar^2\frac{\partial\Psi}{\partial x}$ this is $\hbar = \frac{h}{2\pi}$ correct.

So, now the question is very simple, question is very very simple. Let me just see what I how best I can do that ok, question is very very simple. So, I can write down the this equation very simply ok like this. So, $-j\hbar^2\frac{\partial\Psi}{\partial t} = \frac{\hbar^2\partial^2\Psi}{\partial x^2} + V_x\Psi_x$.

So, V_x is basically the potential and Ψ_x is the wave function. Remember that Ψ_x is nothing but the wave function. So, that is something you should not forget these are the very standard terms and it is in x directions and t is the time, $\hbar = \frac{h}{m}$ is the mass of the particle.

So, now the question is this. How do you solve this equation in case of this potential well? Obviously, inside this potential well V_x right with in this domain, $0 \leq x \leq L$. So, we can write down $E\psi = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$ right or basically it is it can be written like this correct or you can write down like E or we can write down this very simply.

$\frac{\partial^2 \Psi_n}{\partial x_n^2} + k_n^2 \Psi_n = 0$, where $k_n^2 = \frac{2mE_n}{\hbar^2}$ is nothing but twice $m E_n$ by a square. So, now you can assume the psi for this equation the solution of $\Psi_x = A \sin k_n x + B \cos k_n x$ right or its basically you can also do $\Psi_x = C_1 e^{jk_n x} + C_2 e^{-jk_n x}$; please do not ask me how I am getting this. These are all elementary plus 2 level differential equation solution.

Remember this is a ordinary differential equation. This is not a partial differential equation ok. Why? Because it is 1-D that is why. So, 1 dimensional case this will be ordinary differential equation. So, such a kind of ordinary differential equation if you have it can have such a kind of solutions ok.

So, now once you know these are the two solutions possible you can apply boundary condition right. What are the B.Cs here? Very simply B.C is what are the B.Cs? You can see that at $x=0$, at $x=L$, $\Psi=0$, right. So, what does it mean? That mean $k_n L = n\pi$. Yes because if it is $Y(0)=0$, $B=0$. So, $x=L$, $Y=L$, $\cos 0=1$, $\sin 0=0$ right.

So, then $k_n \pi$ right. So, therefore, and this is the boundary condition therefore, we get $\Psi(0)$ to be 0 when $B=0$ right. So finally, you can clearly see after doing applying similarly one other boundary condition is what? Another boundary condition at $x=L$ $\Psi=0$ right that is also true.

So, therefore, $\Psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x$ right that is what it is. This is the wave function. Similar energy is given as a $E_n = \frac{\hbar^2 \pi^2}{2mL^2} n^2$ here; obviously, because its 1-D, this is energy, this is the wave function. So, if you can solve such a kind of expression very easily very easily you can solve such a kind of expressions, it is not difficult.

And if you are not able to do that so, please get back to me we can do that, but solving this Schrodinger equation in 1D is a very elementary things in physics. It is not at all a difficult term and you know we have already considered such a kind of system. So, at $x=0$, $V=0$ as $x=L$, $V=\infty$. So, therefore, at this position less electron cannot stay.

So, therefore, $\Psi(0) = 0$ here there right that is very clear. So, now, you have clearly. So, this is what you got this is the same expression we have got there ok. Or we have got something else ok, we have not, we have not got anything.

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The 1d (infinite) Potential Well ("particle in a box")

$$E\Psi = \hbar\omega\Psi = \hbar\hbar\frac{\partial^2\Psi}{\partial t^2} \quad \hbar = \frac{h}{2\pi}$$

$$-\hbar\hbar\frac{\partial^2\Psi}{\partial x^2} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi(x)$$

B.C.s
 At $x=0$ $\Psi=0$
 At $x=L$ $\Psi=0$
 $V(x)=0$ $0 < x < L$

$$E\Psi_n = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi_n}{\partial x^2}$$

$$\Psi(x) = A\sin k_n x + B\cos k_n x$$

$$= C_1 e^{jk_n x} + C_2 e^{-jk_n x}$$

$$k_n L = n\pi$$

$$k_n = \frac{n\pi}{L}$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

So, something wrong here, I am sorry, I made a mistake. Root, this is basically root this is ok. So, that is the solution of the equation. So, if you put the solution it will be ok.

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The 1d (infinite) Potential Well ("particle in a box")

$$E_n = \left[\frac{\pi^2 \hbar^2}{2mL^2} \right] n^2$$

where $\hbar = h/2\pi$, h is Planck's constant, m is the mass of the electron, L is the width of the potential well (thickness of 2-D nanomaterial), and n is the principal quantum number.

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

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

$$p = mv$$

So, now what happens in case of nanomaterials let us discuss. In case of 2D nanomaterials thickness at which the thickness at the nanoscale basically thickness is the nanoscale. So, therefore, quantum confinement will occur along the thickness dimensions right. Simultaneously carrier motion is or electronic motion the whole motion is uninterrupted along the plane of the sheet. What is that mean?.

So, if you have a if you have a 2D thin film like this on a substrate the small thickness right and this is what is your thickness is. So, I can write down this is my x, this is y and this is your z right, the thickness in the z direction. So therefore, you can see the quantum confinement or the electron such a kind of thing. So, just now I discussed the electron is in a potential well. Such situation only happening in the thickness directions ok, this aspect this aspect happening only thickness direction, thickness direction is confined ok.

This direction, as a length, which is almost close to the electronic energy bands or the lambda actually. So, therefore, but other two direction electron can move uninterrupted ok without any problems. So that means, along the planar sheet of the I mean the plane of the surface electron can move very easily.

And in fact, as the thickness decreases wave function of electrons will be substantially limited by the; wave function will function will be substantially limited by the what? By the specific value along the cross section. Why it will be specific value? It is very simple. So, if this is the length. The value of wave you can see this is energy at n equal to 1 or this is basically how the wave functions will look like not the energy ok.

So, electron can have specific wavelengths. You have see this is $L/2$, this is $L/4$, $L/6$, $L/8$, $L/10$ right that is what will happen. You remember that one wave is this right. Am I clear right? So, it is something like that. This is half of the wave $2L/C$. So, not $L/2$, this is half of the wave the $2L$ ok this is L then L/C , $L/2L$ by this is $2L$ and this is 2 and L correct $8L/2$ am I clear. So, 3.5 sorry $5L/2$ that is very clear.

So, this is because electronic wavelengths are multiple integers of the thickness that is very clear. The wave lengths of the electrons this is the lambda that is multiple integers of the thickness. So, all the other electron wavelengths will not be present they will be absent. In

other words there is a reduction in the number of energy states available for the electronic conduction along with thickness.

So, you have discretized now the energy levels such a way only few energy levels are allowed electron can stay there. Electron cannot stay in all the energy level like in a continuous system continuous kind of spectrum right. So, electron become trapped; obviously, they are trapped in a well and width of width is equal to thickness.

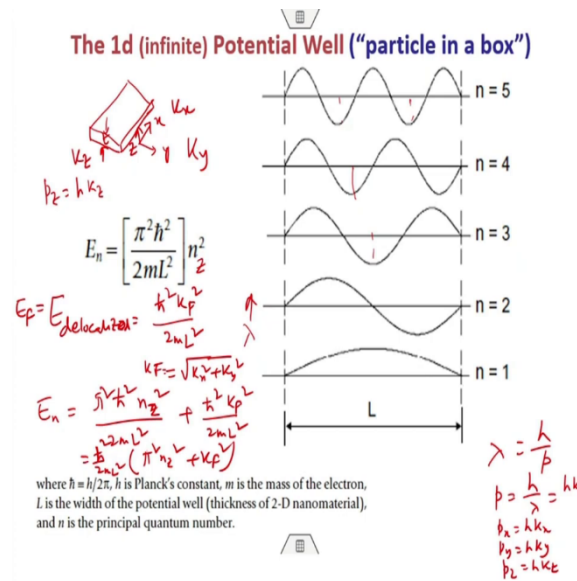
So, in a general electron containment of the energy states in 2D nanomaterials with thickness nanoscale is given by this expression $E_n = \frac{\pi^2 \hbar^2 m L^2}{2 m L^2} n^2$ and we have discussed about everything. Now, this particular expression is assumes an empty infinite depth potential well, but carriers are free to move along the x and y directions right.

So, therefore, total energy of the carrier will have two components; one along the thickness other one is because of the uninterrupted movement of the electrons along the plane of the system. So, understand this energy levels or energy associated unrestricted motion. So, let us assume z is the thickness that we have already done ok. If you assume z is thickness and x and y are the in plane that is what exactly I drawn in this picture x and y the in plane and z is the thickness right.

So, now the question is very simple under these conditions unrestricted movement of the electrons are characterized by 2 vectors k_y and k_x are restricted when the electron is characterized by k_z correct they are the wave vectors. So, you can see that we can write down the momentums $p = \hbar k_z$ to what, $\hbar k_z$ you might be asking how I am getting. That is basically from the de Broglie's equation what is lambda is equal to P/mv right, am I correct. So, mv is what? P/λ correct.

So, now you know that this can be written as a so, this is the momentum. So, p is equal to yeah p is equal to that ok h/λ sorry h by lambda is h/P right ok. So, h of something wrong I have written right sorry, I am writing something wrong, let me correct it.

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So, actually de Broglie's equation λ is equal to what? $\lambda = h/p$. So, $p = h/\lambda$. So that means, is written as a $1/\lambda = k$. So, So, $p_x = \hbar k_x$, $p_y = \hbar k_y$, $p_z = \hbar k_z$ these are the momentums. So, we can write down that. The energy corresponding to this with this kind of uninterrupted electrons or the de localized electrons is given for the energy of the delocalized electrons.

This we can write down de localized is given as by the Fermi's energy E_n that is nothing but

what? $E_n = \frac{\hbar^2 K_F^2}{2mL^2}$. You must be thinking where from the K_F^2 coming very simple, n^2 is replaced by k_F right and so, therefore, you can write down this is what is known as actually Fermi energy also. This is the highest occupied energy levels or Fermi energy levels ok.

So now, therefore, I get this is what is the unfetter energy and here K is what? $K =$

$\sqrt{K_x^2 + K_y^2}$ correct because these are the two directional electron can move unfettered or

uninterrupted. So, therefore, total energy of system is E_n , $E_n = \frac{\pi^2 \hbar^2}{2mL^2} (K_F^2 + n_z^2)$ is right.

So, one can actually take a common of $2mL^2$ and you can see this become or $E_n = \frac{\pi^2 \hbar^2}{2mL^2}$

$(K_F^2 + n_z^2)$, this is what it is. So, since the electrons electronic states are confined along these

thickness directions electron movement is only movement of machine only relevant in the in plane directions other directions is not important.

So, as a result scattering by phonons and impurities can occur in the in plane direction. Like electrons which are moving along a plane they can only undergo scattering because of phonons or because of you know grain boundaries or because of impurity atoms many other things ok. So however, for the two nanometer nano crystalline structure will have a line number of grain boundaries also. So, this grain boundaries also act as scattered. Am I clear?.

That is what will happen and so, therefore, smaller the grain size lower will be electrical conductivity for the 2D nano crystalline materials. That is very clear because its confined because of that in z direction it is confined because of that electrical conductivity will decrease, but still electron can have an unfettered undisturbed motion along the plane. But, there also depending on the grain size this motion will be hindered because of the scattering effects, but that is classical effect actually.

So, you have both the quantum confinement effect classical level presence together that is what happens ok. I hope I am made it clear. So, this is something which is very unique for the 2D materials and it is easy to understand that is what I started with 2D materials and described the whole things. So, first you solve the Schrodinger equations for a 1 dimensional case because 2D is 1 dimensional quantized other 2 dimension, it is not quantized and is easy to do this calculations.

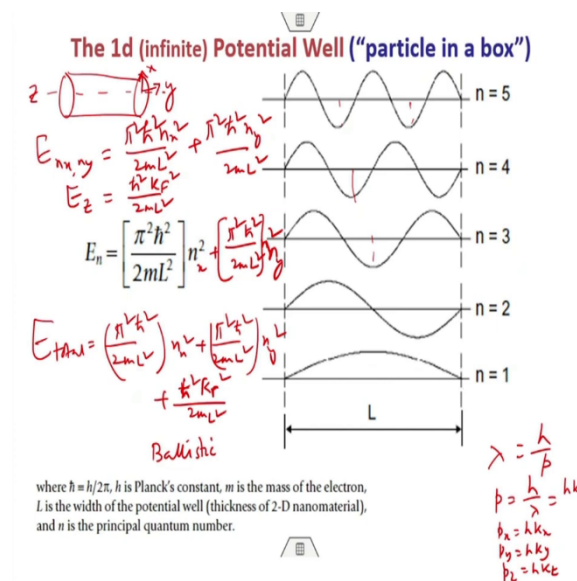
And then you can bring about this concept of motion of electrons confine along z directions, but unconfined or undisturbed or uninterrupted along the plane of the material that is something which is very important. So, what happen in case of 1D materials right? Let us see that ok. Well, so, we will come back to these equations later. Say in case of 1D materials quantum confinement will occur in the 2 dimensions.

1D material like a nano tube nano wire, it will happen at two directions, where unrestricted motion can occur only along the axis of the nanotube rod or wire. So, contrary to 2D material 2D nanomaterials which allows only one value of the principal quantum number for the each energy states, you have seen it is only in z. In this case here you have a 2 dimensional

confinements and two quantum numbers will be used for that. So, how it will be, let us do that. I will erase it.

So, it is like a nanowire or nanotube. Let us draw this nanowire and do that again the mathematical part so that you can understand without any problems. Obviously, you will always have some questions. So, for that only you need to read the books and understand the things very clearly ok.

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So, I first draw a nano tube. So, in this nanotube this is the z directions ok. I am changing ok directions now z and this and this is the two directions x and y ok, y is not z it is a 3D ok you have to understand that. So, because there will be confinement along x and y directions and z direction is unfettered movement of the electrons or undisturbed movement of electron will happen. So, what will happen?.

We can always write down $E_{n_x, n_y} = \frac{\hbar^2 \pi^2 n_x^2}{2mL^2} + \frac{\hbar^2 \pi^2 n_y^2}{2mL^2}$. This is what will happen and along the z directions it will not be. So, along z directions E_z rather or it it will be like this the earlier case right.

So, $E_{nx,ny} = \frac{\hbar^2 \pi^2 n_x^2}{2mL^2} + \frac{\hbar^2 \pi^2 n_y^2}{2mL^2}$ right that I have written right that is what is E_n . So, total energy of the system then $E_{\text{total}} = \frac{\hbar^2 \pi^2 n_x^2}{2mL^2} + \frac{\hbar^2 \pi^2 n_y^2}{2mL^2} + \frac{\hbar^2 \pi^2 n_z^2}{2mL^2}$ right.

So, it states the 1 dimensional nano materials will not. So, it is a single energy band, but it will spread into sub bands that is what it tells you. It will spread into sub bands it will not even have one single bands because you have discretization happening in two direction x and y. So, you will have sub bands. Because of these confinement effects nanoscale dimensions of 1D act as a reflector they will act as a reflector. You know what happen in reflector?.

A reflector if you put a beam it will come back reflected same thing will happen here. So, it will not allow electron to exit the surfaces. They will they cannot go beyond that this surfaces of the materials ok or rather not upto the material per se from the energy bands actually because each energy band this sub band will act as a surface. So, in addition scattering of impurities and obviously, phonons will also be happening along the long axis or z axis of this nanotube.

And therefore, what will happen? And you know this will happen and the scattering will be more as the size decreases further that is the length of the tube decreases further the wire decreases further. As a consequence transport of electrons on the tube will occur without significant loss of kinetic energies or in other words transport along the electron transport along z direction will be ballistic ok. Remember this word ballistic.

Ballistic means very high speed. You have probably heard of intercontinental ballistic missiles. So, ballistic means very high speed transport will happen and this is more generally found in case of 2D nanometer 1D nano materials in at low temperatures, so, like since you have nanotubes. How many nanotubes are metallic ok, what does it mean?.

The conductivity is extremely high you know. How high? It is 1 billion amperes per centimeter square. In this a copper it is only 1 million. So, you have a three orders to magnitude increase of the electrical conductivity along the z direction or the length of the tube can happen in case of metallic carbon nanotubes ok.

So, we will discuss later on what is metallic and what is non metallic carbon nanotubes that is part we have not yet talked about it. But for the sake of understanding assume that the electronic motion will happen in a ballistic way a very fast manner unfettered undisturbed manner along the tube or the length of the tube and therefore, they have a huge thermal electrical conductivity.

Same thing happened with thermal electrical conductivity process also. Phonons can move very easily we have discussed about that. So, in addition to this effect carbon nanotubes also exhibit very low density of defects and high thermal dissipation. So, therefore, thermal dissipation heat will be moving also fast. As you pass the current there will be joule effect because the heat will be produced. So, if heat is also dissipated electrical conductivity will also increase ok.

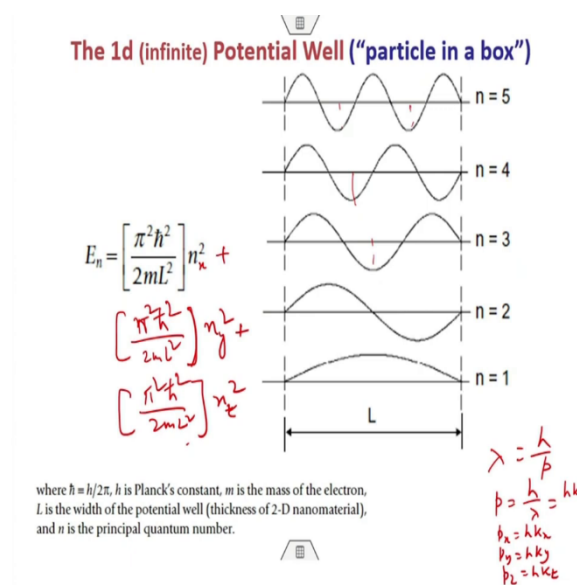
So, because of the low concentration of defects and high thermal conduct heat dissipations again lateral conductive will further rise in case of nanotubes along the direction of the length of the tube, correct. So, this is something which is very important in case of nanotubes, nanowires or even in case of rods actually. This is very frequently observed that is why these materials become very important in 90s. There are they are very highly considers important aspect of subjects.

And after that metallic nanowire scheme like gold, silver, platinum nanowires they are these effects are even stronger because you have a metallic things coming into picture. Your nanotubes that is not always the case, but in case of metals electrons are free. So, therefore, you have addition of that. So, you can have very high electrical conductivity in some metallic nanowires.

Well so, that is something which is important to know for the 2D sorry 1D nanometers. What happen in 0D or quantum dots ok? So, let us discuss about that. So, quantum dots they are all the three dimensions are in nanoscale. So, this quantum confinement will happen in three directions, all together right, it is bound to happen. So, if that is what is going to happen in all the three dimensions. So what will happen?.

The 0 0 dimension nanomaterials the motion of electrons is totally confined along the three dimension directions like x, y and z.

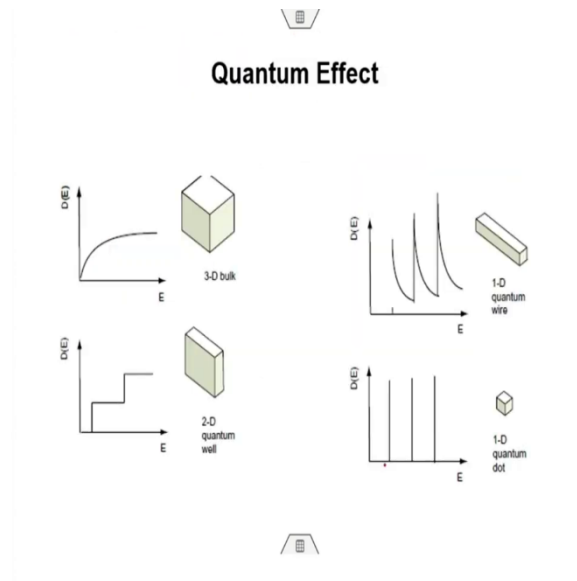
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So, therefore, energy $E_n = \frac{\pi^2 \hbar^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2)$ can be given as this equation right. Take one final three directions. So, under this conditions metallic system will behave like a insulator because electron will be electro motion will be confined in the three surfaces x, y, z correct. They will not be able to move because of discretization of the bands.

See you can imagine in 1 dimensional confinements, that is in 2D nano materials you have confinement only happening in one direction. So, this will lead to such a kind of energy band structure. In 2D you have 2 dimensional confinements. So, therefore, there will be sub band formation. In 3D 0D nano materials you have been in the three directions basically confinement happens.

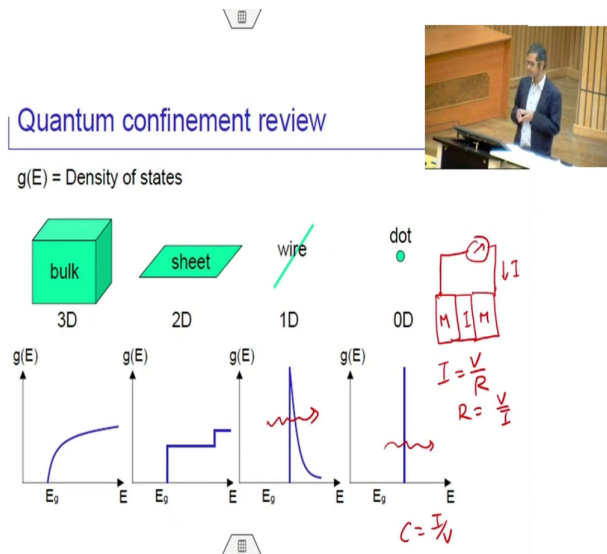
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So, sub bands will divide into more and more sub bands that is why in 0D you have discrete complete discrimination or delta function type energy bands. So, electron can only stay in this portion in this portion electron cannot stay, it is not allowed because of this they behaves like insulator in all the three directions. So, you can make an insulating metallic nanomaterials by making them quantum dots. So, that is very very important.

So, that is what I have showing you in a 3D you have a density of states continuous function of x if energy levels, in a 2D you have step functions and in 1D you have such a kind of things and in 0D it is completely discretized. This is something which is very very easily formed ok.

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So that is because in the sheet (Refer Time: 41:10) it can unfettered movements and the length of the wire it has unfettered movement of the electrons and quantum dots it cannot move at all. So, far we have been discussing electrical properties of this different dimensions of nano materials like 0D, 1D, 2D and 3D in isolated entities.

But, you know from the particle point of view these materials need to be coupled to the external circuits if I want to use by electrodes right. If you want to use this you have to connect with electrodes, for 2D and 3D nanomaterials this will be like a ohmic kind of a contacts right.

The moment you contacting with the wire for 2D and 3D it will be like a ohmic contacts there will be voltage stops, but for 0D and one nano materials the contour resistance for the nanometers and the connecting leads will be extremely high, it will be extremely high ok. So, therefore, one mechanism providing conduction is so, you cannot use it right one motion conducting this is wire that is by electron tunneling.

And this is a quantum mechanical effect in which electron can penetrate a potential well a barrier due to high energy conduction layer which is higher than the kinetic energy of electrons ok that is possible, the electron tunneling is possible. So, you have a very high energy barrier electronic can actually tunnel through this that is what it is tunneling.

Same thing happen here electrons can turn into that correct that is what you have to use. So, how do you understand that? Well, that is can be easily understood by by have a like such a kind of structure. Like you have a one metal and one insulator there is insulator stand with between two metal wires, this is metal, this is insulator, this is metal then we have to connect with leads ok.

The simple way achieving this is to apply voltage V across this circuit to rest the Fermi energy correct, one of the metals. You apply voltage, Fermi energy amount of metals increase because obviously, with the moment you put energy electrons will move from the valence band and go above much of the valence band and the height of the upper level of electrons in a conduction while we will move up right.

So that is what is called Fermi energy level. Fermi energy will go up and because of that what will happen? Because of these electrons that can tunnel from one metal with the highest energy Fermi level to the metal with the lowest Fermi energy level that is a you are creating a you know upper and lower sides to jump electrons from the jump from the highest occupied Fermi level in the metal which is on which on which is applied because one on which this an electron levels are lower.

This is something which is very unique and widely found ok. So you know regular electronic circuits we all know that regulation circuits. This is what is ohmic torque is or rather $R=V/I$ right and however, in this case the resistance is permanent due to electronic tunneling because of electron resistance is happening. So, as an example if I have a gold around gold nano particles which are electrically coupled by connecting the nano particles to each other by organic molecules.

You can put organic layers around this that is nothing but a capped layer. A nanoparticle can act as a metal electrode, whereas, the organic molecule can play as a thin insulator. Under this conduction condition conduction conductance basically $C=I/V$ ok and this is will increase due to electron tunneling are compared to in case of nanoparticles were not connected by the organic molecules.

If there is no organic layer around it the conduction will increase in this case. Well, so, that is something which is very important. In the next lecture I will primarily talk about the

magnetic properties of the materials. It is easy to discuss about these aspects, but there are some things of the electrical conductivity I will finish if off then I will talk about the this aspect of magnetic properties ok. So, keep in mind that this discussion requires you to understand the basics of quantum mechanics.

So, please do study that because law all these things like electrical properties, thermal property, electrical properties, magnetic properties and optical properties will be basically based on the quantum mechanical statements that is solutions of Schrodinger coordinate equations and other aspects also and electron the confinement effect quantum confinement effects very strongly will come into picture. So, please do study these aspects and we will get back to you.

Thank you.