Nanomaterials and their Properties
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Lecture - 22
Thermal Properties of Nanomaterials (III) Cont.

Students, let us start the lecture 22. And this will be extension of lecture 21 that is on Thermal Properties of Nanomaterials.

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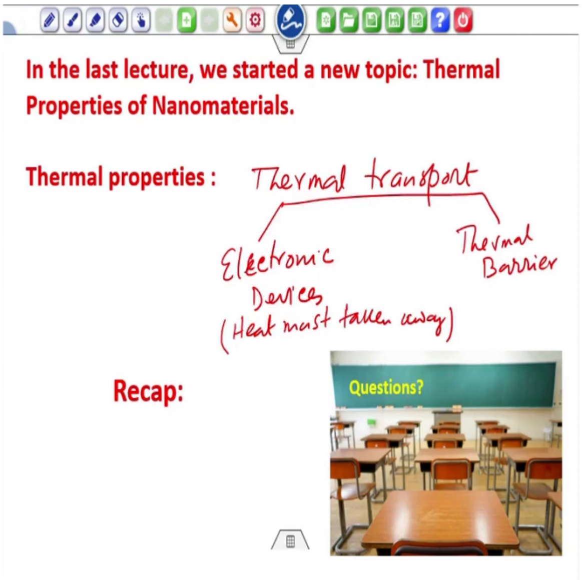

So, you know that the last lecture, we have been discussing about thermal properties especially the thermal conductions, ok. That is what is we have been discussing, a thermal transport. Thermal transport is very important in electronic devices, right. Electronic devices as like computers, laptop, mobile phones, etcetera, the thermal transport is equally important.

So, there are two things which is required in while thermal transport is considered. One that is the heat must be conducted away or heat must be taken away, or there will be situation where you need to put a barrier to the heat transport. These are known as a thermal barrier. In both the cases, important aspect is the thermal transport. So, there are few aspects we have already discussed. Let us first have some recap of those.

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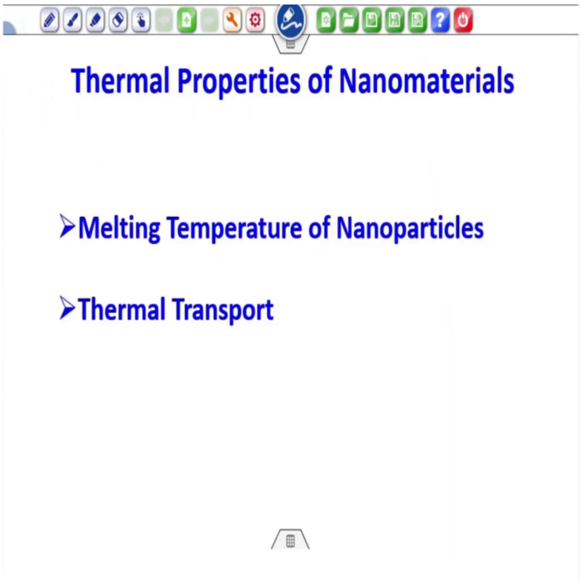

As you know, thermal transport and the melting temperature of nanomaterials are important aspects to be considered while designing any component using nanomaterials.

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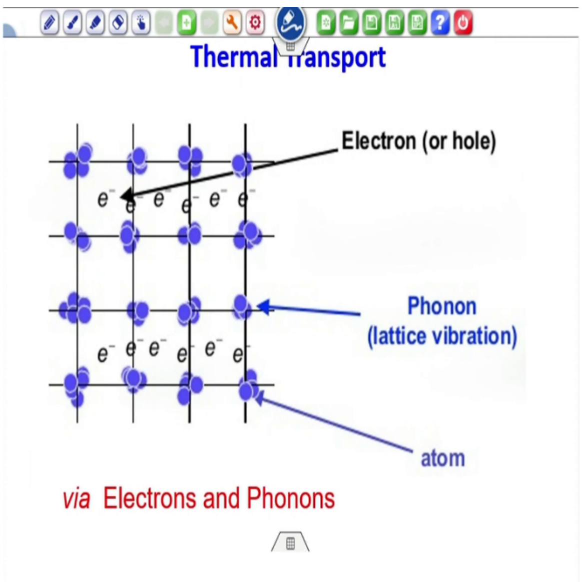

So, in a any device, heat is transported by either electrons or holes and phonons which are nothing but lattice vibration. So, electrons in a metal are free. They are not bounded or they are actually not localized. Rather they are delocalized electrons which can move from one place to other place without much of hindrance.

But hindrance can come from the scattering of electrons by different kind of scatterer like grain boundaries or even it can be scattered by the heavy atoms. So, therefore, there will be some kind of a loss of because of these scattering events. On the other hands, phonons or lattice vibrations are more important for non-metals where electronic conductions are not possible. So, these are actually travelling waves which are propagated to the material because of the vibrations of the atoms.

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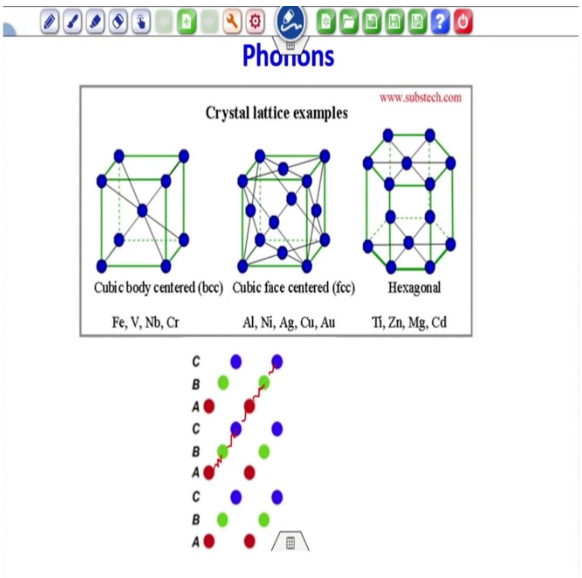

So, as you heat the material, atom starts to vibrate, and because atoms start to vibrate, they push and pull each other during the vibration, and that is leads to the motion of a wave or travelling of a wave in the material. And this is what is known as a phonon which we have discussed in the last lecture already. So, in a standard material like FCC, atoms are arranged in a chain, right like this A, B, C layers.

Now, these atoms can be considered to be connected by springs, right. So, as they are connected by spring, now during heating about the material the atoms will vibrate from the mean or equilibrium positions. So, as is vibrate like this, from the both the directions what will happen? The atom one atom can push the other atom or it can pull the other atom in the neighborhood, and this can lead to a travelling wave, and that is what is known as a phonon.

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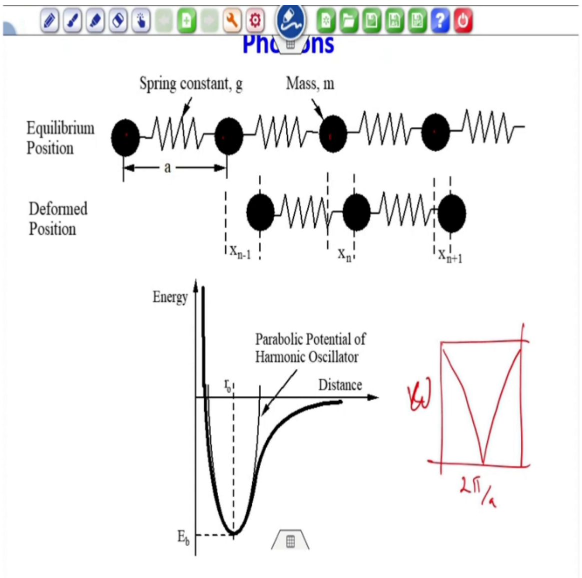

This is shown something is shown here. So, you have suppose chain of atoms 1, 2, 3, 4, and they connect by spring. Now, if they move small distance X_{n-1} atom suppose, it moves by small distance from its equilibrium positions, what will happen? This spring will get pushed or pulled, and this can lead to a travelling wave. That is what we are talking of phonons.

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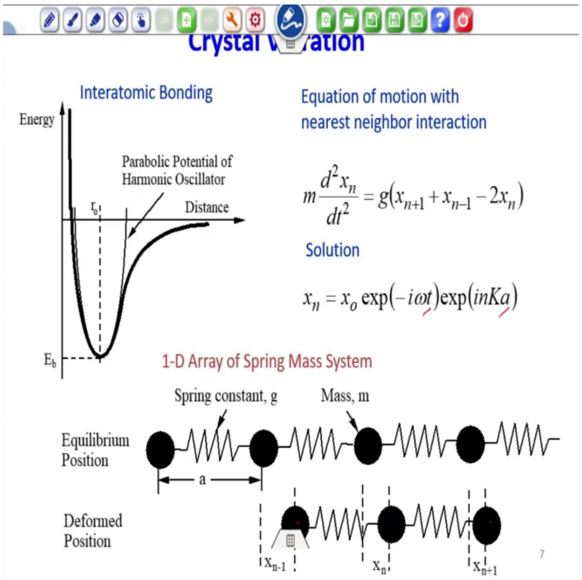

So, well, one can actually design equations of motion taking 3 neighbors, x_{n-1}, x_{n+1} and x_n, ok. So, central atom will be pulled by both the corner atoms or the atoms at these positions x_{n-1}, $x_{n+1,}$ and x_n, and this can lead to a kind of a motion equation in terms of force, where m is the mass of the atom and then this is the double derivative with respect to time is acceleration, and this is nothing but the push and pull.

So, therefore, this is the force this is also force, and g is a spring constant, right. Hence, we can solve this equation and we can get two important exponential solutions, one in terms of t, time; other in terms of amplitude a, a is the equilibrium distance between the two atoms when they are not scattered or they are not moving from equilibrium positions, ok.

So, hence, if we plot these things, ok we can get some sort of a scattering things like that. I do not know whether I have as you where I have shown in the last class. So, you have a two branches of the thing, this is k, and sorry, this is omega and this is twice pi by a. So, you have a two branches of the travelling waves, correct. So, that is leads to motion of phonons from one part of the crystal to the other part of crystal.

Now, this way heat can be transmitted. So, now, the question is this. Whether it is a electron or a phonon, whatever may be the carrier of heat, carrier of the thermal transport ways and means of that, important aspect is what? Important aspect is the size effect of nanomaterials on the electronic or the phonon energy levels. That is what is going to dictate or control the heat transport in nanomaterials.

So, before we discuss that let me just tell you again that there is the nanomaterials of different dimensions, 0, 1, 2, or 3. Therefore, the electronic energy levels as well as the phononic energy levels, can get affected significantly by these dimensions. You may ask why. That is very simple as the dimension of the materials becomes small enough to be comparable with the electronic energy levels or the phononic vibrations wavelengths.

What will happen then? Then, they will interfere each other. The dimensions of the material will interfere the energetics of the electrons as well as the phonon wavelengths. And this can significantly affect the thermal movements. So, how does it happen. Let us talk about it. That is what the important aspect comes into picture, ok.

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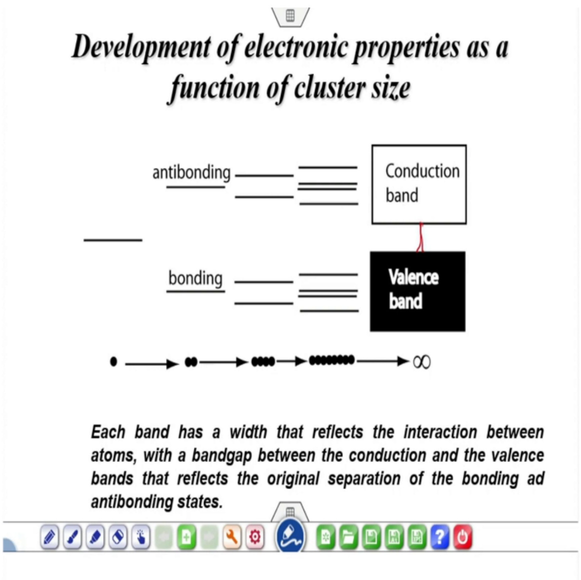

What is that? That is what is known as the confinement effect, ok. So, as you know in a nanomaterial, the you have antibonding and bonding orbitals and electrons are divided between conduction and the valence band, right. And each band has a width that reflects interaction between the atoms with the band gap, between the conduction, and the valence bands that reflect the original separation of the bonding antibonding steps, right. This is the binding band gap.

So, in a metal in a metal actually you do not have any band gap, right. There is no band gap between in a metal because the valence band and conduction band overlap each other. On the other hand, in semiconductors insulator you have a definite band gap. So, in a semiconductor band gap is small compared to the insulators.

So, that is because there is no band gap between the conduction the valence bands. What will happen? Because of overlap of these two bands electrons are free to move there is no barrier. And as you see because there is no barrier, so electrons are delocalized. This is a we have discussed about it.

But in semiconductor you need a definite energy gap between these two bands and therefore, we need to provide that energy to the system, so that electron moves from a valence band to the conduction band. This can be done by using heat or thermal energy or by doping, right. We can modify the band diagrams simply by doping. In insulator, you cannot do that.

There is no electronic conduction is possible in insulator. So, there are only heat conduction is possible is a phonon. Let us think of electronic insulator like diamond. A diamond is a good thermal conductor. So, therefore, in diamond phonons actually are the major heat carriers, correct. So, what are the situations both phonon and electrons can undergo confinement?

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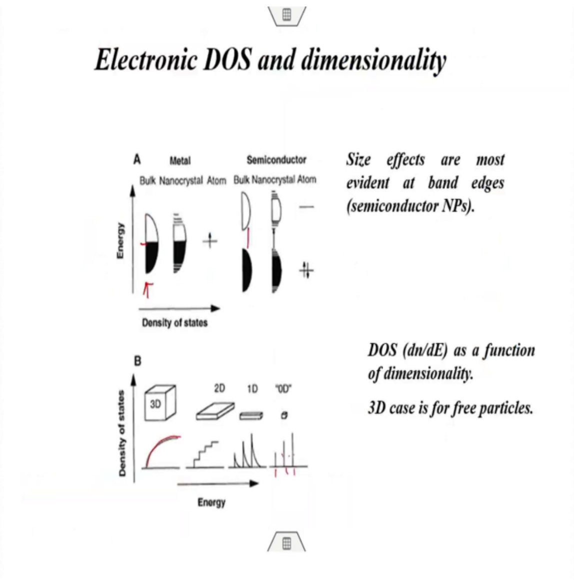

Now, how does it so? So, in a metal as we can see in a bulk material electron, this is what is shown here, the conduction band is completely you know full on and the sorry the valence band is completely full and conduction band is overlapped with the valence band, right. That is what is shown there. The highest energy level is known as a Fermi level. That is can be seen from here which is a completely free energy level.

So, now as you decrease the dimensionality of the material that is what you make a nanomaterial of that these bands will undergo discretization; that means, this bands will no longer remain continuous. As you can see here, density of states is varying continuously with respect to the energy E, right for a 3D nanomaterials. In 3D nanomaterials, all the dimensions are not nanoscale, they are bigger than the nanoscale dimensions.

So, as soon as you make them as a nanoscale dimensions any of these xyz directions, what will happen? The energy levels will undergo discretizations. You might be thinking why it is so. We will come to it very soon why it is so. Energy levels will be discretized, and that means, what? Electrons cannot occupy any energy level continuously like in case of bulk material. Electrons can only occupy those discrete energy levels and because of that motion of electron is affected in a nanomaterial.

In a semiconductor with a definite band gap same thing can happen, ok. In a semiconductor, you see there is a definite band gap in a bulk semiconductor, but energy levels in the conduction as well as the valence band can undergo similar discretization due to effect of nano size. Am I clear?

So, therefore, density of states which is nothing, but dn by dE, if you plot the function of dimensionality like 3D, 2D, 1D or 0D, you will see discretizations happening from 2D to 0D, very severe discretion happens in 0D. Electrons can occupy only very specific energy levels given by this delta function, you can see that, spike at certain value of the energy levels, the density of undergoes source 5 spike.

So, therefore, electrons can occupy only these energy levels. They cannot occupy in between these energy levels. And because of this electron motion is affected energy transfer is affected significantly, right. So, this is the effect of dimensionality on the electronic motion. And this is known as a quantum confinement.

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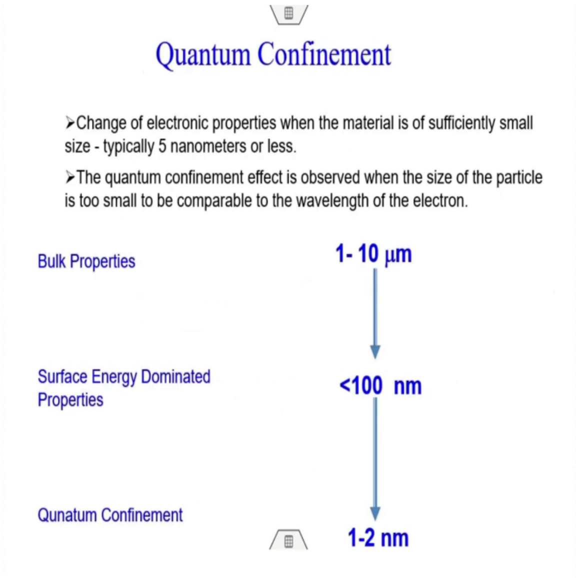

Now, you must be thinking what is it well, what is quantum confinement because this will come keep on coming to us an optical or an electrical or electronics properties also. So, electron confinement means change of electronic properties when the material is of sufficiently small size, typically of the order of 5 and less nanometers, 5 nanometer or less, ok.

As you know, this diagram at the bottom I have shown you earlier in the first one or two lectures. So, quantum confinement is observed when the size of particle is too small to be comparable with the wavelength of the electron. This is something which you must remember. This is only observed when the particle size is comparable with the wavelength of the electron, right.

Same thing can happen in phonons also. The phonon wavelength is compared with the dimension of the material this can be also important aspect for the thermal transport. And this is clear that this size effect will happen only when or the size effect will be dominant only when the size will be 1 to 2 nanometers, preferably below 5 nanometers. This effect can be observed.

So, normally at the higher size between 100 to about 5 nanometers, we will see effect of surface energy dominated aspects. We do not see much effect of quantum confinements. We only observe quantum confinements when sizes becomes much smaller of the order of 1 to 2 nanometers. That is when the wavelengths of the electrons will be comparable with the dimensionality of the material. Now, you must be thinking how does it happen.

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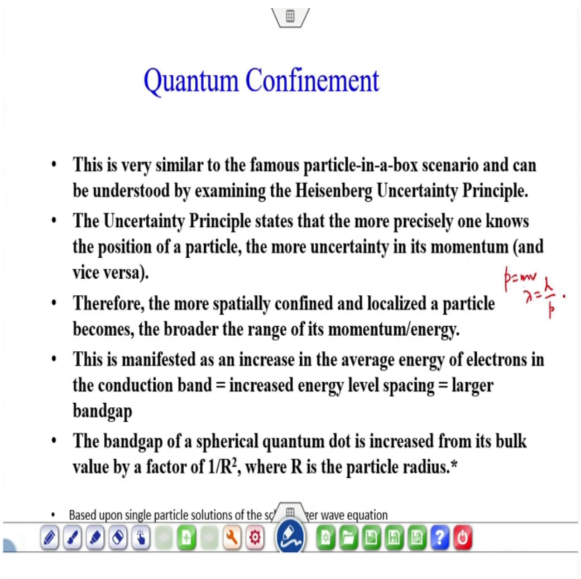

Well, so, this is very similar to a particle in a box problem, ok, very simple. And can be understood simply by invoking the concept of Heisenberg uncertainty principle. What is it? Uncertainty principle states you very clearly that more precisely you know the position of a particle more is the uncertainty in its momentum. Momentum is what? Momentum is p, p is m into v, right.

And p is related to wavelength of the particle by the de Broglie's equation, right. That is lambda is equal to h by p. So, therefore, as you more spatially or space wise you confine and localize a particle broader will be momentum or energy, that is right. Broader means what? The breadth of the momentum energy will be much much larger. So, more you confine the particle to the dimensions like if you from 2D to 0D, the broader will be range of momentum energy.

And this is manifested as an increase in the average energy of electrons in the conduction band that is increase of energy level spacing or larger band gap. Normally, band gap on a spherical quantum dot is increase from a bulk by $1/R^2$, where R is the radius of the spherical nanoparticle. This has been observed.

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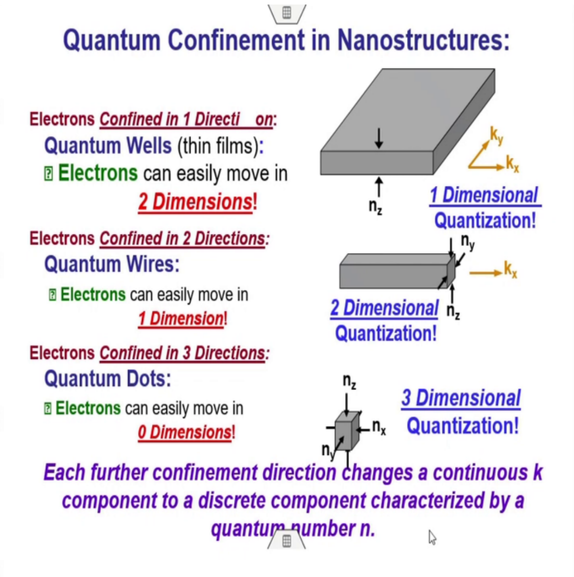

Well, you know, so quantum confined nanostructure can be explained in much better way. So, suppose you have a thin film, ok then your only one-dimensions are nanoscale, other two-dimensions can be micron scale or anything more than 100 nanometers. So, this is a 1D nanomaterials. So, in electrons can easily move in two-dimension like x and y.

So, therefore, k_x and k_y, there is a wave vectors of the x and y directions that can be anything. Wave vector is what? $\frac{2\pi}{\lambda}$ and λ is electron energy or momentum. So, therefore, electron can take any energy or any momentum in x and y directions. But in a z direction, it cannot take, because it is confined. Dimension is smaller in the z directions.

So, in case of 2D nano material, like a nano wire and nano tube, it is electrons are confined in two directions. So, it can freely move in one directions, like in the z direction in case of nanotubes. In 3D, like quantum dots or in 0D nanomaterials in all the 3 directions are confined actually, there electrons movements is confined in 3 directions. So, each further confinement direction changes a continuous component to a discrete component of k by quantum number n, ok.

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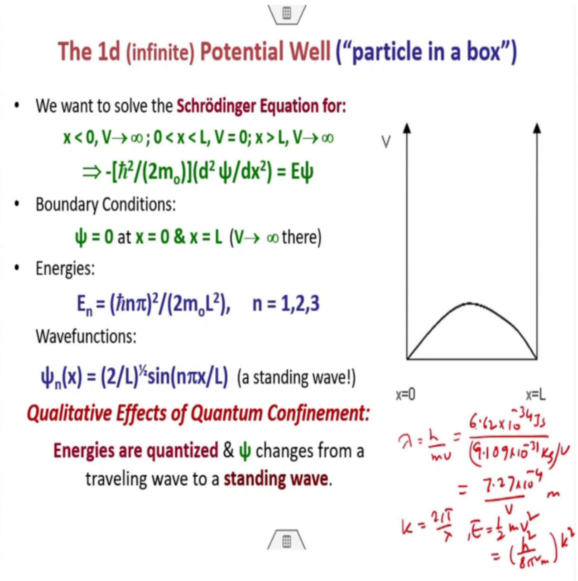

How it is so? Well, let us consider particle in a box problem. Well, before that let me just tell you in a free electron theory the outermost electrons are conserved to take part in the conduction, right. And these electrons are assumed to be free to the move to the solid. And potentials which are periodic actually in a 3D nano materials, due to nano cores or iron cores actually are almost constant.

The potential energy of the electron is not a function of the positions. The Kinetic of the electron is much lower than this potential energy, right. So, as you know, we know that let us do this simple thing. I can give de Broglie wavelength $\lambda=\frac{h}{mv}$, . And therefore, if you consider the electronic mass h as a value of what?

h as a value of 6.62×10^{-34} joule second, and m is mass of the electron is (9.109×10^{-31} kg ×v) and that becomes $\frac{7.27\times10-4}{v}$ meter, correct. You can see that. So, now you can clearly see the V become like V is always of the order of velocity is very high.

So, you can see lambda will be in the range of nanometers actually by the way because 10^{-9} is meter nanometers. So, V is 1000 kind of a meter/second. So, it will be, lambda will be about

7 nanometers or so. So, not 1000, 10000, now 10000, 1 lakh actually. Then, it will be you can calculate. It has to be 10^5, 10 to 10^{-9}.

And we know that wave vector is always defined as twice pi by lambda. So, E is basically $\frac{1}{2}mv^2$, you know that. So, I can write down then it is because $\frac{ħ^2}{8π^2 m}k^2$. This you know, right. This is very simple, correct. So, you can always define relativistic and non-relativistic things.

So, by the way, in a relativistic design its $\frac{ħ^2}{8π^2 m}k^2$. And many times, we write these things as what? You can write this thing. I will erase it out. You can write that a square pi square into as a h cross. So, therefore, energy can be written in a very simple way.

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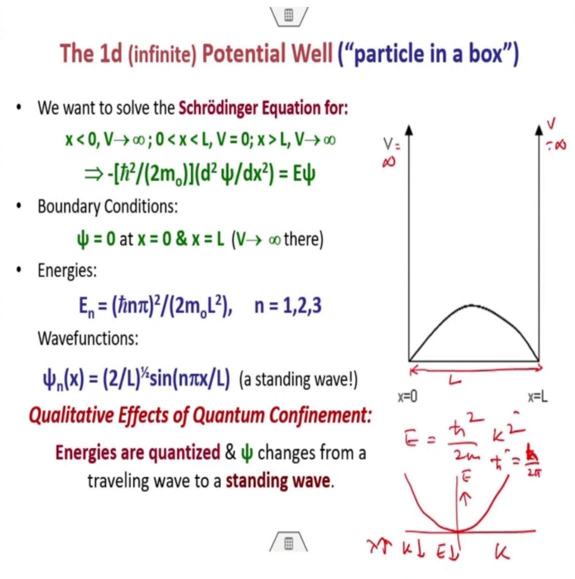

E= $ħ^2/2mK^2$. What is ħ? ħ is nothing but h/2π. That is what ħ is. So, the $ħ^2=h^2/4π^2$, and it is a $E = ħ^2/8πmK^2$, so, therefore, it becomes 2m this is something which you should remember that, right.

And the plot of these the if you plot E versus k, that you know that E versus k diagram looks like what. E versus k diagram will look very simple, like a parabola, right. So, K^2, so it is a parabolic equation. This is something all of you know that. So, if I plot, this is my k, and this is E so that it will look like a this kind of plot. Am I clear? This all of you should know that.

So, as the λ increases, what will happen λ increase k decrease, right, and E also decrease. That is understandable. Am I clear? So, this is something which is very simple in a mathematical formation. Now, let us consider the same problem in a particle in a box. Why you are talking about confinement? Let us consider a box whose length is L in only one dimension, that is, x dimension.

So, if dimension varies from x=0 to x=L, and we can always consider that for x≤0, V is ∞, you can see here, V=∞ at x=0, V is also ∞ at x=L. So, that means, what? You have a two, it is like a well, with the two big barriers, ok. And you are sitting in the well, so you cannot come out from that, right. That is what the meaning of this.

So, we can always consider between x=0 to x =L, well is the potential v=0, correct. More than x= L potential is very high; x<0 potential is also very high. So, we can write down this Schrodinger equation like this format. As you have seen here $(\hbar^2/2m_0)\frac{d^2\varphi}{dx^2} = E\,\varphi$ in one-dimension, right. That is what it is, ok. There is potential energy; there is no kinetic energy part; potential energy obviously, depends on the double derivative of the psi.

Now, if you apply boundary condition $\varphi = 0$ at x=0 and x=L because this infinity the electron cannot stay there, you will see $E_n = (\hbar n\pi)^2/2m_0 L_0{}^2$ is coming to be at $\frac{sCos(n\pi^2)}{2m_0 L^2}$ right, where n is the principal quantum number or values can be 1, 2, 3, right.

So, we can clearly see that electron energy levels, electron energy levels will be as a function of n and you can actually plot the energy levels. So, that means, what? Qualitative effect of quantum confinement very easily seen by plotting the wave function. So, once you know E_n, then you can easily get wave function and wave function $\Psi_n(x)=\sqrt{\frac{2}{L}}\,\sin\frac{n\pi x}{L}$. This is nothing but a standing wave, right.

So, energy levels or energies are required to be quantized by the value of n and psi changes from traveling wave to a standing wave. That is what is taught to you in your class 2 or maybe in the first, first year of your physics in the basic level of engineering or science, right.

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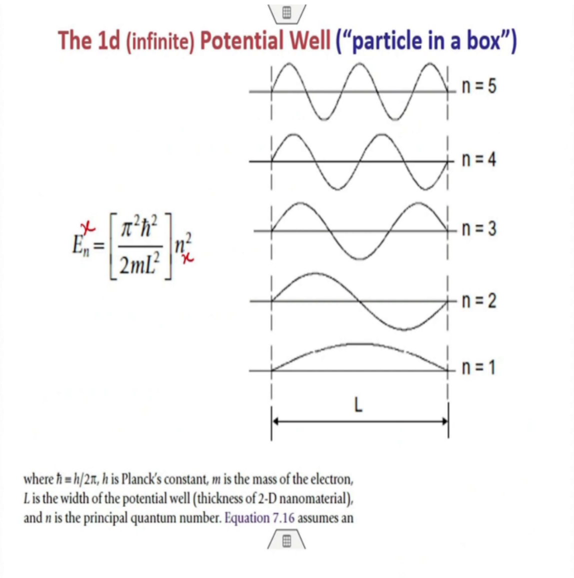

So, now, you can clearly see that if I have a n=1, then I have a standing wave like this wave length equal to L. If n= 2, it will be L/2, n= 3, it will be L/3 and so on. So, that means, what energy levels are highly quantized and $E_n = \frac{\pi^2\hbar^2}{2mL^2}\left(n_x^{\ 2}\right)$, right. This is some thing which is always happen.

And because this is one-dimension. So, we can write down n_x, we can write down E_n (x), right. That is very simple. So, because energy levels are quantized, electron can only take these energy levels, electron motion is dictated by the values of n, so therefore, it cannot be continuous any further, right.

So, L is the dimension of the material. So, if you make L to be nanoscale, that means, what? If it is a 2D nanomaterial, that means one of the dimensions are nanoscale, but the other two-dimensions are non-nanoscale, then L become thickness of the thin films. So, then you can easily get the wavelengths of the electrons will follow this kind of things, right.

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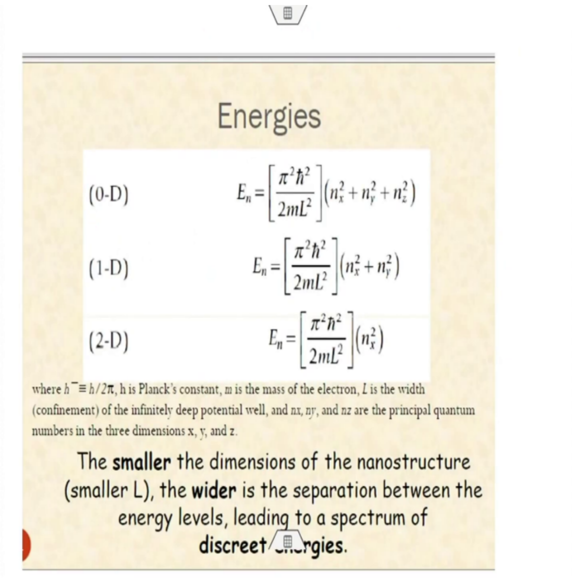

Well, so, in we can do the same mathematics for 2D and 3D, right. So, in a 2D it will be $E_n = \frac{\pi^2\hbar^2}{2mL^2}(n_x^2 + n_y^2)$, then 3D it will be $E_n = \frac{\pi^2\hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$, correct. Am I clear? Remember there here, m is the mass of the electron, ok, it is not 0 mass. It is a relativistically, corrected mass. L is the length or width of the confinement of the infinitely deep potential well n_x, n_y, n_z are the principal quantum numbers in the x, y, z directions, respectively.

So, smaller dimension of a nanostructure has smaller value of L. It will be wider will be the separation between the energy levels, right. Am I clear? This is very clear. As the L become bigger why there will be separation between these energy levels, right. You have energy levels for these different values of n will be separated much larger way.

That is what you have seen in case of this. This energy levels which you see here at the both the valence band and the conduction band in the metal, they are because of these characteristics, ok. You can have only those values of energy levels which are allowed, others are not allowed. Am I clear?

Others in other energy level electron cannot stay. So, we come back to the same concept as the Heisenberg's uncertainty principle. The moment you define the spatial dimension very clearly, the uncertainty momentum increases so much, it becomes very very broad energy becomes very broad, ok. That is the concept which is applied here. So, now, if it is very clear, same thing can be applied for phonons, right. Phonons can also undergo similar kind of things, right, similar kind of confinement effects, ok. I am not going to discuss about that.

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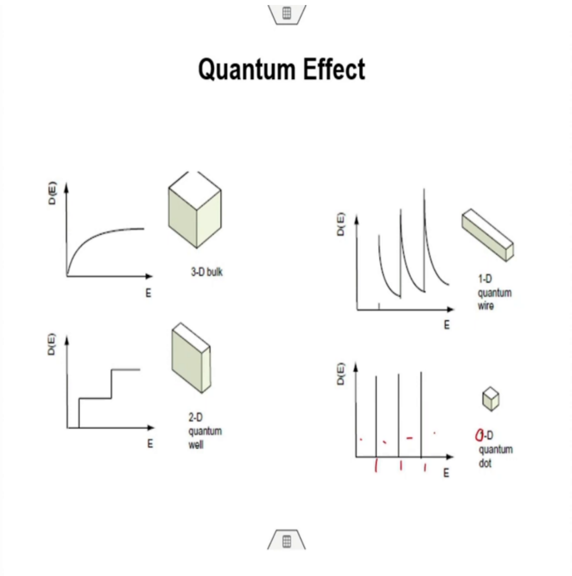

So, the quantum confinement effect thus can be put in this way in a bulk material, the density of states versus energy curves will be looking continuous. In 2D, there will be like a step function. In a 1D, they are like a X-ray refraction pattern, right almost looks like. And in a 1D sorry, in 0D, not 1D, this is 0D, in a 0D they are like a Dirac delta functions.

So, electrons can occupy only these energy levels in between they cannot stay. Similarly, electron cannot stay probability of finding electrons in these things are much smaller than the spikes. So, you can clearly see that a continuous curve is slowly breaking into a discrete energy level.

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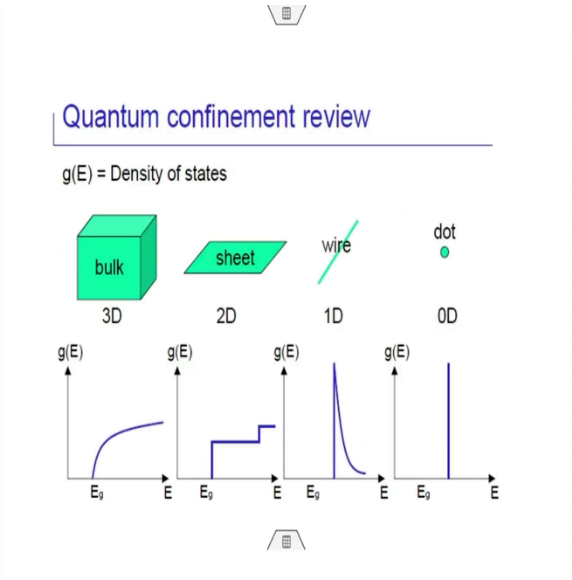

And this is same thing as shown here in a nice manner. The bulk to sheet to wire to dots, ok.

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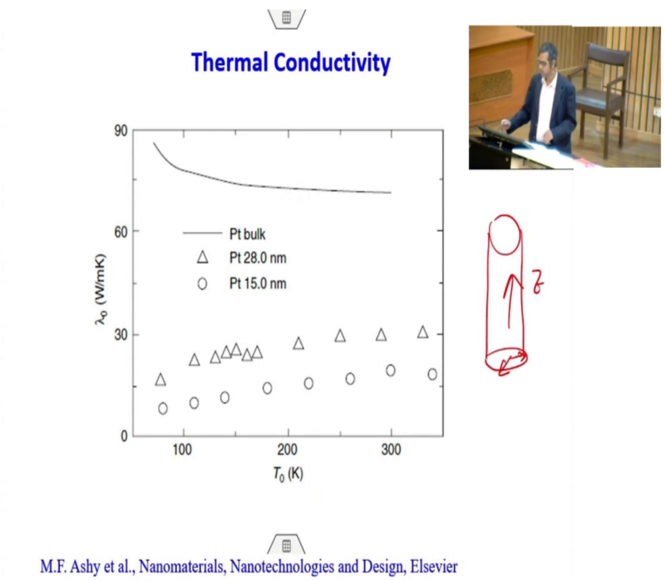

So, let us come back to the situation now, ok. We will talk about this thin films little later. First let me explain, let me reiterate for the case of 0D, 1D, and then we go to a 2D. Well, so, a good way of understand this quantum confined effects to consider the presence of nearby surfaces of 0D, 1D, and 2D nanostructures.

They can cause changes in the distribution of the phonon frequencies, ok. Like electron it is can phonon frequency will be affected also, as a function of a phonon wavelength as well as appearance of surface modes. This process can lead to change in the velocities of the phonons. Say phonons are traveling waves. So, they are moving at a velocity.

Phonons can interact with each other unlike the quantum, I mean the photons. And once they interact each other, they will form a group velocity. This is similar to the ring of waves forming when you drop a stone into the into a water pool, ok. So, hence on the basis phonon bottleneck or the electron bottleneck or phonon bottle both will occur in a 0-dimensional nanomaterials, ok.

Why? Because electrons cannot move any directions, their energy levels are confined in the all 3 directions. Only in fixed wave lengths or discrete energy levels, electrons can remain or the phonons can remain. And because of these many of the 3D, 0D nanomaterials even metallic can be insulators. They will not be able to conduct heat at all

What happens in one dimensional? In one-dimension nanomaterials two dimensions are nano scale. One-dimension is what? One-dimension is non-nanoscale like a carbon nanotubes. And it has been found that in carbon nanotubes, the conductivity can increase in the tube, length of the, length of tube to a very high value like 3000 watt per meter per kelvin compared to the other two directions, like in the plane of direction.

So, you know nano tubes, right. They are like this. So, we are talking about thermal conductivity in this direction as compared to this or this, right. So, this direction like z direction thermal conductivity can have significantly higher, 5 to 6 times or 10 times higher than or in the plane of the sheet or the tube, ok. That is this surface.

Now, it is can be as high as 3000 watt per meter per kelvin. As you know for pure copper the value of thermal conductivity is only 400 watt per kelvin meter, ok. So, therefore, there is a substantial increase of the thermal conductivity because of this confinement effects not taking place at the z direction because z direction dimensions are pretty high.

So, phonons and electrons can easily find ways to move faster, and they can conduct heat very fast. But nanotubes may not have many free electrons available, but phonons will be

(Refer Time: 30:48) a lot for the thermal conductivity. So, now, what about 0D nanomaterials? Now, sorry 2D nano materials not 0D.

Let us talk about that in 2D nanomaterials you have great number of lot of interest are there in thermal properties of material. Because you have large number of applications in terms of the handle PCs, electronic cellular phones, everyday home appliances or various modern medical devices, coatings for sedation shielding, wire resistance coating, thermal barriers, or even flat panel display like a TV or a computer screen, this is this is very important, ok.

So, it should be in this regard we should distinguish between different types of 2D nanomaterials. One is 2D single-layer nanomaterials with thickness in nanoscale, ok. You have given I have already asked a question in your mid-sem exam on that, ok or you can have multi-layer thin films composed of several nano layers, ok or you can have thin film comprised of collection of nano structure units, ok.

These nano structure thin film materials can be subdivided into nano crystalline materials or nanoporous materials. So, the moment you have you know what is called multi-layer thin films, each layer grain structure can be nano scale or micron scale, both are possible. The fact that each layer is of a thickness of nanometric scale it is a nanomaterial.

You can also have nanometric poles in the layers. So, you have this 3 or 4 different type situation, first one is single-layer 2D nano material, then you have multi-layer nanomaterials in which you have several things one is multi-layer nanomaterials in which the grain size in each layer is nanometric or grain size is micrometric or micron scale or you can have nanopores in each of the micron size grain materials, right. So, all are possible.

So, as you know nano porous materials are used as a dielectric material in microelectric industry because of their low dielectric constants, ok. Because the moment you use a pore dielectric constant will go down. However, the thermal conductivity are also low which can cause a serious problem for these dielectric materials.

So, let us start with a single-layer nanometric materials, right. This is what is shown here. The platinum bulk and platinum thin films of dimensions 15 nanometers and 28 nanometer this is a data which has been published by a group of authors, ok, yeah, like Zhang et al, Zhang et al, in 2005, applied physics, Chinese physics letter, ok.

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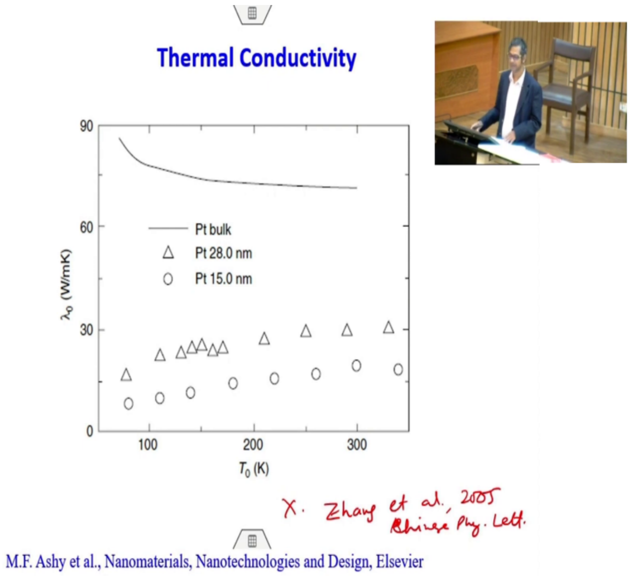

So, what you see here the thermal conductivity of the thin films are much lower than the bulk of platinum, correct. So, that means, what? The thermal conductive has substantially reduced in case of bulk, in case of thin films. And the second thing you see is that the thin film thickness decreases, the thermal conductivity also decreases. So, compared to 20 nanometers, 50 nanometers, thin film has a lower thermal conductivity, right. That is what is the question is.

Now, why does it so? That is very simple as the thickness decreases the energy levels are getting confined and therefore, platinum is a metal the majority transport is will happen by electrons. So, therefore, electron energy levels gets confined in the thickness directions and electron cannot easily move.

Not only that the moment you create a thin films you have large number of grains, ok nano crystalline or micro crystalline grains compared to the bulk. And these grains will have grain boundaries. The grain boundaries will act as a scattering agent for the electrons. That means, they will be not allowing the electrons to have a smooth passage they will be acting as a scatterer like, very simple.

You have particle in the air the light can get scatter easily, right. Same thing happens when you have a large number of grain boundaries in a material the electrons while moving inside the grain material, they will be coming to contact to the grain boundary and get scatter and move in the other directions. So, therefore, while taking at the heat in the, right, direction, they will be bringing the heat back, right. So, that is why the thermal conductivity decreases. This is first thing for the 2D single-layer materials, right observed.

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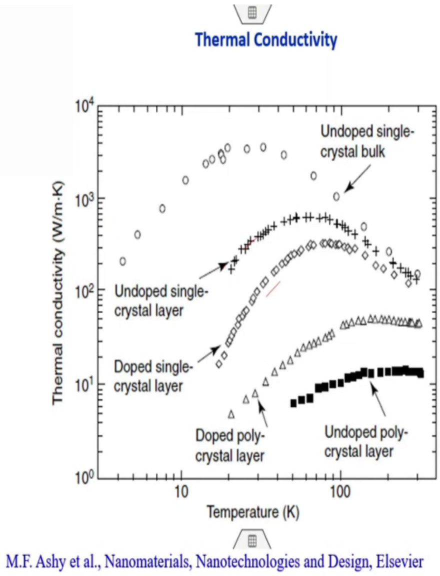

Now, what about multi-layer materials multi-layer thin films and materials with nanoscale grains, in that case you need to consider also the interface between the layers, right. This is not only the grains within the layers, but also you have additional aspect called interface between the two layers. And this interface will act as also scatterer. Whether it is a scattering phonon or scattering electron, that is not only important, but they will act as a scatterer.

So, is you know additionally you have quantum confinements because of the small layers in each case and with that you have a effect of scattering because of interface between the each layers. So, this is because interface constitute a disruption of a regular crystal structure on which phonons can propagate. If a regular crystal structure phonons can easily move, but the moment you have a interface phonons will go and stuck there and they will scatter back.

So, therefore, interface will separate two crystal of the same material which two regions have different distribution of phonons. And on the other hand, interface can also separate 2D similar materials like such a multi-layer structure, for which two different materials have two different densities, and also sound velocities. Phonons are like a you know they move at a velocity of sound in most of the cases.

So, this effect is similar to electron transport in nanomaterials and end result is presence of any interface provides scattering and therefore, reduction of thermal conductivity. What you see? This is the you know, you can see in each cases thermal conductivity this is undoped single-layer you can see, this is a doped single-layer, this is a poly layer, ok.

Forget about doped undoped, compared to single-layer poly layers have, polycrystalline layers have lower thermal conductivity much lower, it is 100 here watt per meter its about 10 or 15 or maybe 20 actually. So, therefore, there is a 5 times reduction of the thermal conductivity, even across the large temperature range.

Well, the effect of doping is serious. Obviously, it will be seriously failed and doping will lead to much change of the energy levels of the electrons as you know and that will affect the thermal conductivity. So, forecast of single crystal, single crystal single you know silicon monolayers which are embedded between two amorphous layers, a strong reduction in thermal conductivity with respect to bulk happen.

This is the bulk, ok. You see the bulk has a thermal conductivity of the order of almost 1000 at about 10 to 100 kelvin degree Celsius, 100 kelvin, ok. So, but you know say same thing is reduced, extensively the moment you have a single-layer silicon. So, especially, at low temperature. This effect is more pronounced for polycrystalline silicon thin films, right. Polycrystalline means polycrystalline layers, ok.

So, for this grain boundary will act as a scatterer over the surface of multi-layer scattering. This is additional scatter. Grain boundary will act as additional scatterer on the top of multi-layers. Multi-layers each layer will be acting separately. So, interface between the layers will act as scatterer and within the layer you have poly crystalline grains that grain boundaries also will act as scatterer. Am I clear?

So, overall, the idea is to take different approaches control the phonon transport in various regions of the phonon spectrum. So, high frequency phonons can be blocked by the alloy scattering because wavelengths are of the order of few atomic speaking, ok. So, phonons can have different wavelengths, and so therefore, their scattering will depends upon what is the relative grain size of the materials.

So, now comes the nanoporous material. The size effect determine the number of and the pores as well as the size, ok. So, due to the porosity these materials have very low permittivity and thermal conductivity also low which I am, ok, that is why it is used in microelectric industry, right. But, you know this can lead to the increase in the temperature of the device and the circuit can fail. So, therefore, they are not considered good materials for applications.

So, the problem is it is not theoretically understood how to treat this nanoscale pores for thermal transport, ok. It is not clear. But, nonetheless, the pores are not good for the thermal transport. That is very clear to understand, ok. So, hence as you can see here the with the 2D nanomaterials, the effect of the dimension is very very distinct and clear on the thermal conductivity. And this can be easily explained by talking considering 3 important aspects.

First, the confinement effect because of electron or phonons. Second, the scattering effect. Single-layer scattering is less, multi-layer scattering is more, ok. Multi-layer each between the two layers, they have interface, interface will acts as scatterer. Secondly, even if you have polycrystalline grains in each layer the grain boundaries will act as a scatterer. So, that will further reduce the thermal conductivity.

So, if you want to have a thermal barrier, you can do that, you can create a multi-layer structure and then within each layer you can have nano crystalline grains. So, substantially thermal conductivity will go down. And that is what is used. But you know then you have a question of this stability of this grain structure comes into picture.

As you increase the temperature of the material, the nano crystalline grains will grow and their grain size will become very large and hence the thermal conductivity will change. So, this aspect is important. So, that is why many people actually many scientists, they do not go up very low size of grains in each layer, but they reduce the thickness of each layer substantially.

And each layer act as a separate layer, so they do not interact much. So, that is something which is very very important you know. So, in a nutshell, I discussed you various aspects of thermal behavior, not only the thermal conductivity, but also very very fundamental concept like electron confinements, phononic confinements, phonon motions, without going into much of mathematics, ok.

I know that too much mathematics may not be good because then it will you need to dig up lot of literature to understand those mathematical equations. But fundamentally, the concepts can be understood simply by following the book of Michael Ashby and others in the chapter 7, nicely given.

So, with this I will stop here. And we will come back in the next class on the electrical properties. That is easy for me now because I have already explained you the electronic confinement. And I will again explain you in a different manner, but electrical properties will be discussed subsequently. Then finally, I will talk about magnetic and optical properties and then wind off the properties of materials, ok. So, in next may be 5-6 lectures, I will wind off the properties and then we will talk about characterization of nano materials.

Thank you.