Micro and Nanoscale Energy Transport
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Lecture - 03
Some Applications of Micro/ Nanoscale Energy Transport

Good morning. Yesterday we had a brief introduction about classification of the different regimes like the macro scale, micro scale and nanoscale based on the Knudsen number, non-dimensional Knudsen number was introduce to be the single most important non-dimensional number that governs basically the effect of as assuming a continue approximation.

Typically in this small Knudsen number values and if you are increasing the Knudsen numbers to larger and larger values this approximation fails, and finally we are going to the free molecular limit at Knudsen numbers going to infinity, where none of the continue approximation work. And therefore, we have to use what we called as Boltzmann transport equation model based hypothesis.

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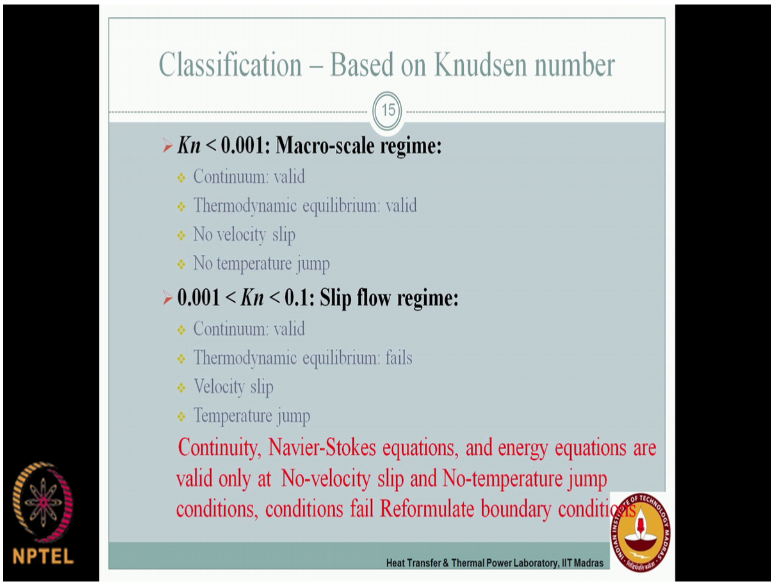

Classification – Based on Knudsen number

- **$Kn < 0.001$: Macro-scale regime:**
  - Continuum: valid
  - Thermodynamic equilibrium: valid
  - No velocity slip
  - No temperature jump
- **$0.001 < Kn < 0.1$: Slip flow regime:**
  - Continuum: valid
  - Thermodynamic equilibrium: fails
  - Velocity slip
  - Temperature jump

Continuity, Navier-Stokes equations, and energy equations are valid only at No-velocity slip and No-temperature jump conditions, conditions fail Reformulate boundary conditions

Therefore, for solving the problems at large Knudsen numbers we have to be little bit careful where the approximation based on continuum hypothesis can be used. And I want to therefore, once again summarize the different regimes where the continuum hypothesis can be valid. If you look at Knudsen number values much smaller than say

0.001. So, this is a thumb rule, but need not be exactly 0.001 sometimes people take it as 0.01. But generally the thumb rule is that for the limiting case of Knudsen number going to 0, this is where the actual continue approximations are valid. And this is called the Macro Scale Regime.

When you say continue approximations are valid, you definitely use the assumption that there is a local thermodynamic equilibrium. It is not globally even at least locally it should be satisfied that is why this is the continue approximation. And at the boundaries of the between the system and the fluid, so you do not have any slip in either the momentum or in the temperature. So, this is what you have been we have been generally dealing with in the classical thermodynamics or classical heat transfer and so on and so forth; classical fluid mechanics.

So now, we can also have systems where the so called mean free path or the length scales. Mean free path could be quite large compared to the length scale or the length scale could be quite small compared to the mean free path. So, this could put the Knudsen number the range between 0.01 or 0.001 to somewhere up to a maximum value of 0.1. This case there is a possibility of using the continuum equations that were still used in the macro scale regime, but with the fact that you have to account for the slip between the fluid and the system boundaries.

So, slip here happens not only for the momentum, but also for the energy equation, the temperature also shows the slip characteristic slip. Therefore, we have the account for the boundary conditions through the accommodation of slip at the boundaries through slip boundary conditions for both velocity and temperature. And therefore you know this regime is called Slip Flow Regime. This is particularly more suited for the gases. So, gases are shown to have pronounced to slip at the boundaries compared to the liquids, and therefore the kind of regime that we are talking about is more suited for gases.

Now for the liquids; since the mean free path is smaller you may rarely find liquids in the micro scale at least which are tending towards Knudsen number of 0.1 are greater than that. Usually gases can approach this quite easily, but not so easily with liquids.

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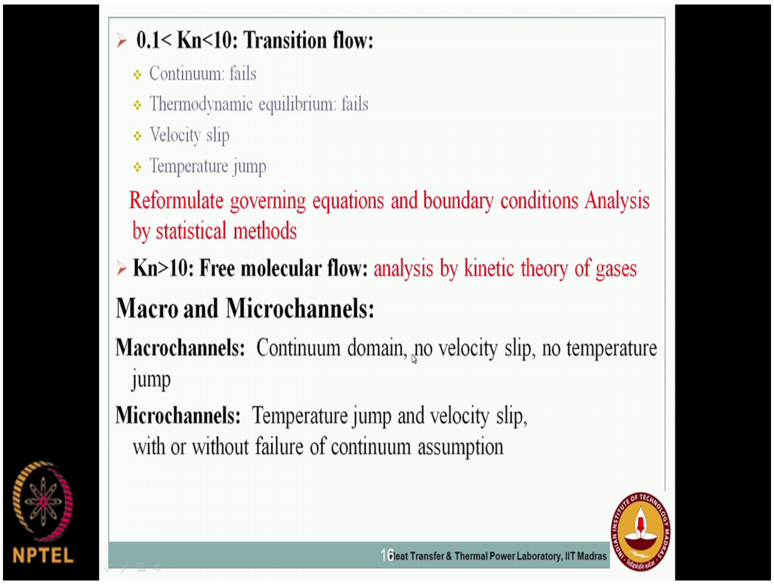

- **0.1< Kn<10: Transition flow:**
  - Continuum: fails
  - Thermodynamic equilibrium: fails
  - Velocity slip
  - Temperature jump

Reformulate governing equations and boundary conditions Analysis by statistical methods

- **Kn>10: Free molecular flow:** analysis by kinetic theory of gases

Macro and Microchannels:

Macrochannels: Continuum domain, no velocity slip, no temperature jump

Microchannels: Temperature jump and velocity slip, with or without failure of continuum assumption

And then we were talking about what is called Transition Flow. Yesterday in the mark that I showed you, so if you are Knudsen numbers are greater than 0.1 and less than 10. I mean there is no question that there is a slip happening at the valve, and apart from that there is also question of the validity of using continue a model outside. So, this is a problem where people have been trying to use different formulations, alternate formulations for the Navier-Stokes equations.

So, some people referred this to the extended Navier-Stoke equations. Although, people have been trying the higher order formulation of Navier-Stokes equation here, but strictly speaking we cannot use continue your model at all and even the extensions of continue models may not give you satisfactory results. And finally, the case where your Knudsen number is greater than 10, is the high Knudsen number case with the respect to gases there rarified highly rarified flows and their refer to as a free molecular flow. And people analyze this by what in the rarified gas dynamics. They refer to as kinetic gases.

So, the same Boltzmann transport equation is used in the kinetic theory of gases. And that can be also used for other energy carriers as well, need not be gas molecule but you know the pronouns which will introduce and then you have electrons for the same Boltzmann transport equation which suppose to be for used for the rarified gas flows in the free molecular limit can be also be used an other media as well.

Generally, these are the different regimes and these are different governing equations and boundary conditions preferred for those particular regimes.

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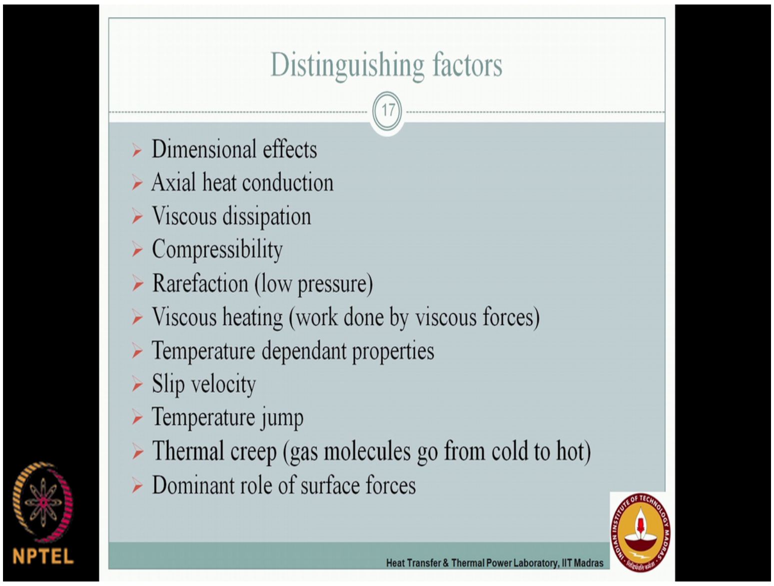

Distinguishing factors

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- Dimensional effects
- Axial heat conduction
- Viscous dissipation
- Compressibility
- Rarefaction (low pressure)
- Viscous heating (work done by viscous forces)
- Temperature dependant properties
- Slip velocity
- Temperature jump
- Thermal creep (gas molecules go from cold to hot)
- Dominant role of surface forces

Then we just also list down what are the distinguishing factors typically in the extreme high Knudsen number limits. So, one is that you have what we call as dimensional effects. This is very particular at nanoscales. For example; if you look at the bulk properties, they are all independent irrespective whatever dimensions you take; for example; thermal conductivity, so good example. So, you measure thermal conductivity and you do not care whether the size is millimeters or centimeters or meters the value is the same. Whereas, if you going to the nanometer dimensions you find that they exhibit strong size effects, so the thermal conductivity becomes function of also the length scale.

So, this is the particular characteristics of high Knudsen number limit. We will see that what it happens. So, why this size effects should happen at nanoscale? And you also have viscous dissipation could be a very important role at small length scales. You have strong heat generation due to viscous dissipation which becomes very significant. If you do the scaling analysis you will find that at small length scales of all the terms in the energy equation, the viscous dissipation will become very significant and cannot be neglected. And sometimes even compressibility can be important, rarefaction is definitely if you look at gases these are associated with low pressures, so high Knudsen numbers so therefore rarefaction will be very important.

So now, slip of both velocity and temperature becomes extremely important as well. We will see that when we go to micro flows, because a slip as such we are still dealing with continuum, outside and just changing the boundary conditions, so this generally is applied to micro flows not nano flows. And we also have what we call as thermal creep. In this case we have a phenomenon call thermo forces. So, a thermo force is a case where your gas molecules can defuse from the hot end to the cold end. So, now you can also have a reverse effect call thermal creep.

And you can also have other surface forces which are playing a very important role, and this could be used also to dry flows at micro scale. We will see some of these effects as and when we going to the particular topic, but you can say that there are number of important factors which come into play at such small link scales which are not so important relevant at the macro scales.

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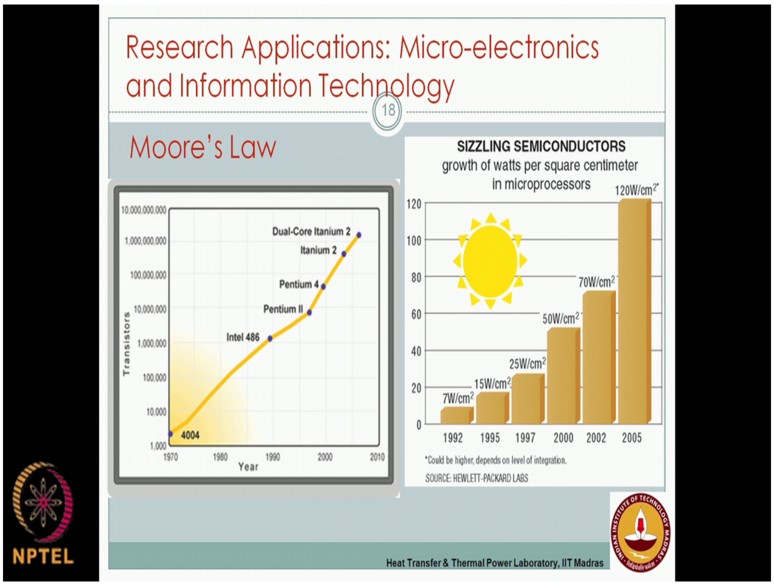

Research Applications: Micro-electronics and Information Technology

Moore's Law

*Could be higher, depends on level of integration.

SOURCE: HEWLETT-PACKARD LABS

Yesterday we talked about the Moore's Law, and the problem associated the bottle neck associated with following the Moore's Law over a period of time now, and also the heat dissipation problem happening in micro electronics. So, we also discussed about the three levels of cooling and so on.

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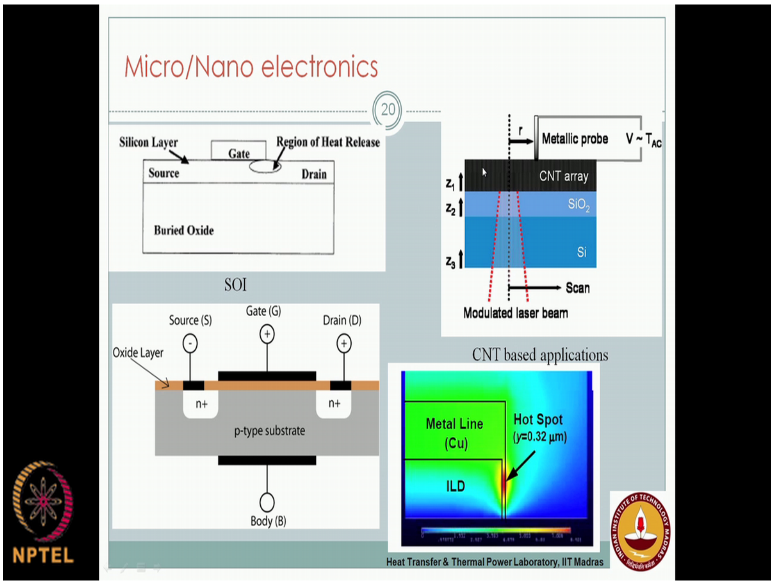

Micro/Nano electronics

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So, if you again once again go back to the micro electronics.

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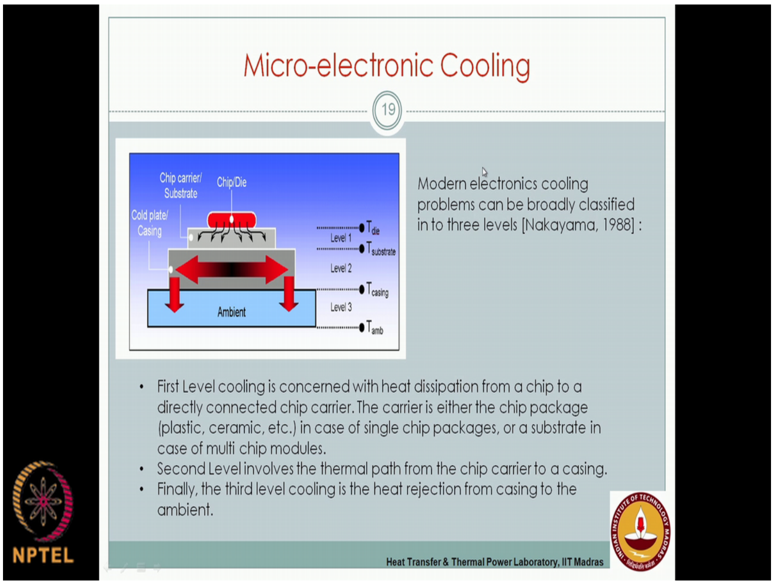

Micro-electronic Cooling

Modern electronics cooling problems can be broadly classified in to three levels [Nakayama, 1988] :

- First Level cooling is concerned with heat dissipation from a chip to a directly connected chip carrier. The carrier is either the chip package (plastic, ceramic, etc.) in case of single chip packages, or a substrate in case of multi chip modules.
- Second Level involves the thermal path from the chip carrier to a casing.
- Finally, the third level cooling is the heat rejection from casing to the ambient.

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We now know these three levels of cooling; out of which the level one is a problem with the materials, level two is something that we can deal with by using the micro technology like using micro channels and so on. If you look at the level one, this is typically within the particular shift and within a particular semi conducted device. We are going into now the nanoscale regime. So, why do we have a heat generation or you know generation of hot spots, what we call as hot spots within the particular semi conducted device that raises this thermal bottle neck problem.

Typically if you take silicon on insulated device, this is the most fundamental semi conducted device where you have a silicon layer which is which is actually deposited over a buried oxide layer. So, this is something like a silicon dioxide S I O 2 over which you have thin silicon layer, this silicon layer could be as thin or as thick of you tens of nanometers. And typically this is your semi conducted device, so you have currents you have a potential at the gate, you have a source, you have a sink, or the drain on then by controlling the potential between the source and drain you can basically control the speed with which the electrons move from the source to the drain. You can also control the channel width through which the electrons tunnel through by adjusting the gate potential here.

Nowadays what is happening is, because of the higher process as speed you need faster electron transfer from the source to the drain. Typically you are applying higher potential differences between the source and drain. And, what is happening the channel sizes are becoming smaller and smaller. The electrons have to move fast, too many of them at the same time they cannot go through very big channel, because the sizes of these silicon layers are becoming is thinner and thinner. Therefore, what happens is the substrate the silicon itself has atoms and therefore we can understand that these electrons have to basically propel through this atomic structure and they usually collide with this latte structure and usually this coalition will result in the generation of heat at the fundamental level.

So therefore, it is not just the electrons are moving without resistant's they are have their phasing resistant's due to the lattes in the background, and therefore this coalition is bound to generate heat. And what we refer to as now usually the source of the generation is around the gate and the drain region. This is where the electrons usually can to get heated up. So, these are hot electrons, typically very high temperatures, and these electron temperatures are typically order of magnitude higher than the base lattes temperature.

So, also these results in generation of what we call as hot spots, so localized hot spot. All this is local thermal non-equilibrium, so everything is non-equilibrium process here. And this once the hot spots are generated you know number one is prediction of these hot spots. If you use the Fourier's equation at this length scales, you will be usually under predicting the hot spot temperature as well as the heat fluxes, so they will fail at this particular scale. And again the next aspect is how do we remove these hot spots? Now these hot spots become also bottle neck when you have the junction between a metal and the dielectric. So, these are the interfaces for example, between a metal line and dielectric. And usually there is also a thermal interface resistance between the metal and dielectric leading to this hot spot generation.

Similarly, people have been trying out lot of novel materials where you can improve the thermal conductivity in a certain direction. And this can be achieved by using typically what we call as carbon nano tube arrays. So, over the last decade or so carbon nano tubes have emerged as very potential materials for micro electronics, because you can tune their electrical and thermal conductivity is certain direction to be enormously high. And they can be grown vertically on substrate like silicon dioxide like this, and you can use them as the thermal interface materials.

And thereby you can actually reduced the amount of interfacial thermal resistance and reduce the size of these hot spot and so on. There are different techniques to measure the thermal interface resistance, so I be will be talking about this towards the end where we will briefly go over the experimental methods that are used in micro and nano scale.

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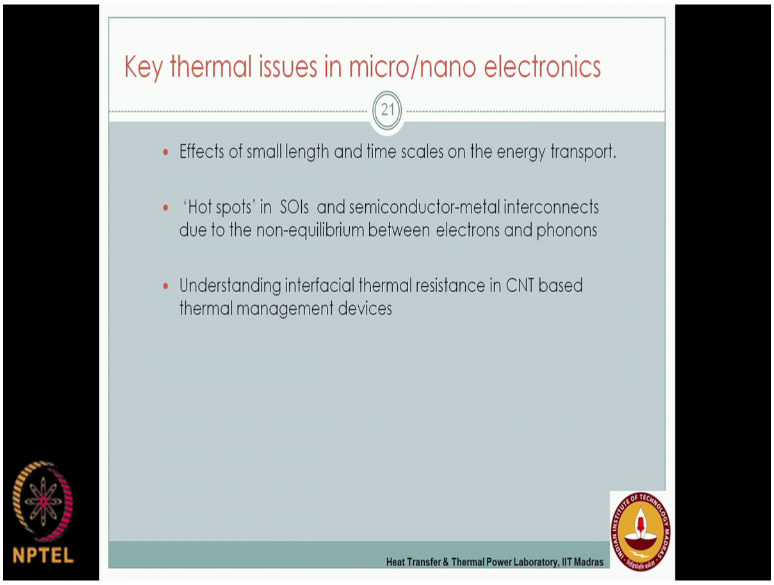

Key thermal issues in micro/nano electronics

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- Effects of small length and time scales on the energy transport.
- 'Hot spots' in SOIs and semiconductor-metal interconnects due to the non-equilibrium between electrons and phonons
- Understanding interfacial thermal resistance in CNT based thermal management devices

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But, what are the key thermal issues therefore? So, one is the effect of small length and time scales on the energy transport. So, you have to understand that that part which cannot be predicted with the classical constitutive two equations; the hot spots especially when you are looking at silicon on insulator kind of devices number one, and semiconductor metal interconnects due to the interfacial thermal resistance. And why do they arise, because of the non-equilibrium between electrons and the background lattes. Right now, we will introduce these background lattes vibrations particularly with some virtual particle call phonons.

So, they are just like photons, they virtual you cannot really find phonon inside metals, so they are just lattes structure and vibrations, since we have a wave particle duality you can always associate this lattes a Vibrational waves with some particle called phonons and you can give them some certain energy and so on.

So, this interaction between electrons and phonons are going to be at non-equilibrium all the time and therefore they result in the generation of these hot spots. So, what is important if you are looking at better thermal management is to understand thermal interface resistance well, generation of these hot spots, and how do we mitigate them by means of efficient material such as using carbon nano tubes.

The other so we have two aspects; one is effect of small length scales which we described by taking an example of a micro or nano electronic device, such as a semi conducted device here the other could be small time scales.

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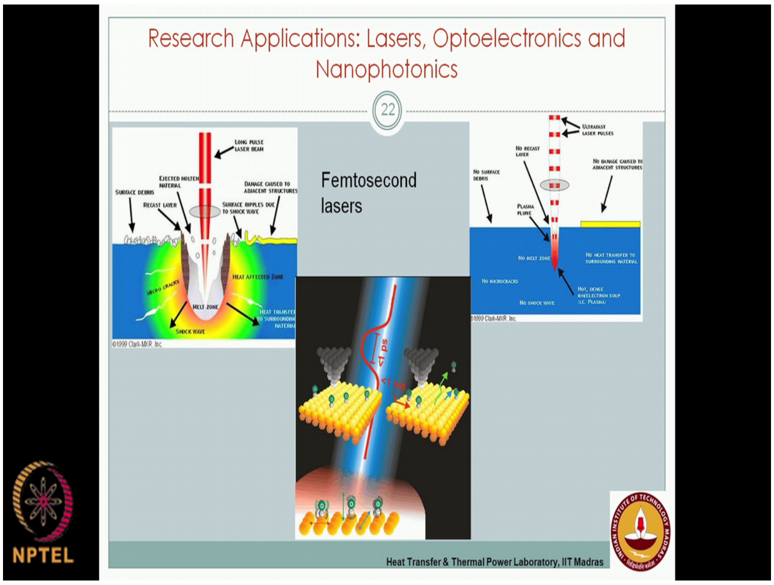

Research Applications: Lasers, Optoelectronics and Nanophotonics

Femtosecond lasers

If you look at lasers for example, there are applications of laser everywhere, and usually the laser pulse width can range from all the way from milliseconds to what we now use in some applications to Femtoseconds; that is 10 power minus 15 seconds.

So, the laser time duration or the pulse width anything less than few nano seconds, so of the order of picoseconds 10 power minus 12 10 power minus 15, again indicate that they are extremely fast times scales compared to what you can actually physically observe. For example, if you are using such kind of lasers to oblate, some issues or metals or whatever, if the actual physical times scale for the heat to penetrate from the surface to subsurface will be actually these times scales are much longer compared to the time scale of the radiation of the pulse.

Therefore, again there is a strong local non-equilibrium that happens. The photons come and just heat and go and by the time the surface responds to it; the photons are all ready gone and there is a big non-equilibrium there. There is also chance that you have a hot spot generated. So, if you look at some of the applications at in nano electronics and some of the applications and also metal cutting and so on, they used Femtosecond lasers.

So, you have a very strong local thermal non-equilibrium. So, it is not only a small length scale problem, but also a small time scale problem here and therefore once again you cannot use the continue approximations.

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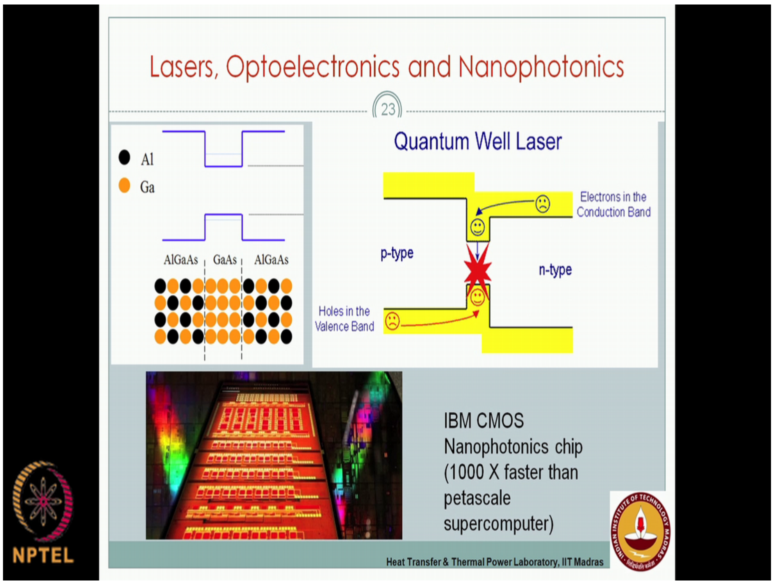

Lasers, Optoelectronics and Nanophotonics

Quantum Well Laser

IBM CMOS Nanophotonics chip (1000 X faster than petascale supercomputer)

So, you also have lot of other applications where you deal with this kind of non-equilibrium, not only in lasers but now what we call as a optoelectronics, nanophotonics and so on. These are advancements that are made to have newer way of creating micro process are chips musing optical based phenomena. So, they say that for example the nanophotonics chip compared to using electrons you are using the light as a medium and you can achieve the processors speeds which can be thousand times faster and what we have as a petascale supercomputers are right now.

So these are all little bit futuristic, but you should understand that non-equilibrium problem can become more challenging in the future when you are talking about higher speeds of propagation.

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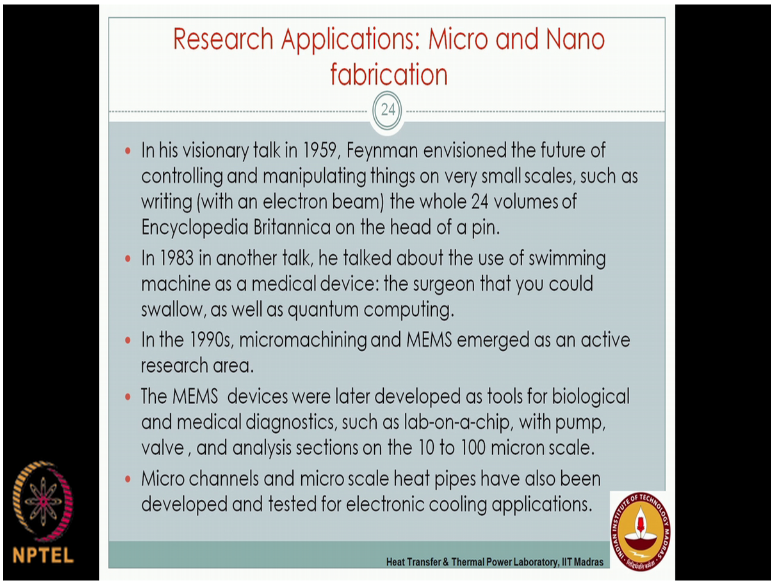

Research Applications: Micro and Nano fabrication

- In his visionary talk in 1959, Feynman envisioned the future of controlling and manipulating things on very small scales, such as writing (with an electron beam) the whole 24 volumes of Encyclopedia Britannica on the head of a pin.
- In 1983 in another talk, he talked about the use of swimming machine as a medical device: the surgeon that you could swallow, as well as quantum computing.
- In the 1990s, micromachining and MEMS emerged as an active research area.
- The MEMS devices were later developed as tools for biological and medical diagnostics, such as lab-on-a-chip, with pump, valve , and analysis sections on the 10 to 100 micron scale.
- Micro channels and micro scale heat pipes have also been developed and tested for electronic cooling applications.

The area of MEMS; MEMS in general so has not been you know very old, so if you are looking at you know Feynman's lecture that there is plenty of room at the bottom. So, in 1959 he was also proposing lot of ideas about controlling and manipulating devices at small scales. Basically, he was coming forward with lot of challenging problems and offering rewards to people who can actually build such kind of micro scale devices.

For example, in 1993 he was talking about quantum computing. That was one of the beginning ideas, later on quantum computing took of very well. In 1990s micromachining and MEMS then took off as a very active research area if you look at many of the professors, I mean during 1990s 2000 was very active period for MEMS. It still continues, but now we have understood the phenomena at micro scale for more than what it was done and that time. They were more eager to build the devices before understanding the phenomena. So now, that there was a bottle neck at the time and again now we have gone back to the fundamentals trying to understand them well and again now we are building more efficient micro fluidic devices.

So some of the MEMS devices, mostly they were focused on medical application, medical diagnostics, for example; lab-on-chip devices and so on. And then also mechanical components, micromechanical components such as micro pumps, micro valves. Once you build such kind of lab-on-chip devices that means, you take as entire lab laboratory and build it on a small chip in the order of microns. So, you need all the associated mechanical components to also make this device possible, such as micro valves, micro pumps.

Then one after the other all these mechanical devices had to be skilled down and you cannot use the conventional principles of pumping for example. You cannot use your conventional pumps; you have to use maybe peristaltic pumps and this kind of devices at such small scales. And again analysis of these devices had to be done in order to understand the fundamental fluid flow and so on.

And then later on I think cooling became very important problems. So, one hand you have the MEMS devices for biomedical applications; on the other hand electronic cooling was becoming a challenging problem, because that was also rapidly advancing we have reduce the sizes of these devices and we have the heat dissipation. Then the use of micro channels and micro heat pipes. So, they have emerged as potential applications for electronic cooling.

These are how you know over a period of time from something as theoretical during Feynman's talk in 1959 to the recent times where we have had a fair amount of understanding and also we have developed applications. I am not very sure whether we have commercial micro channel devices for electronic cooling right now, but still in the research and development stage. But in the MEMS area yes, we have lot of medical diagnostic kits which have based on MEMS which have come up in the last few years.

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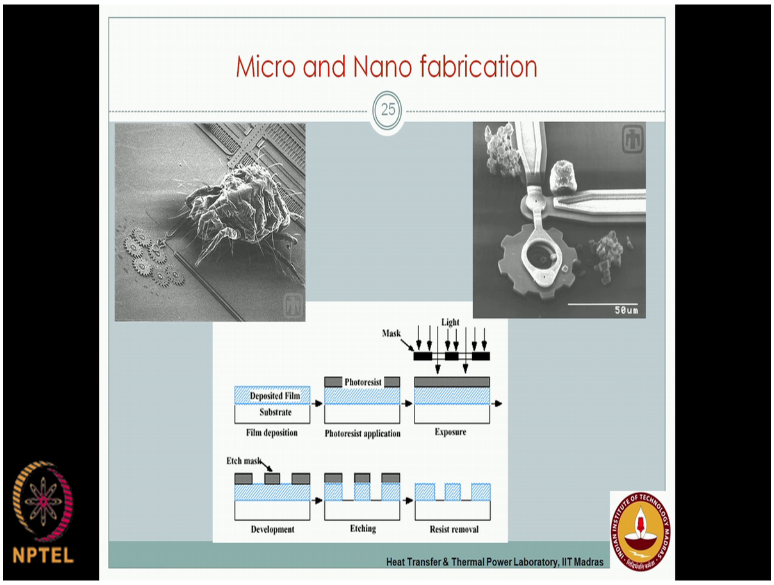
Micro and Nano fabrication

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The other issue that you have to understand at micro nanoscale is a fabrication. So, when you say fabrication of MEMS devices, so you cannot use your conventional machining tools and do this. Now we have recently lot of mechanical based machining which are happening at micro machining device in our IIT, we have purchased big micro machining device a micro milling and micro cutting and so on. So, we have very good equipment in our institute. Apart from that you know micro fabrication; nano fabrication has being existing an electrical engineering for a long time. They do not use the mechanical based machining device, so what do they do? A photolithography; so photolithography has been that to make these microelectronic devices, semiconductor chips.

This can also be used for creating mechanical devices. The MEMS devices typically or the lab-on-chip devices can also be done using photolithography. But, now increasingly being replaced a with the new age micromachining a tools we can make mechanical devices of the order of microns using mechanical cutting rather than the photolithography. Now photolithography has several layers of process; starting from you have to start with a film over a substrate and then you have to prepare a mask, and you have to have a photo resist, you have to put the mask on top of these, you allow the UV light and then it like the exposed areas will be ached out and so on, and finally the pattern will be formed on the particular film.

So, this has several layers, the using of the photo resist and these are little bit expensive. Now, these are good on a really small scale and making small devices, but if you want to make so many of them commercially. So, especially when we talk about mechanical devices, so becomes little bit difficult and therefore slowly the transition has been moving towards using this micromachining devices as well.

For example; this figure shows, this is a dust mite. And this dust mite you cannot see with you naked eye. Now these dust mites are really of the size of microns and there are some gears which are manufactured by MEMS technology and they are just compared to the scale of the dust mite here. So, these are that small. On the right hand side also you have typically some microns size particles, so these are of the scale of 50 microns here and there are some associated micro scale devices compared with those microns size particles.

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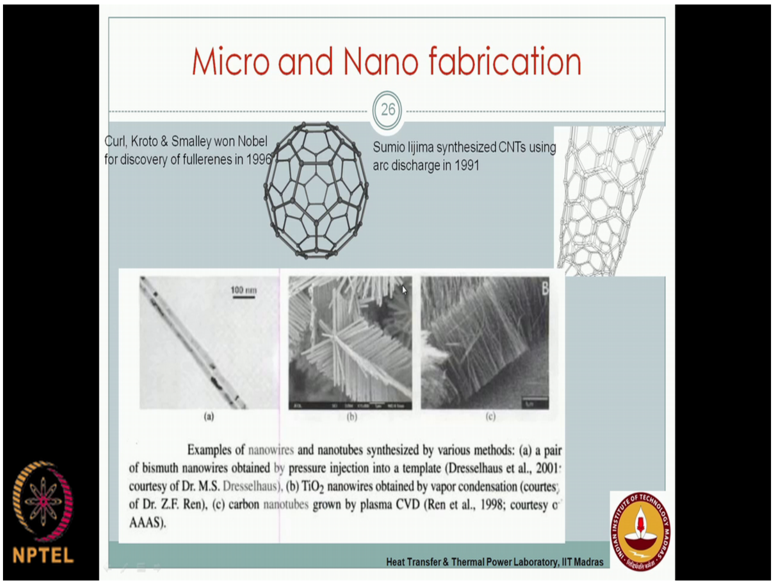

Micro and Nano fabrication

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Curl, Kroto & Smalley won Nobel for discovery of fullerenes in 1996

Sumio Iijima synthesized CNTs using arc discharge in 1991

Examples of nanowires and nanotubes synthesized by various methods: (a) a pair of bismuth nanowires obtained by pressure injection into a template (Dresselhaus et al., 2001 courtesy of Dr. M.S. Dresselhaus), (b) TiO_2 nanowires obtained by vapor condensation (courtes of Dr. Z.F. Ren), (c) carbon nanotubes grown by plasma CVD (Ren et al., 1998; courtesy o AAAS).

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So, lot of fabrication efforts from the material science. So, people from primarily chemistry and material science they have been working over a period of last 30 40 years to develop novel materials, synthesized novel materials, come out with the new processes for synthesizing materials at nanoscale.

For example, carbon nano tubes; carbon nano tubes is carbon nano tubes are nothing but a single layer of graph graphing. So, that is you take graphite and you take a monolayer of graphite, so that is maybe of the order of a few nanometers thickness and then you just role it, so just you role it and then that it becomes your carbon nano tubes. Now it depends on how you role it? If you just take the graphing sheet and you just role it normally like straw you get a carbon nano tube, and you role it like a ball you get what is called as a buckeye ball here. Or there are also called as fullerenes for which you know these people who discover the structure won the Nobel Prize in 1996.

And a Lijima synthesized carbon nano tubes using arc discharge method. Now these were some of the novel materials that paved way for discovering; for example, graphing, synthesize, carbon nano tubes synthesize and so on. And now we have lot of different nano wires, nano particles of different materials that you can imagine. And there are different fabrication techniques using chemical vapor deposition p e c v d plasma enhanced chemical vapor deposition and so on.

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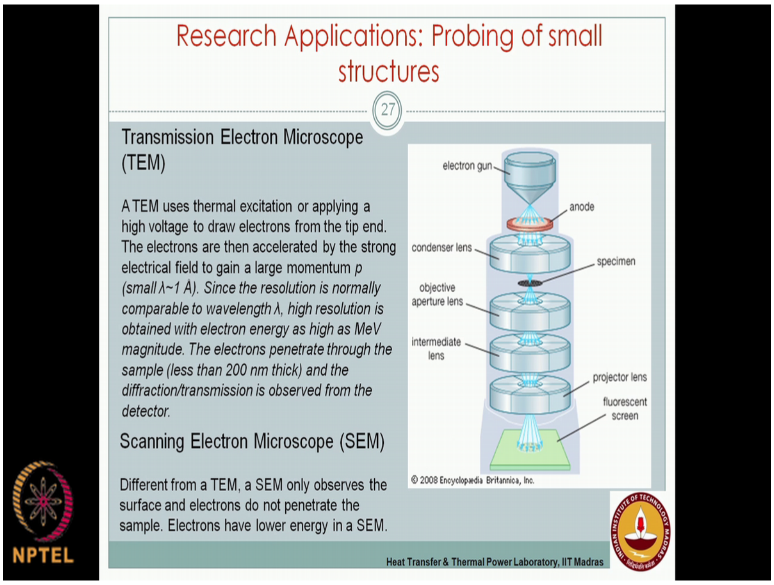

Research Applications: Probing of small structures

Transmission Electron Microscope (TEM)

A TEM uses thermal excitation or applying a high voltage to draw electrons from the tip end. The electrons are then accelerated by the strong electrical field to gain a large momentum p *(small λ~1 Å). Since the resolution is normally comparable to wavelength λ, high resolution is obtained with electron energy as high as MeV magnitude. The electrons penetrate through the sample (less than 200 nm thick) and the diffraction/transmission is observed from the detector.*

Scanning Electron Microscope (SEM)

Different from a TEM, a SEM only observes the surface and electrons do not penetrate the sample. Electrons have lower energy in a SEM.

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Also if you look at the area of characterization, so once you make these nanostructures or carbon nano tubes and nano particles, nano flowers, whatever they called so many names. Once you prepare them you have to characterize them or could be even characterization of particular surface for example. So, you fabricate through micromachining set nanostructures on a surface and now you want to look at the height width patterns and so on. So, how do you characterize this? We cannot use the conventional microscope, because these are nano scale structures we cannot be resolved. Therefore, we have to go to techniques which are based on electron microscope.

Electron microscope is a very novel technique, so you can either use the tunneling effect. So the transmission electron microscope, basically in this case you have the electron tunneling effect used as a principle behind characterizing a particular surface or you can have a scanning electron microscope. In this case the electrons do not have to penetrate into completely through the target sample, but only on the surface level. These are different level.

For example the resolution of the TEM is quite high, so it can actually resolve of the order of angstrom whereas, the SEM can only resolve surface aberrations or whatever characteristics only of the order of few nanometers. So, depending on the kind of resolution that you want to choose by whether you want to go for a scanning electron microscope or a transmission electron microscope.

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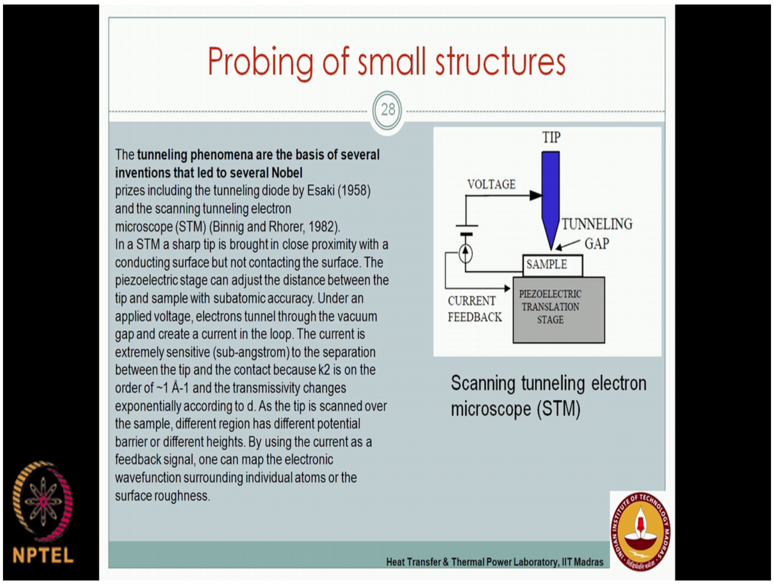

Probing of small structures

The **tunneling phenomena are the basis of several inventions that led to several Nobel** prizes including the tunneling diode by Esaki (1958) and the scanning tunneling electron microscope (STM) (Binnig and Rhorer, 1982).
In a STM a sharp tip is brought in close proximity with a conducting surface but not contacting the surface. The piezoelectric stage can adjust the distance between the tip and sample with subatomic accuracy. Under an applied voltage, electrons tunnel through the vacuum gap and create a current in the loop. The current is extremely sensitive (sub-angstrom) to the separation between the tip and the contact because k2 is on the order of ~1 Å-1 and the transmissivity changes exponentially according to d. As the tip is scanned over the sample, different region has different potential barrier or different heights. By using the current as a feedback signal, one can map the electronic wavefunction surrounding individual atoms or the surface roughness.

Scanning tunneling electron microscope (STM)

And, again you have scanning tunneling electron microscopes. As a said is based on the tunneling phenomena which can happen when you have very very small gaps, so that this becomes just a quantum mechanics theory. And then the electrons can actually rather than flowing, it can just simply appear on the other end. So, this phenomenon is called a Tunneling. We will see that when we do quantum mechanics; how tunneling can happen. Say they do not have to pass through just like a normal atom; they just emerged out of the other end just like that. So, this is called Tunneling Phenomena.

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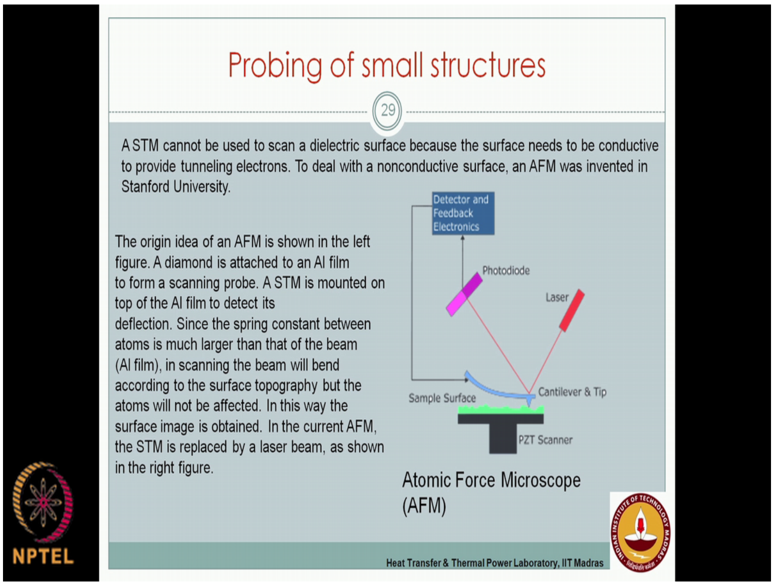

Probing of small structures

A STM cannot be used to scan a dielectric surface because the surface needs to be conductive to provide tunneling electrons. To deal with a nonconductive surface, an AFM was invented in Stanford University.

The origin idea of an AFM is shown in the left figure. A diamond is attached to an Al film to form a scanning probe. A STM is mounted on top of the Al film to detect its deflection. Since the spring constant between atoms is much larger than that of the beam (Al film), in scanning the beam will bend according to the surface topography but the atoms will not be affected. In this way the surface image is obtained. In the current AFM, the STM is replaced by a laser beam, as shown in the right figure.

Atomic Force Microscope (AFM)

There are also other ideas out of which microscopes have been made; the one is called the Atomic Force Microscope. So, here the potential or the interaction potential between atoms is used for characterization of the surface. Here for example, there is a diamond tip here, so we use a diamond tip because the interaction potential between the diamond tip and usually the sample surface could be a metal surface or non metal surface. That potential is very high so that this can be deflected by the potential. Whereas, the spring constant of this particular cantilever over which the diamond tip is placed itself is negligible compared to the interaction potential between the diamond tip and the surface. So, due to this high interaction potential whenever you have a surface aberration, that means there is a change in the height locally the topologies changing, so this potential changes the force changes and therefore there is a deflection of this particular cantilever happening. And this deflection is mainly due to the topology change.

With this you can actually also measure the surface topologies. So, the atomic force microscope is also a very useful technique. And this was actually invented in Stanford University, but the device was built by IBM later on, and I think they collectively won the Nobel Prize for this device.

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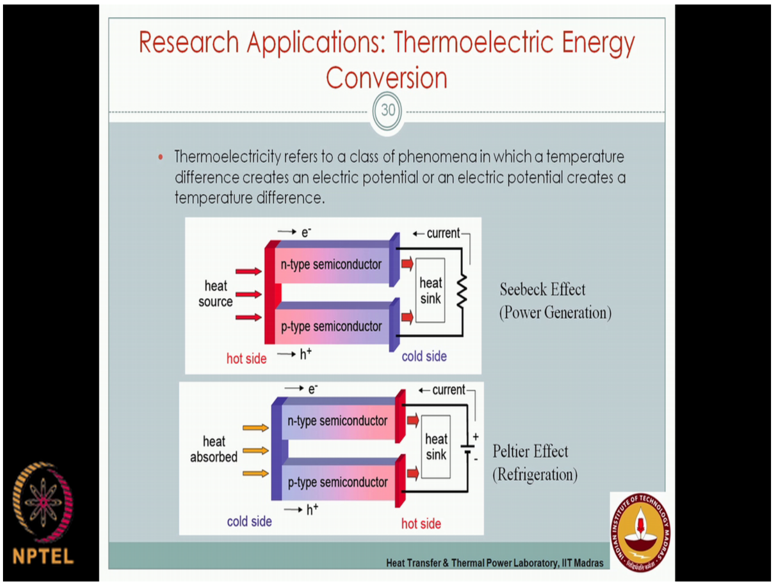

Research Applications: Thermoelectric Energy Conversion

- Thermoelectricity refers to a class of phenomena in which a temperature difference creates an electric potential or an electric potential creates a temperature difference.

Seebeck Effect
(Power Generation)

Peltier Effect
(Refrigeration)

Let us quickly move on to the other applications apart from the micro nano electronics what we discuss. You can also talk about alternate the energy sources. What we called renewable energy, one form of this is called thermoelectric energy conversion. You maybe all aware of the principle of thermoelectricity from your high school physics, so you can use the Seebeck effect for power generation or the Peltier effect for refrigeration.

In Seebeck effect you have a hot side this is the heat source on one end and a heat sink. So, this is the heat engine typically, so you have source and you have a sink. And you are basically transferring heat from the source to sink, and in the process you are doing some work. And the work here is electrical work. This is the current that is generated. And how it is generated here is due to the transfer of electrons in the n-type semiconductor from the source to the sink. And the transfer of holes in the p type semiconductor from the hot side to the cold side. So, collectively it means that the electrons are flowing through this close to loop thereby producing current.

So, this is the principle of Seebeck effect. That means, from the hot side the electrons on holds have enough kinetic energy to move towards the cold end and in the process they flow through a close circuit and there by producing current. Now, the reverse effect is you know it is utilized for refrigeration this is called Peltier effect. In which you actually pass current right and therefore you basically absorbed heat on one side and you deposit heat on the other side.

So in the hot side, so this is the refrigeration process; for example you want to maintain this side cold, therefore you want to absorbed heat from the cold side. So, you can only transfer heat from a lower to higher temperature only if in put in work, otherwise you are violating the second law of thermodynamics. So, the work that you are putting here is current. So, this principle is used in Peltier effect.

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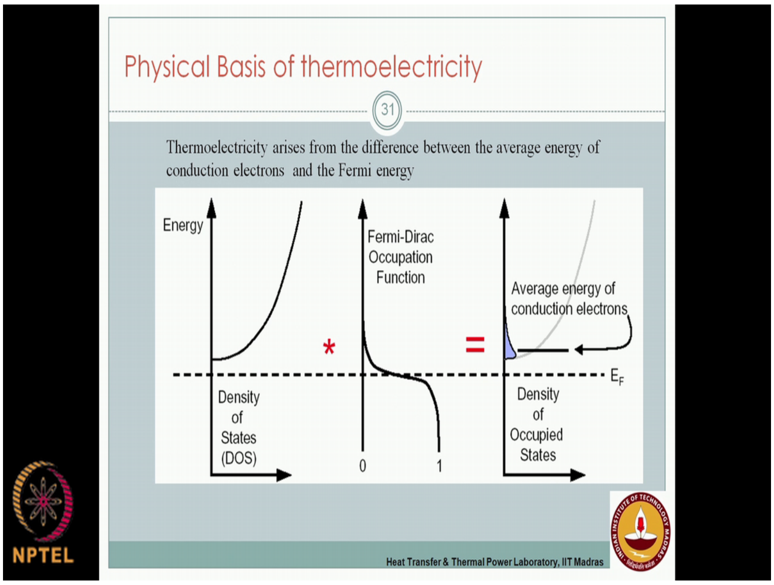

Physical Basis of thermoelectricity

Thermoelectricity arises from the difference between the average energy of conduction electrons and the Fermi energy

Now, what is actually causing the thermoelectricity or the Peltier effect to arise? If you go inside and you do this quantum mechanics solid, state physics and statistical thermodynamics.

So, from the solid state physics we have what is called is density of states. It tells you at each energy level what is average density of electrons that can actually occupy. This is given by curve like this, and on top of that does not mean that all the electrons are only occupying this particular portion here. The actual occupational probability is given by the Fermi-Dirac distribution function; this is coming from the statistical thermodynamics. We will see all these, but you should understand that Fermi-Dirac distribution function is an equilibrium distribution function which governs the probability of occupational distribution of electrons primarily. So, that is given by distribution like this.

Now if you want to calculate what is the density of occupied states; it is like this. You know you have a house which has say 10 rooms, does not mean all the 10 rooms have to be occupied by all the people. We have to now find out how many numbers of people are there in the first place. And what is the preference of each of these persons. So, somebody wants to occupy room number 2, somebody wants to occupy room number 5. So, the number of rooms that are available to you is basically the density of states. The probability of occupying each of this is given by the Fermi-Dirac distribution function.

Once you now take a product of these two, so then you get the density of occupied states. Then you will know two people may it want to occupy say room number 2, so one room maybe completely empty and so on. So finally, you come out with the curve which is density of occupied states and which shows that in fact most of the average energy is focused around this energy band here. And this turns out to be the average energy of the conduction electrons; this turns out to be the conduction band.

If you therefore calculate the average energy; the average energy will come out to be somewhere here given by the solid line. These are the average energy of the conduction electrons. And now you have the reference energy which is called the Fermi energy which is had to given room temperature you have a Fermi energy level which is somewhere here. And this difference between the average energy of conduction electrons and the Fermi energy gives raise to thermoelectricity.

So, the higher the gap between these two the more is the amount of current that you will get for a fixed the temperature difference and so on so. And similarly for the given current you will find greater temperature difference. Therefore, this temperature differences the driving potential or this energy difference between the conduction electrons and the Fermi level is the driving potential for thermoelectricity.

So, we will see this when we talk about solid state physics and then we move on to statistical thermodynamics then we will be able to understand this, how do we get it.

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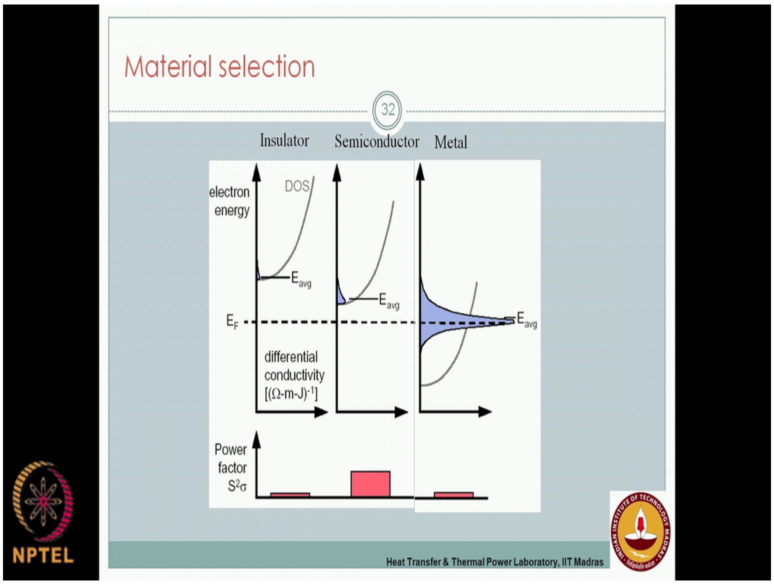

Material selection

If you therefore, look at the kind of materials; so which of these have the largest gap between the conduction band and the Fermi level. So, if you take the case of insulator, semiconductor and metal. The insulator you have probably the biggest band gap and semiconductor it is moderate metal it is almost 0. So that is why you have all the electrons is priming from; the valence to the conduction band in metals very quickly and it is there very good conductors of electricity and so on. Whereas, an insulator hardly any electron can jump from the valence to the conduction bands show so easily.

However, what is happening here is not only this gap but also you should also look at the average energy of the conduction electrons. In the case of insulators you hardly I have any electrons in the conduction band. Therefore, the overall the average energy itself is very small, quite small.

And in the other hand metal, you have very large energy of electrons in the conduction band, but the band gap between the conduction bands on the Fermi levels is almost 0. So, these are two extreme cases. So therefore, we introduce a factor called power factor which is the product of S square. S is called the Seebeck coefficient, which is nothing but in indicator of thermoelectricity. That means, the higher the difference between the conduction band and the Fermi energy indicates the higher value of Seebeck coefficient.

So, we need to have a power factor which is S square times the electrical conductivity sigma. If the electrical conductivity is small as in the case of insulator, although the value of s quite large the product of S square sigma will turn out to be considerably small. And the same with metals, although the sigma is very large so your S quite small and therefore once again you have a very small value of power factor, whereas in the case of semiconductor this is where you have the optimally high values of S square sigma. You have moderately large values of S; you also have moderately large value of the electrical conductivity.

So therefore, what is the most common prefer materials for thermoelectric power generation, they are the semiconductor materials. Therefore, the thermoelectric materials see are use the semiconductor based materials for producing thermoelectricity.

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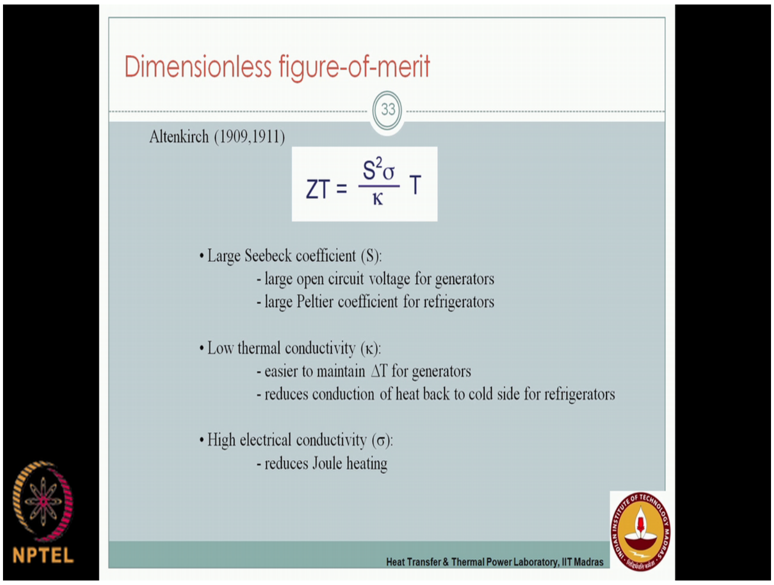

Dimensionless figure-of-merit

Altenkirch (1909,1911)

$$ZT = \frac{S^2\sigma}{\kappa} T$$

- Large Seebeck coefficient (S):
  - large open circuit voltage for generators
  - large Peltier coefficient for refrigerators
- Low thermal conductivity (κ):
  - easier to maintain ΔT for generators
  - reduces conduction of heat back to cold side for refrigerators
- High electrical conductivity (σ):
  - reduces Joule heating

And again, now when you talk about these thermoelectric materials we have to characterize their performance in some way. We know that the Seebeck coefficient is a good indicator of thermoelectricity, nevertheless there is a term called the figure of merit which is denoted by the power factor in the numerator and in the denominator we use the thermal conductivity multiplied by the temperature to make it a non-dimensional number. The unit of S square sigma by k turns out to be 1 our Kelvin. So, in order to make this non-dimensional number it is multiplied by the absolute temperature and therefore it becomes a non-dimensional figure of merit.

Now, if you look at again, if you look at the cases however, in semiconductors the Seebeck coefficient electrical conductivity and thermal conductivity they are all strongly couple to each other. So, you cannot say I take material with a large power factor and a very small thermal conductivity, it turns out that if your power factor is very large your thermal conductivity also turns out be large. Because for example, if you talk about electrons so they the electrical conductivity and thermal conductivity of electrons are directly proportional; so higher the electrical conductivity, higher the thermal conductivity. You do not find a material where electrical conductivity is very high thermal conductivity is very low.

Therefore, the higher the power factor, the higher the thermal conductivity. Now why do we need low thermal conductivity here? Because if you look at this particular example so you do not want the heat to conduct from the hot to the cold side very fast, you want the temperature difference to be maintained only the electrons and holes are suppose to flow not the heat. The heat also flows then the amount of thermoelectricity will naturally reduce.

So therefore, this figure of merit brings in the factor that your thermal conductivity has to be low while the power factor has to be high in order for the performance of the device to be very good. However, these are interconnected and therefore this becomes a problem in designing a very efficient thermoelectric device.

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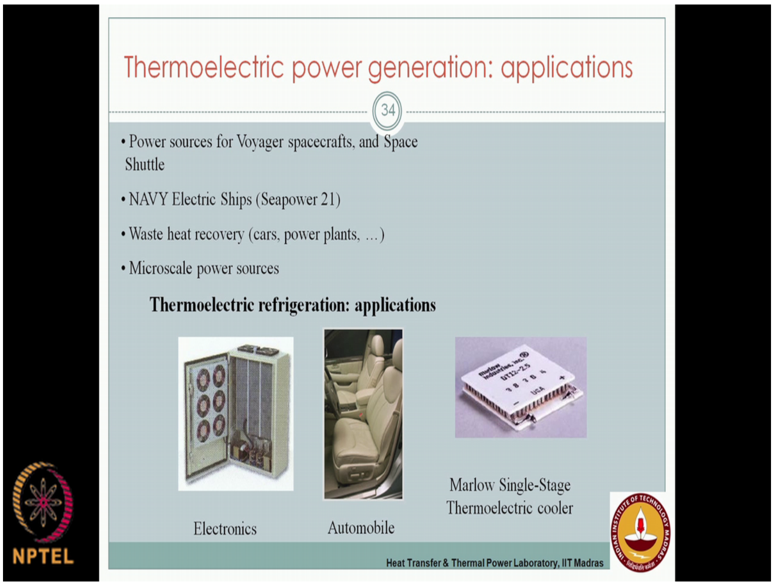

Thermoelectric power generation: applications

- Power sources for Voyager spacecrafts, and Space Shuttle
- NAVY Electric Ships (Seapower 21)
- Waste heat recovery (cars, power plants, …)
- Microscale power sources

Thermoelectric refrigeration: applications

Electronics

Automobile

Marlow Single-Stage Thermoelectric cooler

Therefore, thermoelectric power generation has some applications; for example the voyager spacecrafts their power source because they are so for away from the sun, they cannot be powered by solar panels and therefore the thermoelectricity was used to power these spacecrafts. And some of the navy electrical ships also use thermoelectricity for example.

You can also talk about waste heat recovering in. For example, cars you have so much of heat and temperature difference between the waste heat and the ambient you can use that to power at least some of the devices in a car. At least the dash boat can be illuminated from the rather than from the battery from the thermoelectric power generation and so on. So, you have a lot of applications, refrigerators are also available. In fact, there are some portable thermoelectric refrigerators which cool your fluid you can put your cold drink into that and store it at maybe 5 degrees for a the extended period of time. And all these are based on thermoelectric refrigeration.

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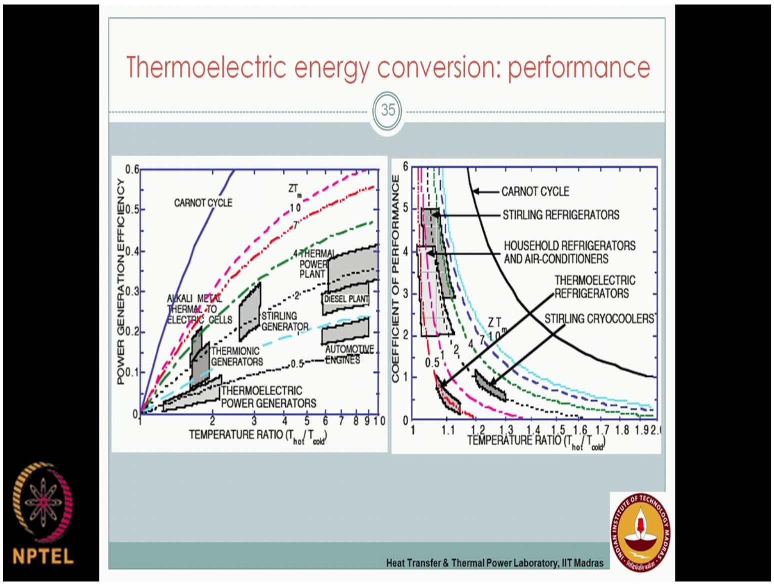

Thermoelectric energy conversion: performance

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Heat Transfer & Thermal Power Laboratory, IIT Madras

However, they are not used at such a large scale. So why, because if you now convert this thermoelectric figure of merit to equivalent engine efficiency, just like you have your car not efficiency so you have your thermal efficiency. And therefore, the power generation efficiency if you plotted you will find this thermoelectric devices or all having efficiency is less than 20 percent. Why, because of the low figure of merit.

So here, these are all plotted for different values of figure of merit. So the figure of merit of all these thermoelectric devices are typically very low and therefore if you look at compared to your thermal power plans which are having efficiency is the order of 30 to 40 percent, so these suffer from low thermal efficiencies.

However, they are very clean energy sources. And if you have good thermoelectric materials so they are the bottle neck. Why they have low figure of merit, because the figure of merit is tie to only three parameters; one is Seebeck coefficient, electrical conductivity, and thermal conductivity. And all these are material properties. So, if you come out it is better materials I think this can be pushed up at least to equivalent to the conventional power plants. And therefore, they can be used more widely in other applications as well.

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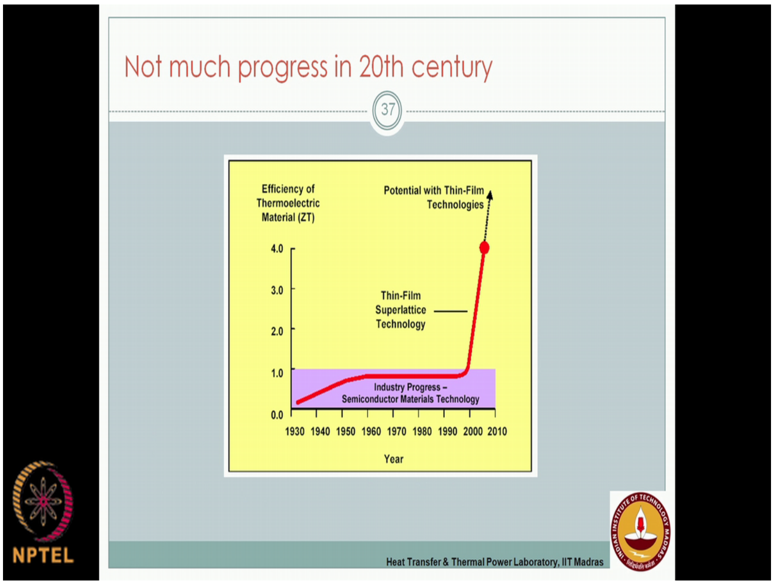

Not much progress in 20th century

So, this is where the nanoscale materials play a role for thermoelectric, because what you see this is the value of ZT plotted in the y axis over period of time. And you see as long as you are using bulk semiconductor materials. So, you are not getting a value of ZT above 1 and you see the value of ZT of 1 will give you efficiency which is always less than 20 percent.

So, suddenly in the year 2000 people started using what is called as thin films a superlattice. These are called as superlatttices you have thin films of 2 different semiconductor materials sandwich together. And based on this they got a value of the thermoelectric figure of merit to be above 4. Now if you see that, if you have a thermoelectric figure of merit of 4 and your operating in the lower temperature range, because the temperature ratios with thermoelectric generation is usually in the lower end you cannot use it like you use your eye internal conversion engines, you do not operated very high temperature ratios.

At this range with the thermoelectric figure of merit of 4 you can push it to 30 percent close to 30 percent and if you are thermoelectric figure of merit of claims to 7 or 10 you are pushing this close towards 30 percent.

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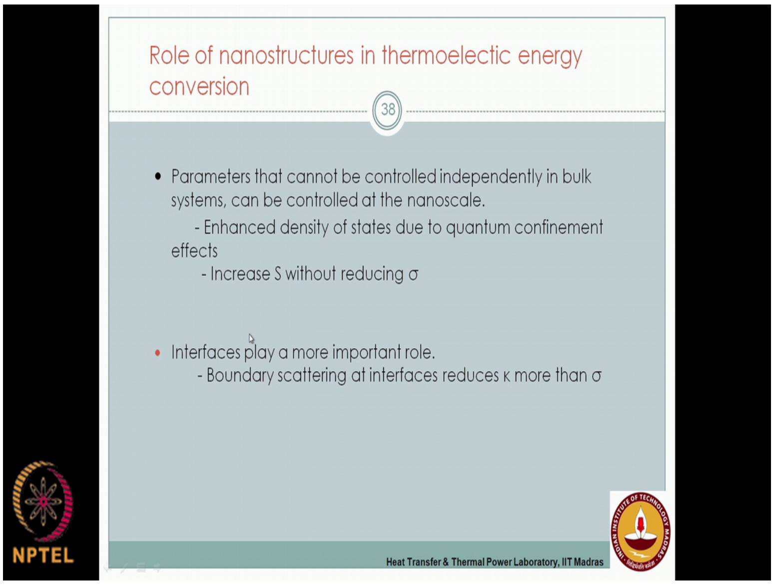

Role of nanostructures in thermoelectic energy conversion

- Parameters that cannot be controlled independently in bulk systems, can be controlled at the nanoscale.
  - Enhanced density of states due to quantum confinement effects
  - Increase S without reducing σ

- Interfaces play a more important role.
  - Boundary scattering at interfaces reduces κ more than σ

So, this is where the role of nanoscale materials comes into picture. You can use these nanscale thin film technology for as potential thermoelectric materials.

I will stop here, I think a have maybe a few more slides to discuss before we stop the power point introduction and go to the bored. So, we will continue this on Tuesday, next week and we will then gradually go to the board and start deriving some basic introductory equations and so on.

Thank you very much.