A Special Tutorial Lecture Series on

Introduction to Nanoscale Heat Transfer

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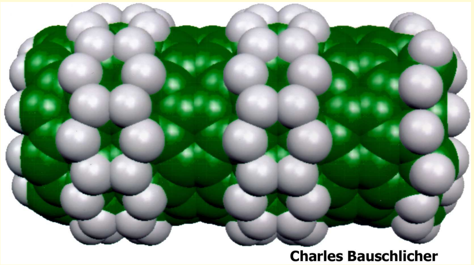
Part 1: **Overview of Nanotechnology**
Part 2: **Atomic Structure & Quantum Physics**
Part 3: **Inter-Molecular Heat Transmission (Nanoscale Heat Transfer)**
Part 4: **Measurements of Thermophysical Properties**



Charles Bauschlicher

An artistic view of a step-shaft
built with atoms

> ***"If I were asked for an area of science and engineering that will most likely produce the breakthroughs of tomorrow, I would point to nanoscale science and engineering."***
>
> -**Neal Lane**
> Former Assistant to the President for
> Science and Technology

Part 1

Overview of Nanotechnology

November 14, 2006

Futuristic Industrial Products in the New Century

Near-term Products	"Dream" Products
• New vaccines and medicines that cure many incurable diseases. • Synthetic antibody-like nanoscale drugs and devices seeking out to destroy malignant cells in human or animal bodies. • In-vivo medical diagnostic and drug delivery systems.	• "Dust" sized super-intelligent computers. • "Needle-tip" sized robots for biomedical applications and for search and rescue. • Spacecraft weighing less than today's family cars.
• Smart surface coating materials with self-adjusting thermal conductance for buildings and refrigeration systems. • Smart fabrics for self-cleaning clothe. • Super-strong materials for light weight airplanes, vehicles and structures.	• Biomedicine, e.g. in-vivo systems and surgery that can sustain human lives to 150 years and longer. • Robots with artificial human intelligence becoming the mainstream workforce in our Society.
• Clean energy conversion systems and super-long life batteries.	• Unlimited supply of clean renewable energies that replace all fossil fuel produced energies on the Earth.
• New breed of crops and domestic animals that can feed entire world population.	• Tele-transportation systems that can transport human anywhere on Earth in seconds. • Spacecraft for human/cargo inter-planet traveling.

HSU-2005

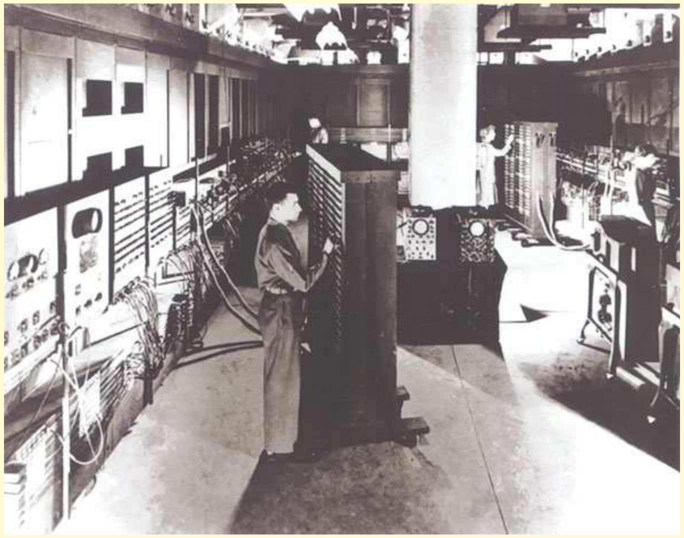
The Core Technology for Producing Futuristic Industrial Products is

MINIATURIZATION

Two phenomenal examples of miniaturization of industrial products in recent years

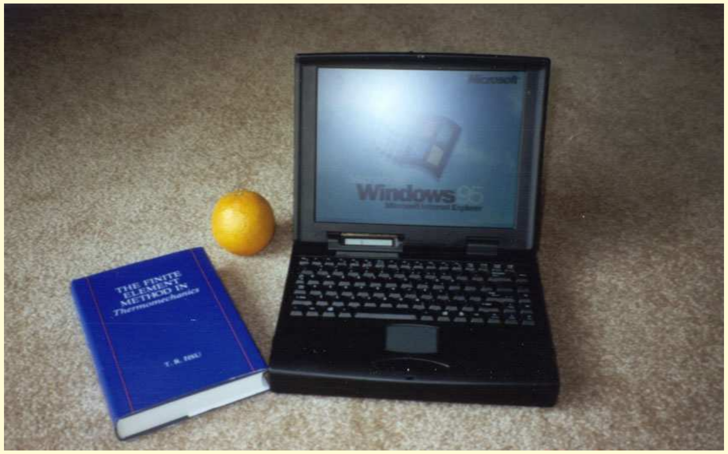
Miniaturization of Digital Computers

- A remarkable case of miniaturization!



The ENIAC Computer in 1946

Size: 10^6 down
Power: 10^6 up



A “Lap-top” Computer in 1996

Size: 10^8 down
Power: 10^8 up

A “Palm-top” Computer in 2001

This spectacular miniaturization took place in 50 years!!

Market Demand for Smaller, Multi-Functional Products

For example, the market development of cellular phones:

Less than 10 Years Ago:

Current State-of-the Art:

Transceived voice only

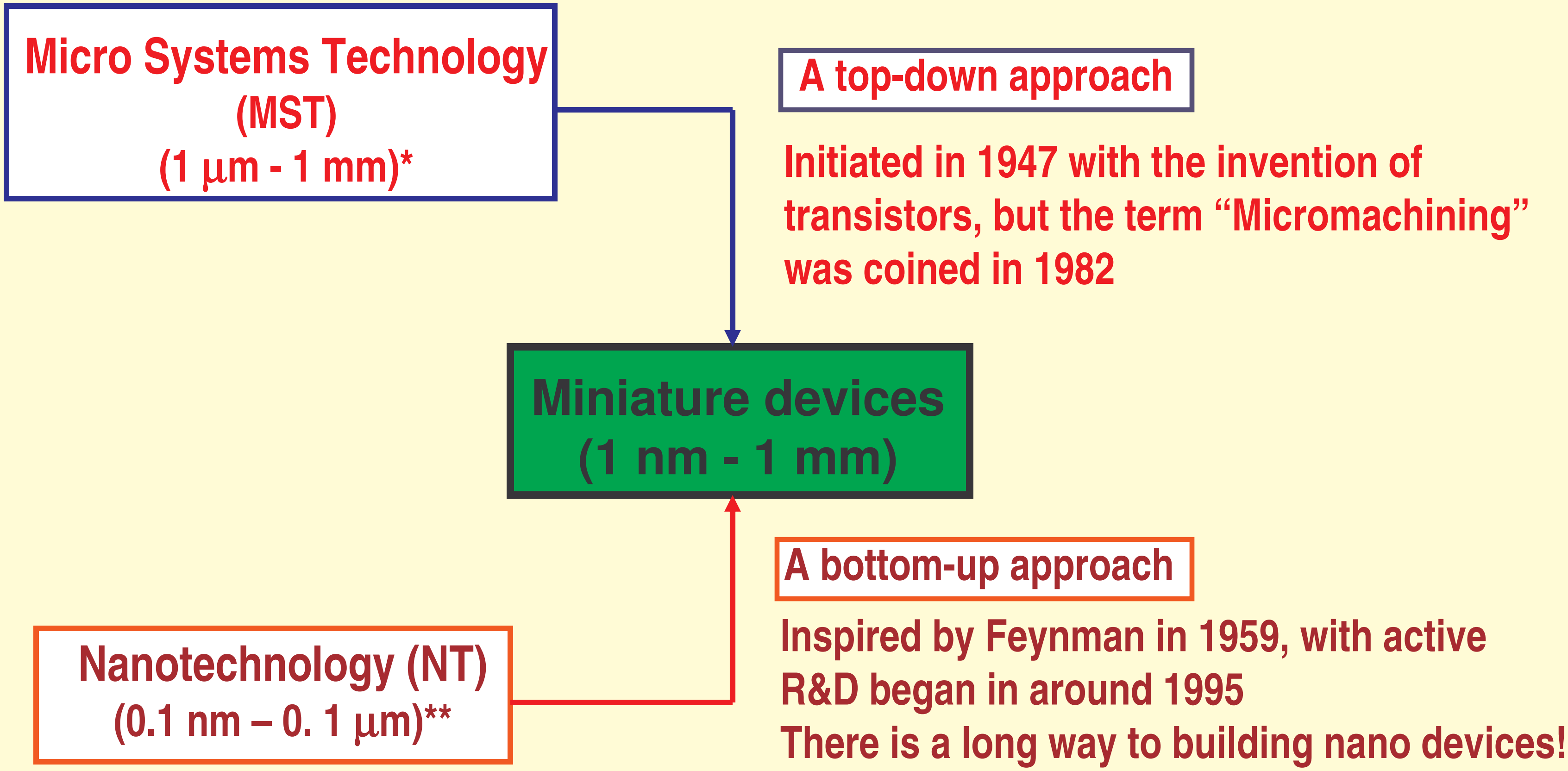
Size reduction

Palm-top Wireless PC

Transceives voice+ multi-media + others
(Video-camera, e-mails, calendar, TV and access to Internet; and a PC with key board)

- **Latest additional function to cell phones: The Global Positioning Systems (GPS)**

Enabling Technologies for Miniaturization



Micro Systems Technology
(MST)
(1 μm - 1 mm)*

A top-down approach

Initiated in 1947 with the invention of transistors, but the term “Micromachining” was coined in 1982

Miniature devices
(1 nm - 1 mm)

A bottom-up approach

Inspired by Feynman in 1959, with active R&D began in around 1995
There is a long way to building nano devices!

Nanotechnology (NT)
(0.1 nm – 0. 1 μm)**

* 1 μm = 10^{-6} m ≈ one-tenth of human hair

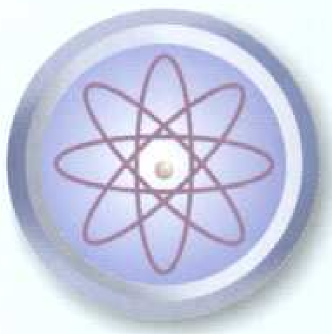
** 1 nm = 10^{-9} m ≈ span of 10 H_2 atoms

What is Nanotechnology?

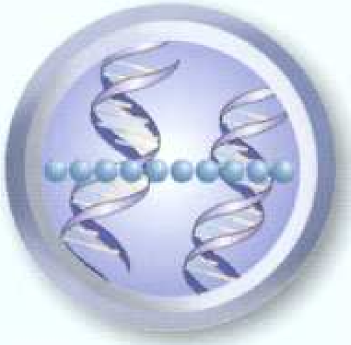
Nanotechnology is the creation of **USEFUL/FUNCTIONAL** materials, devices and systems through control of matter on the nanometer length (nm) scale and exploitation of novel phenomena and properties (physical, chemical, biological) at that length scale.

A Perspective of Nano Scale:

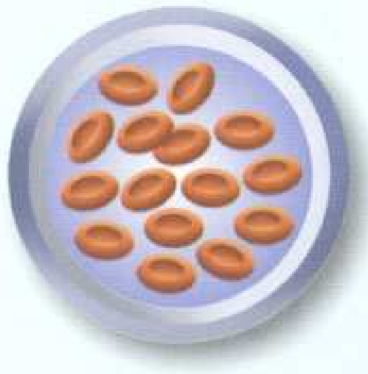
1 nm = 10^{-9} m = 10^{-6} mm = 10^{-3} µm



Less than a nanometer
Individual atoms are up to a few angstroms, or up to a few tenths of a nanometer, in diameter.

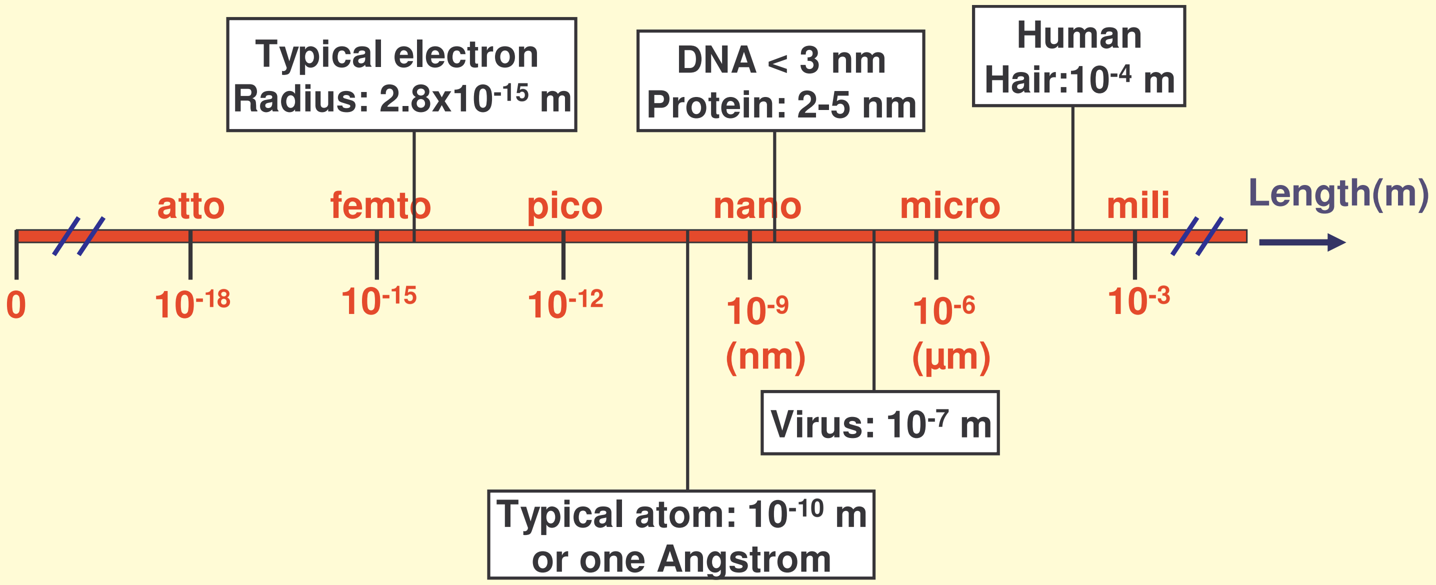


Nanometer
Ten shoulder-to-shoulder hydrogen atoms (blue balls) span 1 nanometer. DNA molecules are about 2.5 nanometers wide.



Thousands of nanometers
Biological cells, like these red blood cells, have diameters in the range of thousands of nanometers.

Length Scale in Nanotechnology



Typical electron
Radius: 2.8×10^{-15} m

DNA < 3 nm
Protein: 2-5 nm

Human
Hair: 10^{-4} m

Virus: 10^{-7} m

Typical atom: 10^{-10} m
or one Angstrom

Why Nanotechnology?

All matters that exist in universe are made of atoms and molecules.

The way molecules of various shapes and surface features organize into patterns on nano scales determines important material properties (e.g. electrical conductivity, optical properties, mechanical strength, etc.)

Nano technology will enable us to synthesize nano structures and control how scale patterning unfolds. From which we can design and create new sets of matters with desired properties and characteristics.

Active R&D in Nanotechnology:

inspired by Richard Feynman's speech in 1959

(1918 - 1988)
A visionary and a Nobel Laureate in Physics, 1965

Feynman, R., **"There's Plenty of Room at the Bottom: An invitation to enter a new field of physics,"** (miniaturization) first presented at the American Physical Society at California Institute of Technology on December 29, 1959. Subsequent publication in 'Engineering and Science', Caltech, February 1960.

The Very First Man-Made Nano Structure -
The “Buckyball”

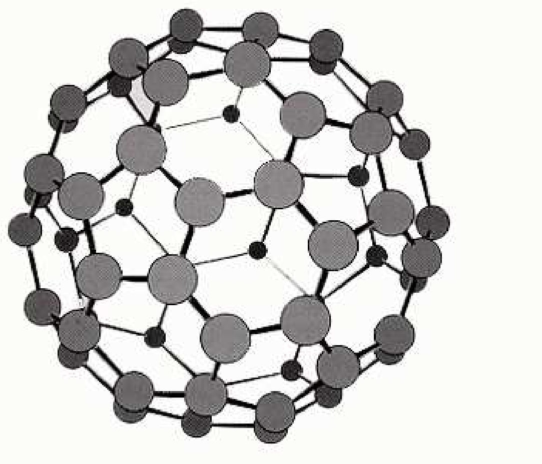
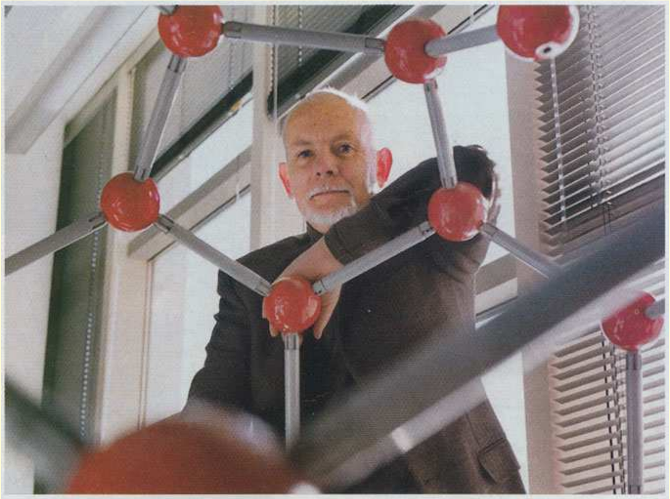


Figure 1.12 Buckminsterfullerene (C_{60}). A third form of pure carbon.

It contained 60 carbon atoms in the shape of a soccer ball with a diameter of 0.7 nano meter.

Made from the Buckminsterfullerene - a third form of pure carbon molecule.
(after the name of a futurist, R. Buckminster Fuller)

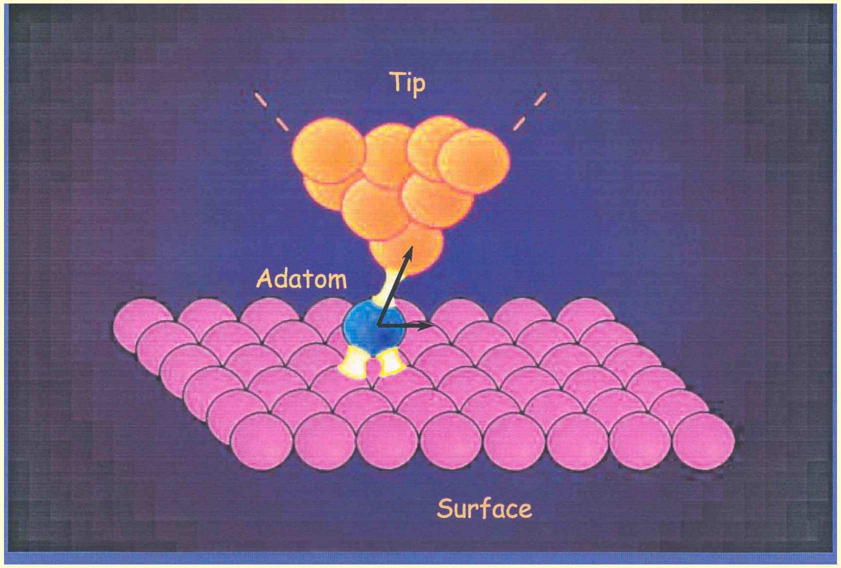
Created in 1985 by a chemistry professor,
Richard Smalley from Rice University -
a Nobel Laureate in 1996.



SMALLEY The buckyballs he discovered can be assembled into shapes that fit onto the receptors of cells

Major Impacts of Nanotechnology

(source: Meyya Meyyappan, NASA Ames)



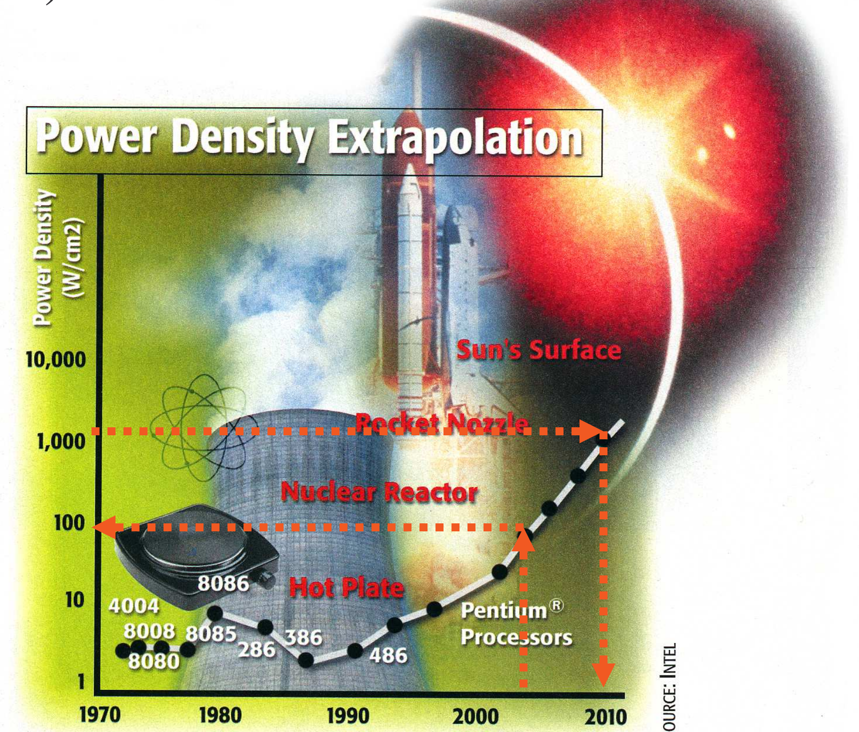
Nanotechnology is an enabling technology

- **Electronics, Computing and Data Storage**
- **Materials and Manufacturing**
- **Health and Medicine**
- **Energy** and Environment
- Transportation
- National Security
- Space exploration
-
-

Nanotechnology Benefits in Electronics and Computing

(source: Meyya Meyyappan, NASA Ames)

- Processors using molecular electronics with declining energy use and cost per gate, thus increasing efficiency of computer by 10^6.
- Small mass storage devices: multi-tera (10^{12}) bit levels.
- Integrated nanosensors: collecting, processing and communicating massive amounts of data with minimal size, weight, and power consumption.
- Higher transmission frequencies and more efficient utilization of optical spectrum to provide at least 10 times the bandwidth now.
- Display technologies.
- Quantum computing.



SOURCE: INTEL

CPU - Computer Power User Magazine

Heat = Horrendous challenge to mechanical engineers !!

TWO DISRUPTIVE HEAT TRANSFER TECHNOLOIES

(1) Nanoscale Heat Transfer in Nano Transistors

(2) Nanoscale Data Storage Systems

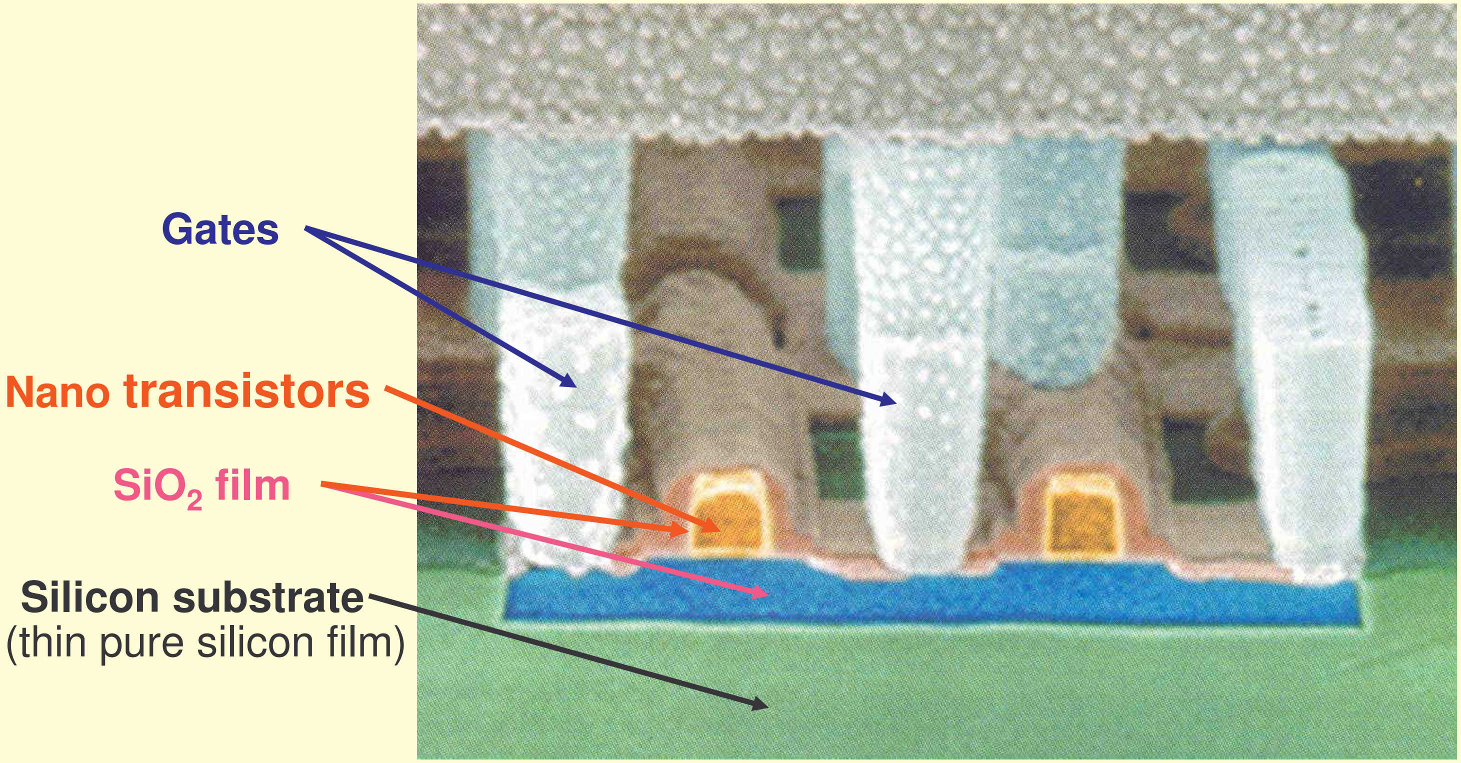
(1) Nanoscale Heat Transfer in Nano Transistors

Nanotechnology Benefits in Electronics and Computing

The Nanochip

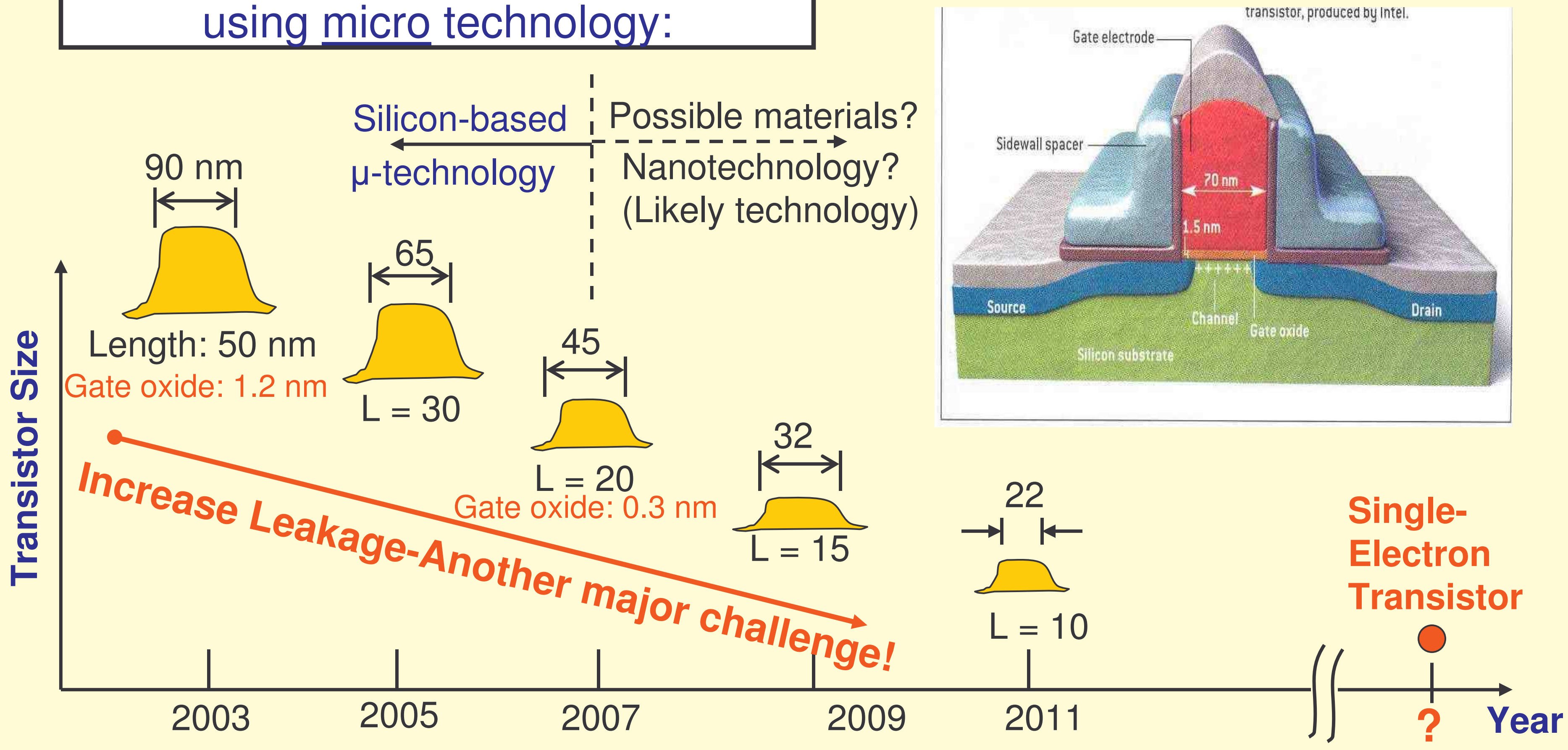
Advantages: (1) Low unit cost.

(2) Narrow gates for faster on-off → boost speed limit of the integrated circuits.



Nanotechnology Benefits in Electronics and Computing

Intel roadmap on nano transistors
using micro technology:



Silicon-based
μ-technology

Possible materials?
Nanotechnology?
(Likely technology)

90 nm
Length: 50 nm
Gate oxide: 1.2 nm

65
L = 30

45
L = 20
Gate oxide: 0.3 nm

32
L = 15

22
L = 10

Single-Electron Transistor

Increase Leakage-Another major challenge!

Heat dissipation and **leak of electricity** are two critical technical problems in further miniaturization of transistors.

Possible Solutions

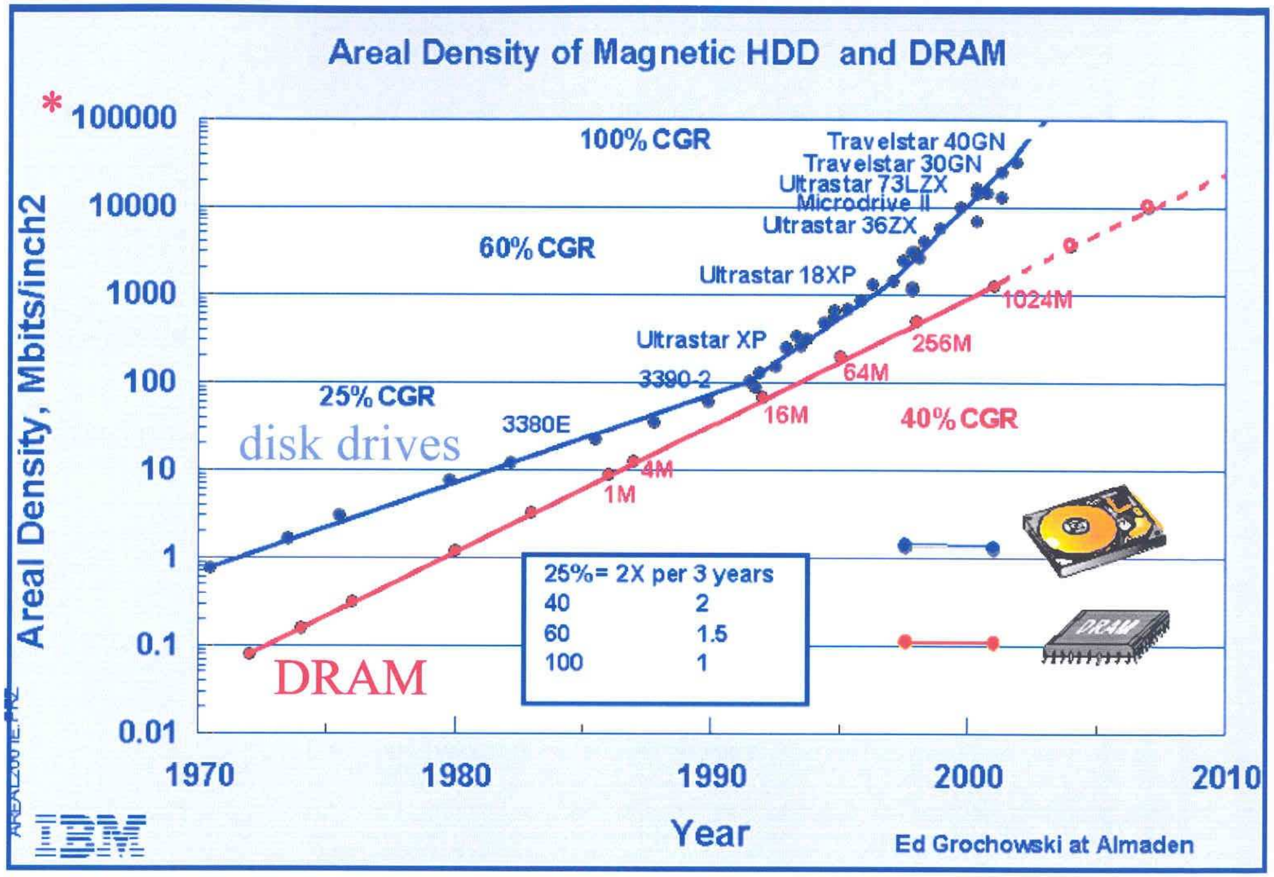
- Cooling by nanofluidics involving nanoscale fluid flow in nanoscale channels.
- Cooling by Nanoscale heat pipes.

(2) Nanoscale Heat Transfer:

Nano Data Storage System

Nanotechnology Benefits in Data Storage-1

The ever-increasing demand for high density information storage:



*80 nm ×80 nm bit cell $\Rightarrow 10^5$ Mbit/in^2

Nanotechnology Benefits in Data Storage-2

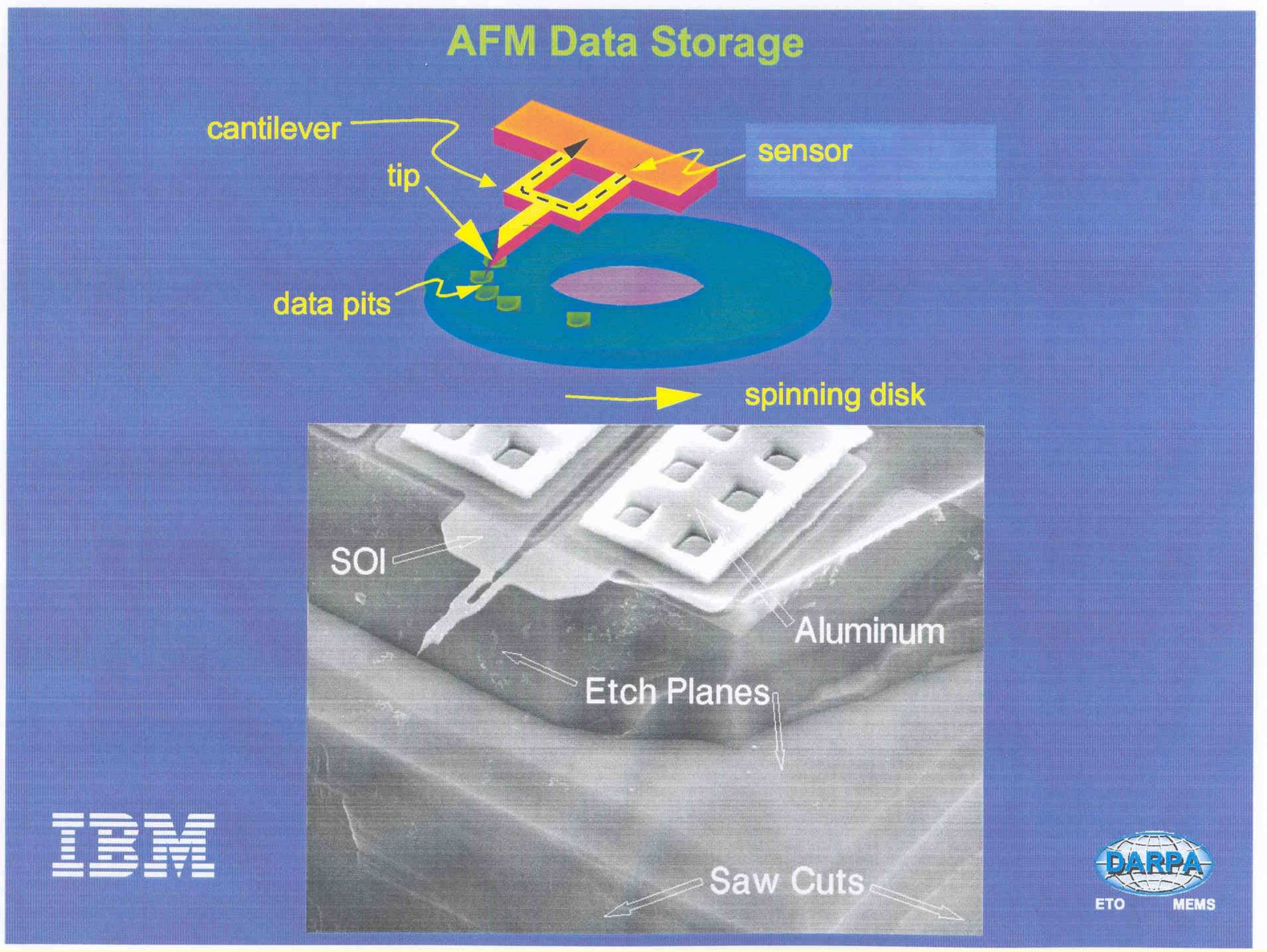
Data Storage Requirements:

- Density
- Error rate
- Re-writability
- Tracking
- Data rate
- Overall reliability
- Data retention
- Cost

Source: “Scanning Probes Microscope & Their Potential for Data Storage,” John Mamin, IBM Almaden Research Center, San Jose, CA. (Private communication)

Nanotechnology Benefits in Data Storage-3

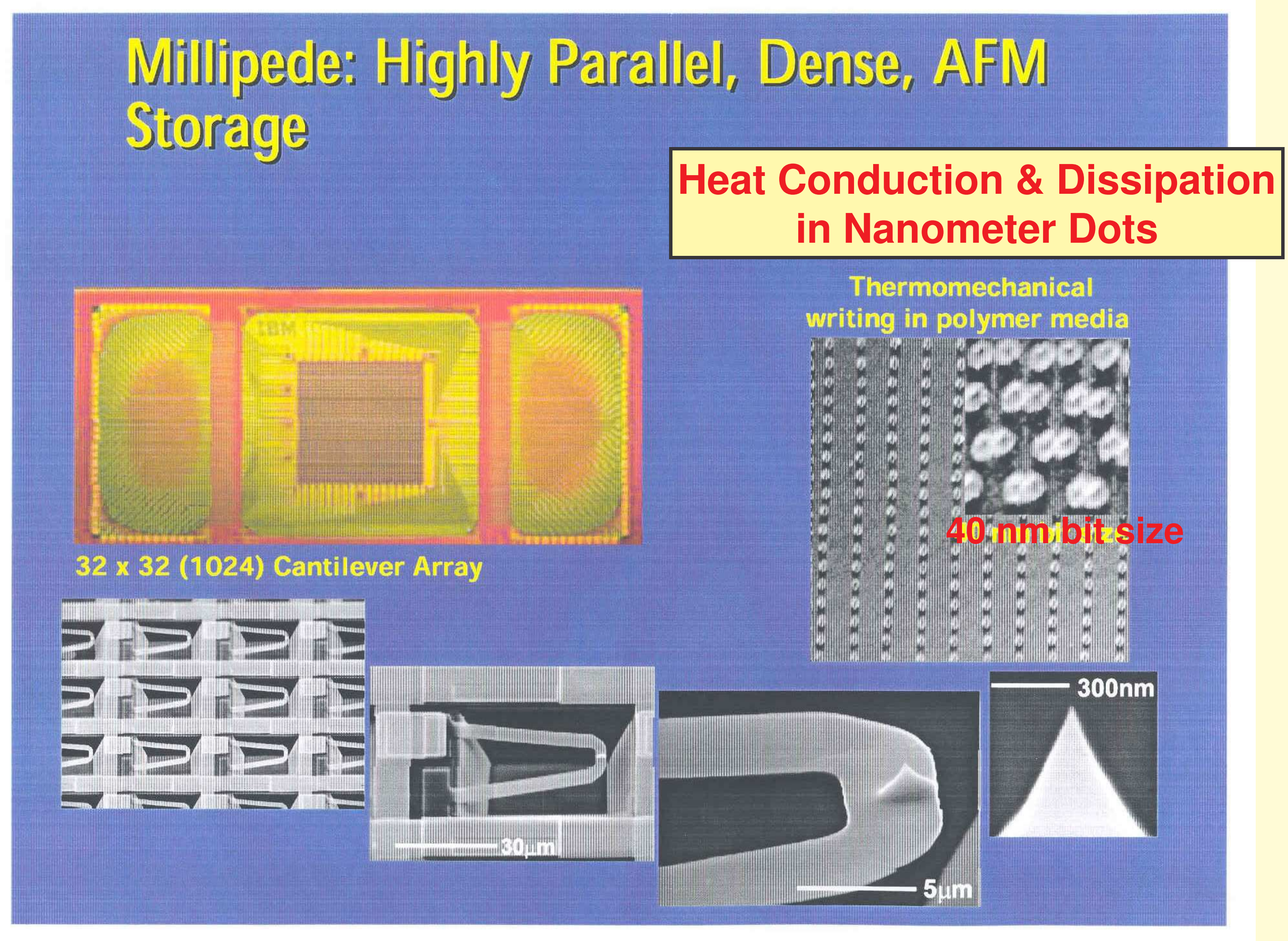
- The continuous demands for high density data storage has passed the limit of traditional electromagnetic means.
- A new concept of “Read-Write” is being developed – the “**Millepede**” project by IBM, San Jose and Zurich, Switzerland.
- Working principle involving indenting the surface of polymer film using AFM.



AFM Data Storage

Nanotechnology Benefits in Data Storage-4

- Encouraging initial results of the Millipede development:



Millipede: Highly Parallel, Dense, AFM Storage

Heat Conduction & Dissipation in Nanometer Dots

Thermomechanical writing in polymer media

40 nm bit size

32 x 32 (1024) Cantilever Array

Both these cases require the use of nanoscale heat transfer techniques - A radically different from macroscale heat transfer techniques that use:

- Fourier law for heat conduction in solids
- Newton’s cooling law for heat convection, and
- Kirchhoff’s law and Stefan-Boltzmann Equation for thermal radiation

Part 2

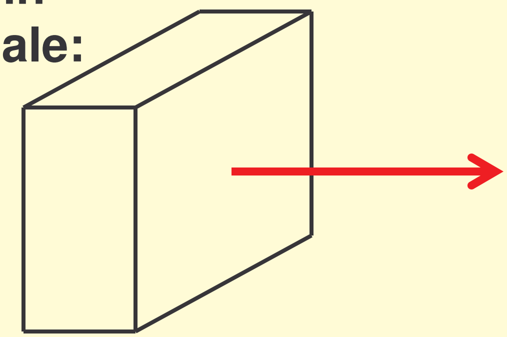
Atomic Structure & Quantum Physics

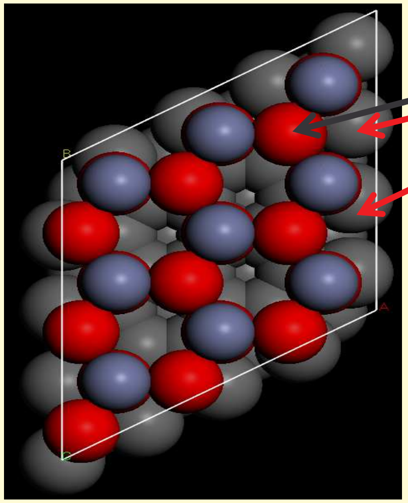
November 16, 2006

The Makes of Matter

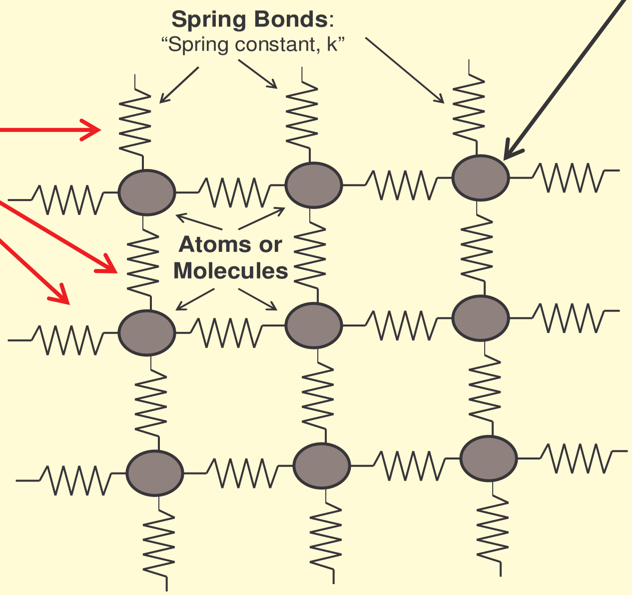
- ALL matter on Earth are made by ATOMS:

A solid in
macroscale:





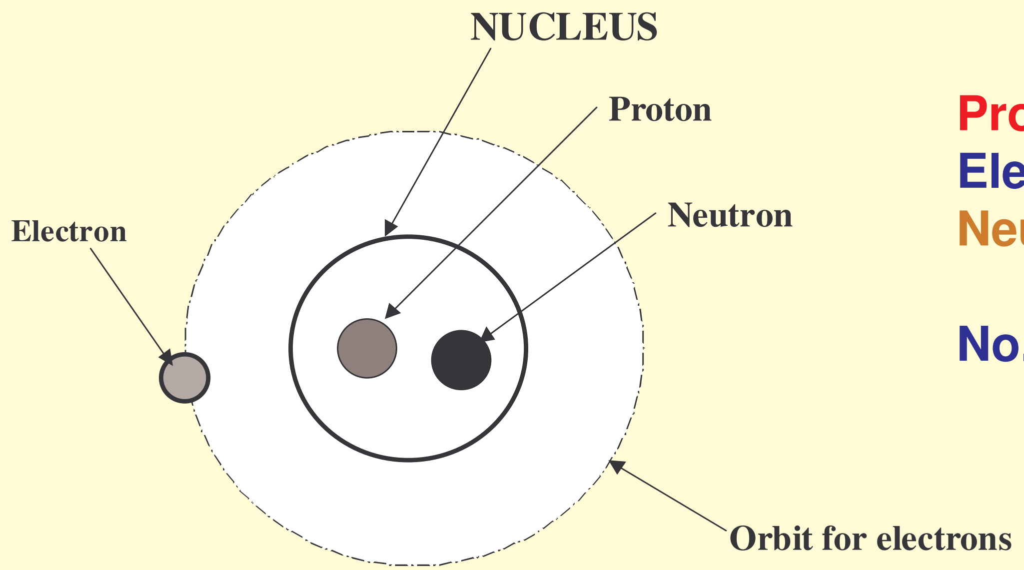
**Packed
Atoms**



- **Atoms are bonded together by "CHEMICAL BONDS," which are treated as elastic bonds simulated by "springs"**
- A "spring" can be stretched or compressed by external energy.
- A deformed "spring" contains energy, that can be released under circumstances.

Atomic Structure of Matter

Basic atomic structure



Protons carry +ve charge
Electrons carry –ve charge
Neutrons carry no charge

No. of protons = No. of electrons

NOTE: There is no neutron in the nucleus of H_2 atoms.

The diameter of outer orbit: 2 to $3x10^{-8}$ cm, or 0.2 to 0.3 nm.

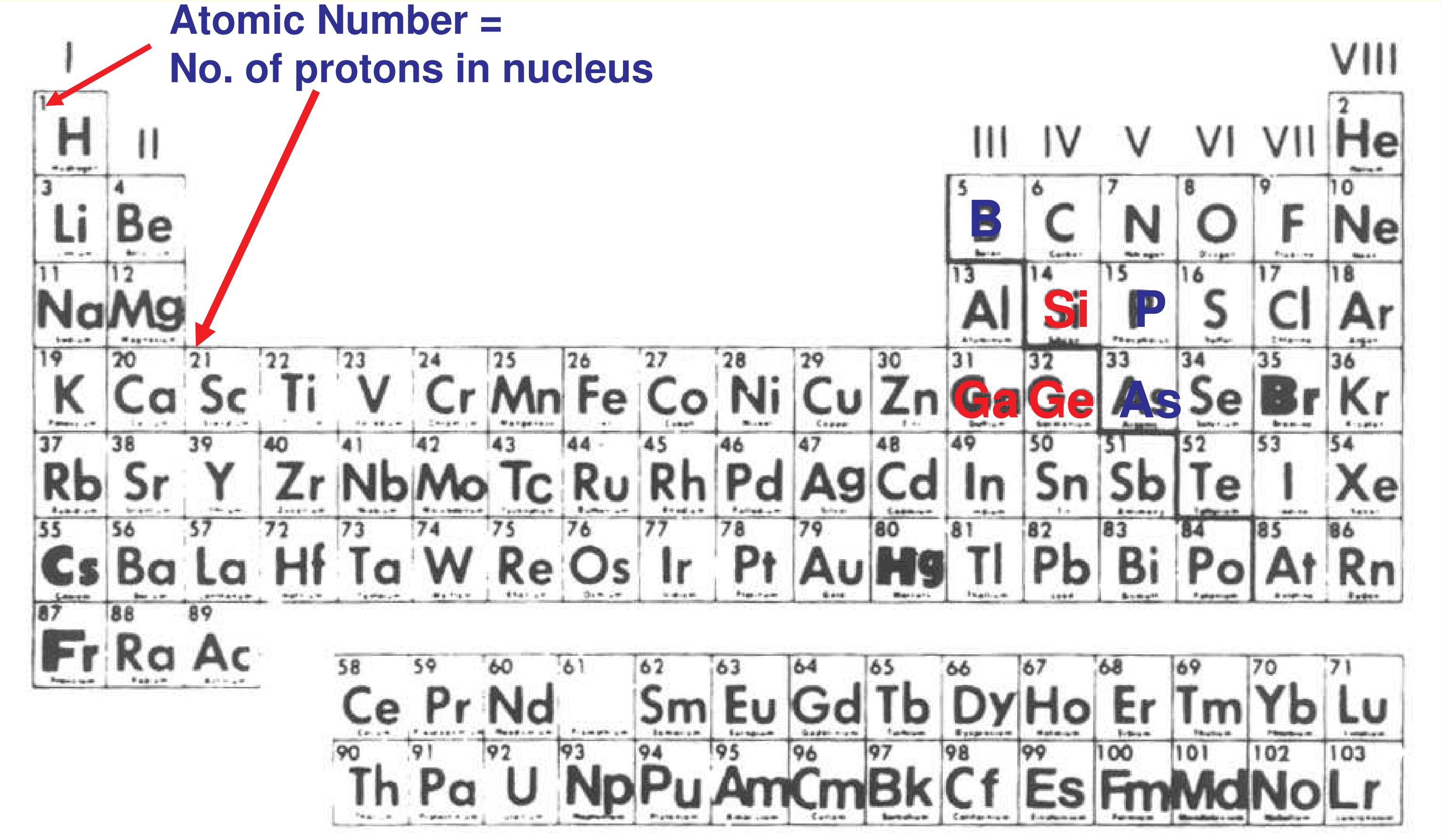
Mass of protons: $1.67x10^{-24}$ g

Mass of electrons: $9.11x10^{-28}$ g

Atomic Structure of Matter-Cont'd

The periodic table of elements

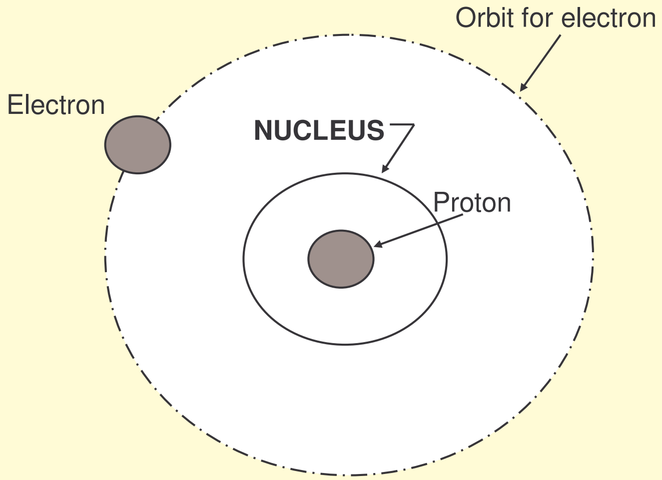
- Every thing on the Earth is made by 96 stable and 12 unstable elements.
- Each element has distinct atomic structure.
- The number of protons (and thus electrons) in the element determines the properties of the element.



Atomic Number =
No. of protons in nucleus

I	II											III	IV	V	VI	VII	VIII
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac															
			58 Ce	59 Pr	60 Nd	61	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
			90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

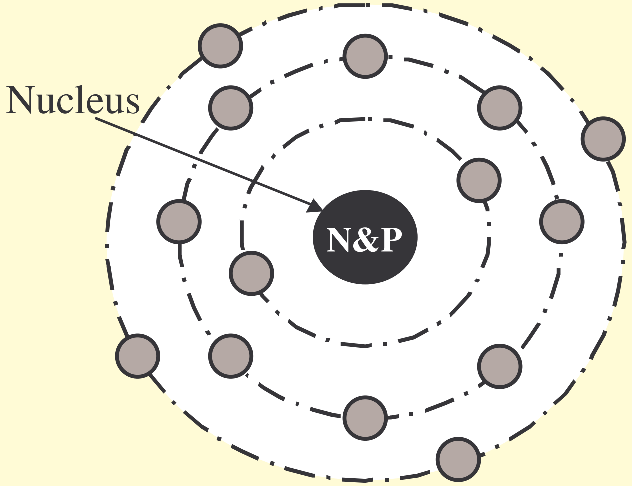
A Hydrogen Atom



One electron
One proton
No neutron

A Silicon Atom

- A common semiconductor



14 electrons**
14 protons
14 neutrons

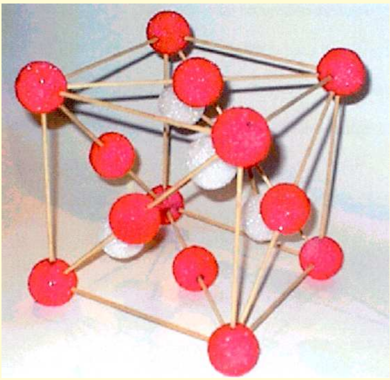
** The 4 electrons on the outmost orbit are shared with 4 neighboring atoms in silicon crystals = covalent solid
– common for semiconductors and dielectric materials.

Grains and Crystals

- Some matter in natural states with single atoms.
- Many others are made with combinations of atoms with different structures = **MOLECULES**

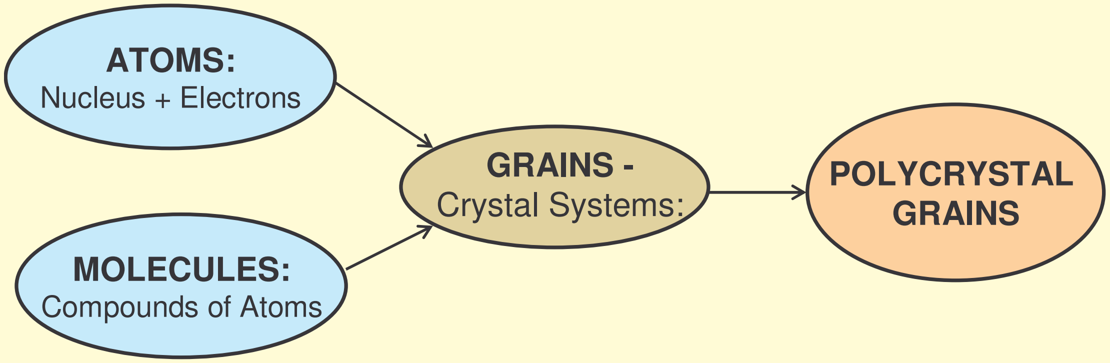
- **Crystals** = aggregations of atoms or molecules.

A single silicon crystal →



Silicon atoms are shown in “red” and “white” balls bonded together by chemical bonds (shown in yellow sticks).

- Most matter are made of congregation of crystals = **Grains** → **Polycrystalline grains**.



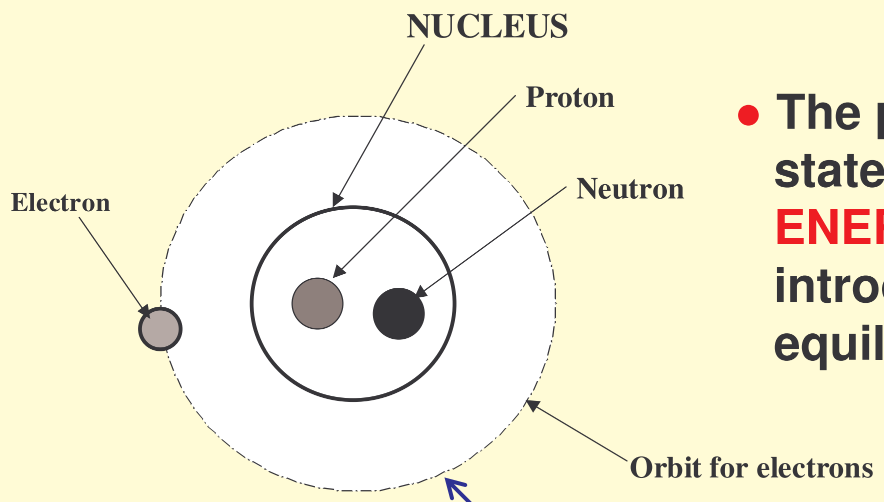
ATOMS:
Nucleus + Electrons

MOLECULES:
Compounds of Atoms

GRAINS -
Crystal Systems:

POLYCRYSTAL GRAINS

Mechanics of Atoms



- **The position of electrons in atoms at natural state becomes UNSTABLE when external ENERGY (thermal or mechanical forms) is introduced → VIBRATIONS from its initial equilibrium position.**

The radii of orbits for electrons in a matter

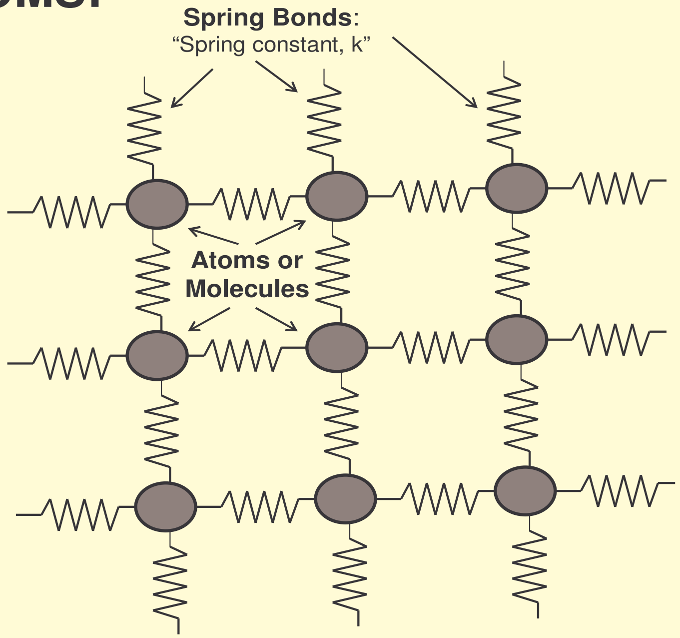
- Expands from its natural state with **sufficient** added ENERGY
- Shrinks with lost ENERGY.

- In the case of covalent solids, the number of electrons at the outmost orbits of a base material may be altered (i.e. increase or decreased) by invasion of foreign atoms by input ENERGY through **diffusion** or **ion implantation** processes – known as **Doping processes** in semiconductor industry.

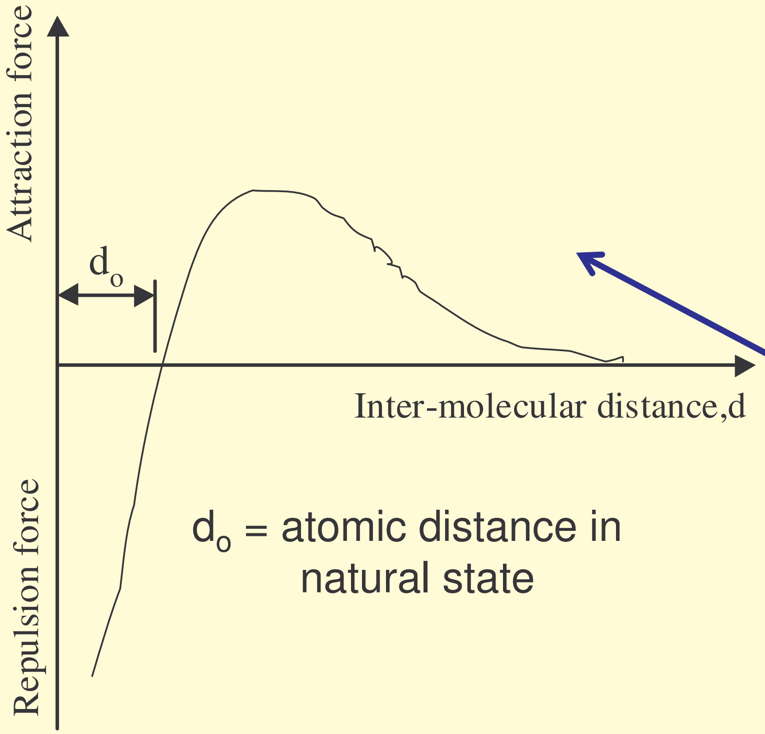
- The base material, after doping, changes its electronic properties.

Mechanics of Atoms – cont'd

- **ALL matter on Earth are made by ATOMS:**



- **Atoms are bonded together by "CHEMICAL BONDS," which are treated as elastic bonds simulated by "springs"**



d_o = atomic distance in natural state

- **Atomic force required to change the natural state.**

Heat Generation by Molecular Vibrations

- **The position of electrons in atoms at natural state becomes UNSTABLE when external ENERGY (thermal or mechanical forms) is introduced → VIBRATIONS from its initial equilibrium position.**

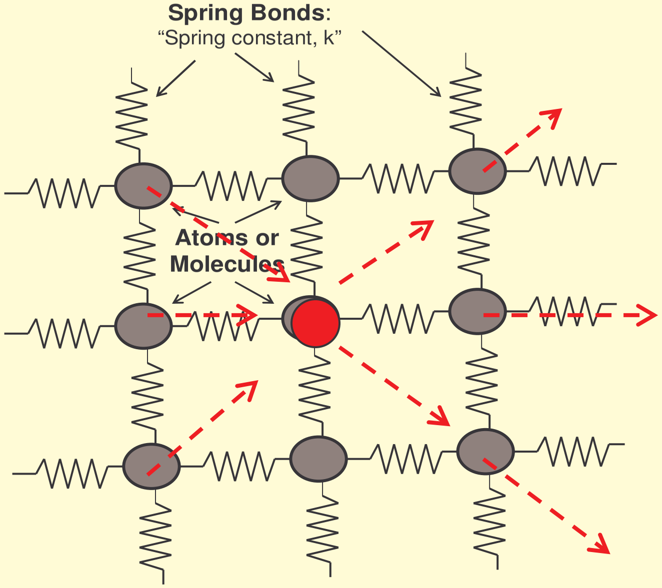
The displacement of any atom in the matter induced by VIBRATION will result in:

(1) Stretching or compression of the "springs" that are attached to that atom, and

(2) The elongation and compression of these "springs" will cause the atoms attached to the other end to displace → Resulting to a "chain reactions" of vibration of other atoms.

(3) The initial vibration of one atom can thus be TRANSMITTED outward and cause many other atoms to vibrate.

Network of Atoms by "Spring Bonds"



- If the external ENERGY that cause initial atomic vibration = **HEAT**, Then, heat is transmitted from one atom or a set of atoms can be **TRANSMITTED** to other atoms in the way as described above.

SUMMARY

Fundamental Mechanisms of Heat Transmission in Matter

- Lattice vibration of atoms generates heat.

- Atomic vibration caused geometry change of lattice (bond) and more atoms to vibrate, and hence transmits thermal energy and thus HEAT.

- For cases with more energy input, or matter with more mobile electrons in the atoms (e.g. metals), there could be release of electrons accompanying the transmission of energy among atoms.

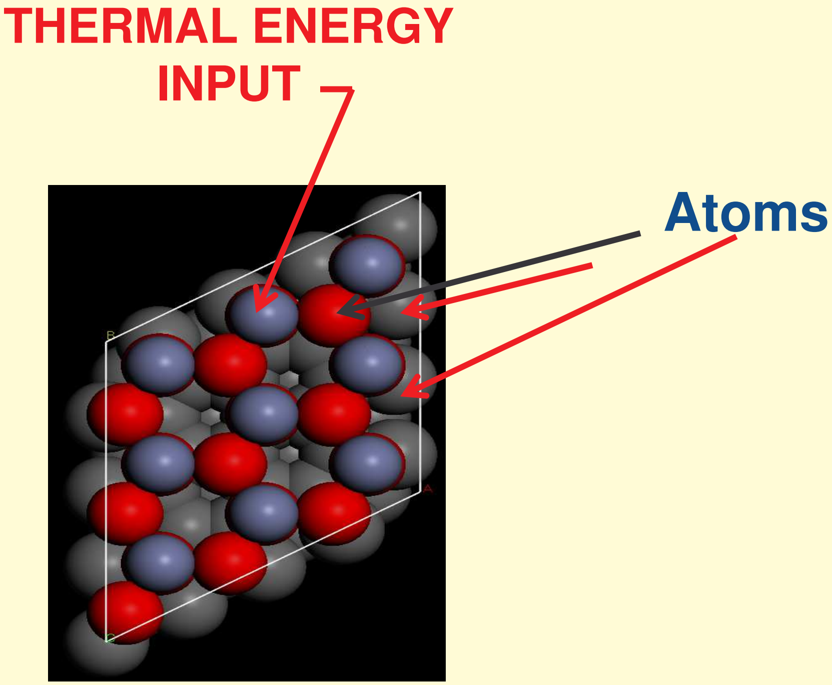
Part 3

Inter- Molecular Heat Transmission

(Nanoscale Heat Transfer)

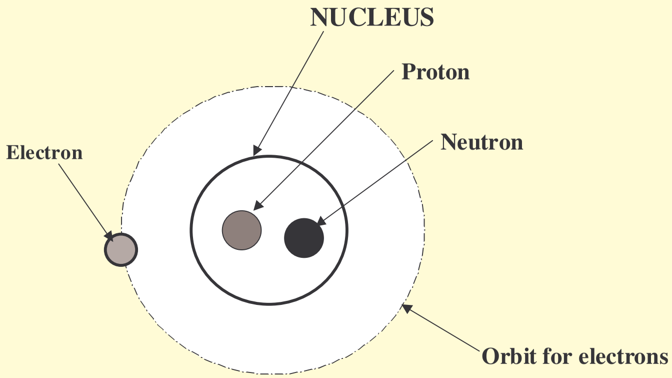
November 21, 2006

PHONONS – The Thermal Energy Carriers

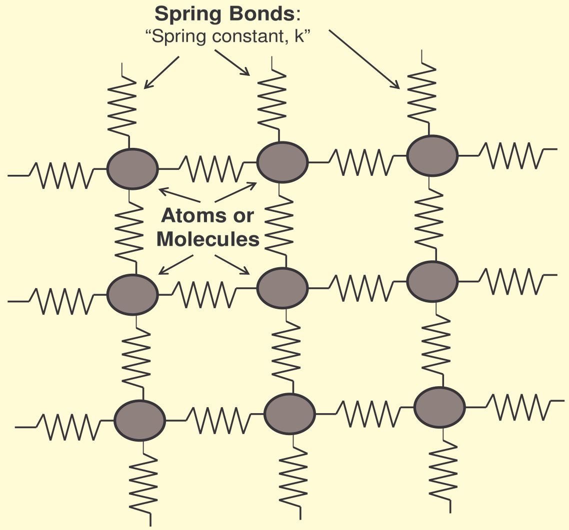


Consequences

- Electrons are energized into motion (metals)
- The atom is energized to vibrate (semi-conductors or insulators)



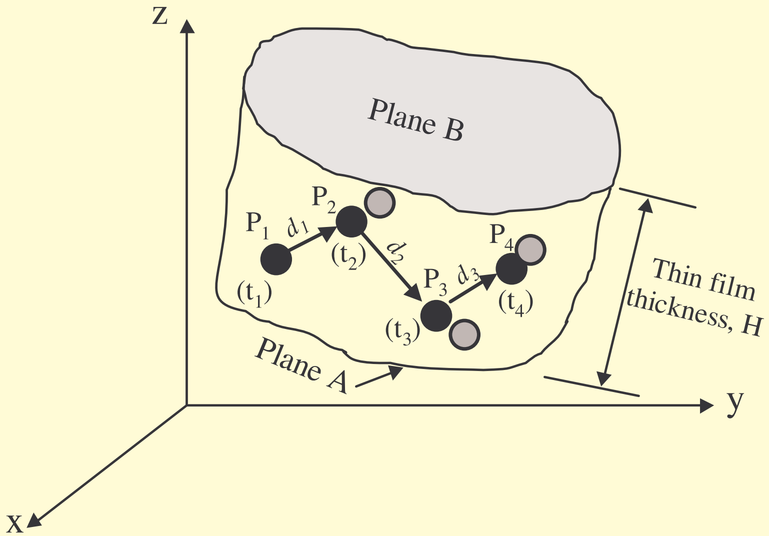
- The vibrating atom results in ENERGY generation in the attached bonds (e.g. stretching and compression of the “springs”) - **PHONONS**
- The energy in bonds causes more atoms to vibrate → more PHONONS
- **Transferring thermal energy (heat) = PHONON traveling (in semiconductors or insulators).**



- **Transferring thermal energy (heat) = phonon and ELECTRONS in metals. The carrier in radiation is PHOTONS.**

Collision of Traveling Phonons

- PHONON is like Photon physically exists as energy induced by vibrating atoms.
- They are treated as “particles” with <u>virtual</u> size and mass.
- There are zillions of atoms in a substance → possible zillion of phonon particles.



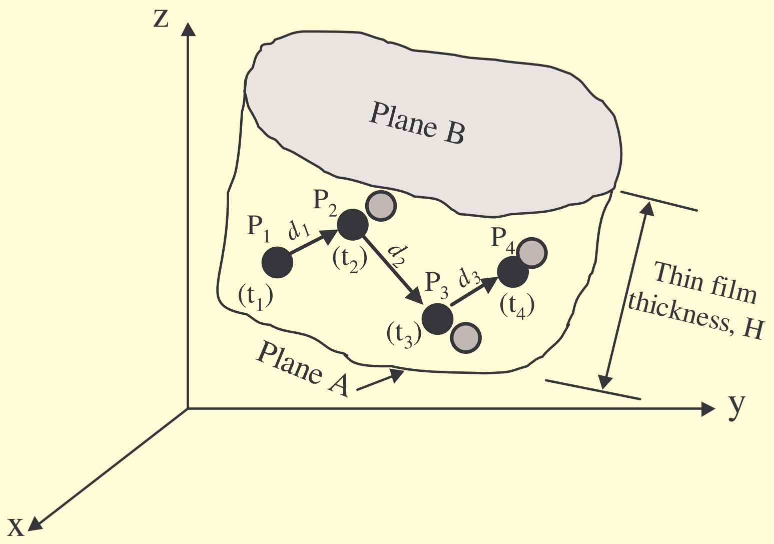
When an energy-carrying phonon travels from one position (Plane A) to another position (Plane B) in a solid, it encounters zillion times collision with other phonon particles.

The traveling phonon would change its course after each collision → No direct and clear path from Plane A to Plane B.

Free path The distance of free traveling of phonons without collision with other phonon.

Free time The time required for a phonon traveling without collision with another phonon.

Collision of Traveling Phonons – Cont’d



Average “mean free path” (**MFP**)

$$\lambda = \frac{d_1 + d_2 + d_3}{3}$$

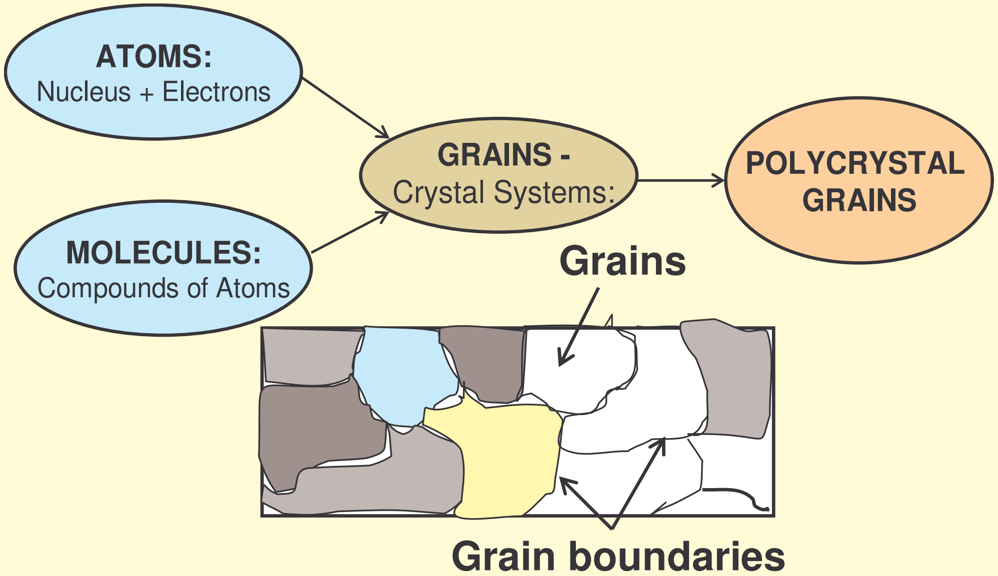
Average “mean free time” (**MFT**)

$$\tau = \frac{(t_2 - t_1) + (t_3 - t_2) + (t_4 - t_3)}{3} = \frac{t_4 - t_1}{3}$$

The MFP and MFT in Nanoscale Heat Transmission

Magnitudes of MFP and MFT depend on:

- Molecular structures
- Congregation molecules
- Grain geometry
- Grain boundaries
- Temperature



	Electrons	Phonons	Gases	Liquids
MFP	10^{-8} m	$>10^{-8}$ m ($=10^{-7}$ m for diamond)	65 nm	130 nm
MFT	10^{-12} s			

- The effect of both MFP and MFT are negligible in magnitudes in macroscale heat transmission even with millions of collisions of phonon and electrons because of the low magnitudes of MFP and MFT, and their effects even out in the size of the domain.
- **In nanoscale solids, the effects of MFP and MFT become more significant and need to be accounted for in the analysis → DELAY IN HEAT FLOW.**

Heat Transmission in Solids of Nanoscale

Heat transmission in solids is achieved by:

- **Traveling of phonons in semiconductors or dielectric materials, or**
- **Traveling of phonons and electrons in metallic materials.**
- **Traveling of photons in radiative heat transmission.**

- Traveling of phonons and electrons in solids induced by thermal energy involves collisions and scatterings along their ways.

- In solids in **macroscale**, such alterations of paths of traveling is “AVERAGED” with “big” sizes. So, the effect of altered paths is not significant. In solids of **nanoscale**, this factor becomes significant in heat transmission because of much shorter distance (i.e. small size) for phonon to travel.

- Time associated with the traveling of phonons and electrons in different **size** of solids is significant in solids of nanoscale for the same reason as in the alteration of paths in heat transmission.

- **Thus MFP and MFT have significant effect in heat transmission in solids of nanoscale.**

Observations

All nanoscale heat transmission is time-dependant because of MFT. So, there is no such thing as steady-state heat transfer in nanoscale domains.

Solids of nanoscale is a poorer heat conductor than the same material in macroscale.

This implies that solids of nanoscale has LOWER thermal conductivity than that of the same material in macroscale.

This size-dependent thermophysical property of nanoscale solids make the heat conduction analysis nonlinear in nature.

Thermal Conductivity (k) of Thin Films

A. Model by Rohsenow and Choi [1961]:

$$k = \frac{1}{3} C V \lambda$$

Parameters for Thermal Conductivity of Thin Films

	Materials	**Dielectric and semiconductors**
Specific heats, C	Specific heat of electrons, C_e	Specific heat of phonons, C_s
Molecular velocity, V	Electron Fermi velocity, $V_e \cong 1.4 \times 10^6$ m/sec	Velocity of phonons (sound velocity), $V_s \cong 10^3$ m/sec
Average mean free path, λ	Electron mean free path, $\lambda_e \cong 10^{-8}$ m	Phonon mean free path, $\lambda_s \cong$ from 10^{-7} m and up

References: Flik et.al. 1992 and Tien and Chen 1994

Thermal Conductivity (k) of Thin Films – Cont'd

B. Model by Flik and Tien [1990]:

Normal to the thin film:

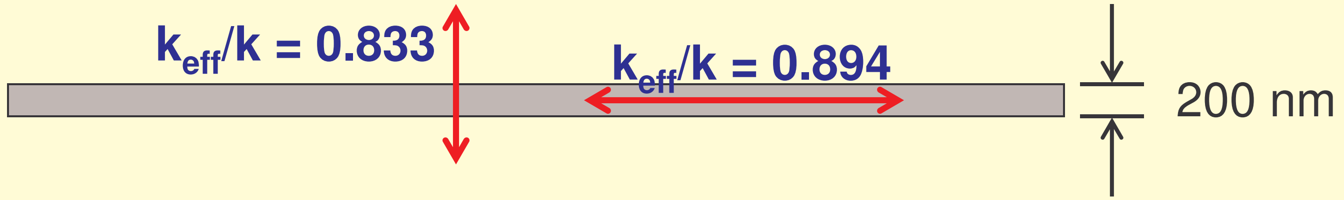
$$\frac{k_{eff}}{k} = 1 - \frac{\lambda}{3H}$$

Along the thin film:

$$\frac{k_{eff}}{k} = 1 - \frac{2\lambda}{3\pi H}$$

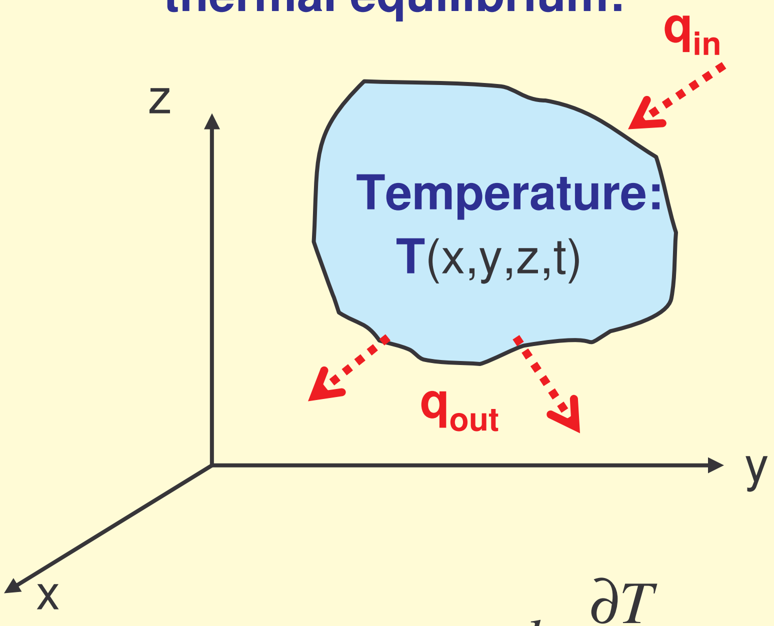
where k_{eff} = thermal conductivity of thin film.
k = thermal conductivity of the same material in macroscale.
H = thickness of thin film. λ = Mean free path (MFP)

Example: For silicon thin film at H = 0.2 μm or 200 nm thick, with MFP, $\lambda = 10^{-7}$ m, we have:
$k_{eff}/k = 0.833$ normal to the thin film and $k_{eff}/k = 0.894$ along the film.



The Heat Conduction Equation for Macroscale Solids

Temperature in a solid in thermal equilibrium:



The heat conduction equation can be derived from the Fourier law of heat conduction and the First law of Thermodynamics.

The Fourier law of heat conduction:

The heat flux in the solid:

$$q = -k\nabla T(\vec{r},t)$$

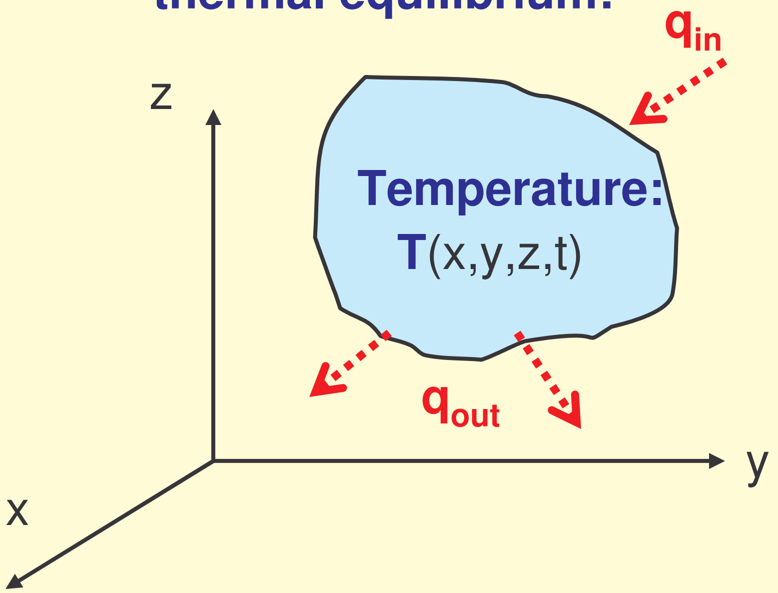
In the Cartesian coordinate system, we have:

$$q_x = -k_x \frac{\partial T}{\partial x} \qquad q_y = -k_y \frac{\partial T}{\partial y} \qquad q_z = -k_z \frac{\partial T}{\partial z}$$

in x, y, and z-direction respectively.

The Heat Conduction Equation for Macroscale Solids –cont'd

Temperature in a solid in thermal equilibrium:



The First Law of Thermodynamics relates energy and work as:

$$\Delta U = \Delta W + \Delta Q$$

in which

ΔU = change of internal energy;
ΔW = difference between the input and output work; and
ΔQ = net heat flow in the solid.

In a non-flow system, such as this, ΔW = 0 that leads to: ΔU = ΔQ→ $\Delta \dot{U} = \Delta \dot{Q}$

Rate of change of internal energy, ΔU = **Rate of net heat input to the solid, ΔQ**

$$\Delta \dot{U} = \rho c v \frac{\partial T}{\partial t}$$

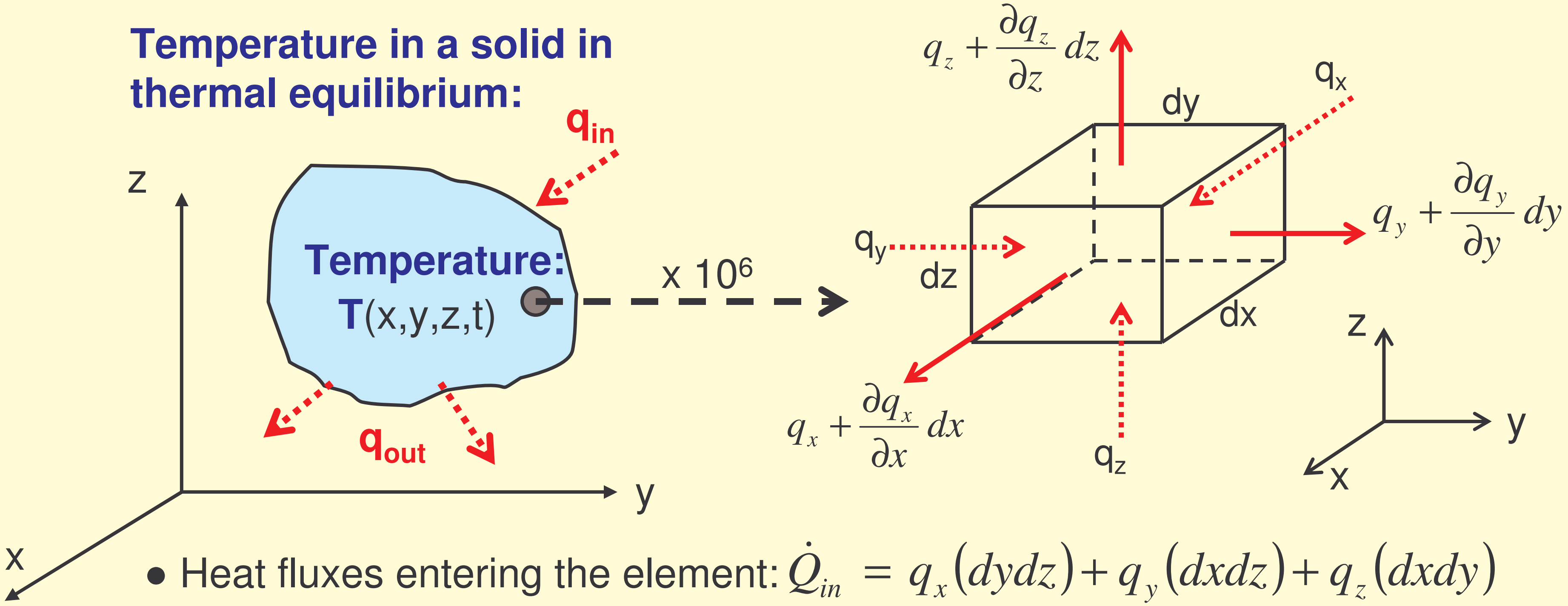
Heat flux in and out,Δq

Heat generation by the material,Q

ρ = mass density, c = specific heat, v = volume

The Heat Conduction Equation for Macroscale Solids –cont'd

Temperature in a solid in thermal equilibrium:



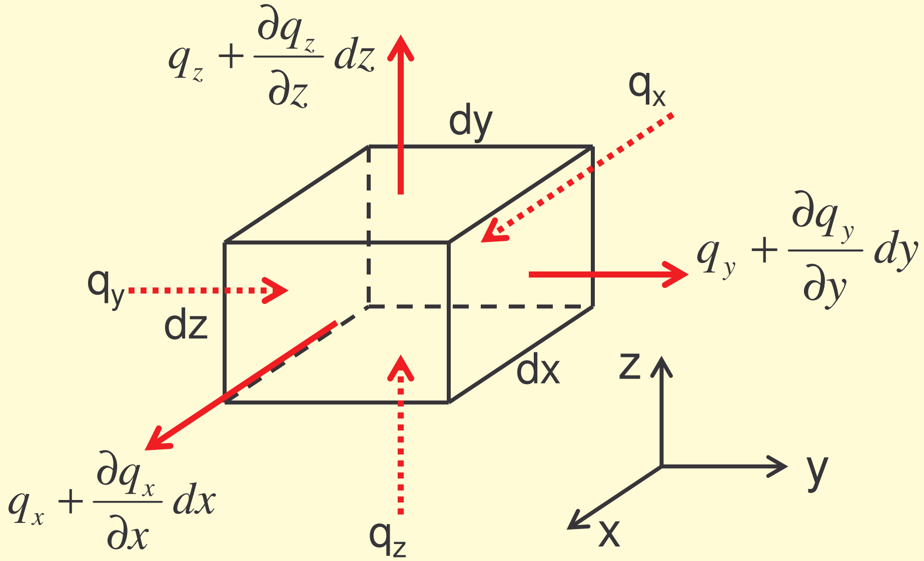
- Heat fluxes entering the element: $\dot{Q}_{in} = q_x(dydz) + q_y(dxdz) + q_z(dxdy)$
- Heat leaving the element is:

$$\dot{Q}_{out} = \left(q_x + \frac{\partial q_x}{\partial x} dx\right)(dydz) + \left(q_y + \frac{\partial q_y}{\partial y} dy\right)(dxdz) + \left(q_z + \frac{\partial q_z}{\partial z} dz\right)(dxdy)$$

- The net heat flux flow in the element is:

$$\dot{Q}_{in} - \dot{Q}_{out} = -\frac{\partial q_x}{\partial x}(dxdydz) - \frac{\partial q_y}{\partial y}(dydxdz) - \frac{\partial q_z}{\partial z}(dzdxdy)$$

The Heat Conduction Equation for Macroscale Solids –cont'd



Let Q(x,y,z,t) = heat generated by the element in unit volume and time.

and the change of internal energy in the element to be:

$$\Delta \dot{u} = \rho c \frac{\partial T}{\partial t} dv = \rho c \frac{\partial T}{\partial t} (dxdydz)$$

From the relationship: $\Delta \dot{Q} = \Delta \dot{u}$ in the element, we have:

$$\dot{Q}_{in} - \dot{Q}_{out} = -\frac{\partial q_x}{\partial x}(dxdydz) - \frac{\partial q_y}{\partial y}(dydxdz) - \frac{\partial q_z}{\partial z}(dzdxdy)$$

$$+ Q(x, y, z, t)(dxdydz) = \rho c \frac{\partial T}{\partial t}(dxdydz)$$

$$\longrightarrow \quad -\frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y} - \frac{\partial q_z}{\partial z} + Q(x, y, z, t) = \rho c \frac{\partial T}{\partial t}$$

The Heat Conduction Equation for Macroscale Solids –cont'd

But from Fourier law of heat conduction:

$$q_x = -k_x \frac{\partial T}{\partial x} \qquad q_y = -k_y \frac{\partial T}{\partial y} \qquad q_z = -k_z \frac{\partial T}{\partial z}$$

The heat conduction equation in a macroscale solid can be obtained by substituting the above relations into the last expression derived from the First Law of Thermodynamics:

$$\frac{\partial}{\partial x} k_x \left(\frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} k_y \left(\frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} k_z \left(\frac{\partial T}{\partial z} \right) = \rho c \frac{\partial T}{\partial t}$$

For isotropic solids, $k = k_x = k_y = k_z$, the heat conduction equation becomes:

$$\nabla^2 T(\vec{r},t) + \frac{Q(\vec{r},t)}{k} = \frac{1}{\alpha} \frac{\partial T(\vec{r},t)}{\partial t}$$

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is the Laplacian operator;

$$\vec{r} = position\ \ vector = (x, y, z)\, in\ a\ Cartesian\ coordinate\ system$$

$$\alpha = \frac{k}{\rho c} = Thermal\ diffusivity\ of\ \ material$$

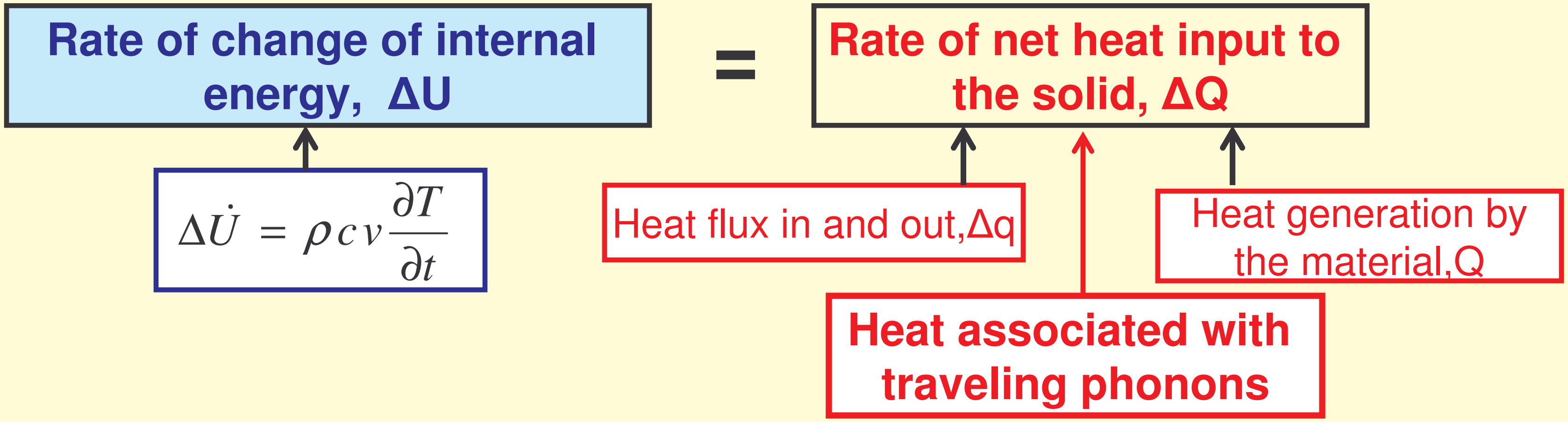
The Heat Conduction Equation for Nanoscale Solids

Heat transmission in nanoscale solids is achieved by:

- Traveling of phonons in semiconductors or dielectric materials, or
- Traveling of phonons and electrons in metallic materials.
- Traveling of photons in radiative heat transmission.

- Thus MFP and MFT have significant effect in heat transmission in solids of nanoscale.

The heat conduction equation for nanoscale solids thus needs to account for the heat carried by traveling phonons (and electrons). Consequently, we have The following additional term in heat generation in the solid:



Rate of change of internal energy, ΔU = **Rate of net heat input to the solid, ΔQ**

$$\Delta \dot{U} = \rho c v \frac{\partial T}{\partial t}$$

Heat flux in and out,Δq

Heat generation by the material,Q

Heat associated with traveling phonons

The Heat Conduction Equation for Nanoscale Solids-cont'd

The modified Fourier Law for thermal wave propagation in solids [Cattaneo & Vernotte]:

$$\vec{q} + \tau \frac{\partial \vec{q}}{\partial t} = -k \nabla T(\vec{r}, t)$$

Expanding the above in (x,y,z) coordinate system:

$$q_x + \tau \frac{\partial q_x}{\partial t} = -k_x \frac{\partial T(x, y, z, t)}{\partial x}$$ in the x-direction

$$q_y + \tau \frac{\partial q_y}{\partial t} = -k_y \frac{\partial T(x, y, z, t)}{\partial y}$$ in the y-direction

$$q_z + \tau \frac{\partial q_z}{\partial t} = -k_z \frac{\partial T(x, y, z, t)}{\partial z}$$ in the z-direction

where τ is the “relaxation time” accounting for the traveling of phonons

The Heat Conduction Equation for Nanoscale Solids-cont'd

Following the similar procedure in the derivation of heat conduction equation for macroscale solids, using the modified Fourier law of heat conduction, we will get the following equation for heat conduction in nanoscale solids:

$$\frac{\partial}{\partial x}k_x\left(\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}k_y\left(\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}k_z\left(\frac{\partial T}{\partial z}\right)=\frac{1}{\alpha}\frac{\partial T}{\partial t}+\frac{\tau}{\alpha}\frac{\partial^2 T}{\partial t^2}$$

In this equation, the thermal diffusivity, $\alpha = \alpha(k_x,k_y,k_z,c_x,c_y,c_z)$, in which c_x, c_y, and c_z are specific heats of the material in x-, y- and z-direction respectively.

The relaxation time: $\tau = \frac{\lambda}{v}$

with λ = average mean free path, and V = average velocity of heat carrier (i.e. phonon or electrons)

We may find that $\tau \approx 10^{-10}\ \sec onds\ \ for\ semiconductors$

Such a small value is insignificant in heat conduction analysis in macroscale Solids.

The Heat Conduction Equation for Nanoscale Solids-cont'd

The variation of thermophysical properties of materials in x-, y- and z-directions is induced by the variation of MFP and MFT of energy carrier of phonons in these directions.

We have shown the difference of thermal conductivity k in the normal (z-direction) and the plane direction (x- or y-direction) of a thin silicon film before.

Variation of thermal diffusivity α is another property that vary with directions.

Measurements of thermophysical material properties of nanoscale solids thus present major challenges to research community in nanotechnology, and design engineers.

Concluding Remarks

Almost all miniature electromechanical devices encounter serious over heating problems. Over heating is a major stumbling block of nanoscale engineering such as molecular electronics.

Excessive heating is detrimental to reliability of devices in:
(1) Drastic deterioration of material strength,
(2) Develop excessive thermal stress, leading to structure failure, and
(3) Develop significant thermal distortion, leading to malfunctioning of the device.

It is thus imperative that engineers having reliable analytical models when are involved in the design of micro and nanoscale devices.

Properly derived heat conduction equation with reliable material properties will provide engineers with such tool.

The solution of this equation will enable engineers to assess the temperature variations within the thin films, and thereby accurately assess the induced **thermal stresses** distribution for strength, and **thermal strain** for dimensional stability.

Concluding Remarks-Cont'd

The heat conduction equation for nanoscale solids are applicable to thin films that are common in many concurrent high tech devices and many of these thin films are subjected to change of thermal environments.

The solution of this equation requires the availability of thermo-physical properties of thin film materials of k and α, as well as accounting for the wave motion of the energy carriers of phonons and electrons.

Nanoscale metrology is thus an emerging challenging technology for engineers.

Part 4

Measurements of Thermal Conductivity of Thin Films

November 28, 2006

Overview

Thermal conductivity k of a material is a measure of how well it can conduct heat.

Metals are better heat conductors than semiconductors and insulators.

Thermal conductivity is considered to be a material property of solids in macroscale in moderate temperature ranges.

For solids of nanoscale, k is size-dependent.

Database of k of nanoscale materials, e.g. thin films is thus of critical importance for performance and structural design analyses.

Credible measurement techniques for k of semiconductors and insulators has become a major R&D activity of nanotechnology.

Principle of k- Measurements

Thermal conductivity of solids k is usually determined by measuring the temperature gradient produced by a steady flow of heat in a one-dimensional geometry.

Reliable and accurate measurements of k rely on the one-dimensional heat flow.

Theoretical Background

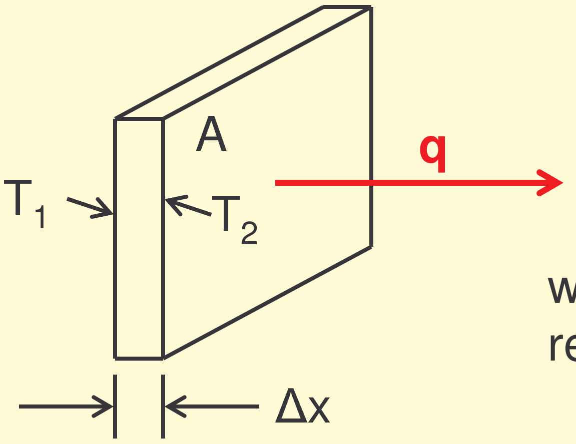
Heat conduction in solids is governed by
Fourier law of heat conduction:

$$q_x = -kA \frac{\partial T(x,y,z)}{\partial x}$$

where q_x = heat conduction rate, BTU/h, or Watt
A = area through which the heat is transferred, ft^2 or m^2
k = thermal conductivity of the material, BTU/h-ft-^{o}F or W/m-^{o}C

$\frac{\partial T}{\partial x}$ = Temperature gradient in the direction of heat flow, ^{o}F/ft or ^{o}C/m

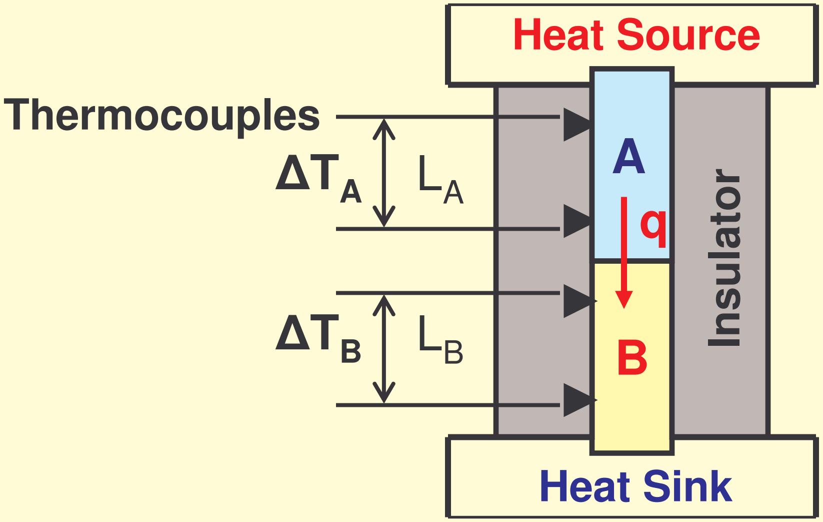
Measurement of k may be conducted on a flat slab:



$$k = \frac{q\,\Delta x}{A(T_1 - T_2)}$$

where T_1 and T_2 are temperature of the rear and front surfaces respectively

Measurement of k of Conductors, e.g. Metals



Two metal rod samples:

Sample A with known k_A

Sample B with K_B to be determined.

From Fourier law of heat conduction: $q = \dfrac{k_A\, A_A\, \Delta T_A}{L_A} = \dfrac{k_B\, A_B\, \Delta T_B}{L_B}$

where $A_A = A_B$ = cross-section of the Sample A and B.
$L_A = L_B$ = the distances between thermocouples in
Sample A and B
$\Delta T_A, \Delta T_B$ = measured temperature differences in
Sample A and B respectively.

Hence the thermal conductivity of Sample B is determined by:

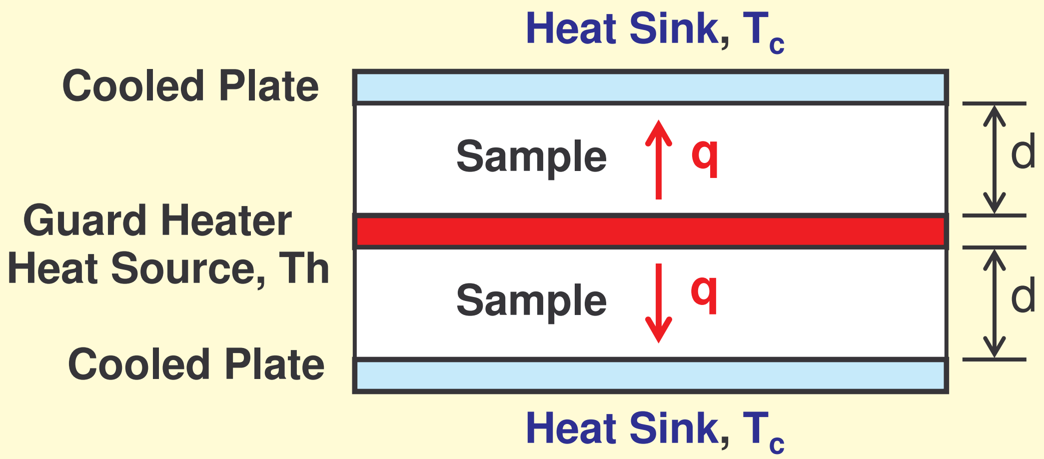
$$k_B = \frac{\Delta T_A}{\Delta T_B} k_A$$

Measurement of k of Semiconductors and Insulators

These materials typically have low k-value.
Maintaining one-dimensional flow of heat in the samples is a major issue.

Measurement set-up requires strict control of temperatures in both heat source (guard hot plate) T_h and heat sink T_c.

One-dimensional heat flow is ensured by the difference of T_h and T_c.



The thermal conductivity of the samples $k = \frac{d}{A(T_h - T_c)} q$

where A = cross-sectional area for heat flow; q = heat output of the heater

Measurement of k of Semiconductors or Insulators in Sub-micrometer and Nanometer Scale

Major issues

- These materials have low k-values. Consequently, require high precision measurement techniques with high resolutions.
- Samples are normally thin and small in size. Proper positioning and stationing in the fixture are difficult.
- Being thin in sample size (e.g. silicon wafers), it is not possible to ensuring one- dimensional heat flow.
- The temperature gradient along the sample thickness is too small to be measurable.
- There is no place for thermocouples in the samples.

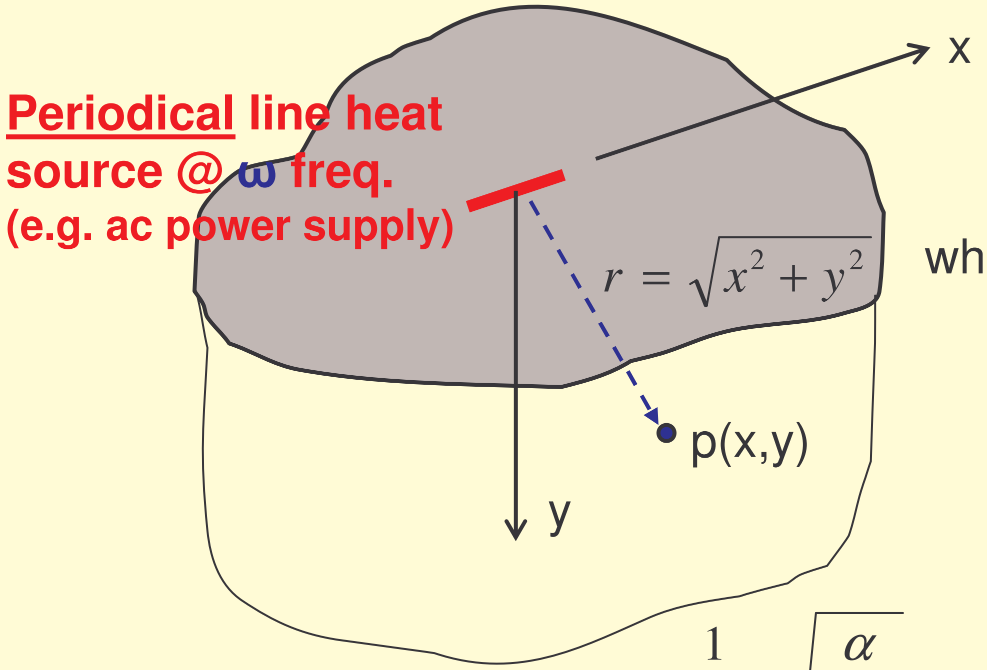
Two Principal Techniques for Measurements of k in Thin Films of Semiconductors and Insulators

- The 3 – Omega Method
- Scanning Thermal Microscope

The 3-Omega Method for Semiconductors and Dielectric Materials

Theoretical basis of 3-Omega method [Cahill 1990]:

Temperature distribution of a semi-infinite solid induced by a finite line heat source [Carslaw and Jaeger 1959]



The temperature rise at point P inside the half-volume is:

$$\Delta T(r) = \frac{1}{\pi k}\left(\frac{P}{L}\right) K_o(qr)$$

where P = the amplitude of the power generated at a angular frequency ω in the line source.

L = length of the line heat source

k = thermal conductivity of the solid

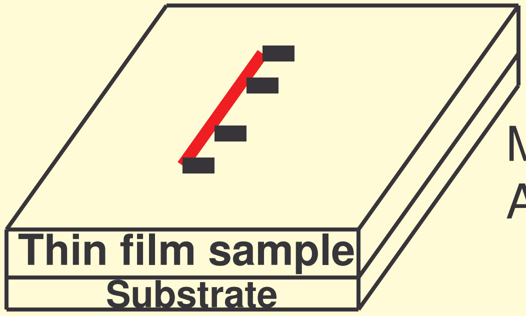
$K_o(r)$ = Modified Bessel function of second kind at zeroth order

$$\frac{1}{q} = \sqrt{\frac{\alpha}{i2\omega}}$$

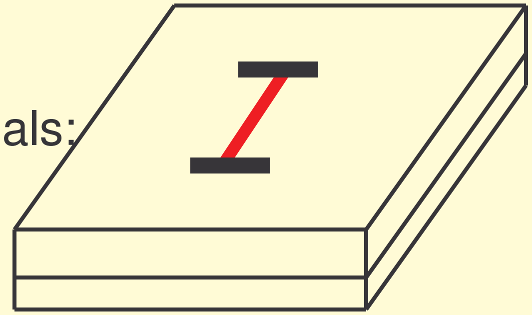
= wavelength of the diffusive thermal wave with α to be the diffusivity of the solid

The thermal conductivity k may be calculated from the measured temperature rise as shown above

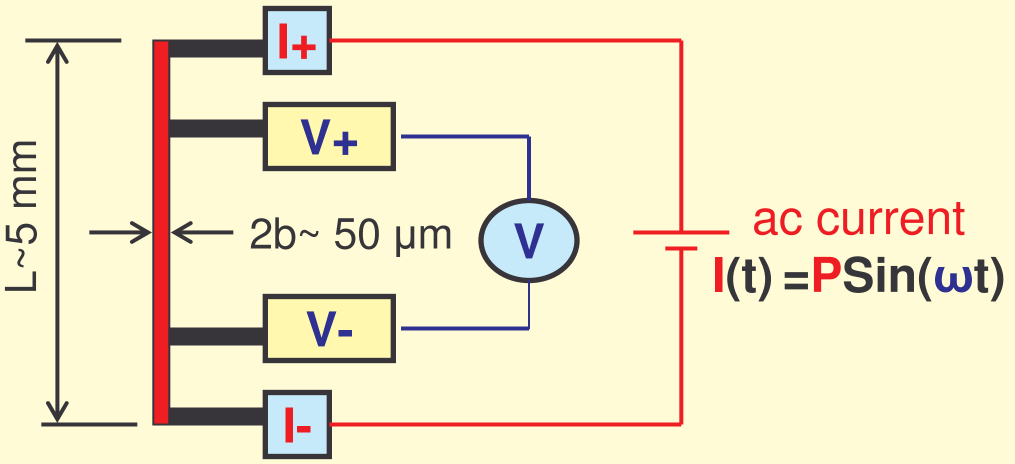
The 3-Omega Method –
Experimental Set-up



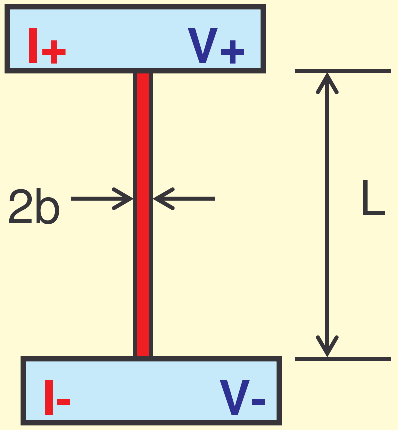
Metal line materials:
Au, Ag, Pt, etc.



Metal line by photolithography:



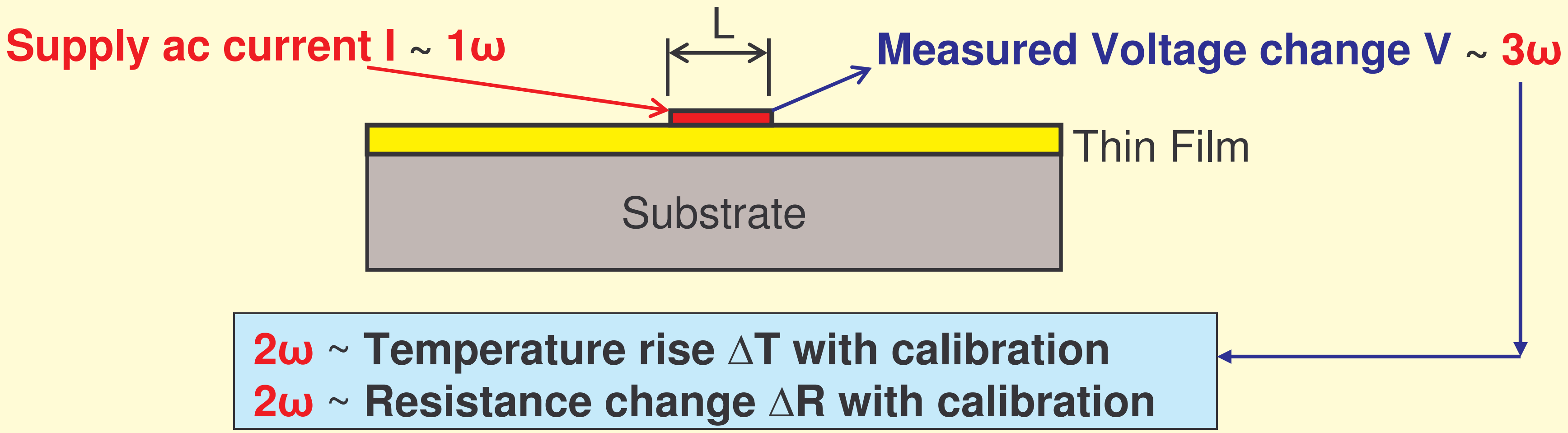
Metal line by evaporation:



- **Supply current I ~ 1ω**
- **Temperature rise T ~ I^2 ~ <u>2ω</u>**
- **Resistance in metal line R ~ T ~ 2ω**
- **<u>Measured</u> voltage output V ~ IR ~ 3ω**

The 3-Omega Method

k-Measurements



2ω ~ **Temperature rise ΔT with calibration**

2ω ~ **Resistance change ΔR with calibration**

The thermal conductivity of the thin film is:

$$k = \frac{V^3 \, \ell n\left(\frac{\omega_2}{\omega_1}\right)}{4\pi L R^2 \left(V_{3,1} - V_{3,2}\right)} \frac{\Delta R \; (\leftrightarrow 2\omega)}{\Delta T \; (\leftrightarrow 2\omega)}$$

ω_1, ω_2 = Measurements with two angular frequencies of supply current
R = resistance in the line heat source
V = voltage across metal line at ω
$V_{3,1}$ and $V_{3,2}$ = measured voltages across the heater @ 3ω
with ω_1 and ω_2 power supplies respectively.

Thermal Microscopy of Micro-Nano Devices

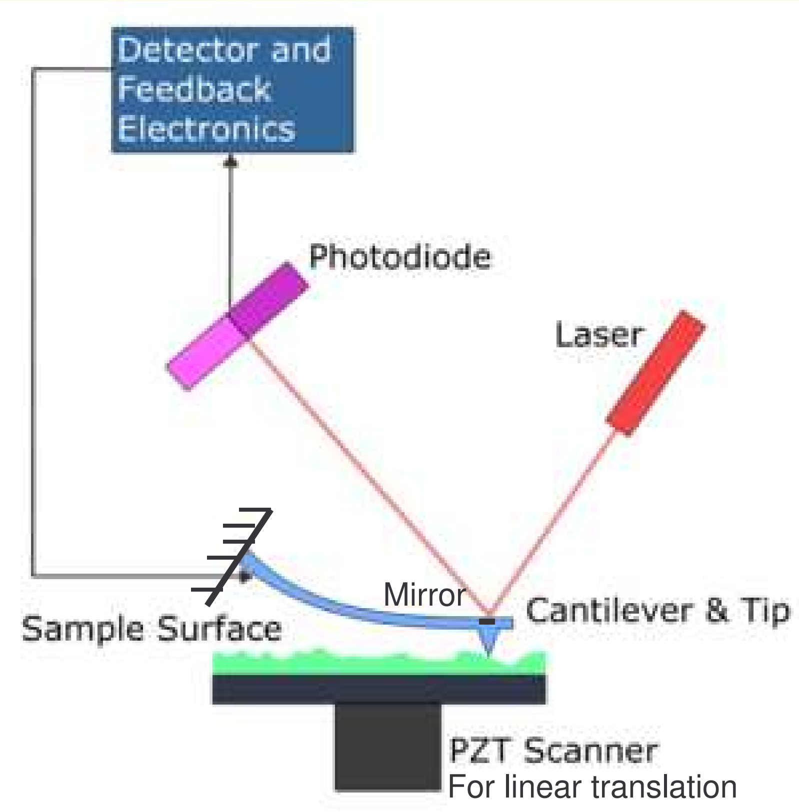
Techniques	Spatial Resolution
Infrared thermometry	1-10 µm
Laser Surface Reflectance	1 µm
Raman Spectroscopy	1 µm
Liquid Crystals	1 µm
Near-Field Optical Thermometry	< 1 µm
Scanning Thermal Microscopy	< 100 nm (= 0.1 µm)

Scanning Thermal Microscope

- For measuring k for thin films in the thickness range of 10 nm to 10 µm.
- The method is based on heated tip that scan across the surface of the sample.
- The heat flowing into sample is correlated to local thermal conductivity of the sample.
- Modified version of scanning thermal microscope – called thermoreflectance thermometry can measure k of thin films in both normal and lateral directions.
- Atomic force microscope (AFM), laser beam, photo- and thermal sensors are major components in this type of measurement systems.

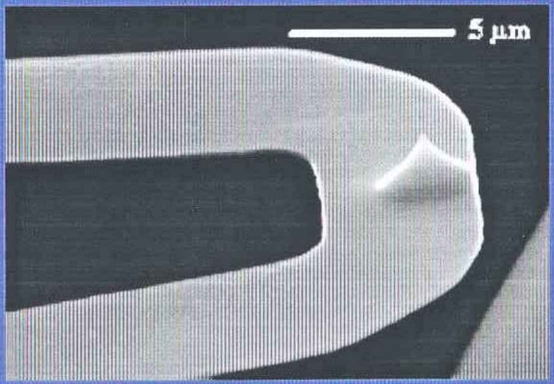
Atomic Force Microscope (AFM)

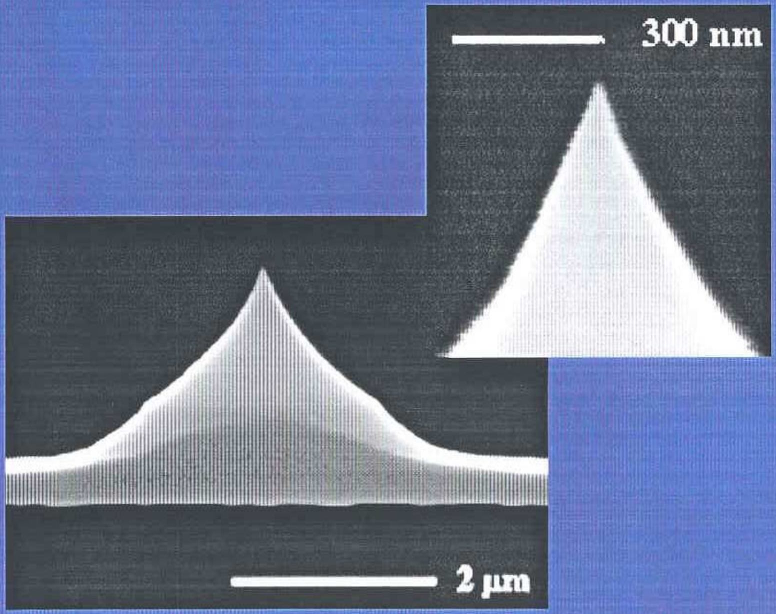
- The **AFM** consists of a microscale cantilever with a sharp tip (probe)
- Its end is used to scan the specimen surface.
- The cantilever is typically silicon or silicon nitride with a tip radius of curvature on the order of nanometers.
- When the tip is brought into proximity of a sample surface, forces between the tip and the sample lead to a deflection of the cantilever by Hooke’s law
- Depending on the situation, forces that are measured in AFM include:
    - mechanical contact force,
    - Van der Waals forces, capillary forces,
    - chemical bonding, electrostatic forces,
    - magnetic forces,etc.
- Typically, the deflection is measured using a laser spot reflected from the top of the cantilever into an array of photodiodes.



For linear translation of sample in x-, y- and Z-direction

Tip Characteristics





Tip Height: ~1.7µm

Tip Height Homogeneity in an Array: ± 50 nm (± 0.5%)

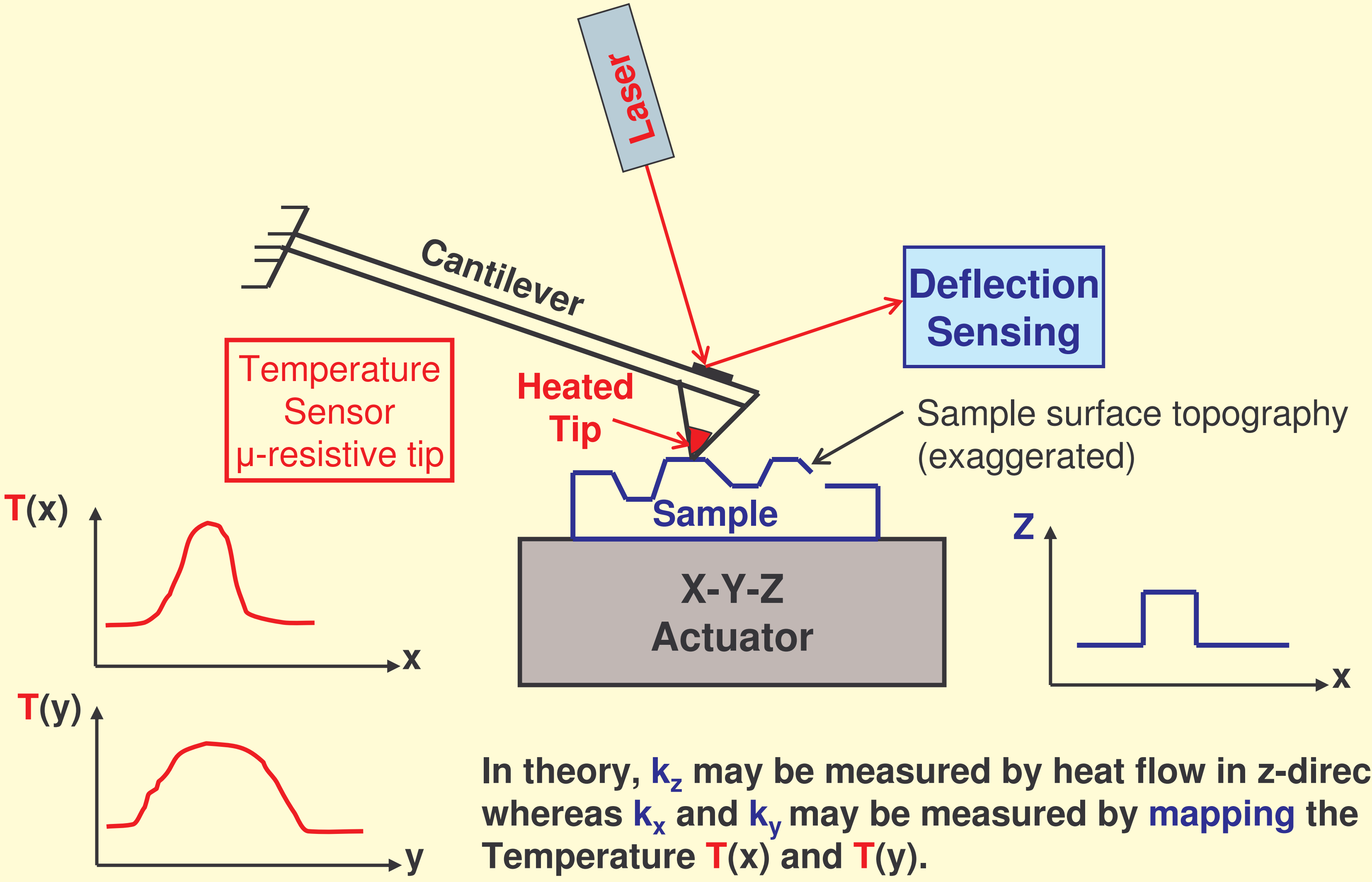
Tip Radius: <20 nm

IBM

Zurich Research Laboratory
Micro- and Nanomechanics Team

Major Components of Scanning Thermal Microscope

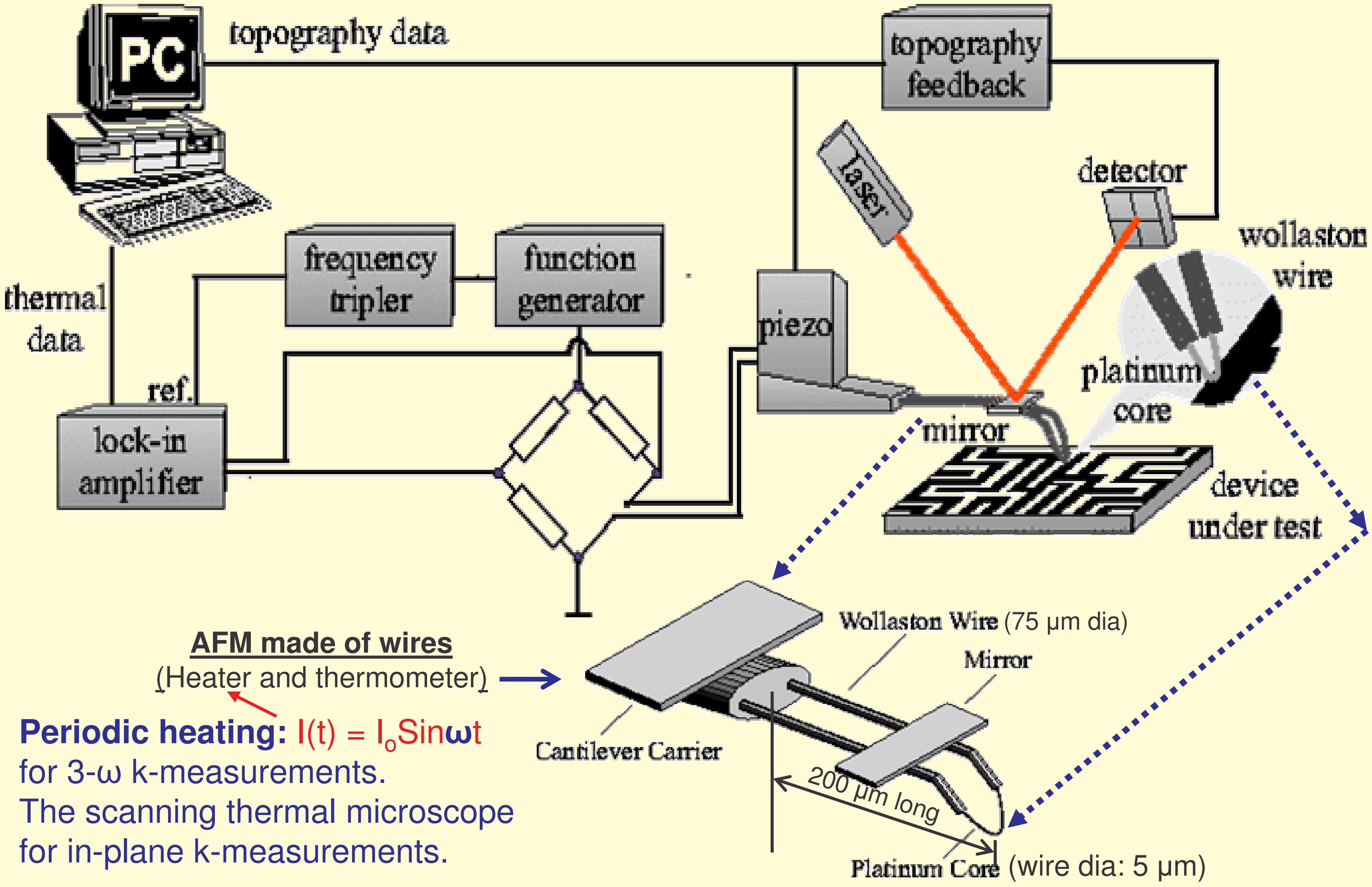
AFM + **Thermal Probe**



In theory, k_z may be measured by heat flow in z-direction whereas k_x and k_y may be measured by **mapping** the Temperature T(x) and T(y).

Measurement of k of Thin Film Using 3-Omega Method and Scanning Thermal Microscope

Fiege, G.B.M, Altes, A., Heiderhoff and Balk, L.J. "Quantative thermal Conductivity Measurements with Nano Resolution," J. Physics D: Applied Physics, vol. 32, No. 5, 1999.

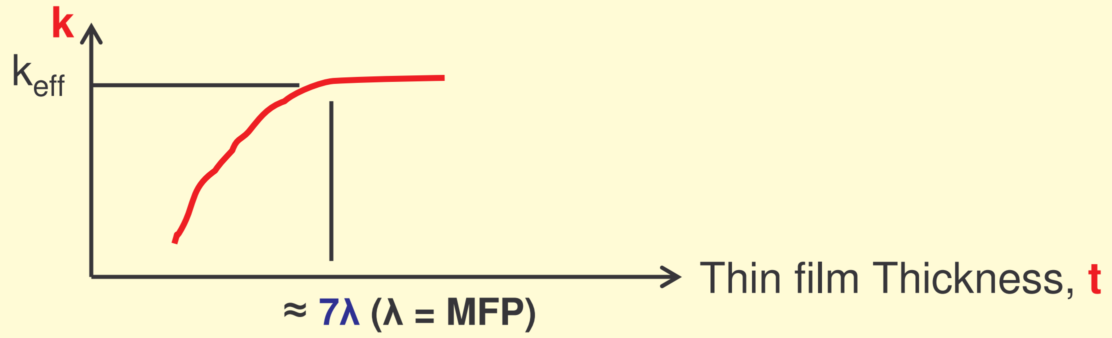


AFM made of wires
(Heater and thermometer) →

Periodic heating: $I(t) = I_o \mathrm{Sin}\omega t$
for 3-ω k-measurements.
The scanning thermal microscope
for in-plane k-measurements.

SUMMARY

- Thermal conductivity is an important material characteristic in micro and nanoscale device design.
- Heat transmission in matter rely on the traveling of energy carriers, such as phonons, electrons and photons.
- The ability of conducting heat by matter, i.e. thermal conductivity, depends on how free these energy carriers can travel in the matter.
- Thermal conductivity of matter k, depends on the size of the matter:



- Measurements of k for thin films presents a major challenge to engineers.

- Two principal methods for measuring k of thin films are:
  - The 3-Omega method using periodic line heat source, and
  - Scanning thermal microscope using scanning AFM with heated contact tips.

- Combined 3-Omega method and scanning thermal microscopy was used to measure the k-values of thin films of 30 nm thick in both normal and lateral directions.