



DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY SRM INSTITUTE OF SCIENCE AND TECHNOLOGY

21PYB102J –Semiconductor Physics and Computational Methods

MODULE 5

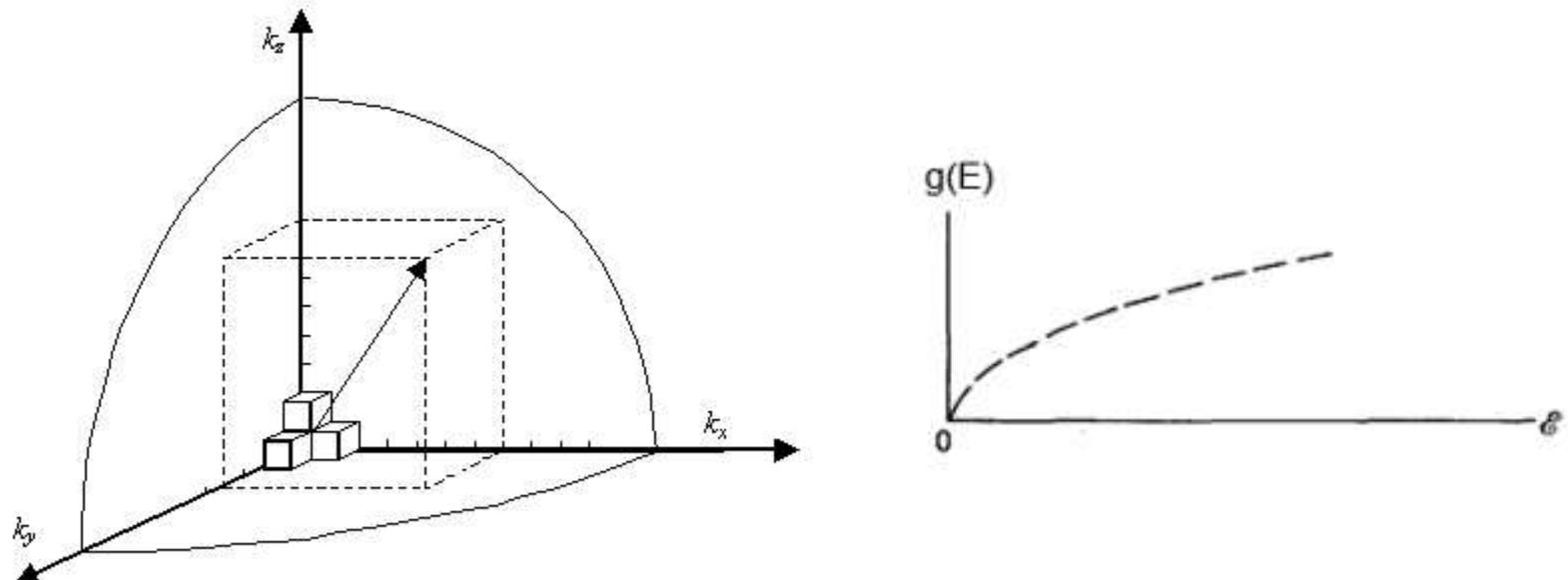
Density of states in 2D, 1D and 0D

Density of States

- The density of states function describes the number of energy states that are available in a system and is essential for determine the carrier concentrations and energy distributions of carriers within a semiconductor.
- In semiconductors, the free motion of carriers is limited to two, one and zero spatial dimensions. When applying semiconductor statistics to systems of these dimensions, the density of states in quantum well (2D), quantum wires (1D) and quantum dots (0D) must be known.

Density of states in 3D (Bulk Material)

The **density of states** is defined as the number of allowed electronic energy states per unit energy range per unit volume of the material.



$$g(E) = \frac{1}{V} \frac{dN}{dE} = \left(\frac{8\pi\sqrt{2}m^{3/2}}{h^3} \right) \sqrt{E}$$

Density of states in lower-dimensional systems

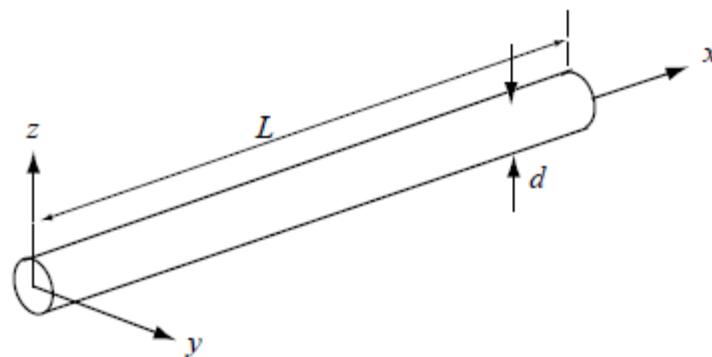
- Three-dimensional electron or hole obtained by doping semiconductors are not ideal for studying quantum effects for two reasons: (i) they are strongly disordered owing to the background of ionized impurities and (ii) the most quantum effects are more pronounced in lower-dimensional systems than those of bulk constituents.
- Therefore, reduction in the dimensionality of a physical system has profound consequences on its profile and new types of electronic and photonic devices can be designed. These devices make use of electron motion through potentials that change rapidly on a length scale comparable to the wavelength associated with the electron and they operate on the rules of quantum mechanics.
- The low dimensional semiconductor systems play a critical role in determining the properties of materials due to the different ways that electrons interact in two-dimensional, one-dimensional and zero-dimensional structures.

Density of states in lower-dimensional systems

- A low-dimensional system is one where the motion of microscopic degrees-of-freedom, such as electrons, phonons or photons, is restricted from exploring the full three dimensions of the present world.
- In the low dimensional quantum systems such as Quantum well, Quantum wire and Quantum dot, the charge carriers are free to move in two, one and zero dimensions respectively.
- This high confinement brings out new effects of great technological potential applications. Quantum mechanics plays a major role as the semiconductor size approaches the nanoscale.
- The main advantages of these low dimensional semiconductor systems are in the realizations of important devices, like the double heterostructure lasers with low threshold at room temperature, high effective LEDs, bipolar transistors, p-n-p-n switching devices, high electron mobility transistors (HEMT) and many other optoelectronic devices.

Density of states in 1D

- Quantum effects in systems which confine electrons to regions comparable to their de Broglie wavelength. When such confinement occurs in two dimensions only (say, by two restrictions on the motion of the electron in the z- and y-directions), with free motion in the x-direction, a one-dimensional system is created.



Density of states in 1D

- Consider a systems where electrons are free to move in one direction and confined in the other two directions (Quantum wire).
- In one dimension two of the k -components are fixed, therefore the area of k -space becomes a length and the area of the annulus becomes a line.

Density of States in 1D

- For a 1D box of width L eigenenergies are given by

$$E_n = n^2 E_1 \quad (1)$$

where E_1 is given by

$$E_1 = \frac{h^2}{8mL^2}$$

- The **density of states** defined so that $g(E)dE$ gives the number of energy states in the interval E and $E+dE$ per unit volume

Density of States in 1D

$$g_1(E) = \frac{1}{L} \frac{dn}{dE}$$

Here the subscript 1 denotes one dimension.

Using Eq (1), we can find

$$g_1(E) = \frac{\sqrt{2m}}{h} \frac{1}{\sqrt{E}}$$

We need to multiply the above expression by a factor of 2 because in each state n , two electrons, one with spin-up and one with spin-down can be accommodated.

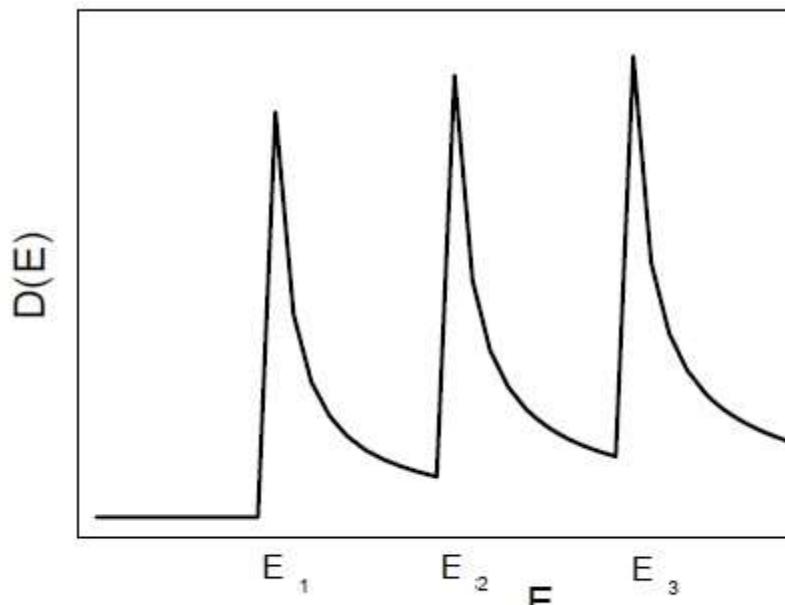
Density of States in 1D

Hence the final expression for density of state in 1D is given by

$$g_1(E) = \frac{2\sqrt{2m}}{h} \frac{1}{\sqrt{E}}$$

- Thus for an electron confined to 1D box, the density of states is a decreasing function of E and vanishes in the limit of large energy.

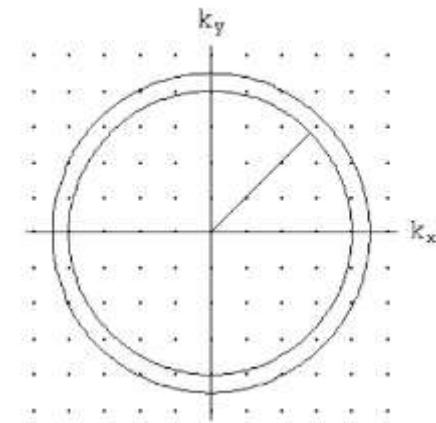
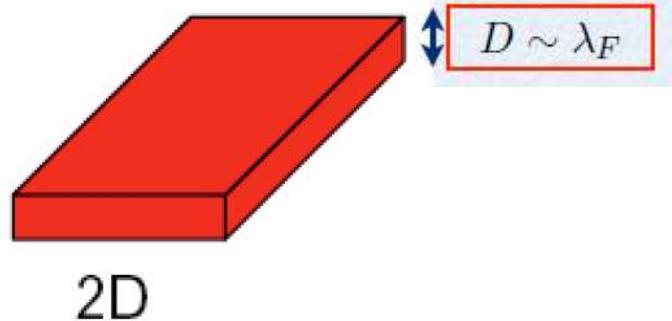
Density of states in 1D



Density of states of a 1D system.

Density of states in 2D

- Quantum effects arise in systems which confine electrons to regions comparable to their de Broglie wavelength. When such confinement occurs in one dimension only (say, by a restriction on the motion of the electron in the z-direction), with free motion in the x- and y-directions, a two-dimensional system is created.
- Consider a slab of material that has macroscopic dimensions in the x- and y directions while the thickness is small (in the nanometer range-Quantum Well).

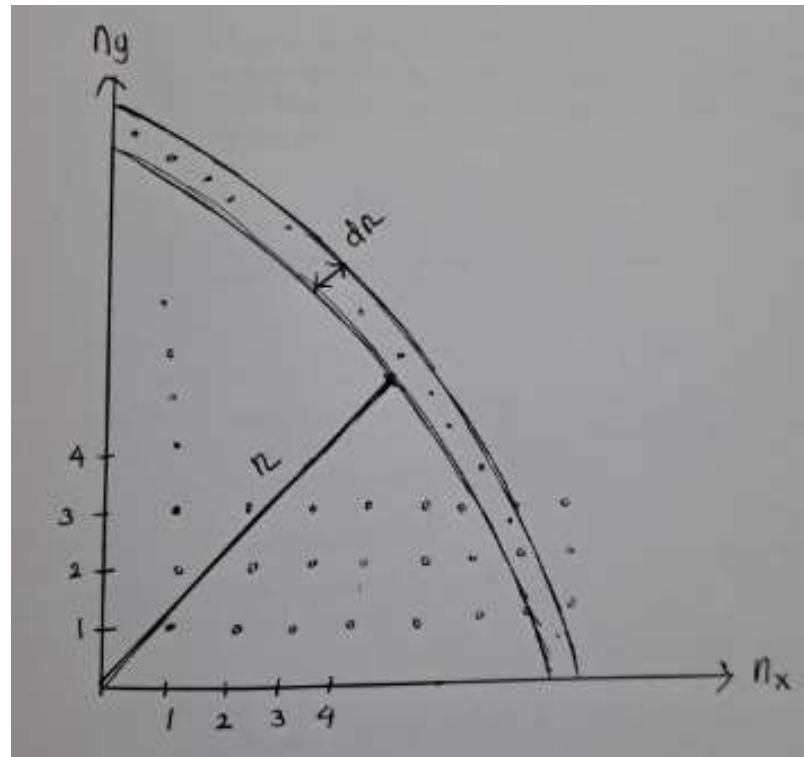


Density of states in 2D

The two-dimensional square-box has energy eigenvalue equation

$$E_{n_1, n_2} = E_1(n_1^2 + n_2^2) \quad (2)$$

It follows that in Cartesian $n_1 n_2$ space, there is an energy eigenstate at every point (n_1, n_2) of this space (Fig)



Density of states in 2D

Let

$$n = \sqrt{n_1^2 + n_2^2}$$

denote the radius vector in this space. The area of this strip is given by

$$dA = \frac{1}{4} 2\pi n dn$$

The factor (1/4) is necessary since the quantum numbers n_1 and n_2 can only take positive values.

Since each quantum state occupies one unit of area in $n_1 n_2$ space, the number of states available in the strip dN is equal to dA .

$$dN = \frac{1}{2} \pi n dn$$

We need to multiply the above expression by a factor of 2 because in each state , two electrons, one with spin-up and one with spin-down can be accommodated.

$$dN = \pi n dn \quad (3)$$

Density of states in 2D

Eq (2) can be written as

$$E = n^2 E_1$$

Taking differential on both sides we can find that

$$ndn = dE/2E_1$$

Substituting the above expression in Eq (3), we get

$$\frac{dN}{dE} = \frac{\pi}{2E_1} = \frac{4\pi m L^2}{h^2}$$

The density of states in two dimension is defined as

$$g_2(E) = \frac{1}{L^2} \frac{dN}{dE}$$

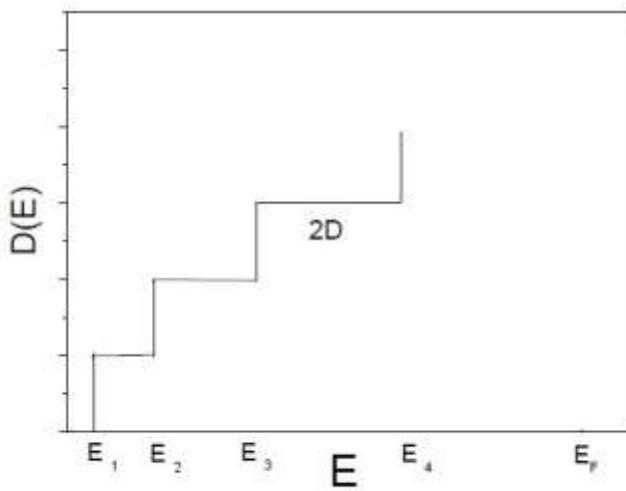
Hence

$$g_2(E) = \frac{4\pi m}{h^2}$$

In two-dimensions, the density of states is a constant, independent of energy. 15

Density of states in 2D

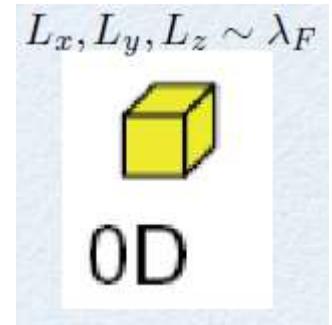
- It is important to notice that the 2D density of states is independent of the energy. However, DOS depends on the number of levels and is thus a sum of the contributions from the discrete levels appearing as a result of the quantization.



Density of states for a 2D system.

Density of states in 0D

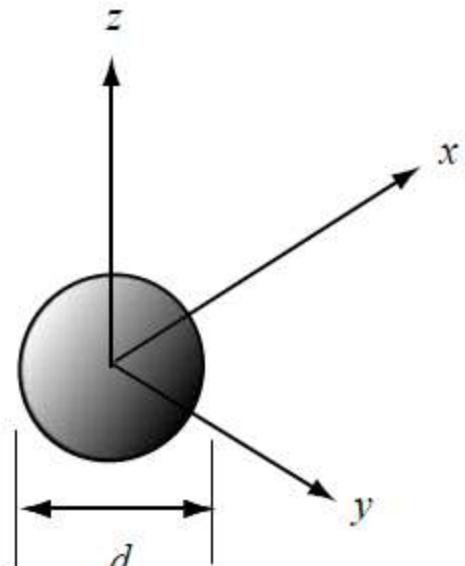
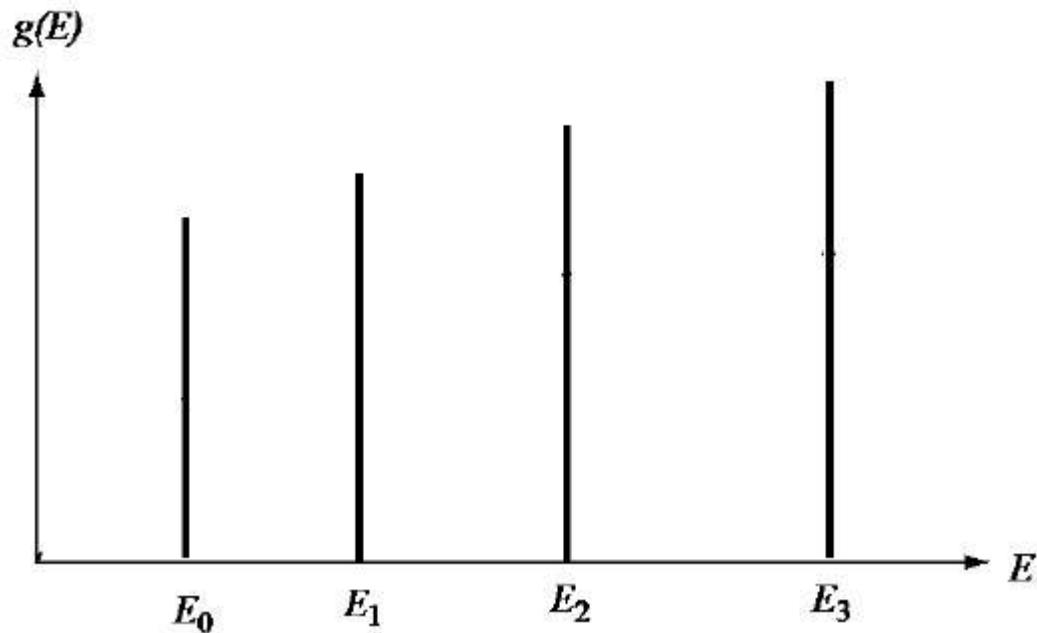
- Electrons can be confined in all three dimensions in a dot. The situation is analogous to that of a hydrogen atom: only discrete energy levels are possible for electrons trapped by such a zero-dimensional potential. The spacing of these levels depends on the precise shape of the potential.
- When considering the density of states for a 0D structure (Quantum dot), no k – space is available as all dimensions are reduced.



Density of states in 0D

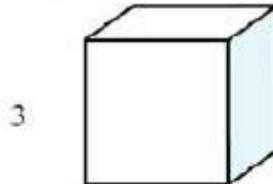
- Therefore DOS of 0D can be expressed as a delta function

$$g(E)_{0D} = 2\delta(E - E_c)$$

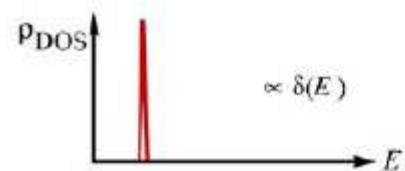
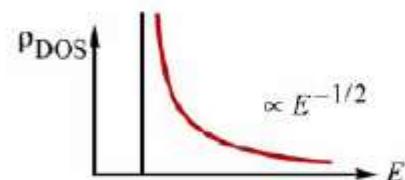
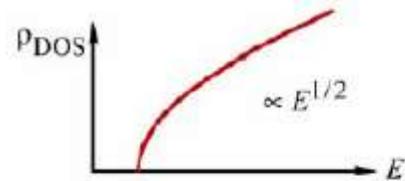


Conclusion

Degrees of freedom



Density of states





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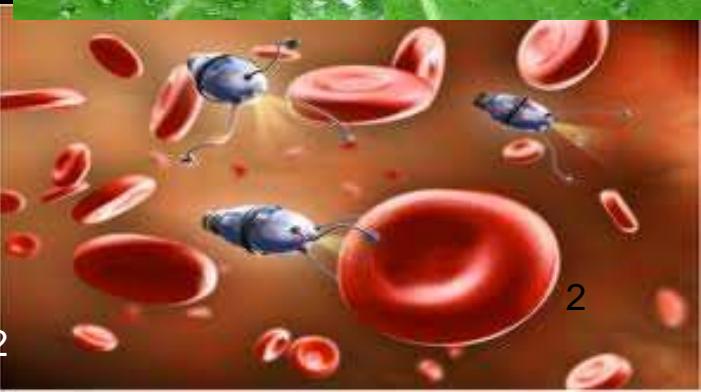
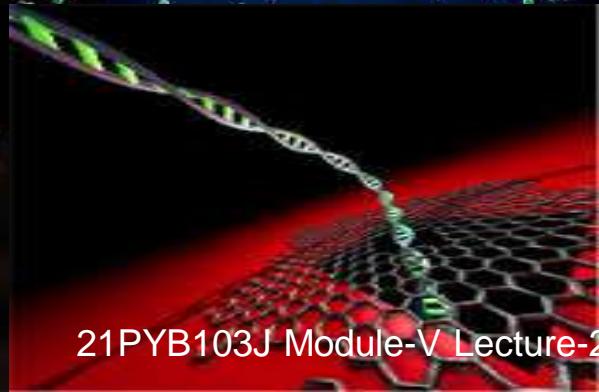
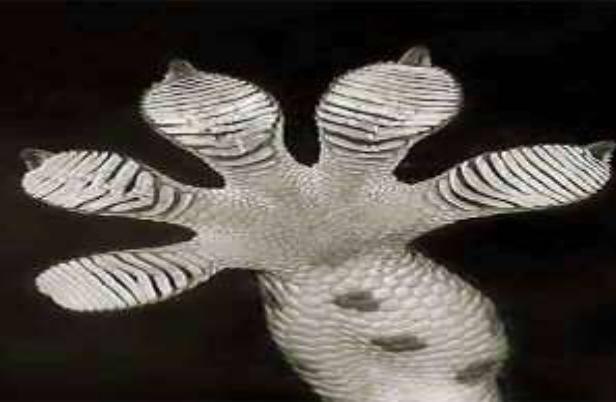
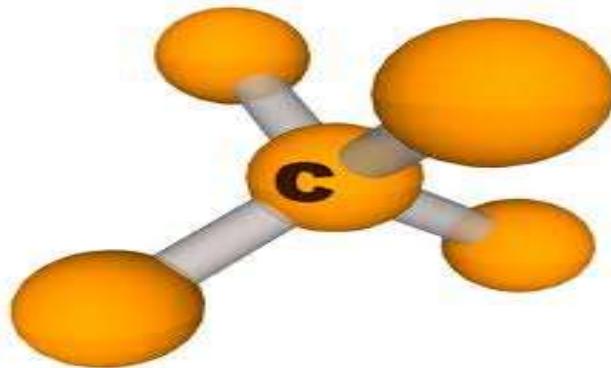
21PYB103J –Semiconductor Physics and Computational methods

MODULE 5 Lecture – 50

**Introduction to Low dimensional systems
Quantum Well, Wire, Dot**

Nanoscience & Nanotechnology

What is happening at a very, very small length scale?





"Nano": How small is that, really?



Mountain
1 km
1000 m

 $0.001 \text{ km} = 1 \text{ m}$

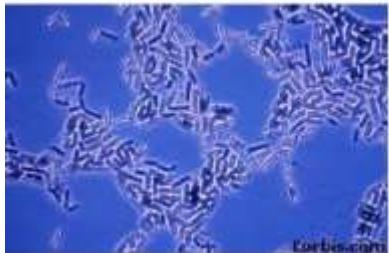


Child
1 m



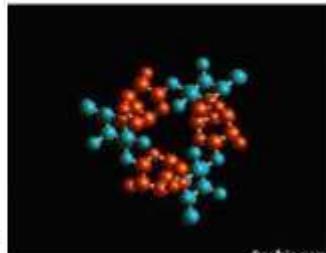
Ant
1 mm
0.001 m

 $1,000 \text{ mm} = 1 \text{ m}$



Bacteria
1 μm
0.000001 m

 $1,000,000 \mu\text{m} = 1 \text{ m}$



Sugar Molecule
1 nm
0.000000001 m

 $1,000,000,000 \text{ nm} = 1 \text{ m}$

What is Nano ?



-

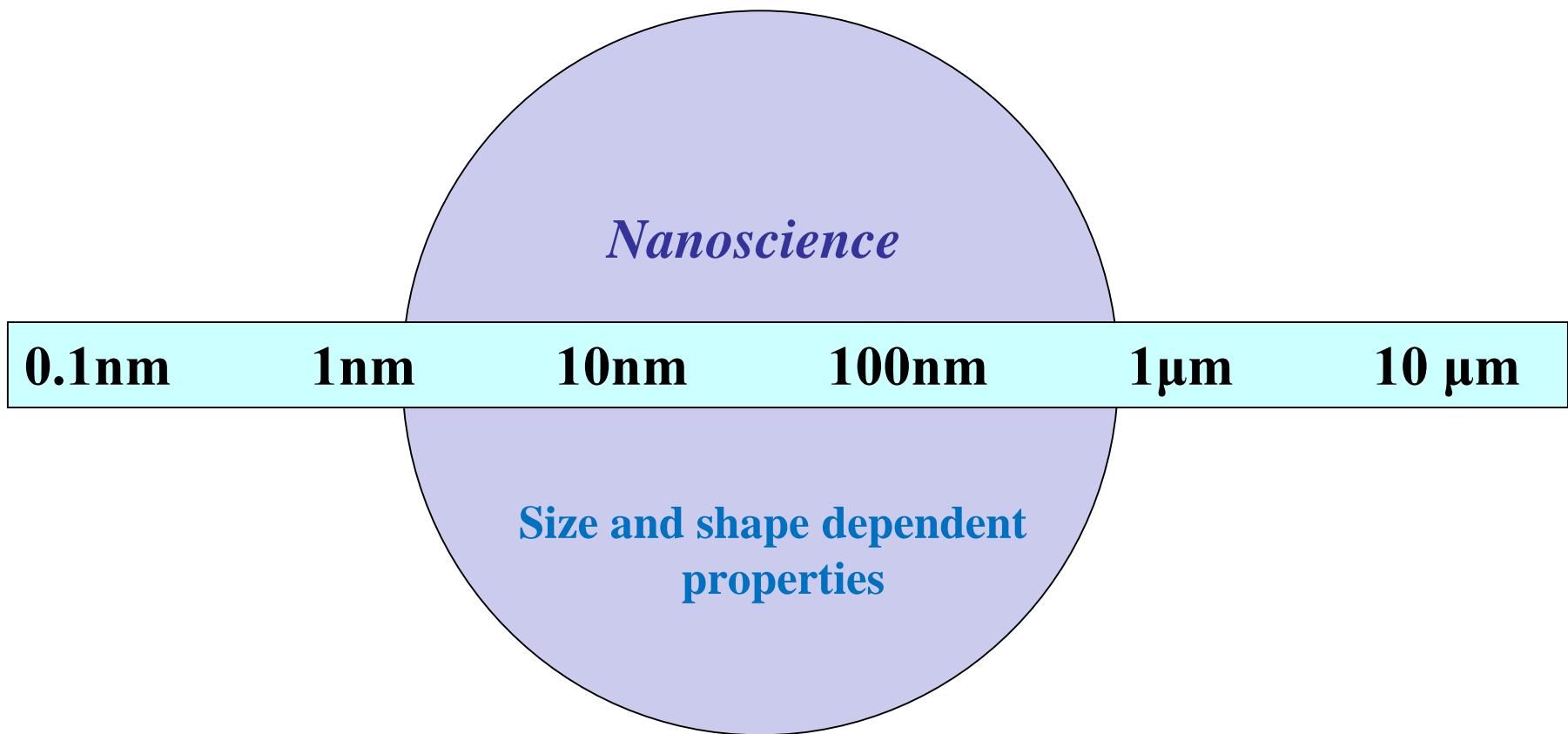
Nano - a prefix that means ***very, very, small !***

- *Question : How small is ‘Nano’ ?*

*Answer: “One billionth” of something, or
0.000000001.*

$$\frac{1}{1000000000} = 10^{-9}$$

Actual physical dimensions relevant to Nanosystem



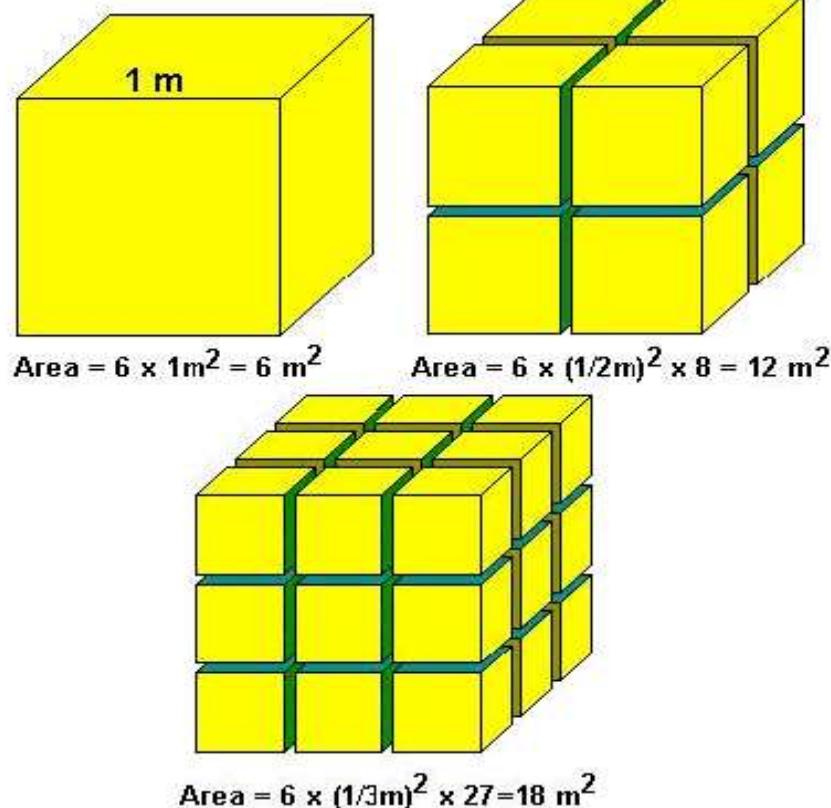
Nanometer scale : The length scale where corresponding property is size & shape dependent.

Surface to Volume Ratio

Increases

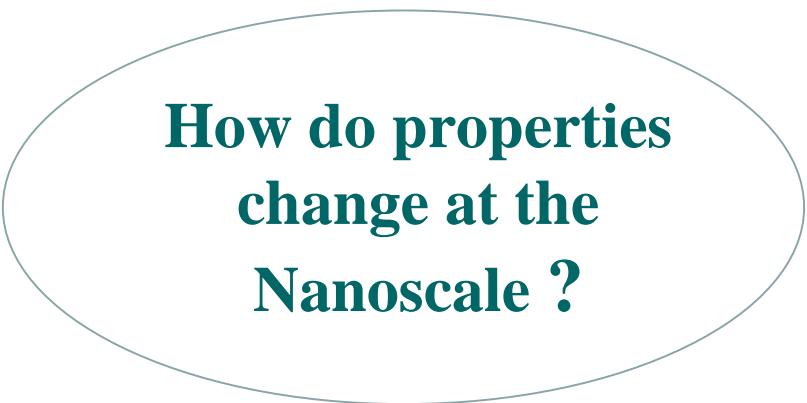
As surface to volume ratio increases

- A greater amount of a substance comes in contact with surrounding material.
- This results in better catalysts, since a greater proportion of the material is exposed for potential reaction.



What's interesting about the nanoscale?

- Nano sized particles exhibit different properties than larger particles of the same substance.
- Nano sized particle exhibit size & shape dependent properties.



**How do properties
change at the
Nanoscale ?**

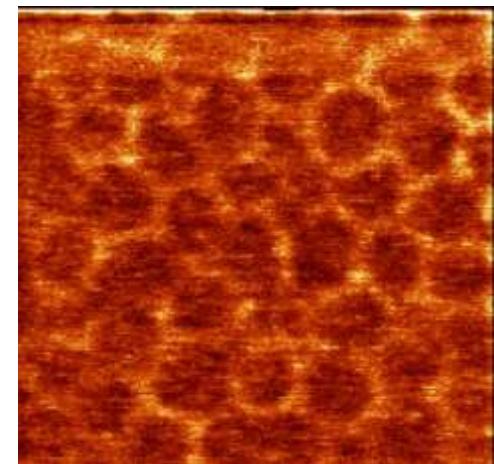
Optical Properties: Colour of Gold

- **Bulk gold**
appears **yellow** in colour.



- **Nano sized gold**
appears **red** in colour.

The particles are so small that electrons are not free to move about as in bulk gold. Because this movement is restricted, the particles react differently with light.



12 nanometer gold clusters of particles look red.

Sources:

<http://www.sharps-jewellers.co.uk/rings/images/bien-hccncsq5.jpg>
<http://www.foresight.org/Conferences/MNT7/Abstracts/Levi/>

21PYB103J Module-V Lecture-2

Nanoscience: Nanometer scale science

- A part of science that studies small stuff

So, what is ***Nano science*** ?

- It is not only Biology.
- It is not only Physics .
- It is not only Chemistry.
- It is **all sciences** that work with the very small.

➤ ***Nanoscience is not physics, chemistry, engineering or biology. It is all of them.***

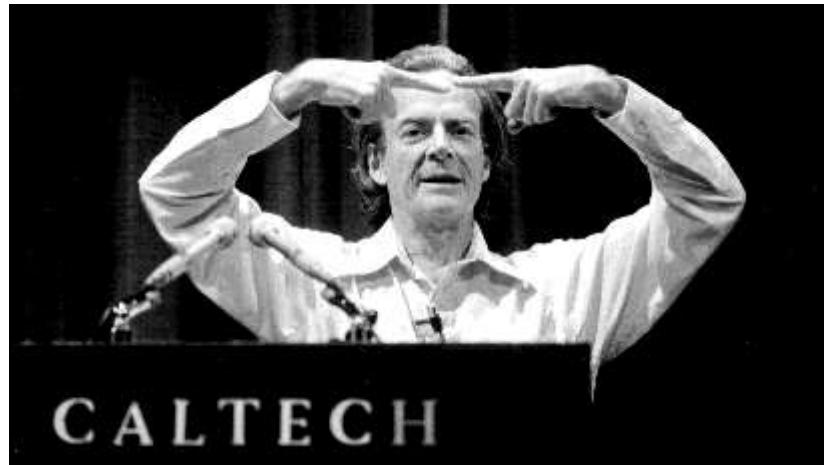
S.M. Lindsay, Introduction to Nanoscience,
Oxford University Press (2009).

Interdisciplinary

- *Physicists: physical forces between the individual atoms composing them – quantum effects*
Chemists : The interaction of different molecules is governed by chemical forces.
Biologists : creation of small devices (encoding informations in DNA to perform multitasks
Computer Scientists : Steady miniaturization : - Moore's Law and its corollaries, the phenomena whereby the price performance, speed, and capacity of almost every component of the computer.
Electrical Engineers : a steady supply of power. A control of electric signals is also vital to transistor switches and memory storage.
Mechanical Engineers: nanolevel issues such as load bearing, wear, material fatigue, and lubrication

What makes the nanoscale special?

- 1) High density of structures is possible with small size.
- 2) Physical and chemical properties can be different at the nano-scale (e.g. *electronic, optical, mechanical, thermal, chemical*).
- 3) The physical behavior of material can be different in the nano-regime because of the different ways physical properties scale with dimension (e.g. area vs. volume).



Prof. Richard Feynman
“There’s plenty of room at the bottom”

Dr. Richard P. Feynman

- *“Why cannot we write the entire 24 volumes of the Encyclopedia Britannica on the head of a pin?”*

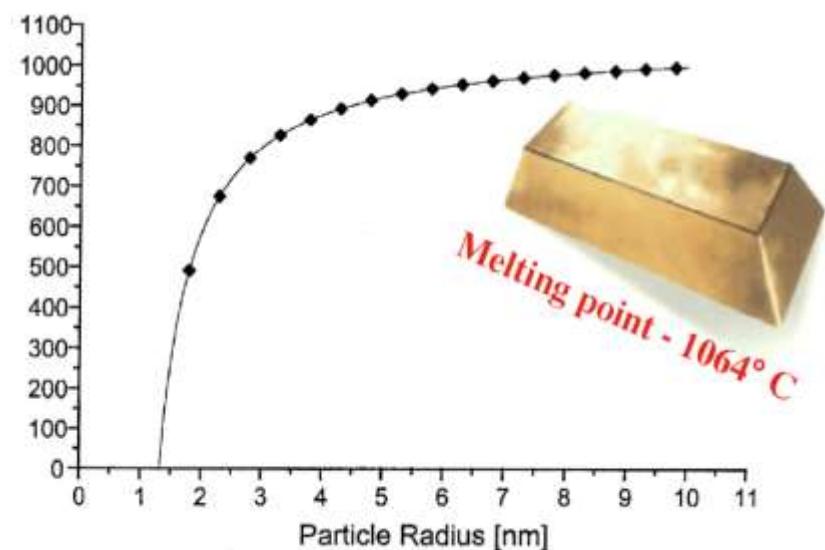
Dr. Richard Feynman, one of America's most notable physicists, 1918-1988.



Figure 1.11: Richard Feynman.

Physical/chemical properties can change as we approach the nano-scale

Melting point of gold particles



K. J. Klabunde, 2001

Fluorescence of semiconductor nanocrystals



M. Bawendi, MIT: web.mit.edu/chemistry/nanocluster
Evident, Inc.: www.evidenttech.com

By controlling nano-scale (1) composition, (2) size, and (3) shape, we can create new materials with new properties **New technologies**

The Lycurgus Cup

A Roman Nanotechnology

Reflected, transmitted



The Lycurgus Cup represents one of the outstanding achievements of the ancient glass industry. This late Roman cut glass vessel is extraordinary in several respects, firstly in the method of fabrication and the exceptional workmanship involved and secondly in terms of the unusual optical effects displayed by the glass.

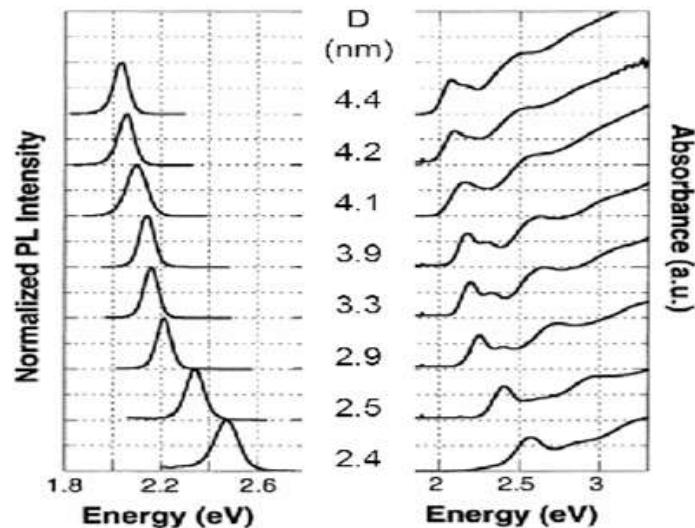
Chemical analysis showed the glass to be of the soda-lime-silica type, similar to most other Roman glass (and to modern window and bottle glass) containing in addition about 0.5% of manganese. In addition, a number of trace elements including silver and gold make up the final 1%. It was further suggested that the unique optical characteristics of the glass might be connected with the presence in the glass of colloidal gold



Optical properties of semiconductor NP

Since the promoted electron and the VB hole have opposite charges, a strong electrostatic attraction causes them to remain relatively localized within a nanometer-sized region. The exciton volume can be calculated for a given material, and the corresponding radius is known as the Bohr radius.

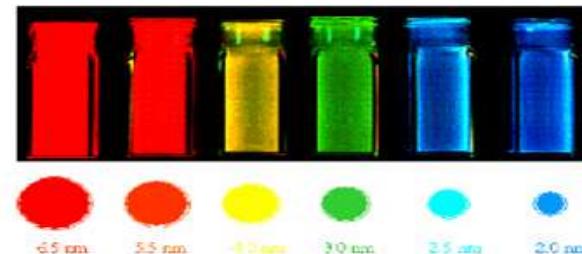
For a semiconductor particle, quantum confinement occurs when the nanocrystal radius becomes comparable to the Bohr radius. For CdSe the Bohr radius amounts to ca. 5.6 nm.



Emission and absorption spectra of CdSe nanocrystals of different sizes. The change in the emission width is due to the decrease in the nanocrystal diameter distribution with increase in diameter.



Vials of CdSe nanocrystals from NN-labs (www.nn-labs.com)



Size tunable fluorescence emission from CdSe/ZnS core shell nanocrystals synthesized by Quantum Dot Corporation (www.qdots.com). The size of the CdSe core dictates the emission wavelength through quantum confinement.

- The semiconductors like PbS, GaAs, CdS etc., can be synthesized in the nanometer level and they are called as semiconductor quantum dots. Their properties like band gap, luminescence etc., always differs from their bulk counterpart.

The quantum structures are useful in the fabrication of high efficiency solar cells, infrared detectors, quantum dot lasers etc.

- **Properties of Nanomaterials**
Unique properties

They have very high magneto resistance

They have lower melting point, high solid state phase transition pressure, lower Debye temperature and high self diffusion coefficient

They have high catalytic activity and lower ferroelectric phase transition temperature

Variation of physical properties with size

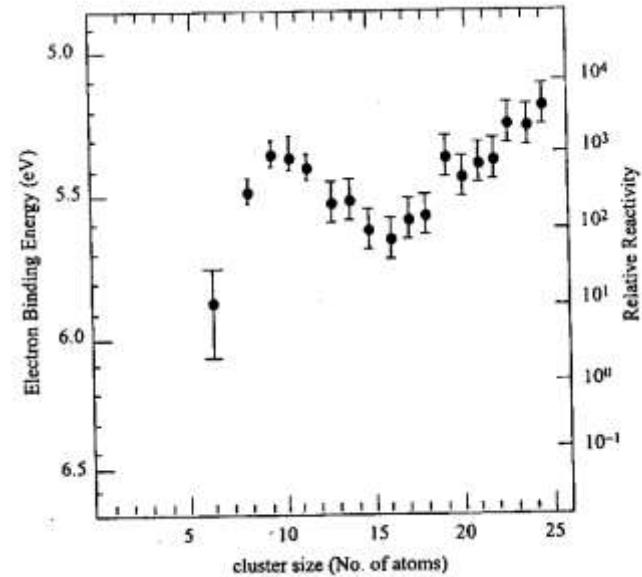
It is well established that mechanical, electrical, optical, chemical, semi conducting and magnetic properties of a material depend strongly upon the size and the arrangement of the constituent clusters or grains.

(i) Electron affinities and chemical properties

Variation in electronic properties with size occurs only when there is a variation in inter particle spacing and geometry. As the size is reduced from the bulk, the electronic bands in metals become narrower and the delocalized electronic states are transformed to more localized molecular bonds.

- Variation in electronic properties with size occurs only when there is a variation in inter particle spacing and geometry.
As the size is reduced from the bulk, the electronic bands in metals become narrower and the delocalized electronic states are transformed to more localized molecular bonds.

- Fig shows the ionization potential and reactivity of Fen clusters as a function of size.
- The ionization potential are higher at smaller sizes than at the bulk work function .
- The large surface – to – volume ratio and the variation in geometry and electronic structure have a strong effect on catalysis properties.



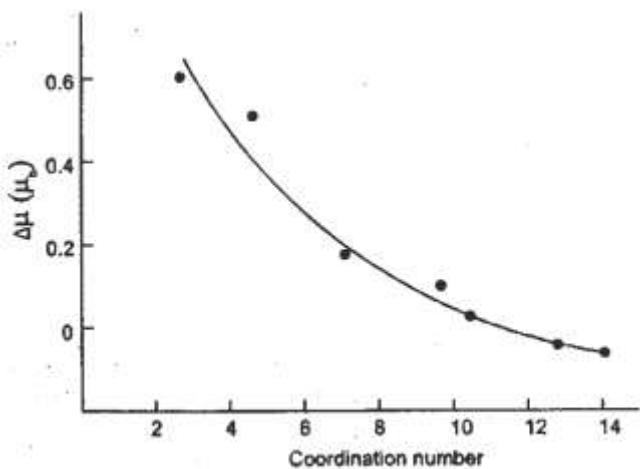
Ionization potential and reactivity of Fen clusters as a function of size

(ii) Magnetic properties

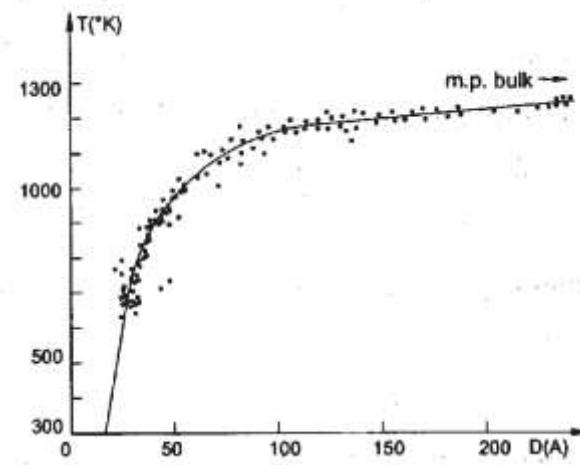
- Nano particles of magnetic and even non magnetic solids exhibit a totally new class of magnetic properties.
- Table gives an account of magnetic behavior of very small particles of various metals.
- Ferro magnetic and anti ferromagnetic multilayers have been found to exhibit *Giant Magneto Resistance (GMR)*.
- Small particles differ from the bulk in that these atoms will have lower co-ordination number.
- From the Fig, it is inferred that the small particles are more magnetic than the bulk material

Metal	Bulk	Cluster
Na, K	Paramagnetic	Ferromagnetic
Fe, Co, Ni	Ferro magnetic	Super paramagnetic
Gd, Tb	Ferromagnetic	Super paramagnetic
Rh	Paramagnetic	Ferromagnetic

Table Magnetism in bulk and in nano particles



**Change in bulk magnetic moment
versus co-ordination number**



**Melting point of gold as a function of
grain size**

(iii) Mechanical behaviour

From the Fig. it is evident that the melting point reduction is not really significant until the particle size is less than about 10nm.

- Nanophase metals with their exceptionally small grain size are found to be exceptionally strong.
- It is because clusters and grains in nanophase material are mostly free from dislocations.
- The variation of hardness with diameter of copper nano crystals is shown in Fig.
- From the Fig. it is revealed that when the grains size was **50nm** in diameter, the copper was twice as hard as usual.
- Thus the material in **nano phase** has **very high strength and super hardness**.

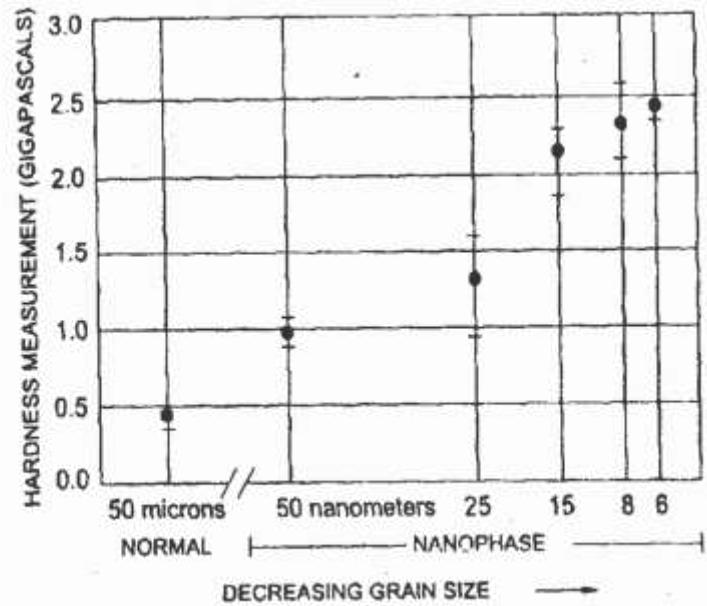
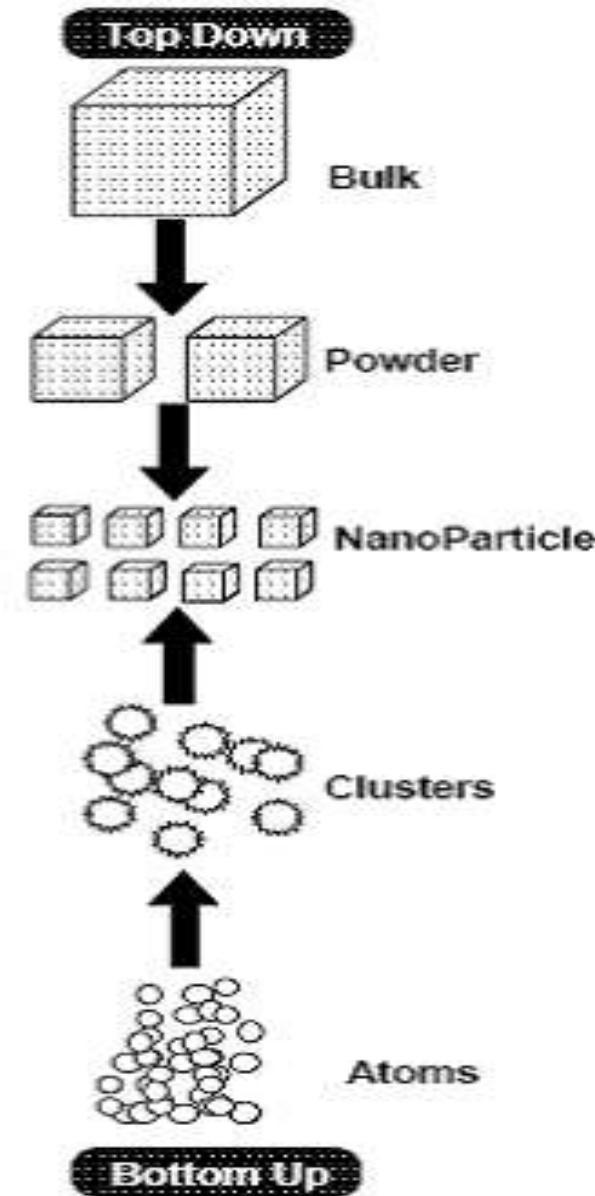


Fig. Strength of nanophase copper as a function of grain size

- The basic principles of nanotechnology is positional control.
- At the macroscopic scale, it is easy to hold parts in our hands and assemble them by properly positioning them with respect to each other.
- At the molecular scale, the idea of holding and positioning molecules is new and almost shocking.
- It is possible to continue the revolution in computer hardware right down to molecular gates and wires -- something that today's lithographic methods (used to make computer chips) could never hope to do.
- One can inexpensively make very strong and very light materials: shatterproof diamond in precisely the shapes we want, by the ton, and over fifty times lighter than steel of the same strength.
- It is possible to make surgical instruments with high precision and deftness that one could operate on the cells and even molecules from which we are made - something well beyond today's medical technology
- Nanotechnology makes almost every manufactured product faster, lighter, stronger, smarter, safer and cleaner.

- The general synthetic pathways to synthesize nanomaterials are top-down and bottom-up approach
- In the later method, chemistry plays a unique role in assembling and building up nanometric units from smaller ones.



Low-Dimensional Systems

A low-dimensional system, also called confined system, is any quantum system in which the carriers are free to move in two, one, or zero dimensions. In these systems, the spatial dimensions are of the order of the De Broglie wavelength of the carriers and therefore the carrier energy states and density of states become quantized. As a result the electronic, electrical, and optical behavior of the carriers are governed by quantum mechanical principles or mechanisms.

different techniques

Classification

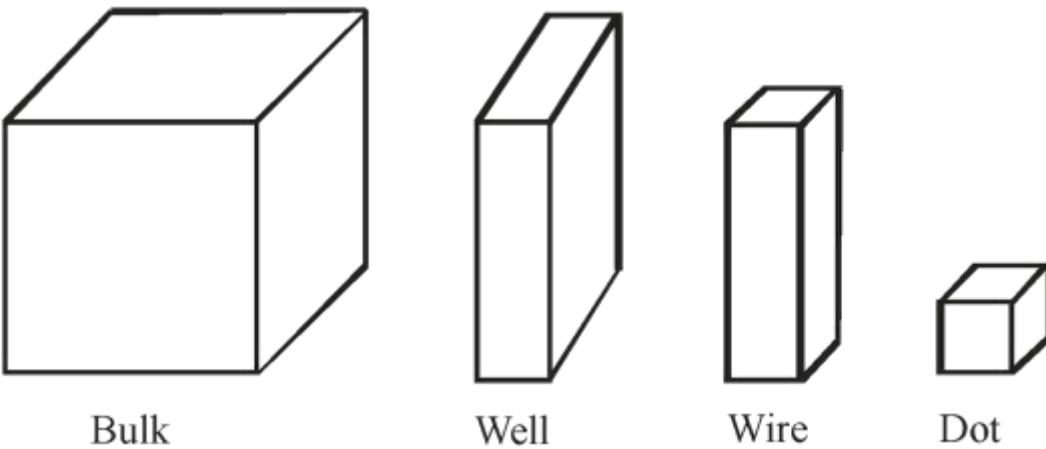
- Classification is based on the number of dimensions, which are
 - not confined to the nanoscale range (<100 nm).
 - (1) zero-dimensional (0-D), (quantum dot & spherical)
 - (2) one-dimensional (1-D), (nanorods, nanowires, nanofibers, nanotubes)
 - (3) two-dimensional (2-D), and (flat membranes, nanosheets, nanodisc)
 - (4) three-dimensional (3-D). (bulk materials)

Progressive generation of nanostructures

Well : - e-s move only in 2D

Wire : - only in 1 D

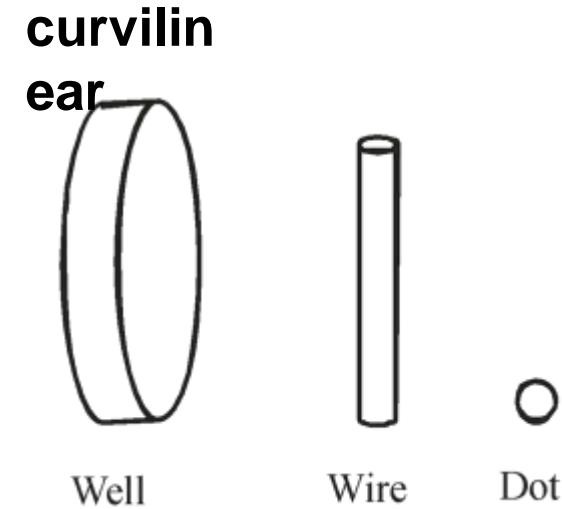
Dots: - confined in all directions, 3D movement



quanta means "how much"

**rectangular
nanomaterials:**

Nanomaterials or nanophase materials are the materials which are made of grains that are about 100nm in diameter and contain less than few ten thousands of atoms



Low-Dimensional Systems Classifications

The most universal classification scheme of low-dimensional system is by considering the number of spatial directions where the particles in the system could move freely. This approach leads.

Quantum-Well Systems. *In these systems the particles are confined in one direction and are free to move in two directions.*

Quantum-Wire Systems. *In these systems the particles are confined in two directions and are free to move in one direction.*

Quantum-Dot Systems. *In these systems the particles are confined in all three directions and can not move freely in any spatial direction.*

Quantum well, Quantum wire and Quantum dots

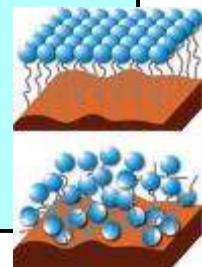
- When the size or dimension of a material is continuously reduced from a large or macroscopic size, such as a metre or centimetre, to a very small size, the properties remain the same at first, then small changes begin to occur, until finally when the size drops below 100 nm, dramatic changes in properties can occur.
- If one dimension is reduced to the nanorange while the other dimensions remain large, them we obtain a structure known as **quantum well**.
- If two dimensions are so reduced and one remains large, the resulting structure is referred to as a **quantum wire**.
- The extreme case of this process of size reduction in which all three dimensions reach the low nanometer range is called a **quantum dot**.

- The word **quantum** is associated with the above three types of nanostructures because the changes in properties arise from the quantum mechanical nature of physics in the domain of the ultra small. The above fig. represents the processes of diminishing the size for the case of rectilinear geometry and the corresponding reductions in curvilinear geometry.
The conduction electrons are confined in a narrow dimension and such a configuration is referred as *quantum well*.
A *quantum wire* is a structure such as a copper wire that is long in one dimension, but has a nanometer size as its diameter. In this case, the electrons move freely along the wire but are confined in the transverse directions.
The *quantum dot* may have the shape of a tiny cube, a short cylinder or a sphere with low nanometre dimensions.

TECHNOLOGICAL ADVANTAGES OF NANOTECHNOLOGY AND NANOMATERIALS

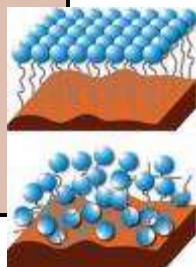
1. IMPROVED TRANSPORTATION

- Today, most airplanes are made from metal despite the fact that diamond has a strength-to-weight ratio over 50 times that of aerospace aluminum.
- Diamond is expensive, it is not possible to make it in the required shapes, and it shatters. Nanotechnology will let us inexpensively make shatterproof diamond in exactly the shapes we want.
- Nanotechnology will dramatically reduce the costs and increase the capabilities of space ships and space flight.
- The strength-to-weight ratio and the cost of components are absolutely critical to the performance and economy of space ships: with nanotechnology, both of these parameters will be improved.
- Nanotechnology will also provide extremely powerful computers with which to guide both those ships and a wide range of other activities in space.



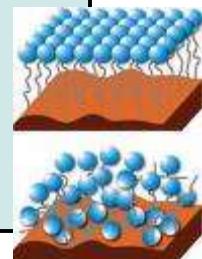
2. ATOM COMPUTERS

- Today, computer chips are made using lithography -- literally, "stone writing."
- If the computer hardware revolution is to continue at its current pace, in a decade or so we'll have to move beyond lithography to some new post lithographic manufacturing technology. Ultimately, each logic element will be made from just a few atoms.
- Designs for computer gates with less than 1,000 atoms have already been proposed -- but each atom in such a small device has to be in exactly the right place.
- To economically build and interconnect trillions upon trillions of such small and precise devices in a complex three dimensional pattern we'll need a manufacturing technology well beyond today's lithography: we'll need nanotechnology.
- With it, we should be able to build mass storage devices that can store more than a hundred billion billion bytes in a volume the size of a sugar cube;
- **RAM** that can store a mere billion billion bytes in such a volume; and massively parallel computers of the same size that can deliver a billion billion instructions per second.



3. MILITARY APPLICATIONS:

- Today, "smart" weapons are fairly big -- we have the "smart bomb" but not the "smart bullet."
- In the future, even weapons as small as a single bullet could pack more computer power than the largest supercomputer in existence today, allowing them to perform real time image analysis of their surroundings and communicate with weapons tracking systems to acquire and navigate to targets with greater precision and control.
- We'll also be able to build weapons both inexpensively and much more rapidly, at the same time taking full advantage of the remarkable materials properties of diamond.
- Rapid and inexpensive manufacture of great quantities of stronger more precise weapons guided by massively increased computational power will alter the way we fight wars.
- Changes of this magnitude could destabilize existing power structures in unpredictable ways.
- Military applications of **nanotechnology** raise a number of concerns that prudence suggests we begin to investigate before, rather than after, we develop this new technology.



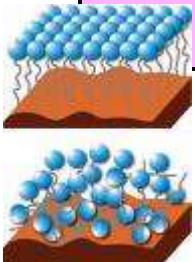
4. SOLAR ENERGY

Nanotechnology will cut costs both of the solar cells and the equipment needed to deploy them, making solar power economical.

In this application we need not make new or technically superior solar cells: making inexpensively what we already know how to make expensively would move solar power into the mainstream.

5. MEDICAL USES

- It is not modern medicine that does the healing, but the cells themselves: we are but onlookers.
- If we had surgical tools that were molecular both in their size and precision, we could develop a medical technology that for the first time would let us directly heal the injuries at the molecular and cellular level that are the root causes of disease and ill health.
- With the precision of drugs combined with the intelligent guidance of the surgeon's scalpel, we can expect a quantum leap in our medical capabilities.



6. Other Advantages

Less Pollution

The problem with past technologies is that they pollute the environment in cases where we humans would die in years.

A good example of a bad polluting invention would be the automobile. The automobile ran on gas and the gas fumes destroyed the ozone layer.



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21PYB103J –Semiconductor Physics and Computational methods

MODULE 5

Lecture- 51

Introduction to novel low dimensional systems



Carbon

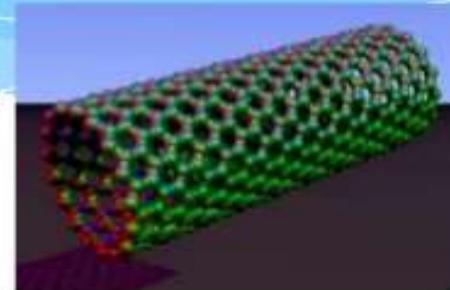
- Carbon is a basic element of life
- Carbon is special because of its ability to bond to many elements in many different ways
- It is the sixth most abundant element in the universe
- The most known types of carbon materials: diamond; graphite; fullerenes; and carbon nanotubes



FULLERENE INTRODUCTION

A **Fullerene** is any molecule composed entirely of carbon, in the form of a hollow **sphere**, **ellipsoid**, or **tube**. Spherical fullerenes are also called **buckyballs**, and cylindrical ones are called **carbon nanotubes** or **buckytubes**.

Discovered by
Buckminsterfuller
in 1960





Buckminster Fuller

Buckminster Fuller	
Richard Buckminster Fuller, c. 1917.	
Born	July 12, 1895 Milton, Massachusetts, United States
Died	July 1, 1983 (aged 87) Los Angeles, United States
Occupation	Visionary, designer, architect, author, inventor
Spouse	Anne Fuller
Children	2: Allegra Fuller Snyder and Alexandra who died in childhood



Richard Buckminster Fuller, c. 1917

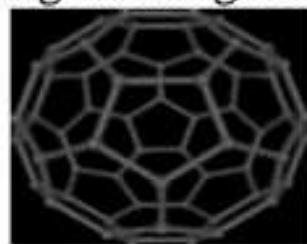


The [Montreal Biosphère](#) by Buckminster Fuller, 1967

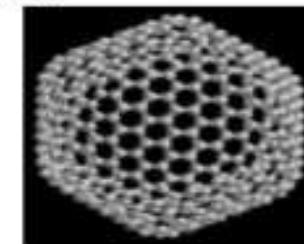


HISTORY

- The existence of C_{60} was predicted by **Eiji Osawa** of Toyohashi University of Technology in a Japanese magazine in 1970
- With mass spectrometry, discrete peaks were observed corresponding to molecules with the exact mass of sixty or seventy or more carbon atoms. In 1985, **James R. Heath, Robert Curl** and **Richard Smalley**, from **Rice University** discovered C_{60} , and shortly thereafter came to discover the fullerenes.
- **Kroto, Curl, and Smalley** were awarded the 1996 Nobel Prize in Chemistry for their roles in the discovery of this class of compounds.
- Minute quantities of the fullerenes, in the form of C_{60} , C_{70} , C_{76} , and C_{84} molecules, are produced in nature, hidden in soot and formed by lightning discharges in the atmosphere.



Buckminsterfullerene C_{60}



The Icosahedral Fullerene C_{540}

NAMING OF FULLERENE

Buckminsterfullerene (C_{60}) was named after Richard Buckminster Fuller, a noted architectural modeler who popularized the geodesic dome.

The shortened name 'fullerene' is used to refer to the family of fullerenes. The suffix "ene" indicates that each C atom is covalently bonded to three others.

Most abundant form of fullerene is C_{60} having 32 facets (12 pentagons and 20 hexagons



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TYPES OF FULLERENE

BUCKYBALL CLUSTERS: smallest member is C_{20} (unsaturated version of dodecahedrane) and the most common is C_{60} .

NANOTUBES: hollow tubes of very small dimensions, having single or multiple walls; potential applications in electronics industry.

MEGATUBES: larger in diameter than nanotubes and prepared with walls of different thickness; potentially used for the transport of a variety of molecules of different sizes.

POLYMERS: chain, two-dimensional and three-dimensional polymers are formed under high-pressure high-temperature conditions; single-strand polymers are formed using the Atom Transfer Radical Addition Polymerization (ATRAP) route.

NANO"ONIONS": spherical particles based on multiple carbon layers surrounding a buckyball core; proposed for lubricants.

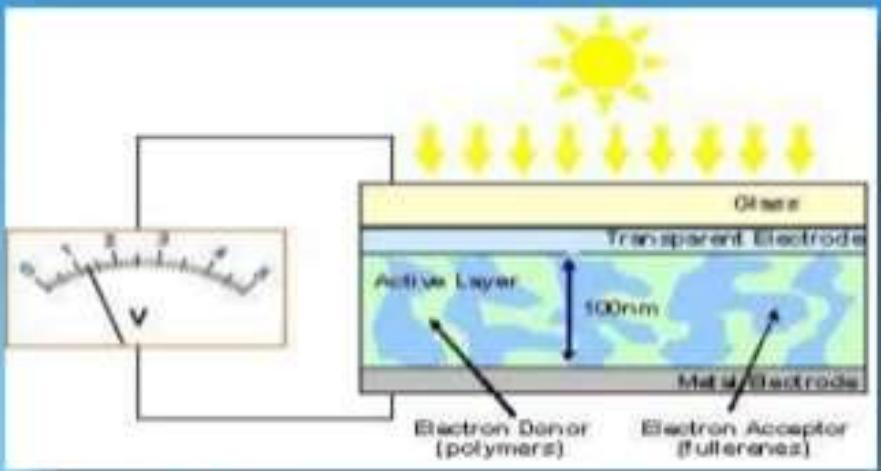
LINKED "BALL-AND-CHAIN" DIMERS: two buckyballs linked by a carbon chain.

a substance which has a molecular structure built up chiefly or completely from a large number of similar units bonded together, e.g. many synthetic organic materials used as plastics and resins



APPLICATIONS

1. Organic Photovoltaics (OPV)



2. Polymer Electronics

The performance of polymer transistors (Organic Field Effect Transistors (OFETS)) and photodetectors has also been increasing, in part due to a great deal of synergy between OFETS and OPVs



Antioxidants & Biopharmaceutical

Fullerenes are powerful antioxidants, reacting readily and at a high rate with free radicals, which are often the cause of cell damage or death. Fullerenes hold great promise in health and personal care applications where prevention of oxidative cell damage or death is desirable, as well as in non-physiological applications where oxidation and radical processes are destructive (food spoilage, plastics deterioration, metal corrosion).

Polymer Additives

Fullerenes and fullerene black are chemically reactive and can be added to polymer structures to create new copolymers with specific physical and mechanical properties. They can also be added to make composites. Much work has been done on the use of fullerenes as polymer additives to modify physical properties and performance characteristics.



OTHER APPLICATIONS

Catalysts

Marked ability to accept and to transfer hydrogen atoms; hydrogenation and hydrodealkylations.

Highly effective in promoting the conversion of methane into higher hydrocarbons.
Inhibits coking reactions.

Water purification & bio-hazard protection

Singlet oxygen catalysis of organics with fullerene C60.

Portable power

Proton exchange membranes for fuel cells.

Vehicles

Enhanced durability, lower heat build-up, better fuel economy with use of fullerene black/rubber compounds.

Medical

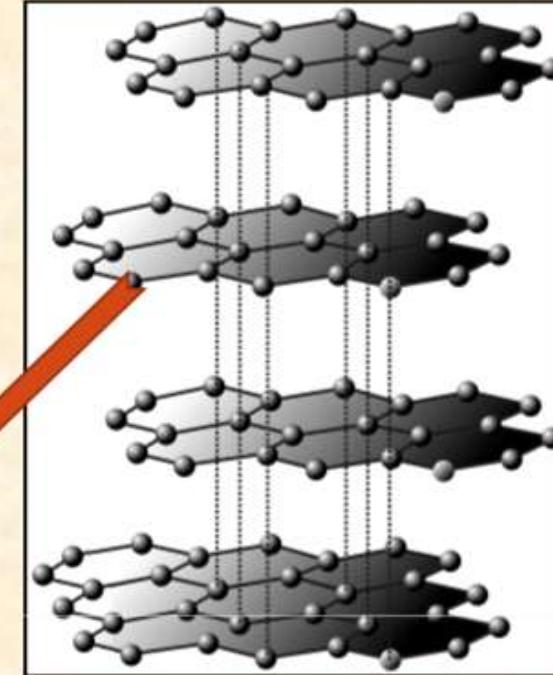
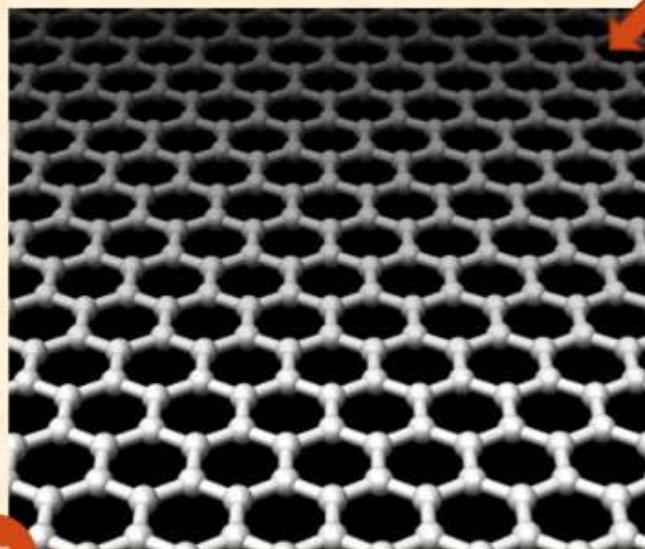
MRI agents.



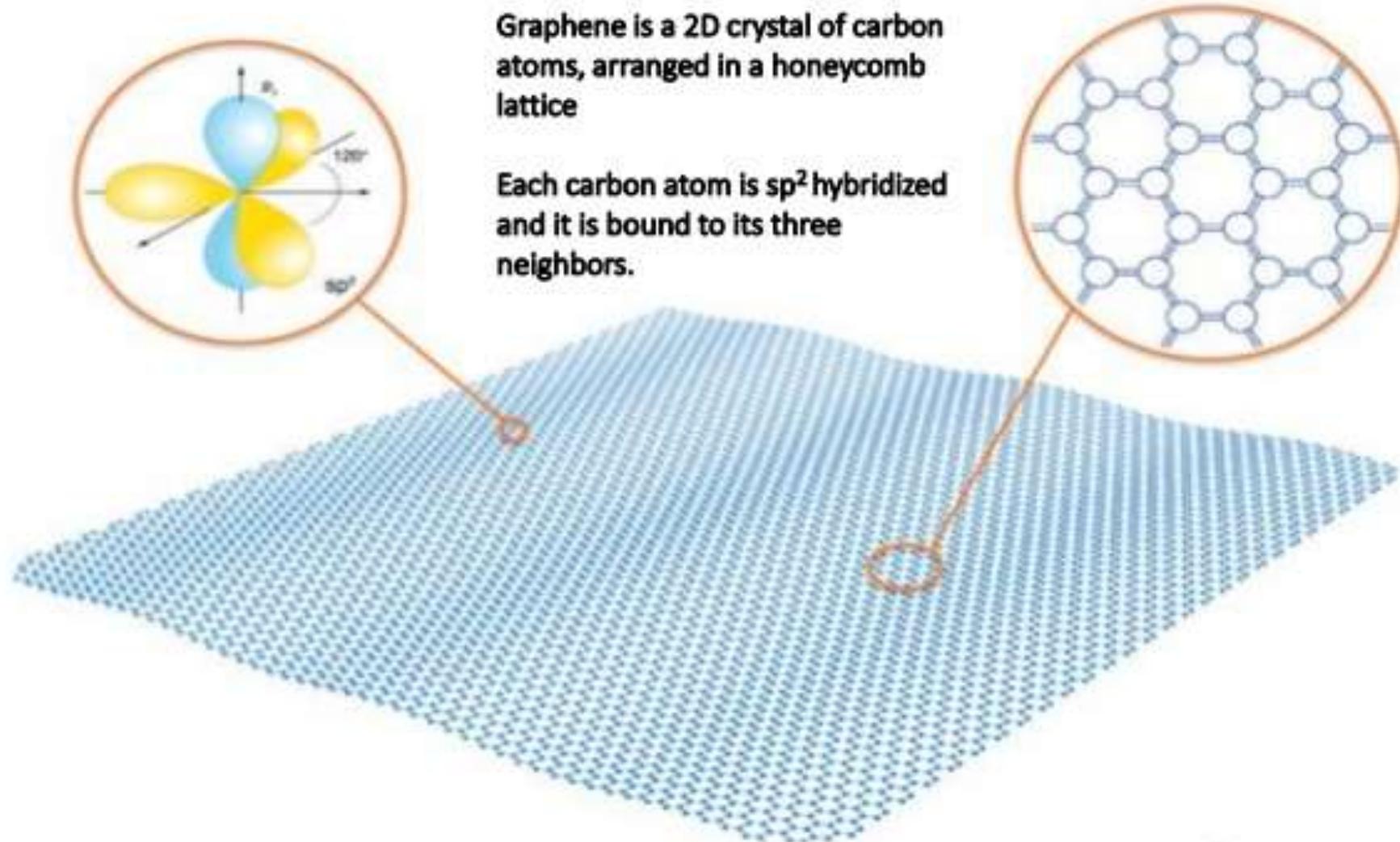
light wire netting with a hexagonal mesh.

Graphene

Graphene is an one-atom-thick planar sheet of sp^2 -bonded carbon atoms that are densely packed in a honeycomb crystal lattice. It can be viewed as an atomic-scale chicken wire made of carbon atoms and their bonds



The carbon-carbon bond length in graphene is about 0.142 nm. Graphene is the basic structural element of some carbon allotropes including graphite, carbon nanotubes and fullerenes.





History

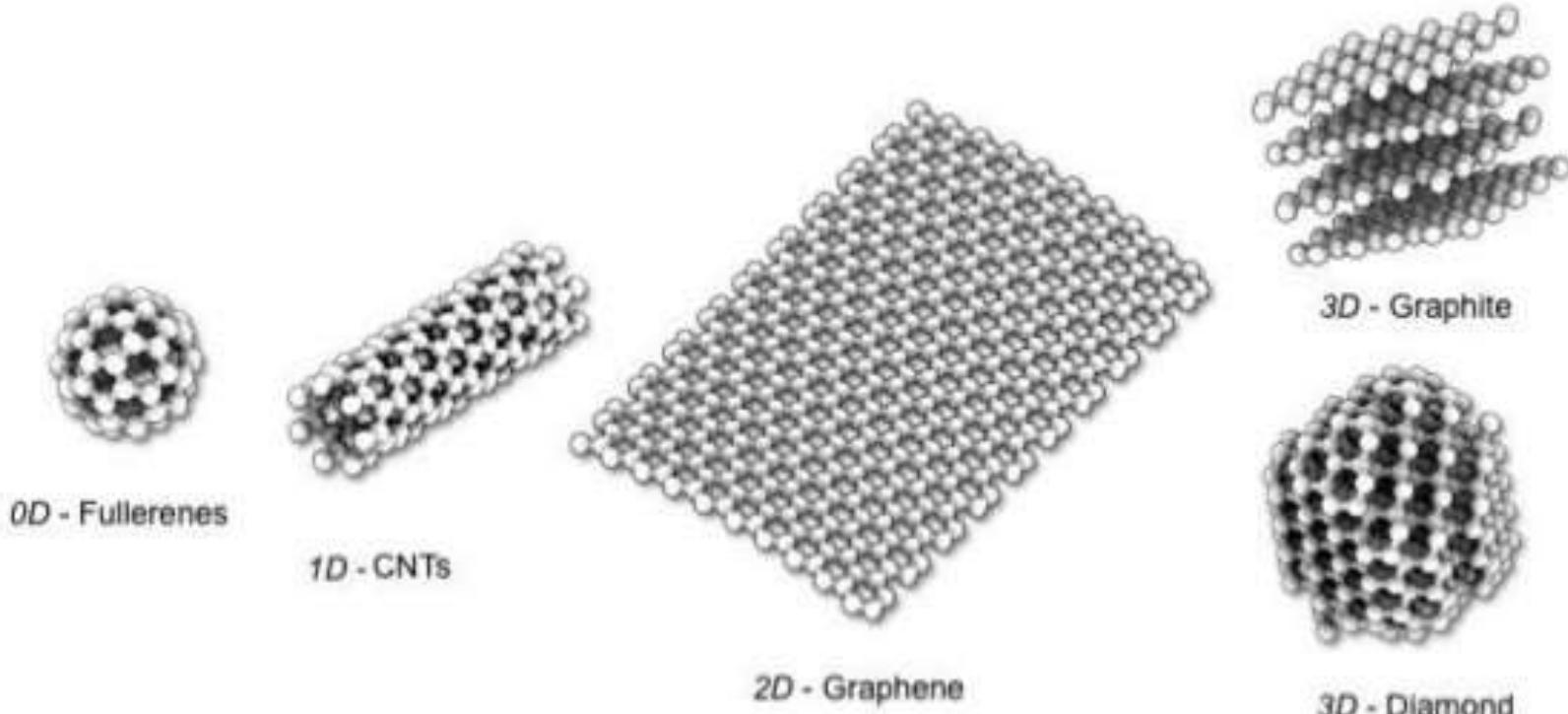
- One of the very first patents pertaining to the production of graphene was filed in October, 2002 entitled, "Nano-scaled Graphene Plates".
- Two years later, in 2004 **Andre Geim** and **Kostya Novoselov** at University of Manchester extracted single-atom-thick crystallites from bulk graphite
- Geim and Novoselov received several awards for their pioneering research on graphene, notably the 2010 Nobel Prize in Physics.

Graphene is million times thinner than paper ($0.33 \text{ to } 0.36 \text{ nm}$)
Stronger than diamond ($\gamma = 1.3 \text{ TPa}$). Better than Copper in electrical conduction ($\rho = 10^{-6} \Omega \cdot \text{m}$ & $\gamma = 2 \times 10^5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$)



Structure

- Graphene is a 2-dimensional network of carbon atoms.
- These carbon atoms are bound within the plane by strong bonds into a honeycomb array comprised of six-membered rings.
- By stacking of these layers on top of each other, the well known 3-dimensional graphite crystal is formed.
- It is a basic building block for graphitic materials of all other dimensionalities.
- It can be wrapped up into 0D fullerenes, rolled into 1D nanotubes or stacked into 3D graphite.
- Thus, graphen is nothing else than a single graphite layer.





Properties of Graphene

- 1) Perfect thermal Conductor ($\kappa > 5000 \text{ W/m/k}$) & thermal Conductivity is isotropic. This helps to fabricate graphene-based electronic device more cool.
- 2) Harder than diamond. (Tensile strength exceeds 1 TPa)
- 3) Graphene can absorb / deabsorb various atoms and molecules ($\text{NO}_2, \text{NH}_3, \text{Kr} \& \text{OH}$)
- 4) High Conducting nature helps to use Graphene as Sensors
- 5) Graphene can be functionalized by several chemical Group forming Graphene Oxides Fluorinated Graphene
- 5) Edge of Graphene has more reactivity than surface



Chemical Properties

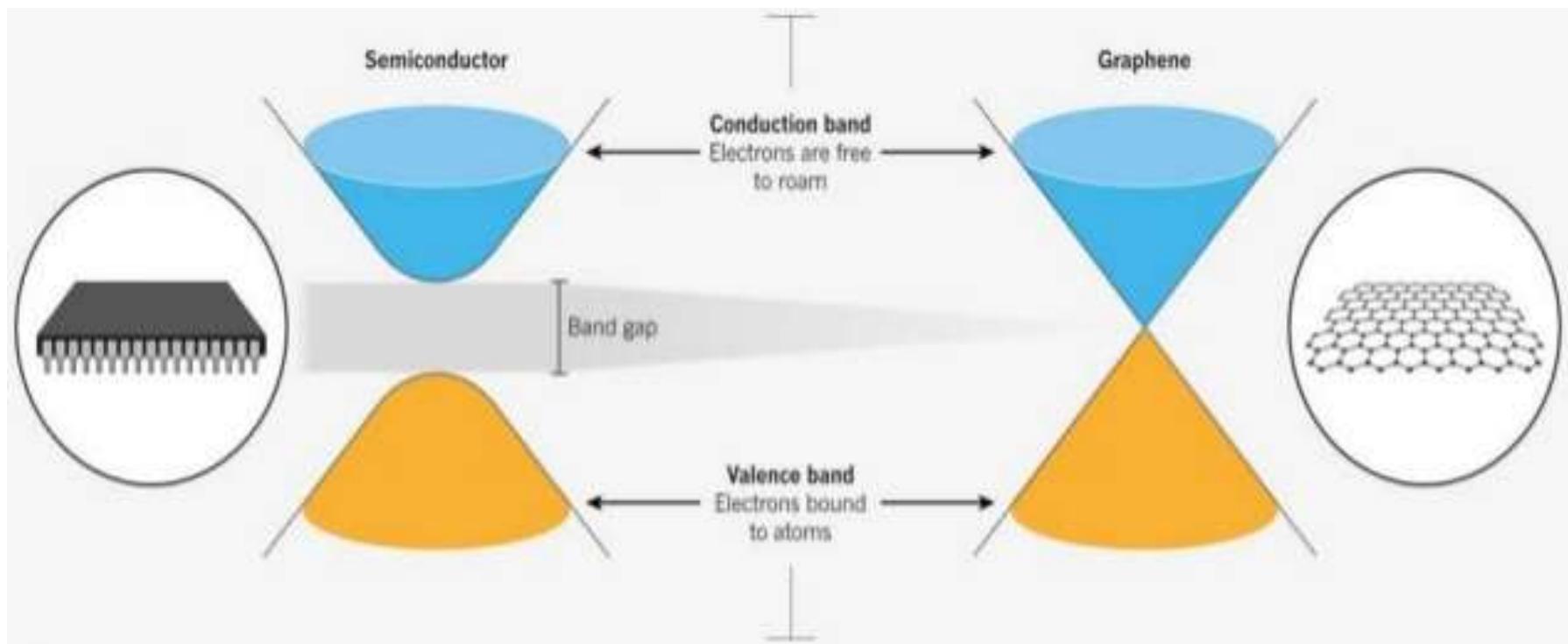
- Graphene is chemically the most reactive form of carbon.
- Only form of carbon (and generally all solid materials) in which each single atom is in exposure for chemical reaction from two sides (due to the 2D structure).
- Carbon atoms at the edge of graphene sheets have special chemical reactivity.
- Graphene burns at very low temperature (e.g., 350 °C).
- Graphene has the highest ratio of edgy carbons (in comparison with similar materials such as carbon nanotubes).
- Graphene is commonly modified with oxygen- and nitrogen-containing functional groups





Electronic Properties

- It is a zero-overlap semimetal (with both holes and electrons as charge carriers) with very high electrical conductivity.
- Electrons are able to flow through graphene more easily than through even copper.
- The electrons travel through the graphene sheet as if they carry no mass, as fast as just one hundredth that of the speed of light.
- High charge carrier mobility, for which values of $10,000 \text{ cm}^2/\text{Vs}$, in some cases even $200,000 \text{ cm}^2/\text{Vs}$ were reported.



In an insulator or semiconductor, an electron bound to an atom can break free only if it gets enough energy from heat or passing photon to jump the 'band gap'. But in graphene the gap is infinitesimal. This is the main reason why graphene's electron can move easily and very fast.



Mechanical Properties

- To calculate the strength of graphene, scientists used a technique called Atomic Force Microscopy.
- It was found that graphene is harder than diamond and about 300 times harder than steel.
- The tensile strength of graphene exceeds 1 TPa.
- It is stretchable up to 20% of its initial length.



It is expected that graphene's mechanical properties will find applications into making a new generation of super strong composite materials and along combined with its optical properties, making flexible displays.



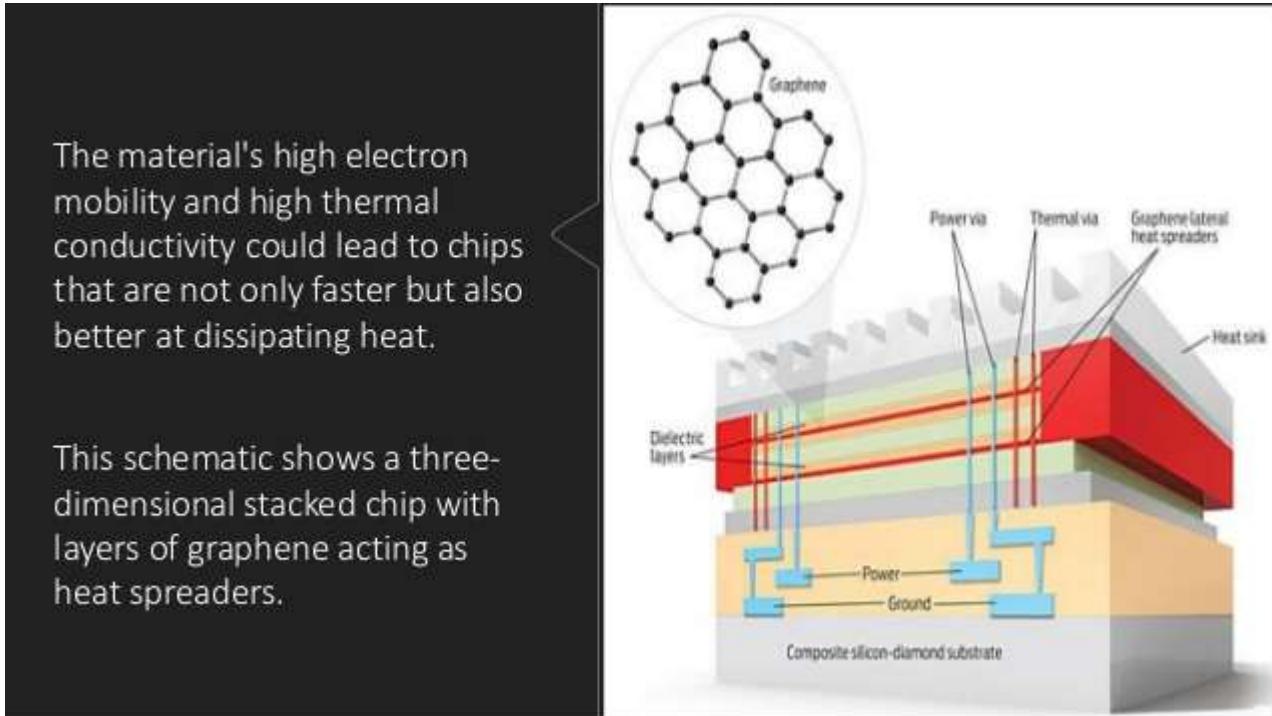


Thermal Properties

- Graphene is a perfect thermal conductor
- Its thermal conductivity is much higher than all the other carbon structures as carbon nanotubes, graphite and diamond ($> 5000 \text{ W/m/K}$) at room temperature
- Graphite, the 3 D version of graphene, shows a thermal conductivity about 5 times smaller (1000 W/m/K)
- The ballistic thermal conductance of graphene is isotropic, i.e. same in all directions

The material's high electron mobility and high thermal conductivity could lead to chips that are not only faster but also better at dissipating heat.

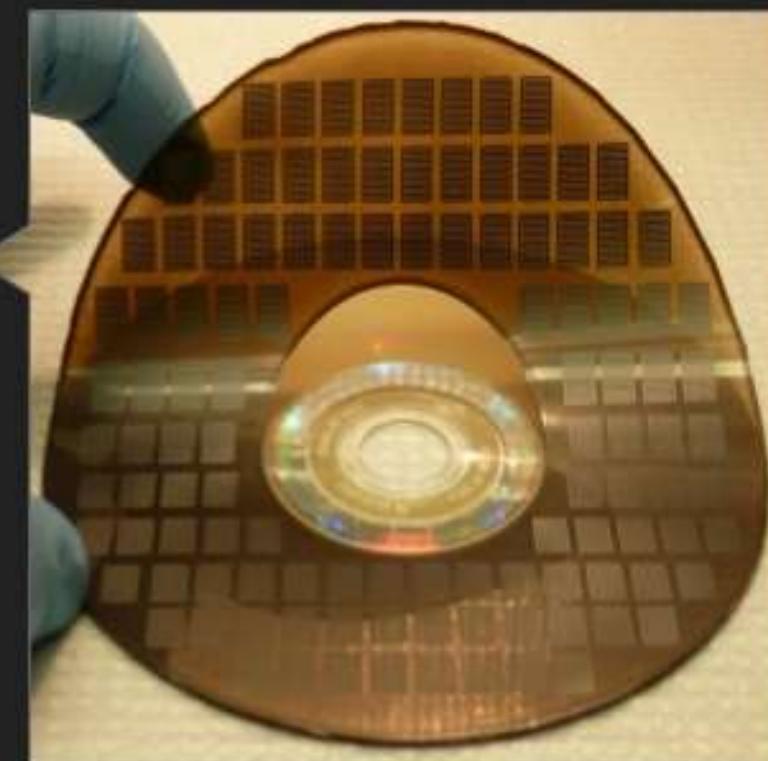
This schematic shows a three-dimensional stacked chip with layers of graphene acting as heat spreaders.





Applications

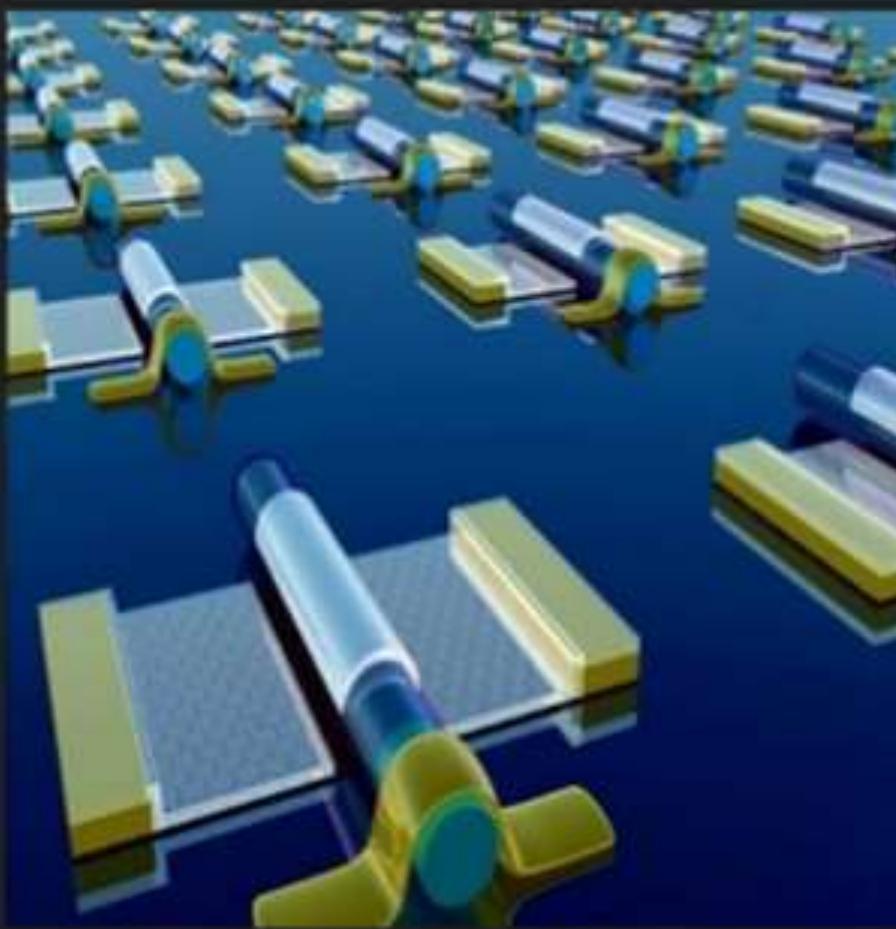
While as of 2014, graphene is not used in commercial applications, many have been proposed and/or are under active development, in areas including electronics, biological engineering, filtration, lightweight/strong composite materials, photovoltaics and energy storage.





Integrated circuits

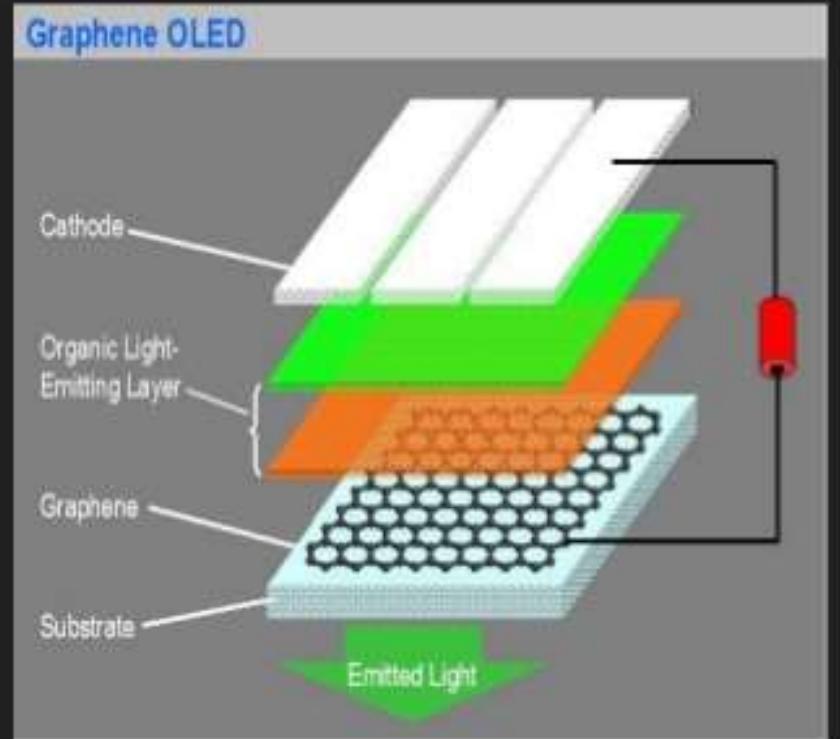
- Graphene has a high carrier mobility, as well as low noise, allowing it to be used as the channel in a field-effect transistor.
- Processors using 100 GHz transistors on 2-inch (51 mm) graphene sheets.
- Graphene-based integrated circuit handled frequencies up to 10 GHz.
- Transistors printed on flexible plastic that operate at 25 gigahertz
- Terahertz-speed transistor





Optical Electronics

- ✓ Graphene's high electrical conductivity and high optical transparency make it a candidate for transparent conducting electrodes.
- ✓ Graphene's mechanical strength and flexibility are advantageous compared to indium tin oxide, which is brittle.
- ✓ So it would work very well in optoelectronic applications: touchscreens, liquid crystal displays, organic photovoltaic cells, and organic light-emitting diodes.



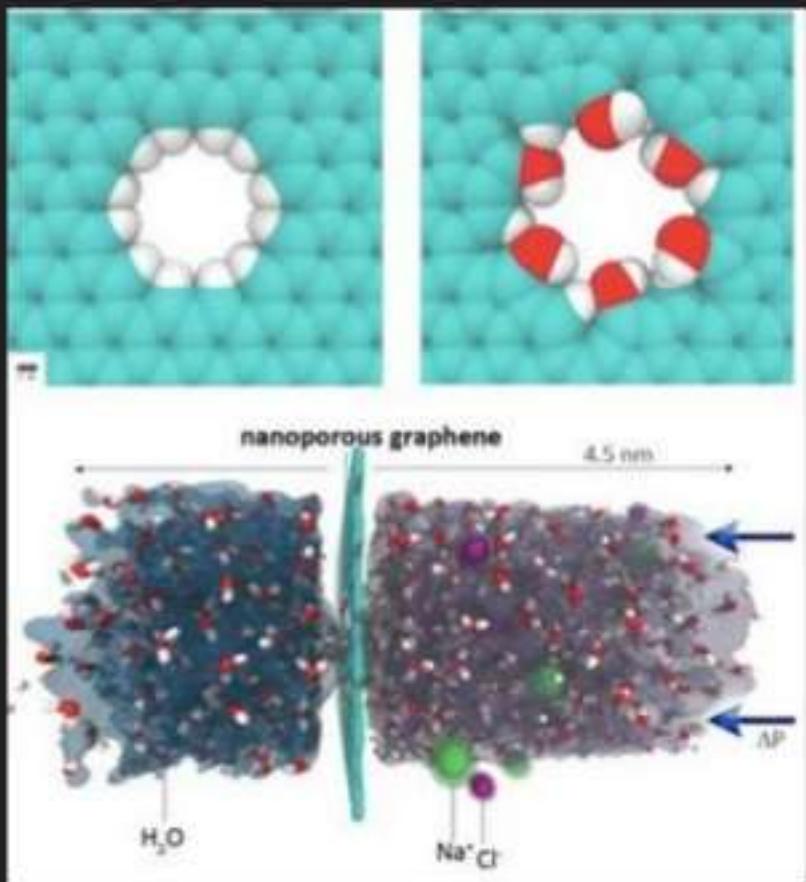


Filters

Desalination: By very precise control over the size of the holes in the graphene sheet, graphene oxide filters could outperform other techniques of desalination by a significant margin.

Ethanol distillation: Graphene oxide membranes allow water vapor to pass through, but are impermeable to other liquids and gases.

Such membranes could revolutionize the economics of biofuel production and the alcoholic beverage industry



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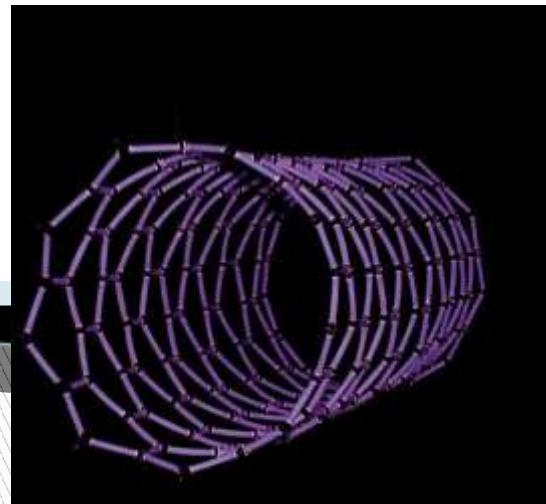
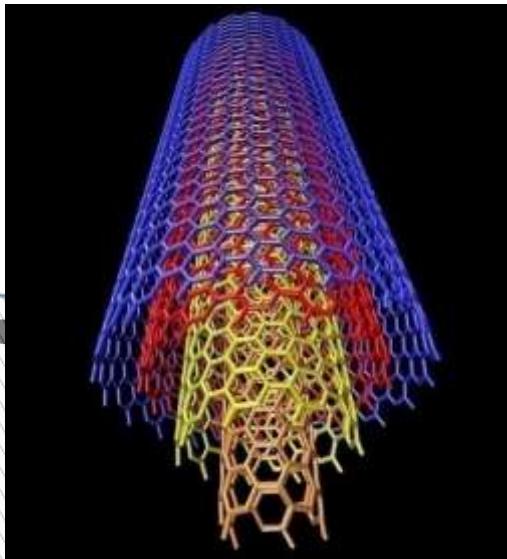
21PYB102J –Semiconductor Physics

Unit-V Lecture-53

Carbon Nano Tubes-Properties, Synthesis and Applications

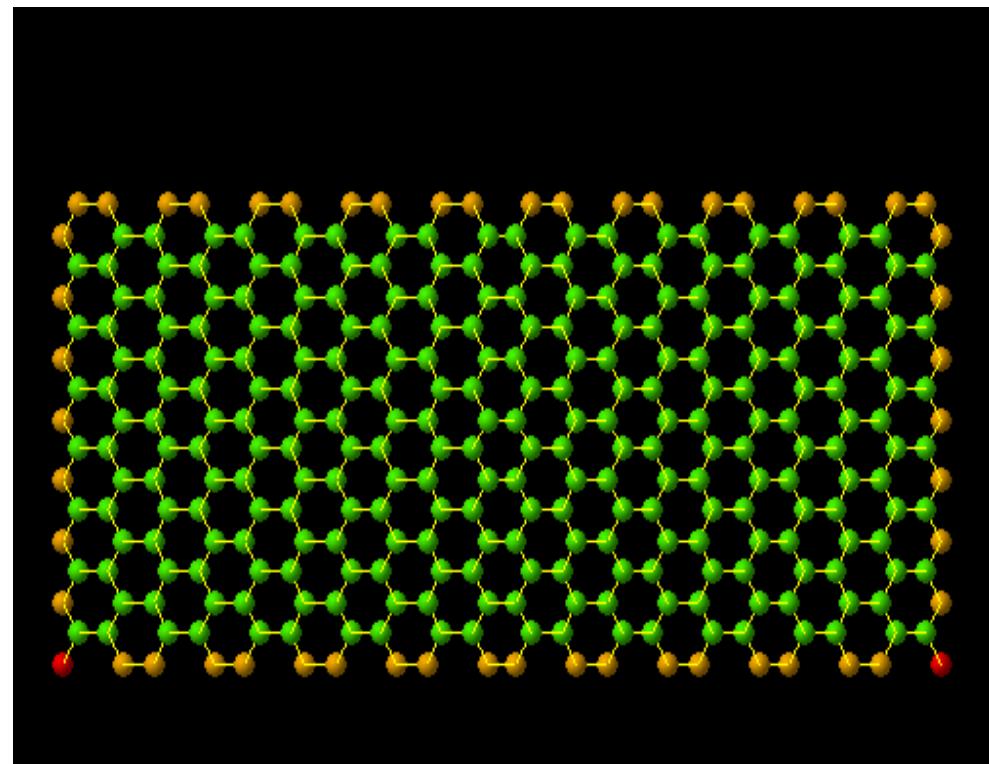
Carbon Nanotubes

Carbon nanotubes (CNTs) are allotropes of carbon. These cylindrical carbon molecules have interesting properties that make them potentially useful in many applications in nanotechnology, electronics, optics and other fields of materials science, as well as potential uses in architectural fields. They exhibit extraordinary strength and unique electrical properties, and are efficient conductors of heat. Their final usage, however, may be limited by their potential toxicity.



What Are Carbon Nanotubes

- CNT can be described as a sheet of graphite rolled into a cylinder
- Constructed from hexagonal rings of carbon
- Can have one layer or multiple layers
- Can have caps at the ends making them look like pills



Discovery

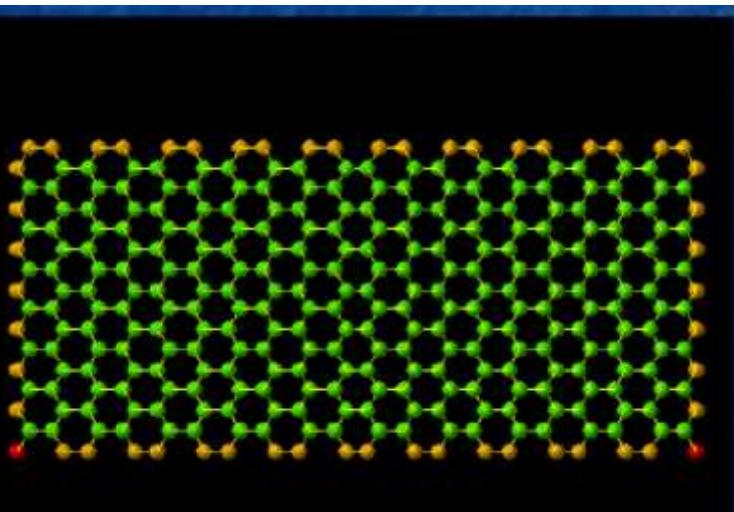
Nano-tubes

They were discovered in 1991 by the Japanese electron microscopist Sumio Iijima who was studying the material deposited on the cathode during the arc-evaporation synthesis of fullerenes. He found that the central core of the cathodic deposit contained a variety of closed graphitic structures including nanoparticles and nanotubes, of a type which had never previously been observed



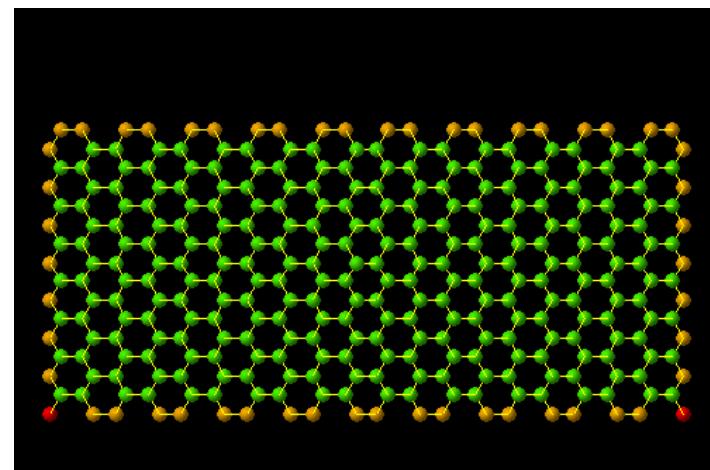


- Carbon Nanotubes are built up using graphite sheet, which is the most stable form of crystalline carbon.
- A carbon Nanotube is obtained by rolling up a plain graphite sheet into a tubular shape.



Graphite Sheet

→
Roll up



Carbon Nano Tube

Carbon Nanotube can be classified into Two type

1. Single wall carbon Nanotube (SWNT)
2. Multiwall Carbon Nanotube (MWNT)

Single-wall carbon Nanotubes (SWCNTs) can be considered to be formed by the **rolling of a single layer of graphite** into a seamless cylinder.

A **Multiwall** carbon Nanotube (MWCNT) can similarly be considered to be a **coaxial assembly of cylinders of SWCNTs**, one within another.

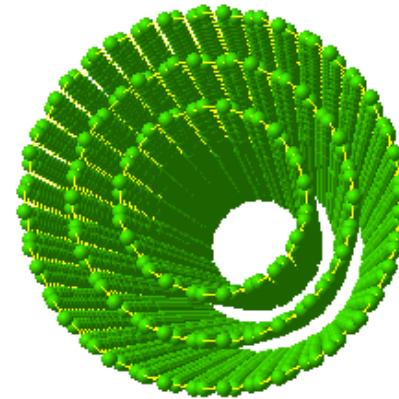
The separation between tubes is about equal to that between the layers in natural graphite. Hence, Nanotubes are one-dimensional objects.

- **MWNT**

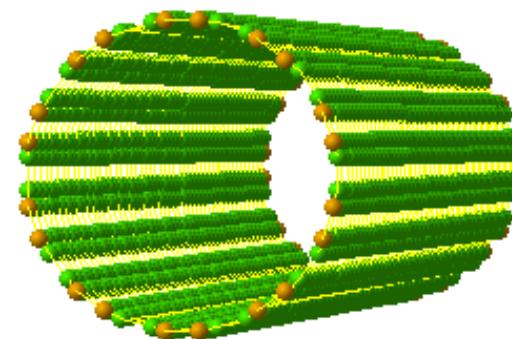
- Consist of 2 or more layers of carbon
- Tend to form unordered clumps

- **SWNT**

- Consist of just one layer of carbon
- Greater tendency to align into ordered bundles
- Used to test theory of nanotube properties



Multi wall CNT



Single wall CNT

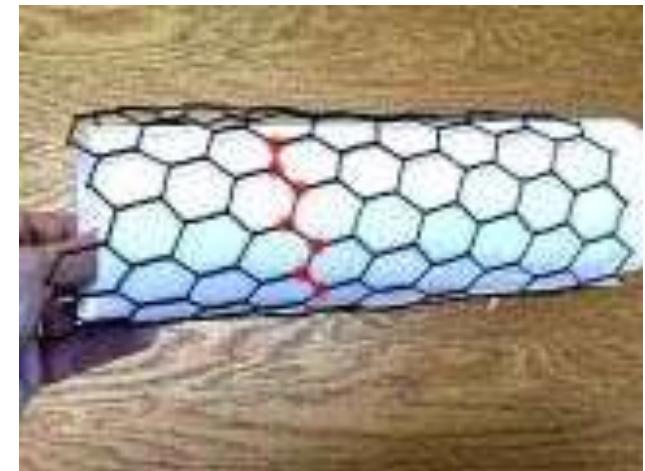
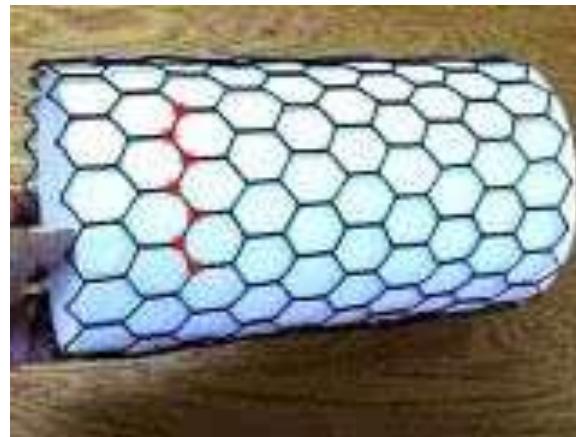
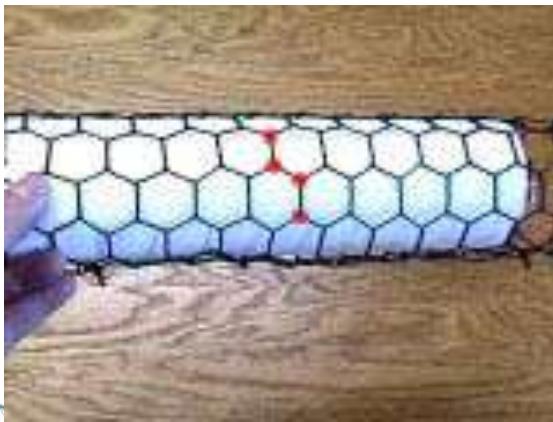


Nanotube's characteristic

- Seemless cylindrical molecules
- Diameter as small as 1 nm.
- Length: a few nm. to several micron
- As a monoelemental polymer: Carbon atoms only
- As hexagonal network of carbon atoms
- CNTs are single molecules comprised of rolled up graphene sheets capped at each end.

NANOTUBE GEOMETRY:

- There are three unique geometries of carbon nanotubes. The three different
- geometries are also referred to as flavors. The three flavors are armchair, zig-zag, and chiral [e.g. zig-zag ($n, 0$); armchair (n, n); and chiral (n, m)]. These flavors can be
- classified by how the carbon sheet is wrapped into a tube

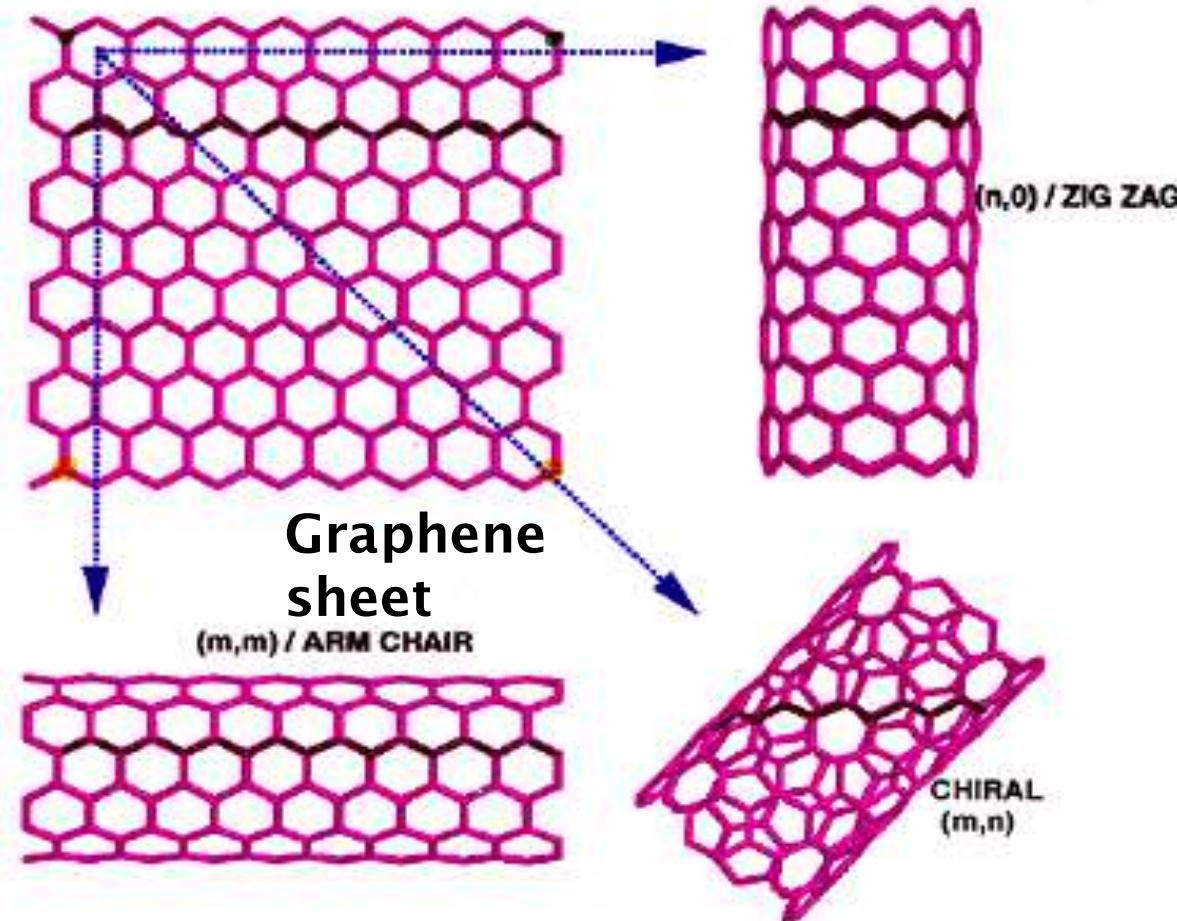


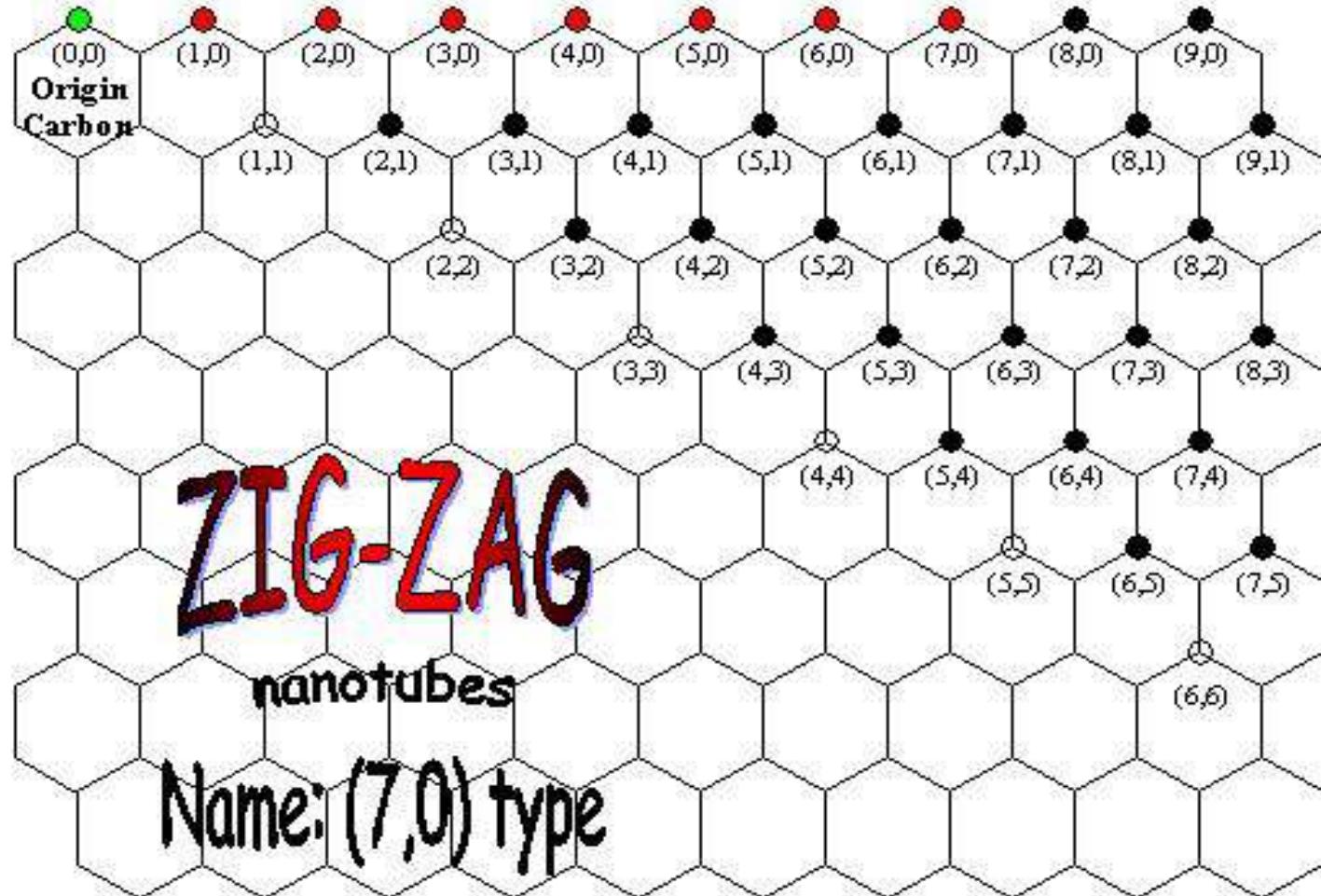
- If the Chiral vector passes through mid point of atomic bonding, it called "zig-zag line" Nanotube
- If the Chiral vector passes through the atoms of six fold axis, it armchair line" Nanotube
- If the Chiral vector line not along a mirror line then it is called chiral Nanotube

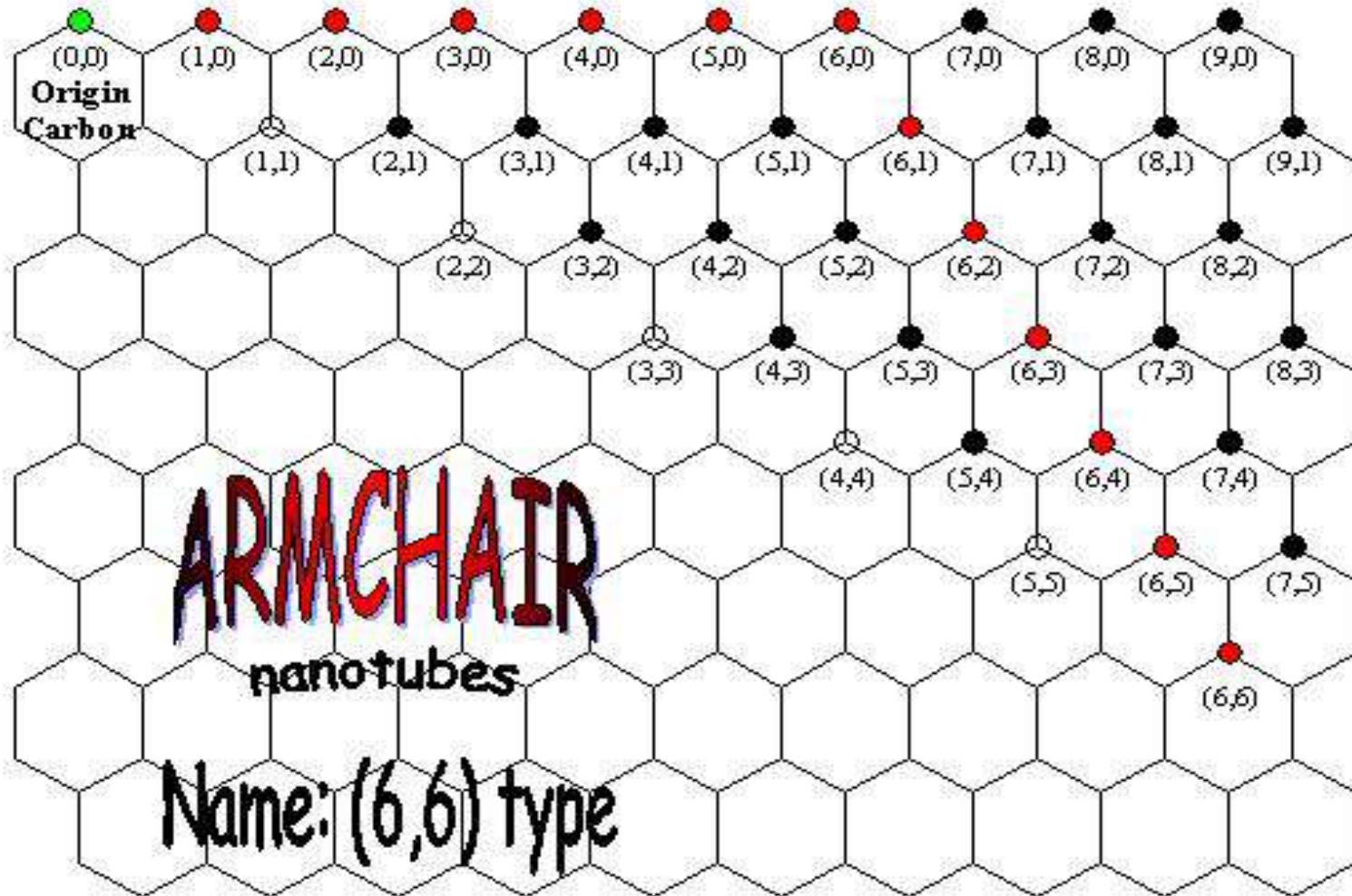
- The Chiral angle and Chiral vector(C_h) of zigzag Nanotubes is 0° and $(n,0)$
- The Chiral angle is 30° and Chiral vector (C_h) is (n,n) for armchair Nanotubes
- The Chiral angle is $0 \leq \theta \leq 30^\circ$
The Chiral vector $n \neq m$ for Chiral Nanotube

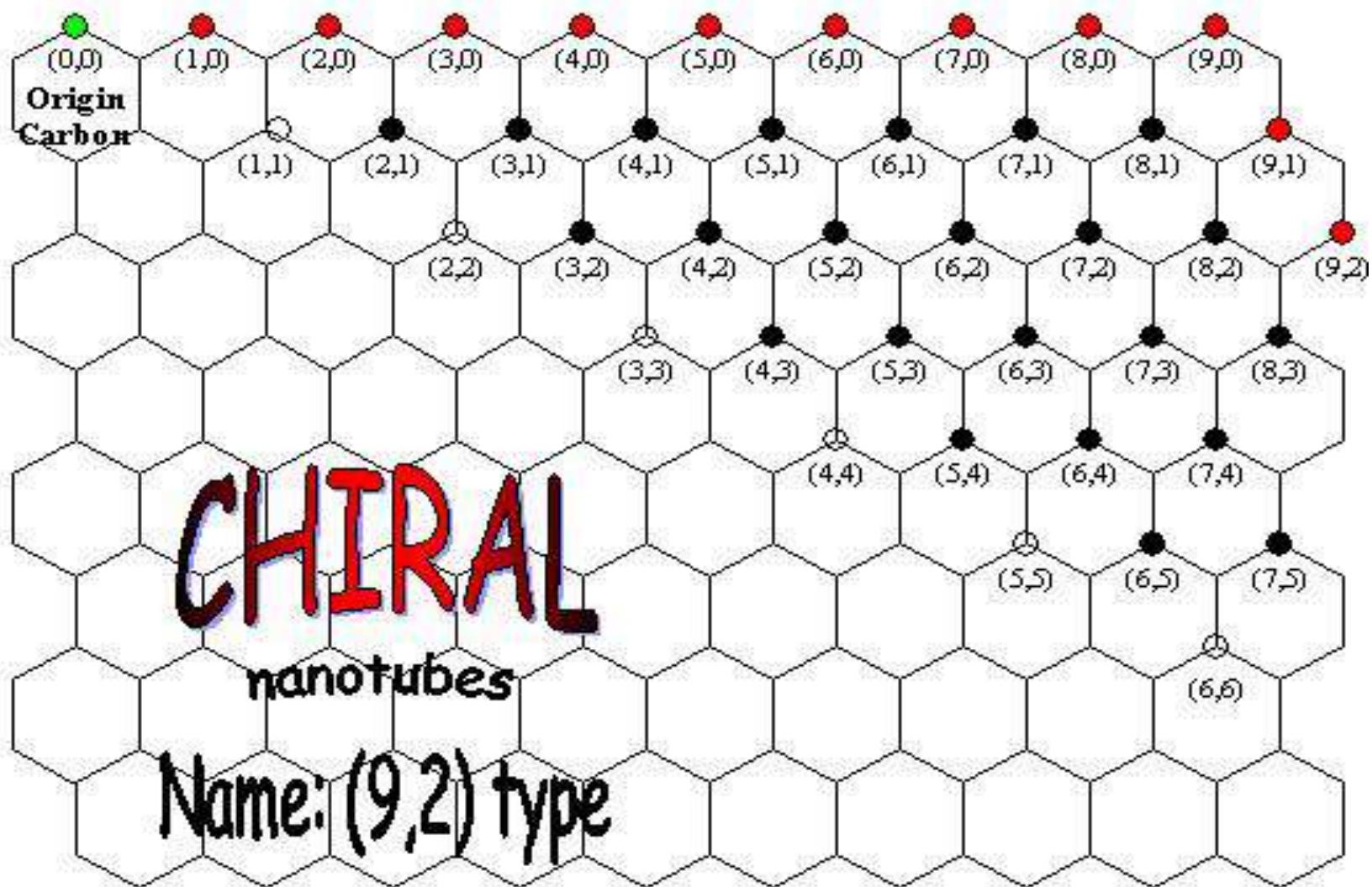


- STRIP OF A GRAPHENE SHEET ROLLED INTO A TUBE









CNT exhibits extraordinary mechanical properties:

- The Young's modulus is over 1 Tera Pascal. It is stiff as diamond.
- The estimated tensile strength is 200 GPa. These properties are ideal for reinforced composites, Nano electromechanical systems (NEMS)

- The dimensions of CNT are variable (down to 0.4 nm in diameter)
- Apart from remarkable tensile strength, CNT nanotubes exhibit varying electrical properties (depending on the way the graphite structure spirals around the tube, and other factors, such as doping), and can be superconducting, insulating, semiconducting or conducting (metallic)

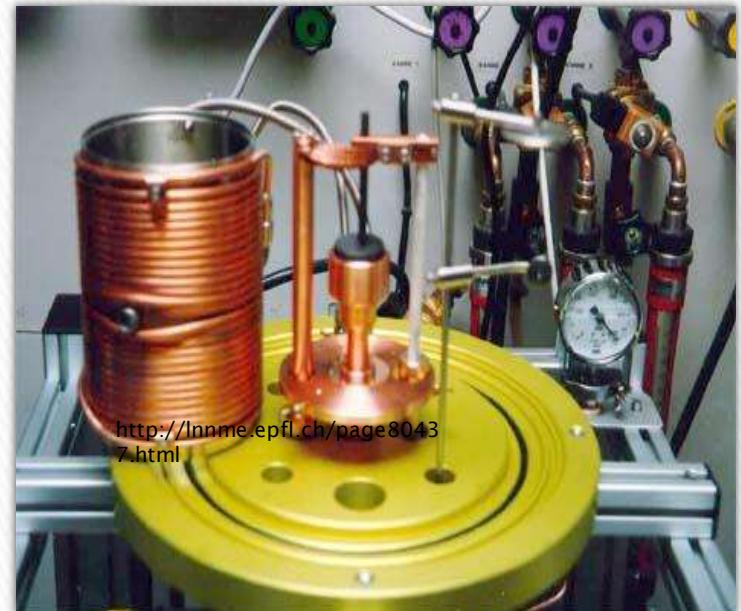
- CNT Nanotubes can be either electrically conductive or semi conductive, depending on their helicity (shape), leading to nanoscale wires and electrical components.
- These one-dimensional CNT fibers exhibit
 - Electrical conductivity as high as copper,
 - Thermal conductivity as high as diamond,
 - Strength 100 times greater than steel at one sixth the weight, and high strain to failure

➤ Chemical reactivity.

- The chemical reactivity of a CNT is very high as compared with a graphene sheet because of its curved surface.
- A Nanotube with smaller diameter results in increased reactivity.

Synthesis of CNTs- Arc Discharge Method

- A direct current creates a high temperature discharge between two electrodes (carbon is vapourized)
- Atmosphere is composed of inert gas at a low pressure
- Originally used to make C_{60} fullerenes
- Cobalt is a popular catalyst
- Typical yield is 30-90%



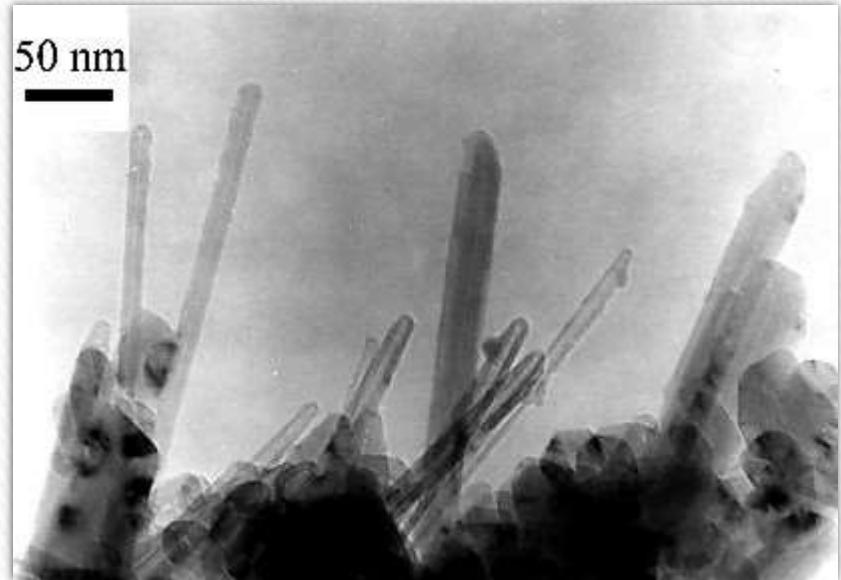
Arc Discharge Method

Advantages

- Simple procedure
- High quality product
- Inexpensive

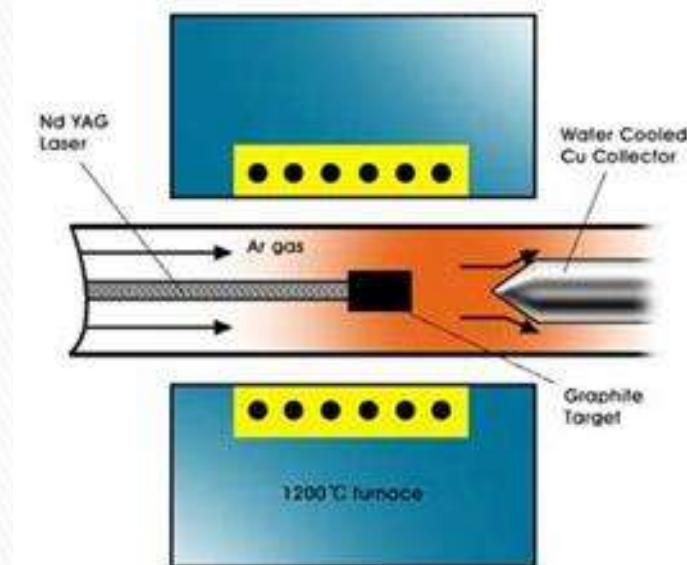
Disadvantages

- Requires further purification
- Tubes tend to be short with random sizes



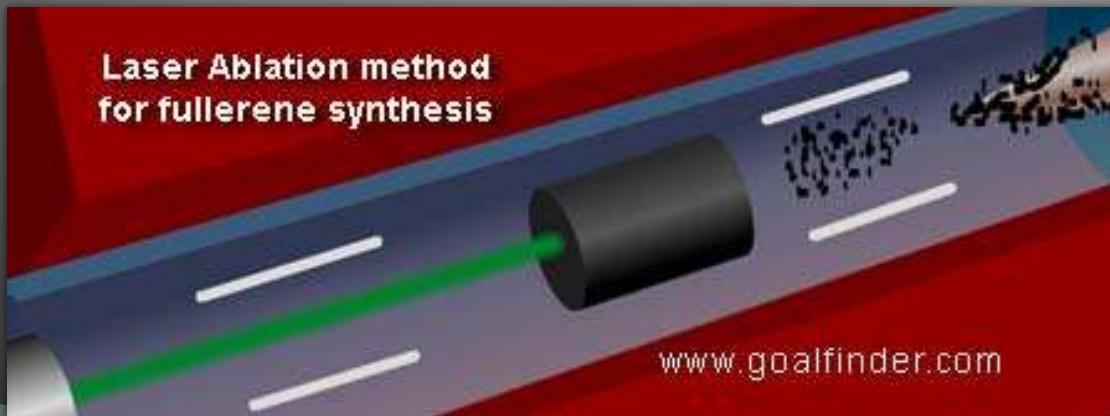
Laser Ablation Method

- Discovered in 1995 at Rice University
- Vaporizes graphite at 1200 °C
- Helium or argon gas
- A hot vapor plume forms and expands and cools rapidly
- Carbon molecules condense to form large clusters
- Similar to arc discharge
- Yield of up to 70%



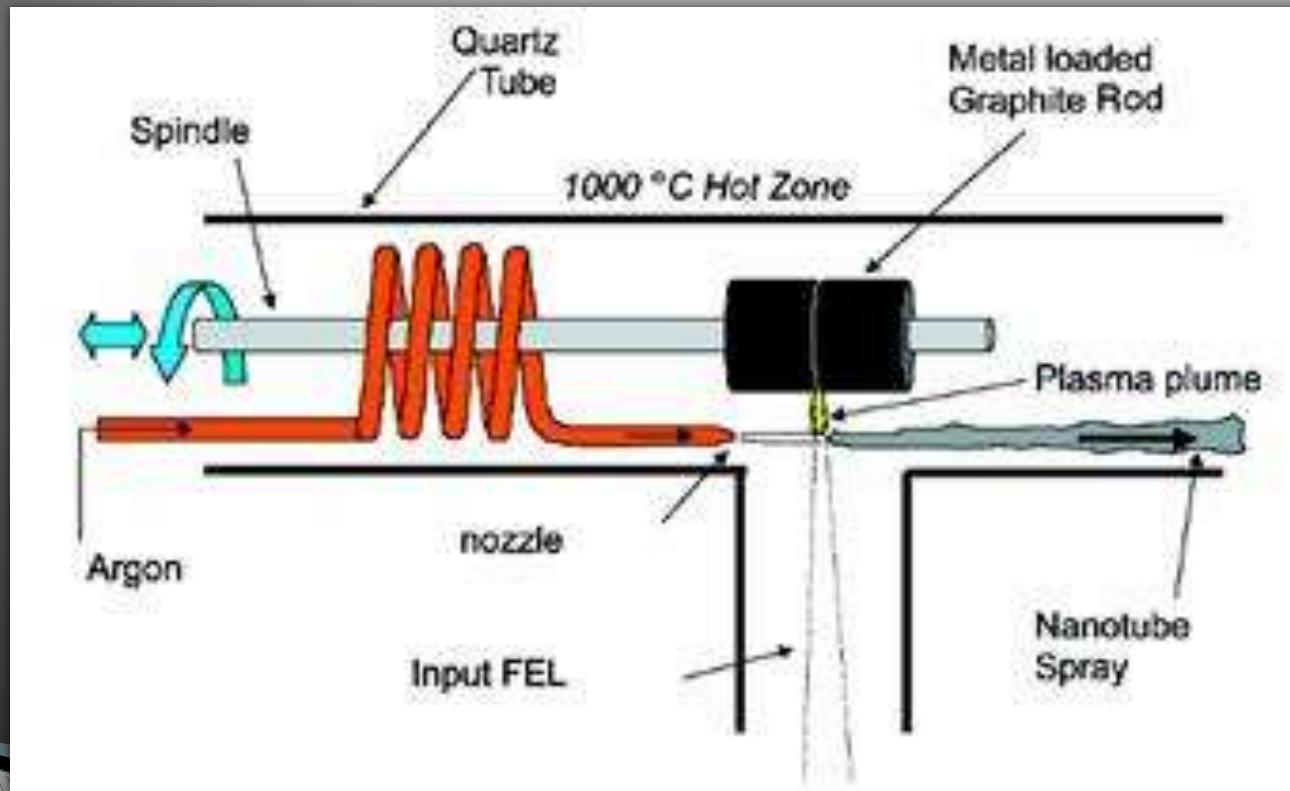
Types of Laser Ablation

- Pulsed
 - Much higher light intensity (100 kW/cm^2)
- Continuous
 - Much lower light intensity (12 kW/cm^2)





Ultra Fast-pulsed Laser Ablation



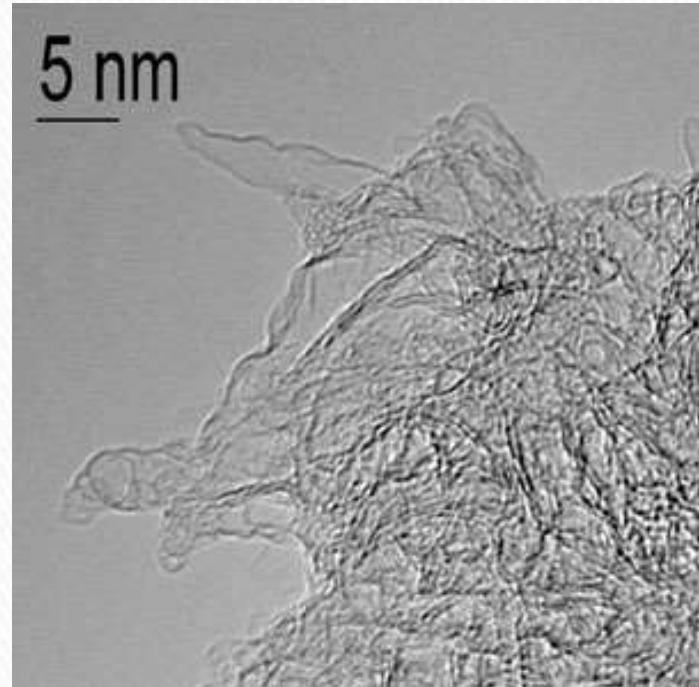
Laser Ablation

Advantages

- Good diameter control
- Few defects
- Pure product

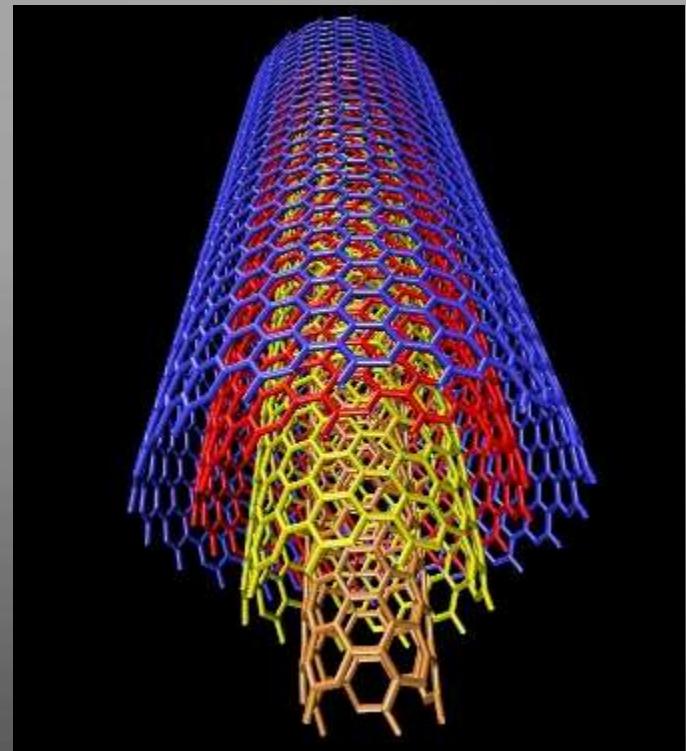
Disadvantages

- Expensive because of lasers and high powered equipment



Chemical Vapor Deposition

- Carbon is in the gas phase
- Energy source transfers energy to carbon molecule
- Common Carbon Gases
 - Methane
 - Carbon monoxide
 - Acetylene





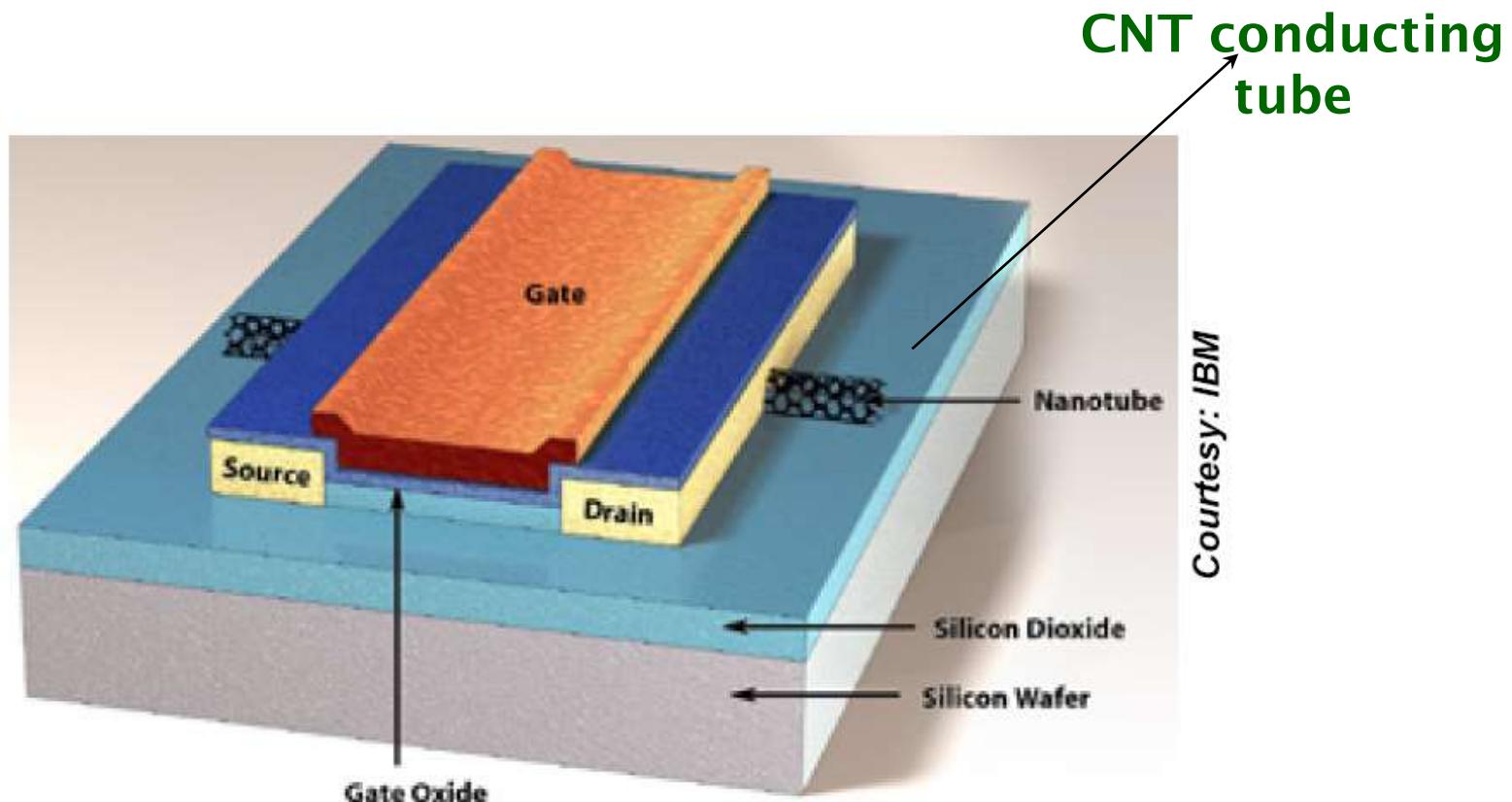
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Applications of carbon Nanotubes

- Carbon Nanotube can be used as a **conducting channel** in Field emission Transistor
- CNT conducting channel result the device with low power consumption



Nanoprobes and sensors

- Because of their flexibility, nanotubes can also be used in scanning probe instruments.
- Since MWNT tips are conducting, they can be used in STM and AFM instruments.
- Advantages are the improved resolution in comparison with conventional Si or metal tips and the tips do not suffer from crashes with the surfaces because of their high elasticity.
- However, Nanotube vibration, due to their large length, will remain an important issue until shorter nanotubes can be grown controllably.
- Nanotube tips can be modified chemically by attachment of functional groups.

1. Electronic Devices

Nanotube TV's

Nano-wiring

2. High Strength Composites

100 times as strong as steel and 1/6 the weight

3. Conductive Composites

4. Medical Applications

Encase drug into nanotube capsule for more predictable time release

Composite materials

- Because of the stiffness of carbon nanotubes, they are ideal candidates for structural applications.
- For example, they may be used as reinforcements in high strength, low weight, and high performance composites.
- Theoretically, SWNTs could have a Young's Modulus of 1 TPa.
- MWNTs are weaker because the individual cylinders slide with respect to each other.
- Ropes of SWNTs are also less strong.
- The individual tubes can pull out by shearing and at last the whole rope will break.

Templates

- Because of the small channels, strong capillary forces exist in nanotubes.
- These forces are strong enough to hold gases and fluids in nanotubes.
- In this way, it may be possible to fill the cavities of the nanotubes to create nanowires.



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21PYB102J –Semiconductor Physics

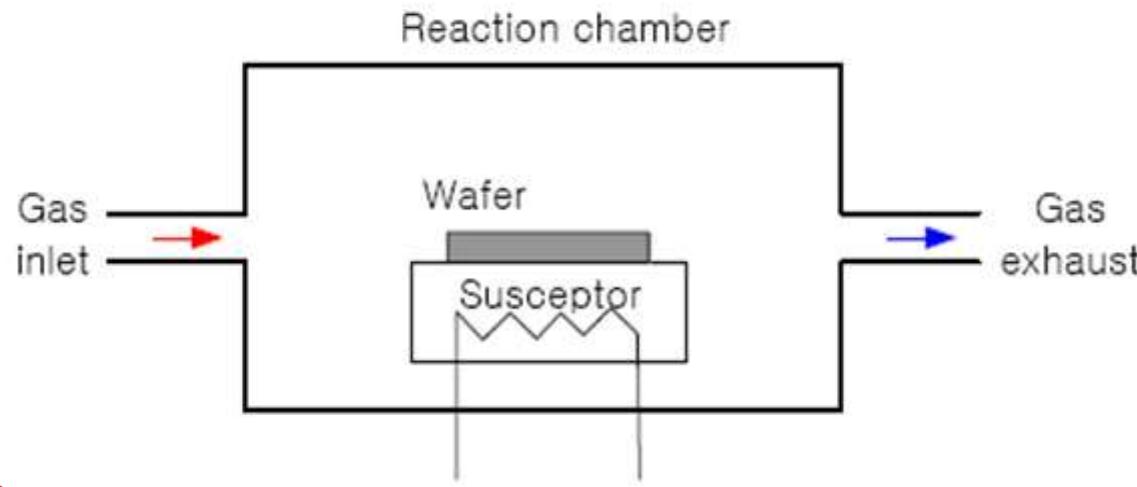
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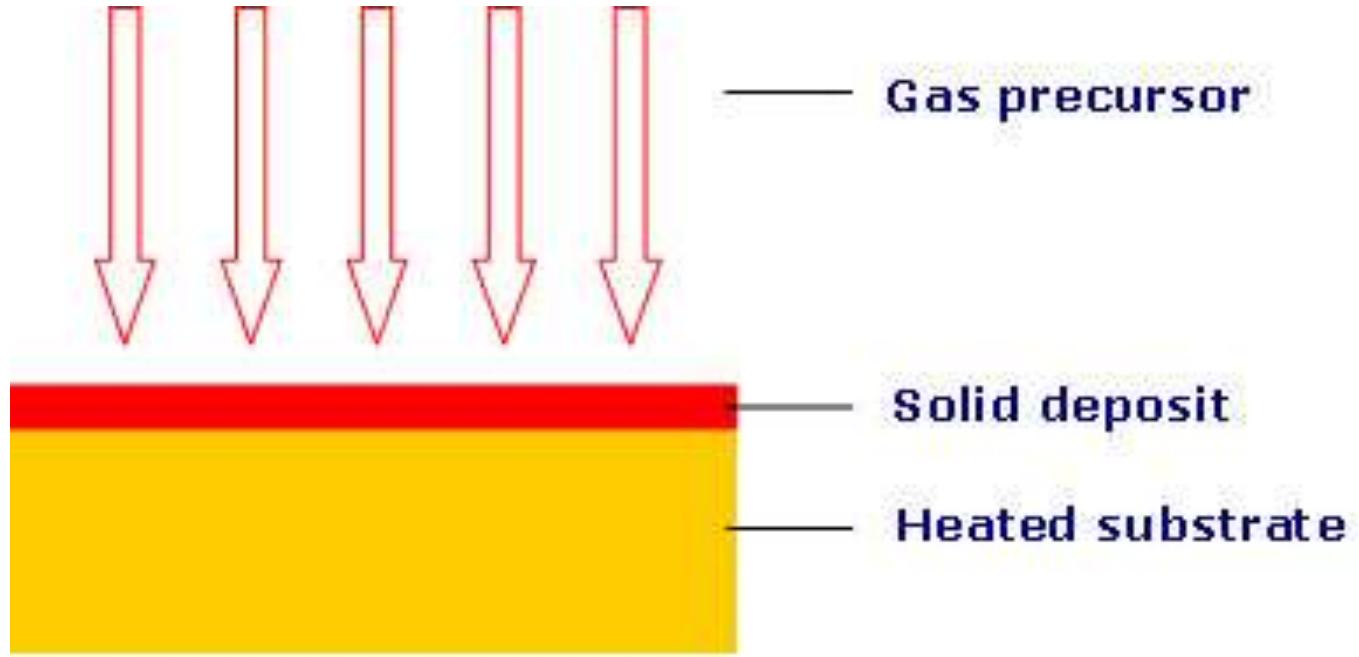
Fabrication Techniques-CVD and PVD



Chemical vapour Deposition

Schematic of CVD





CVD REACTION

A basic CVD process consists of the following steps:

- A predefined mix of reactant gases and diluent inert gases are introduced at a specified flow rate into the reaction chamber;
- The gas species move to the substrate;
- The reactants get adsorbed on the surface of the substrate;
- The reactants undergo chemical reactions with the substrate to form the film; and
- The gaseous by-products of the reactions are desorbed and evacuated from the reaction chamber.

- During the process of chemical vapor deposition, the reactant gases not only react with the substrate material at the wafer surface (or very close to it), but also in gas phase in the reactor's atmosphere.
- Reactions that take place at the substrate surface are known as heterogeneous reactions, and are selectively occurring on the heated surface of the wafer where they create good-quality films.
- Reactions that take place in the gas phase are known as homogeneous reactions.
- Homogeneous reactions form gas phase aggregates of the depositing material, which adhere to the surface poorly and at the same time form low-density films with lots of defects.
- In short, heterogeneous reactions are much more desirable than homogeneous reactions during chemical vapor deposition.

A typical CVD system consists of the following parts:

- sources of and feed lines for gases;
- mass flow controllers for metering the gases into the system;
- a reaction chamber or reactor;
- a system for heating up the wafer on which the film is to be deposited; and
- temperature sensors.

Types of chemical vapor deposition

- A number of forms of CVD are in wide use.
- These processes differ in the means by which chemical reactions are initiated (e.g., activation process) and process conditions.
- For instance, a reactor is said to be 'hot-wall' if it uses a heating system that heats up not only the wafer, but the walls of the reactor itself, an example of which is radiant heating from resistance-heated coils.
- 'Cold-wall' reactors use heating systems that minimize the heating up of the reactor walls while the wafer is being heated up, an example of which is heating via IR lamps inside the reactor.
- In hot-wall reactors, films are deposited on the walls in much the same way as they are deposited on wafers.
- so this type of reactor requires frequent wall cleaning.

- Another way of classifying CVD reactors is by basing it on the range of their operating pressure.
- Atmospheric pressure CVD (APCVD) reactors operate at atmospheric pressure, and are therefore the simplest in design.
- Low-pressure CVD (LPCVD) reactors operate at medium vacuum (30-250 Pa) and higher temperature than APCVD reactors.
- Plasma Enhanced CVD (PECVD) reactors also operate under low pressure, but do not depend completely on thermal energy to accelerate the reaction processes.
- They also transfer energy to the reactant gases by using an RF-induced glow discharge.

- The glow discharge used by a PECVD reactor is created by applying an RF field to a low-pressure gas, creating free electrons within the discharge region.
- The electrons are sufficiently energized by the electric field that gas-phase dissociation and ionization of the reactant gases occur when the free electrons collide with them.
- Energetic species are then adsorbed on the film surface, where they are subjected to ion and electron bombardment, rearrangements, reactions with other species, new bond formation, and film formation and growth.
- Table compares the characteristics of typical APCVD, LPCVD, and PECVD reactors.

APCVD, LPCVD, and PECVD Comparison

CVD Process	Advantages	Disadvantages	Applications
APCVD	Simple, Fast Deposition, Low Temperature	Poor Step Coverage, Contamination	Low-temperature Oxides
LPCVD	Excellent Purity, Excellent Uniformity, Good Step Coverage, Large Wafer Capacity	High Temperature, Slow Deposition	High-temperature Oxides, Silicon Nitride, Poly-Si, W, WSi ₂
PECVD	Low Temperature, Good Step Coverage	Chemical and Particle Contamination	Low-temperature Insulators over Metals, Nitride Passivation

Advantages of CVD

- Can be used for a wide range of metals and ceramics
- Can be used for coatings or freestanding structures
- Fabricates net or near-net complex shapes
- Is self-cleaning—extremely high purity deposits (>99.995% purity)
- Conforms homogeneously to contours of substrate surface
- Has near-theoretical as-deposited density
- Has controllable thickness and morphology
- Forms alloys
- Infiltrates fiber preforms and foam structures
- Coats internal passages with high length-to-diameter ratios
- Can simultaneously coat multiple components
- Coats powders

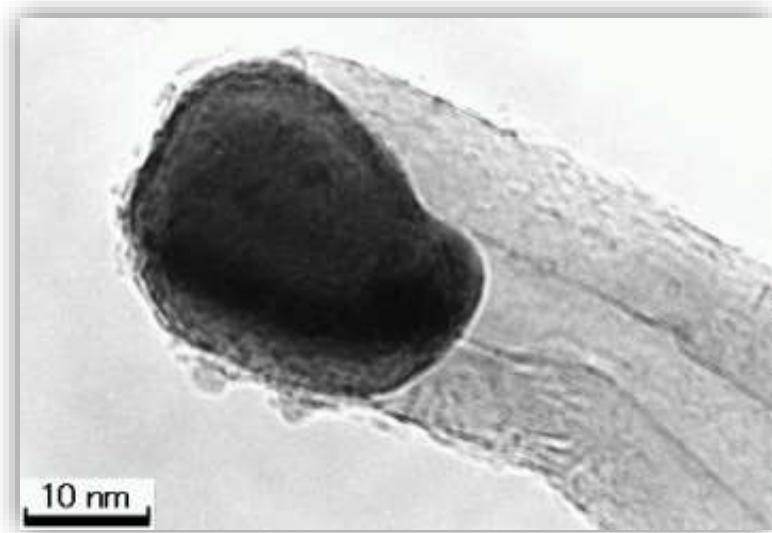
Applications

- CVD processes are used on a surprisingly wide range of industrial components, from aircraft and land gas turbine blades, timing chain pins for the automotive industry, radiant grills for gas cookers and items of chemical plant, to resist various attacks by carbon, oxygen and sulphur.
- Some important applications are listed below.
- Surface modification to prevent or promote adhesion
- Photoresist adhesion for semiconductor wafers Silane/substrate adhesion for microarrays (DNA, gene, protein, antibody, tissue)
- MEMS coating to reduce stiction
- BioMEMS and biosensor coating to reduce "drift" in device performance
- Promote biocompatibility between natural and synthetic materials
Copper capping Anti-corrosive coating

CVD

Advantages

- Easy to increase scale to industrial production
- Large length
- Simple to perform
- Pure product



Disadvantages

- Defects are common

http://endomoribu.shinshu-u.ac.jp/research/cnt/images/cat_cnt.jpg

Physical Vapour Deposition(PVD)

Introduction

1. Physical vapour deposition (PVD) is fundamentally a vaporisation coating technique, involving transfer of material on an atomic level. It is an alternative process to electroplating
2. The process is similar to chemical vapour deposition (CVD) except that the raw materials/precursors, i.e. the material that is going to be deposited starts out in solid form, whereas in CVD, the precursors are introduced to the reaction chamber in the gaseous state.

Working Concept

PVD processes are carried out under vacuum conditions. The process involved four steps:

1. Evaporation
2. Transportation
3. Reaction
4. Deposition



Evaporation

During this stage, a target, consisting of the material to be deposited is bombarded by a high energy source such as a beam of electrons or ions. This dislodges atoms from the surface of the target, ‘vaporising’ them.

Transport

This process simply consists of the movement of ‘vaporised’ atoms from the target to the substrate to be coated and will generally be a straight line affair.

Reaction

- In some cases coatings will consist of metal oxides, nitrides, carbides and other such materials.
 - In these cases, the target will consist of the metal.
 - The atoms of metal will then react with the appropriate gas during the transport stage.
 - For the above examples, the reactive gases may be oxygen, nitrogen and methane.
- In instances where the coating consists of the target material alone, this step would not be part of the process.

Deposition

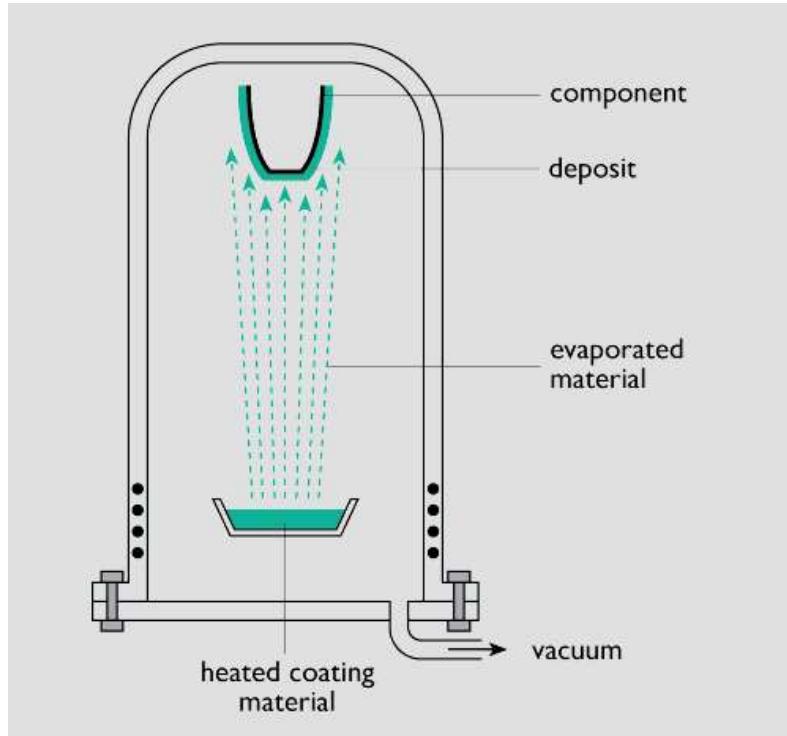
This is the process of coating build up on the substrate surface. Depending on the actual process, some reactions between target materials and the reactive gases may also take place at the substrate surface simultaneously with the deposition process.

Fig. shows a schematic diagram of the principles behind one common PVD method.

The component that is to be coated is placed in a vacuum chamber. The coating material is evaporated by intense heat from, for example, a tungsten filament.

An alternative method is to evaporate the coating material by a complex ion bombardment technique.

The coating is then formed by atoms of the coating material being deposited onto the surface of the component being treated.



The vacuum evaporation PVD process

Variants of PVD include, in order of increasing novelty:

Evaporative Deposition: In which the material to be deposited is heated to a high vapor pressure by electrically resistive heating in "high" vacuum.

Electron Beam Physical Vapor Deposition: In which the material to be deposited is heated to a high vapor pressure by electron bombardment in "high" vacuum.

Sputter Deposition: In which a glow plasma discharge (usually localized around the "target" by a magnet) bombards the material sputtering some away as a vapor.

Cathodic Arc Deposition: In which a high power arc directed at the target material blasts away some into a vapor.

Pulsed Laser Deposition: In which a high power laser ablates material from the target into a vapor.

Merits and Demerits of evaporation methods

Method	Merits	Demerits
E-Beam Evaporation	<ul style="list-style-type: none"> 1. high temp materials 2. good for liftoff 3. highest purity 	<ul style="list-style-type: none"> 1. some CMOS processes sensitive to radiation 2. alloys difficult 3. poor step coverage
Filament Evaporation	<ul style="list-style-type: none"> 1. simple to implement 2. good for liftoff 	<ul style="list-style-type: none"> 1. limited source material (no high temp) 2. alloys difficult 3. poor step coverage
Sputter Deposition	<ul style="list-style-type: none"> 1. better step coverage 2. alloys 3. high temp materials 4. less radiation damage 	<ul style="list-style-type: none"> 1. possible grainy films 2. porous films 3. plasma damage/contamination

Importance of PVD Coatings

- PVD coatings are deposited for numerous reasons. Some of the main ones are:
- Improved hardness and wear resistance
- Reduced friction
- Improved oxidation resistance
- The use of such coatings is aimed at improving efficiency through improved performance and longer component life.
- They may also allow coated components to operate in environments that the uncoated component would not otherwise have been able to perform.

Advantages

- Materials can be deposited with improved properties compared to the substrate material
- Almost any type of inorganic material can be used as well as some kinds of organic materials
- The process is more environmentally friendly than processes such as electroplating

Disadvantages

- It is a line of sight technique meaning that it is extremely difficult to coat undercuts and similar surface features
- High capital cost
- Some processes operate at high vacuums and temperatures requiring skilled operators
- Processes requiring large amounts of heat require appropriate cooling systems
- The rate of coating deposition is usually quite slow

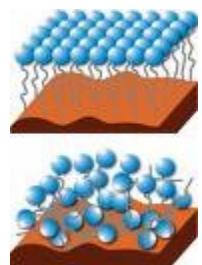
Applications

- PVD coatings are generally used to improve hardness, wear resistance and oxidation resistance.
- Thus, such coatings use in a wide range of applications such as:
- Aerospace
- Automotive
- Surgical/Medical
- Dies and moulds for all manner of material processing
- Cutting tools



LECTURE 55 SCANNING ELECTRON MICROSCOPE -SEM

SEM typically produce resolutions between 1 and 20nm



History of SEM

Limitation of light microscope in resolving fine details of organic cells provided the impetus to develop an electron microscope in the early twentieth century.

The first electron microscope was a transmission electron microscope developed by German scientist Max Knoll and electrical engineer Ernst Ruska in Germany in 1931.

German physicist Max Knoll introduced the concept of a scanning electron microscope in 1935 . He proposed that an image can be produced by scanning the surface of a sample with a finely focused electron beam. Another German physicist Manfred von Ardenne explained the principles of the technique and elaborated upon beam-specimen interactions. He went on to produce the earliest scanning electron microscope in 1937 .



**Davisson-Germer experiment confirm that
Electron do diffract as a wave and it varifies
the De Broglie relation**

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

**And we know that resolution is directly
proportional to wavelength. This is physics
behind any electron microscopy.**

For example, an electron beam (λ of 0.000004 μm) with an accelerating voltage of 100 kV can achieve a resolution of 0.24 nm. The practical limit to resolution is determined by lens aberrations and defects.

SEM

Just like any microscope, the primary function of the scanning electron microscope (SEM) is to enlarge small features or objects otherwise invisible to human sight.

It does that by way of using electron beam rather than light which is used to form images in optical light microscopes. The images are obtained by scanning an electron beam of high energy on the sample surface, hence the name scanning electron microscope.

By virtue of its smaller wavelength, electrons are able to resolve finer features/details of materials to a much greater extent compared with optical light.



SEM

The scanning electron microscope (SEM) is one of the most versatile instruments available for the examination and analysis of the microstructural characteristics of solid objects.

The primary reason for the SEM's usefulness is the high resolution which can be obtained when bulk objects are examined; values of the order of 10 nm (100 Å) are usually quoted for commercial instruments.



Comparision with Other Microscopy

Characteristics	Light microscope	Scanning electron microscope	Transmission electron microscope
Radiation used to form an image	Visible light	Electrons	Electrons
Wavelength of radiation	380–760 nm depending on the color of light	0.008 nm at 20 kV accelerating voltage ^a	0.0028 nm at 200 kV accelerating voltage ^a
Types of lenses used to focus the radiation	Glass	Electromagnetic	Electromagnetic
Useful magnification	1,000×	200,000×	2,000,000×
Possible magnification	Up to 2,000×	1,000,000×	10,000,000 or more
Magnification mode	With lenses	Without lenses	With lenses
Resolution	200 nm	1 nm	0.1 nm
Source of radiation	Tungsten-halogen lamp	Electron gun/emitter	Electron gun/emitter



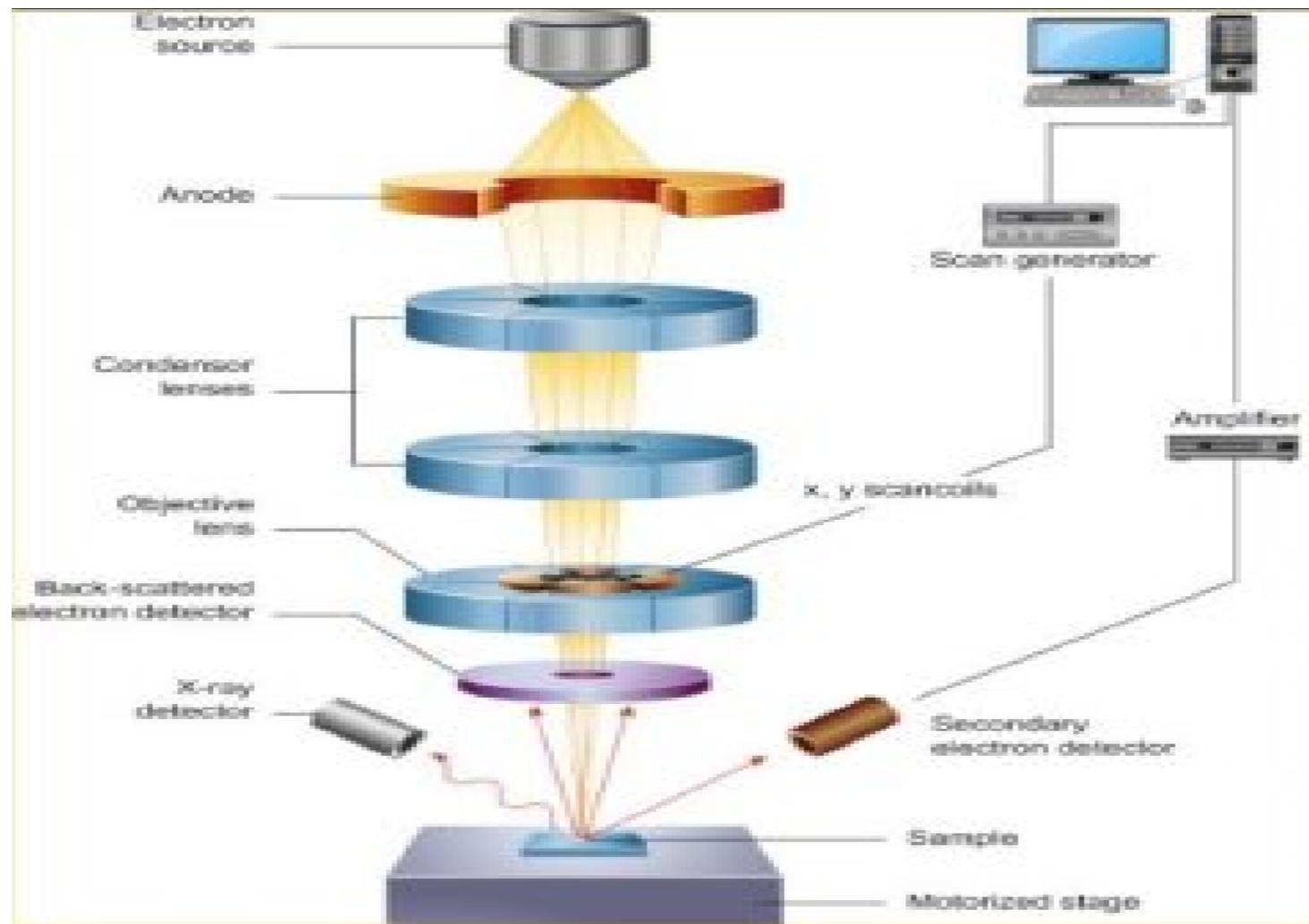
Scanning Electron Microscope (SEM)

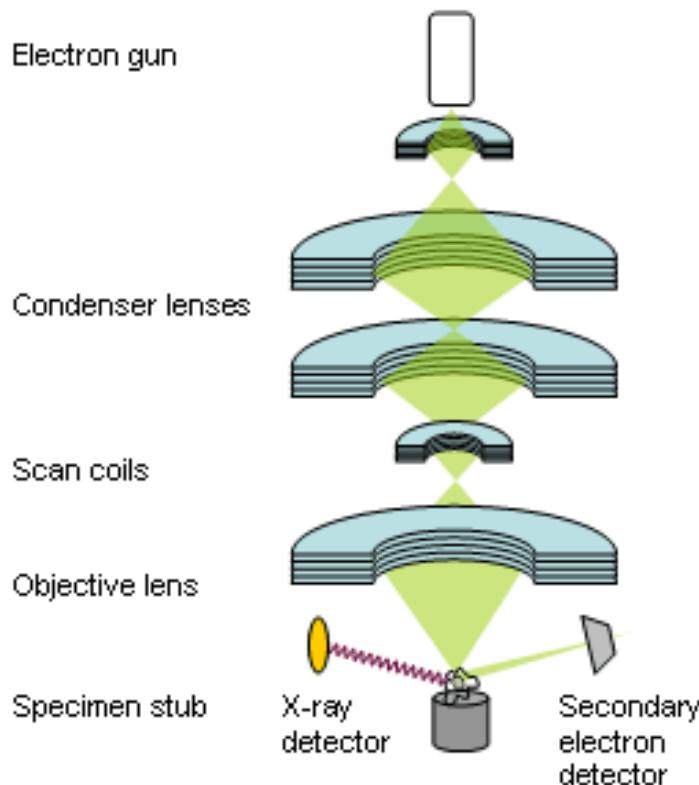
Working Concept

- + **SEM** allows surfaces of objects to be seen in their natural state without staining.
- + The specimen is put into the vacuum chamber and covered with a thin coating of gold to increase electrical conductivity and thus forms a less blurred image.
- + The electron beam then sweeps across the object building an image line by line as in a TV Camera.
- + As electrons strike the object, they knock loose showers of electrons that are captured by a detector to form the image.



SEM diagram





Working concept of SEM



- The "Virtual Source" at the top represents the electron gun, producing a stream of monochromatic electrons.
- The stream is condensed by the first condenser lens (usually controlled by the "coarse probe current knob").
- This lens is used to both form the beam and limit the amount of current in the beam.
- It works in conjunction with the condenser aperture to eliminate the high-angle electrons from the beam
- The beam is then constricted by the condenser aperture, eliminating some high-angle electrons
- The second condenser lens forms the electrons into a thin, tight, coherent beam and is usually controlled by the "fine probe current knob"



- A set of coils then "scan" or "sweep" the beam in a grid fashion (like a television), dwelling on points for a period of time determined by the scan speed (usually in the microsecond range)
- The final lens, the Objective, focuses the scanning beam onto the part of the specimen desired.
- When the beam strikes the sample (and dwells for a few microseconds) interactions occur inside the sample and are detected with various instruments
- Before the beam moves to its next dwell point these instruments count the number of interactions and display a pixel on a CRT whose intensity is determined by this number (the more reactions the brighter the pixel).
- This process is repeated until the grid scan is finished and then repeated, the entire pattern can be scanned 30 times per second.



Specimen Interactions and utilization:

Backscattered Electrons

Formation

- Caused by an incident electron colliding with an atom in the specimen which is nearly normal to the incident's path.
- The incident electron is then scattered "backward" 180 degrees.

Utilization

- The production of backscattered electrons varies directly with the specimen's atomic number.
- This differing production rates causes higher atomic number elements to appear brighter than lower atomic number elements.
- This interaction is utilized to differentiate parts of the specimen that have different average atomic number.



Secondary Electrons Source

- ▶ Caused by an incident electron passing "near" an atom in the specimen, near enough to impart some of its energy to a lower energy electron (usually in the K-shell).
- ▶ This causes a slight energy loss and path change in the incident electron and the ionization of the electron in the specimen atom.
- ▶ This ionized electron then leaves the atom with a very small kinetic energy (5eV) and is then termed a "secondary electron".
- ▶ Each incident electron can produce several secondary electrons.



Utilization

- Production of secondary electrons is very topography related.
- Due to their low energy, 5eV, only secondaries that are very near the surface ($<10\text{nm}$) can exit the sample and be examined.
- Any changes in [topography](#) in the sample that are larger than this sampling depth will change the yield of secondaries due to collection efficiencies.
- Collection of these electrons is aided by using a "collector" in conjunction with the secondary electron detector.
- The collector is a grid or mesh with a +100V potential applied to it which is placed in front of the detector, attracting the negatively charged secondary electrons to it which then pass through the grid-holes and into the detector to be counted.



Auger Electrons

Source

- Caused by the de-energization of the specimen atom after a secondary electron is produced.
- Since a lower (usually K-shell) electron was emitted from the atom during the secondary electron process an inner (lower energy) shell now has a vacancy.
- A higher energy electron from the same atom can "fall" to a lower energy, filling the vacancy.
- This creates an energy surplus in the atom which can be corrected by emitting an outer (lower energy) electron; an Auger Electron.



Utilization

- Auger Electrons have a characteristic energy, unique to each element from which it was emitted from.
- These electrons are collected and sorted according to energy to give compositional information about the specimen



X-rays

Source

- Caused by the de-energization of the specimen atom after a secondary electron is produced.
- Since a lower (usually K-shell) electron was emitted from the atom during the secondary electron process an inner (lower energy) shell now has a vacancy.
- A higher energy electron can "fall" into the lower energy shell, filling the vacancy.
- As the electron "falls" it emits energy, usually X-rays to balance the total energy of the atom so it .
- X-rays or Light emitted from the atom will have a characteristic energy which is unique to the element from which it originated.



SEM Uses

SEM images provide information on:

Topography

Composition

Morphology

Topography is the distribution of features or parts on a surface of a sample.

Composition is what a sample is made of.

Morphology is the form, shape or structure of a sample

Strengths of the SEM

Strengths of the SEM include:

1. A wide variety of specimens can be examined.
2. Relatively easy and quick sample preparation.
3. Ease of use due to user-friendly and automated equipment.
4. Rapid imaging, quick results, time-efficient analysis, and fast turnaround time.
5. Relatively straightforward image interpretation.
6. Large depth of field (ability to focus large depths of samples at one time and produce 3-D like images)
7. Microchemical analysis capability from Be to U.
8. Samples can be dry or wet.
9. Nondestructive (some beam damage may result).

Applications of SEM

Biological Sciences

Uses for SEM in biological sciences include identification of bacterial strains and testing vaccines.

It is also applied in genetics.

SEM can also help to measure the effect of climate change on different species, and to uncover new species.

Forensics

SEM is a reliable method for analysing gunshot residue, and for analysing paint particles and fibres at crime scenes.

Geological Sampling

A scanning electron microscope can identify compositional differences of soil and rock samples, and determine the effects of weathering on materials.

Applications of SEM

Medical Science

SEM is used as a technique to compare blood and tissue samples in patient and control test groups.

It can help to identify viruses and diseases, and to test new medicines.

Electronics

- *SEM supports microchip assembly by enabling detailed examination of designs, and assisting in the development of new fabrication and production methods.*
- *As microchip assembly materials get progressively smaller, the high-resolution capabilities of SEM have become indispensable in design, research and development processes.*
- *The topographical information SEM provides is also essential for inspecting and testing semiconductors for reliability and performance.*
- *Scanning electron microscopes are essential in the quality control process.*



Applications of SEM

Materials Science

In materials science, SEM is applied across a broad range of areas and disciplines, from aerospace and chemistry to energy and electronics.

Applications include research into alloys, mesoporous architectures, nanotubes and nanofibres.

Microscopic Quality Control

- **Much modern development and research across different industries increasingly requires microscopic levels of precise quality control.**



Limitations of SEM

Limitations can be summarized as follows:

1. The sample size is limited.
2. Samples are solid.
3. EDS detector cannot detect H, He, or Li.
4. Poor detectability limit of elements (with EDS) compared to wet analytical methods.
5. Samples need to be examined under vacuum.
6. The instrument typically requires an installation space of 5' 5 m.
7. Non-conductive samples need to be coated.

**DEPARTMENT OF PHYSICS AND NANOTECHNOLOGY
SRM INSTITUTE OF SCIENCE AND TECHNOLOGY**

**21PYB102J –Semiconductor Physics and Computational
Methods
Module-V Lecture-57**

**ELECTRON MICROSCOPY-TRANSMISSION ELECTRON
MICROSCOPE (TEM)
AND ATOMIC FORCE MICROSCOPE (AFM)**

Transmission Electron Microscopy (TEM)

Basic Electron Optics

- Electrons and ions are charged particles; they can be accelerated in an electric field
- The trajectory of an accelerated charged particle can be changed (deflected) by E and/ or B field.
- The accelerated particles also behave like waves (de Broglie)



□Transmission Electron Microscope (TEM) Working Concept

- TEM works much like a slide projector.
- A projector shines a beam of light through (transmits) the slide, as the light passes through it is affected by the structures and objects on the slide.
- These effects result in only certain parts of the light beam being transmitted through certain parts of the slide.
- This transmitted beam is then projected onto the viewing screen, forming an enlarged image of the slide.
- TEMs work the same way except that they shine a beam of electrons (like the light) through the specimen (like the slide).
- Whatever part is transmitted is projected onto a phosphor screen for the user to see.

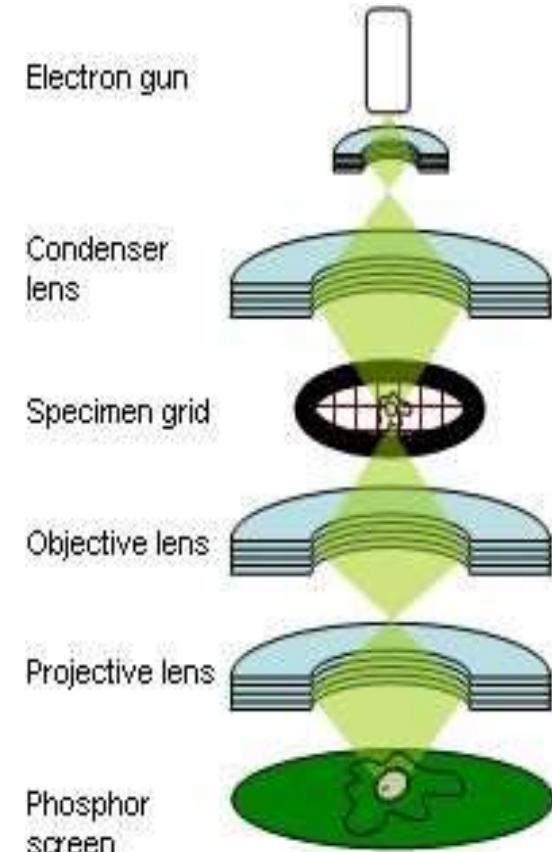
Common Modes of Operation of TEM

- **Bright Field (BF) Microscopy**
- **Selected Area Diffraction**
- **Dark Field (DF)**



Construction and working

1. The virtual source at the top represents the electron gun, producing a stream of monochromatic electron.
2. The stream is focused to a small, thin coherent beam by condenser lens 1 & 2. First one decides the size and second one decides the brightness
3. The beam strikes the specimen and parts are transmitted. The transmitted position is focussed by objective lens into an image.
4. The image is passed down the column through the projector lenses being enlarged and finally strikes the phosphor screen where light is generated, allowing the user to see the image



Unscattered electrons:

Incident electrons which gets transmitted through the specimen without interacting with the sample

Utilization:

Thicker sample- fewer transmitted electrons-appear darker

Thinner sample- more transmission- appear brighter

Elastically scattered electrons:

Incident electrons which gets scatterred by the atoms in the sample elastically (no loss of energy). Then they are transmitted

Utilization:

All electrons follow Braggs condition for scattering

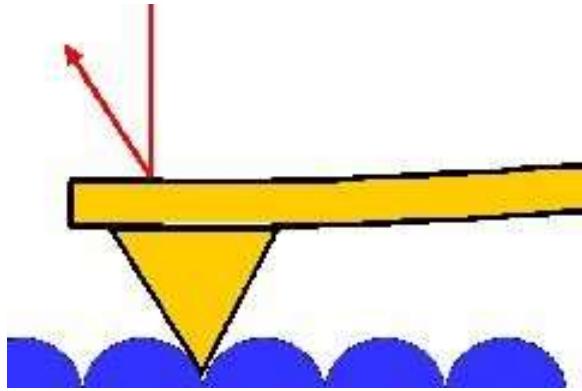
Inelastically Scattered Electrons :

Incident electrons interact with the sample inelastically (loss of energy) and gets transmitted into the specimen

Kakuchi Bands: - Bands of alternating light and dark lines that are formed by inelastic scattering interactions that are related to atomic spacings in the specimen

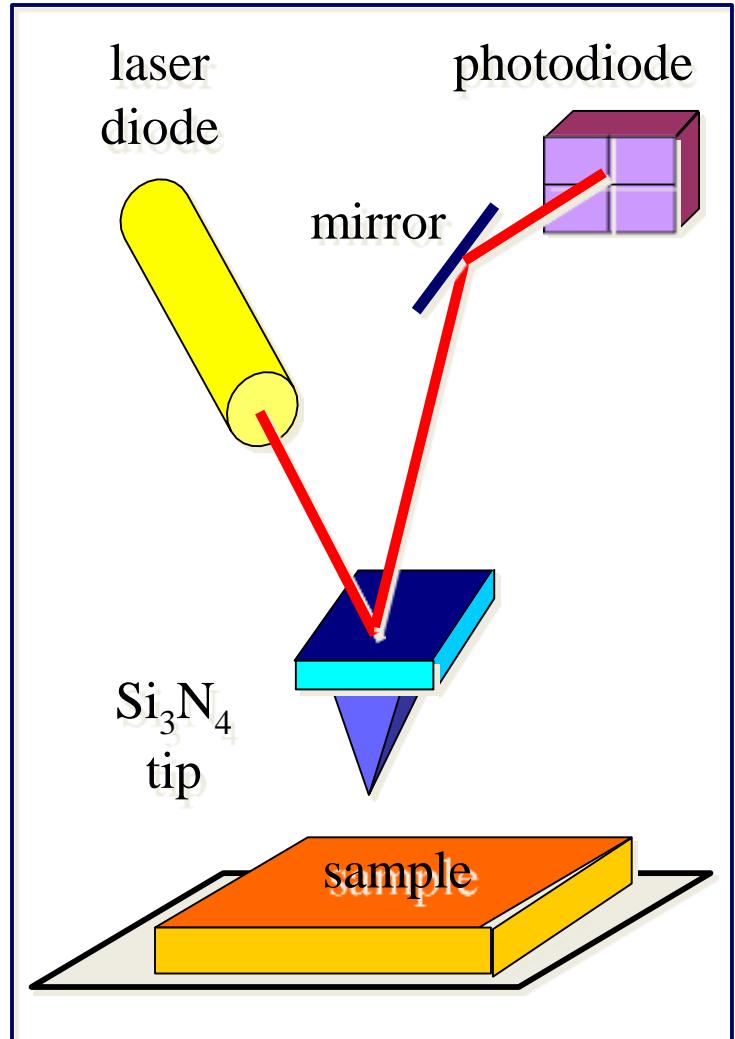


How does the microscope work?



Tip Scans Sample

Up & down movement of the tip is
recorded by position sensing
photodiode

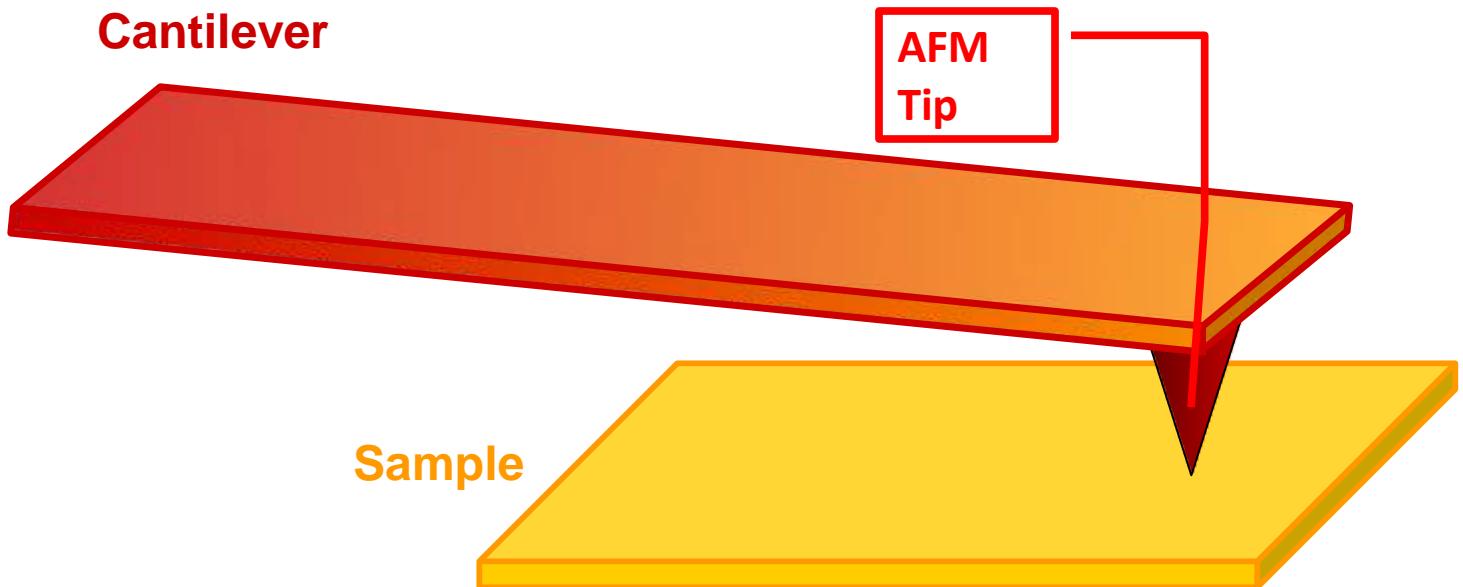


Scanning Probe Microscopy—the Atomic Force Microscope (AFM)

The AFM like the STM is a scanning microscope, but the mechanism depends on the force of attraction between molecules

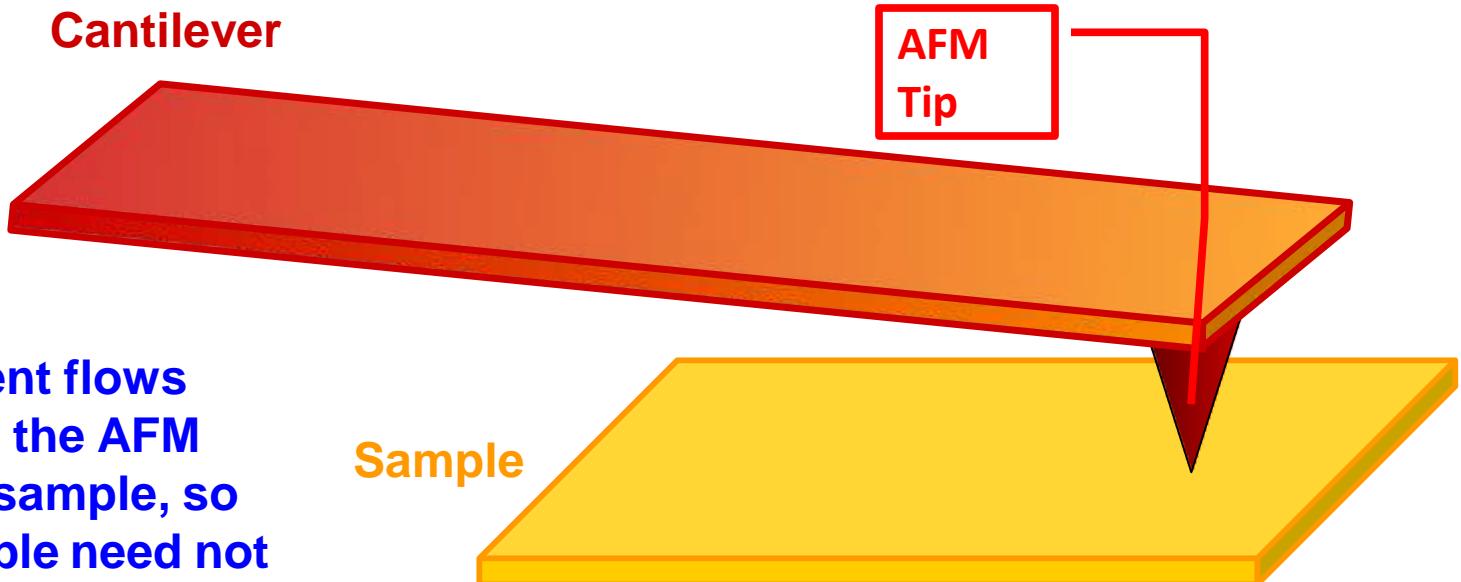
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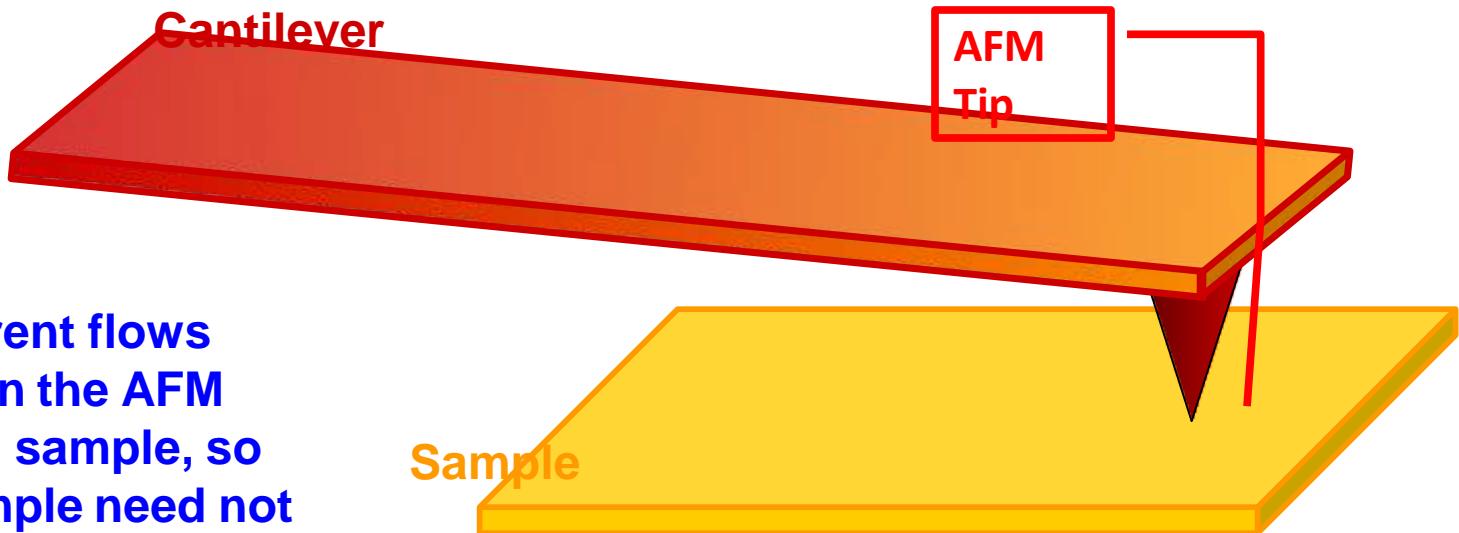
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No current flows between the AFM Tip and sample, so the sample need not be conducting [a requirement for the STM].

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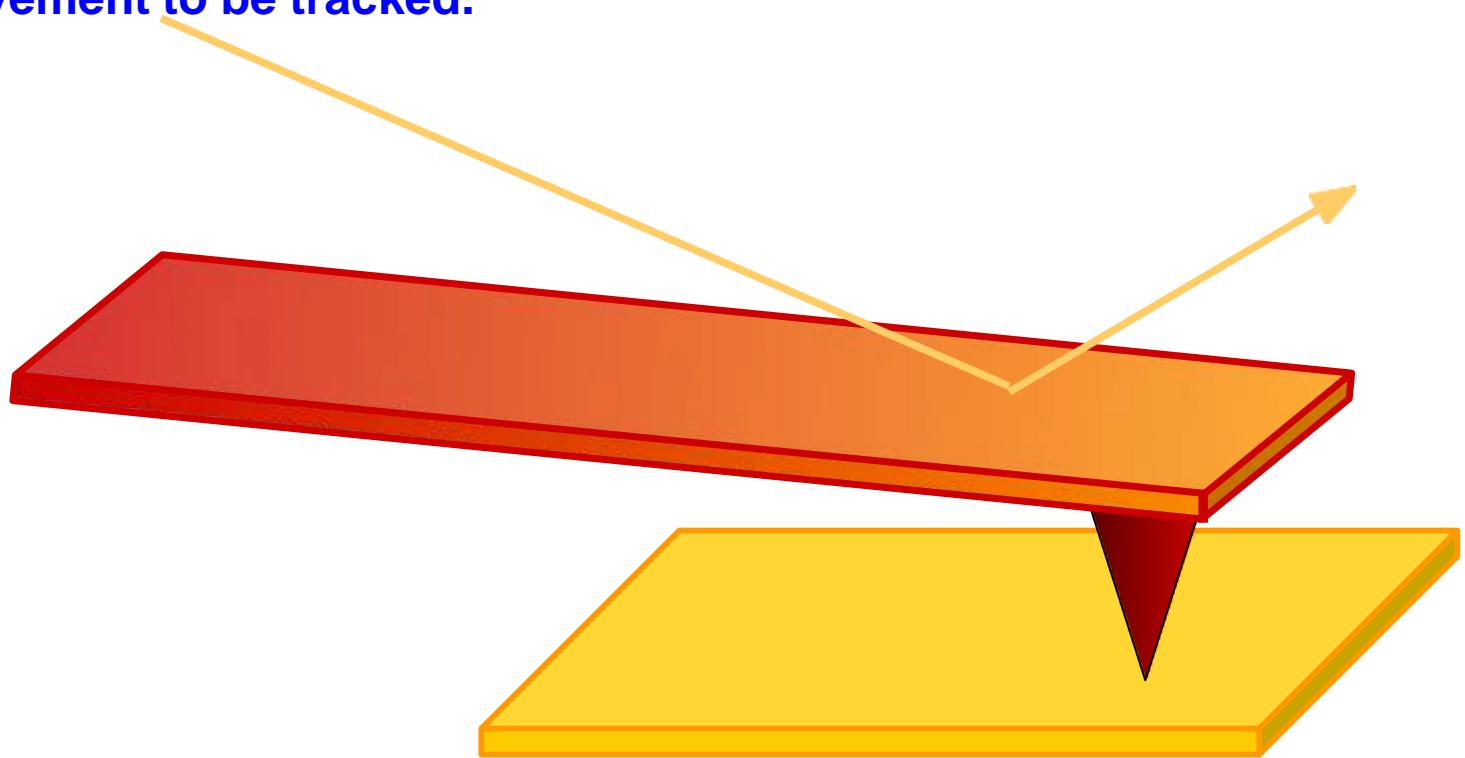
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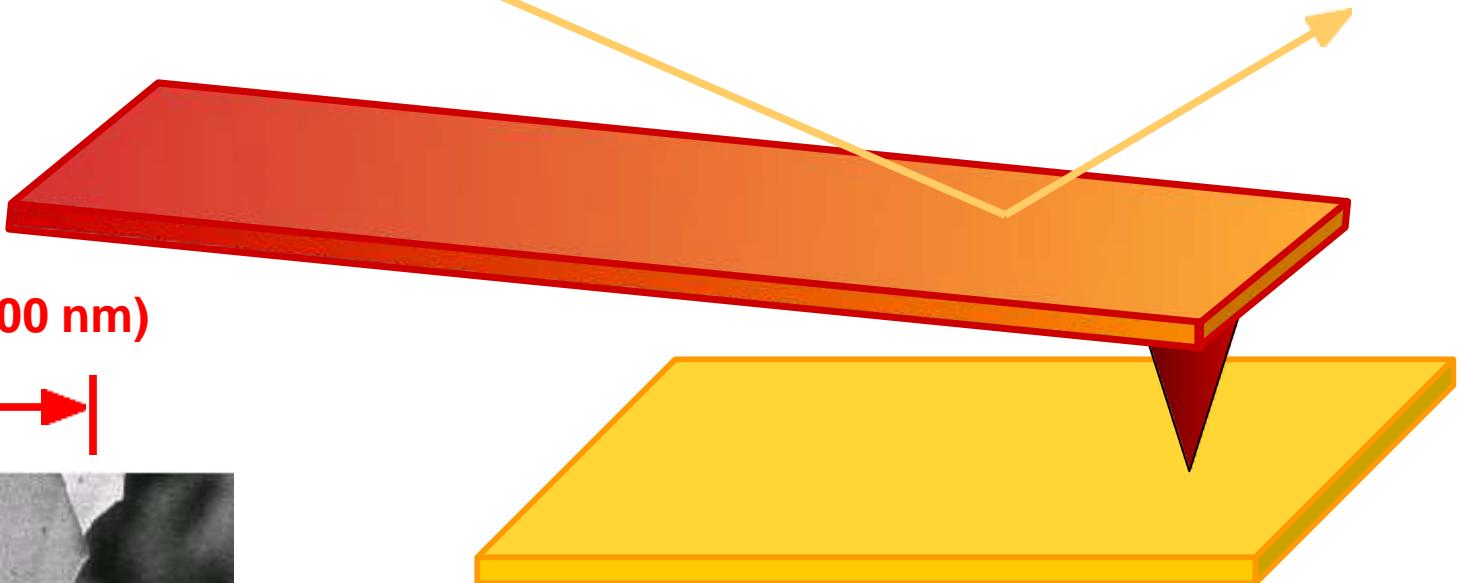
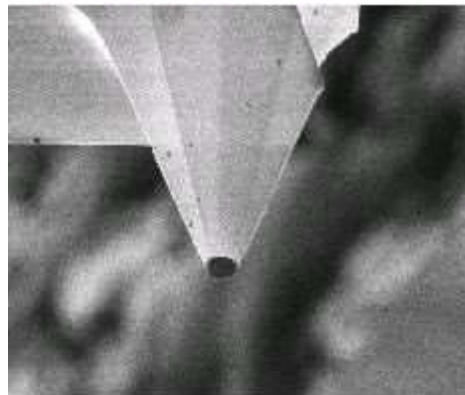
The atoms of the Tip are attracted to the atoms of the sample by the van der Waals interaction.

As the AFM tip is attracted to the surface (causing the cantilever to bend), a laser beam bounces off the end of the cantilever—allowing the tip's movement to be tracked.



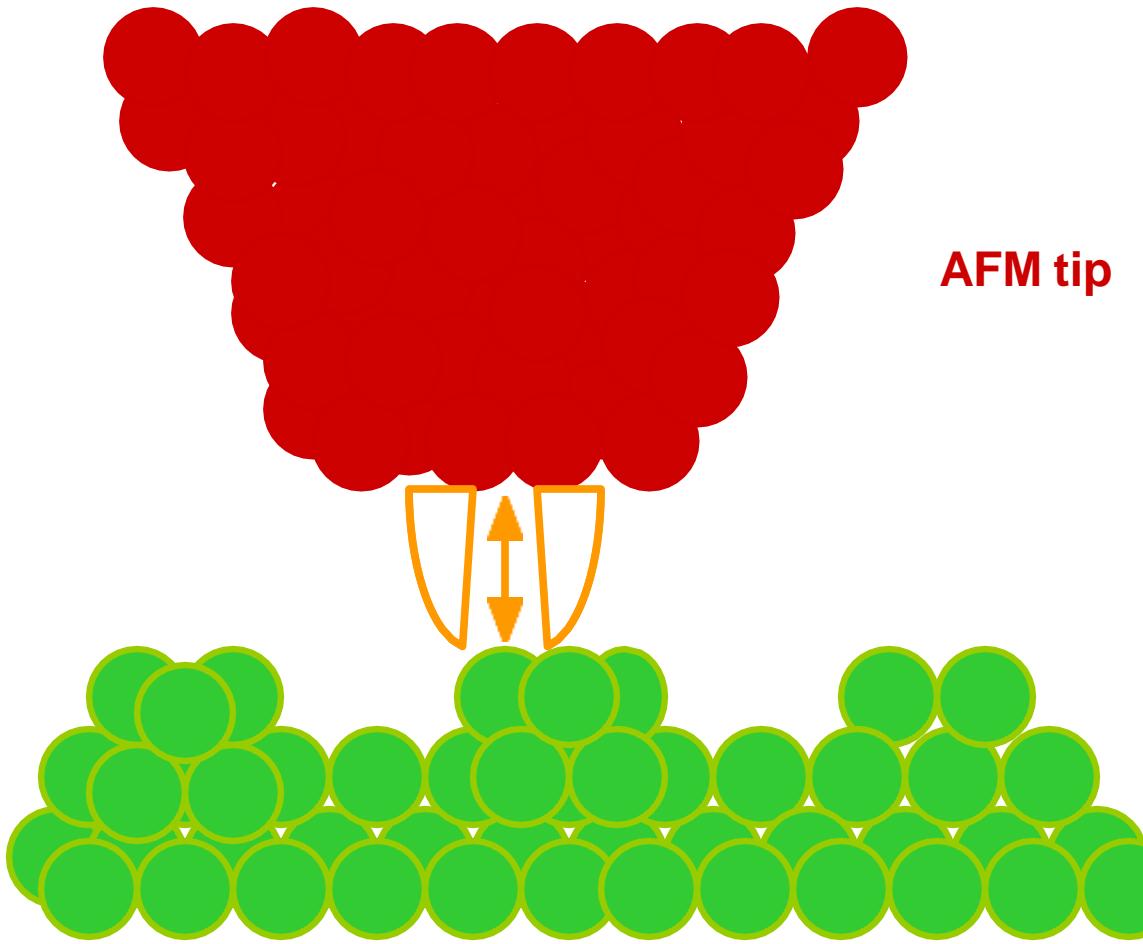
As the AFM tip is attracted to the surface (causing the cantilever to bend), a laser beam bounces off the end of the cantilever—allowing the tip's movement to be tracked.

~1 μm (1000 nm)

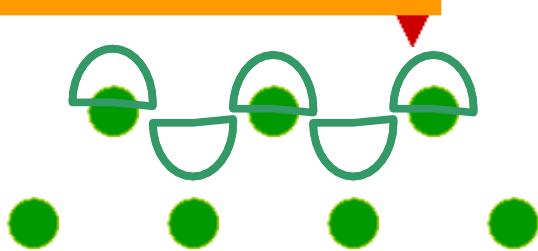


The cantilever is visible to the naked eye but the AFM tip is too small to see without magnification.

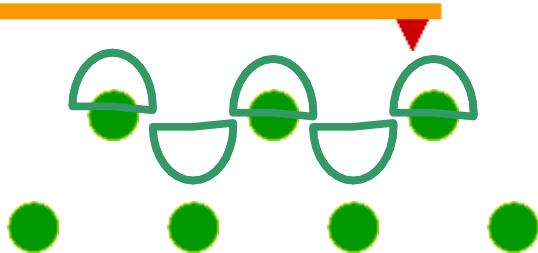
Surface of
sample



The attractive van der Waals interaction acts at a molecular and atomic level, between the AFM tip and the local atoms at the sample's surface.



As the AFM tip scans the surface, its up and down motions map the contour of the sample—scanned line by line.

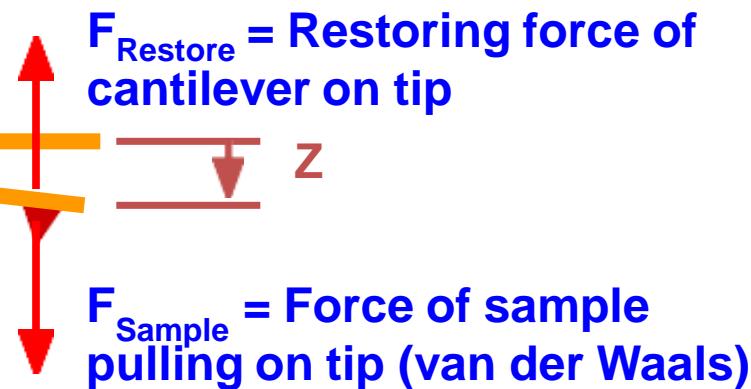


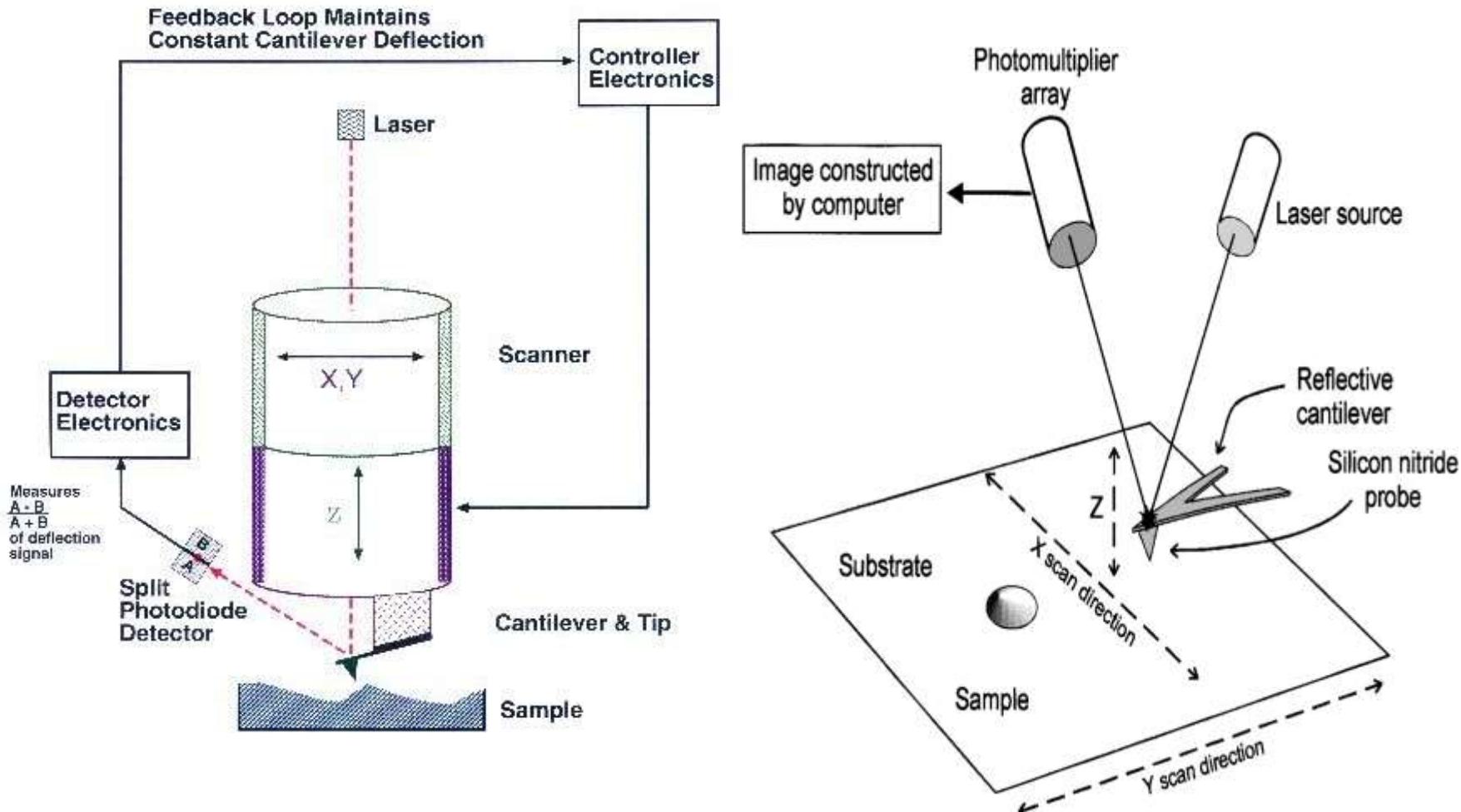
As the AFM tip scans the surface, its up and down motions map the contour of the sample—scanned line by line.

The force on the AFM tip is harmonic (spring like): the tip is displaced toward the surface a distance (Z) proportional to the van der Waals force.

$$F_{\text{Restore}} = -kZ$$

$k \sim 1 \text{ N/m} \Rightarrow$ An AFM can measure forces of pN (10^{-12} Newton) & even fN (10^{-15} N) size!





IMAGING METHODS

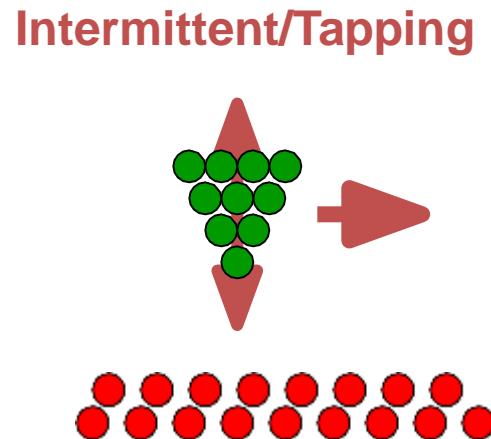
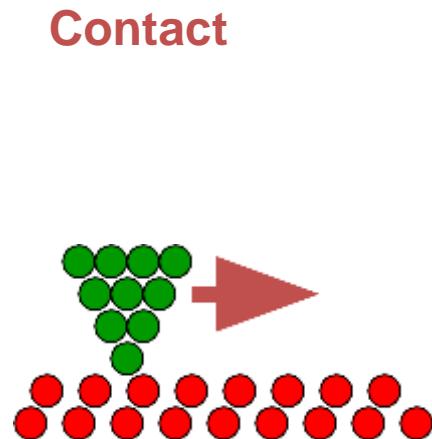
What types of forces are measured ?

- Modes of operation
 - contact
 - noncontact
 - tapping

The AFM can operate in three different ways

Contact Mode—the tip is dragged along a sample's surface; the cantilever deflection is measured and translated into surface shapes. Take care: this mode can damage the surface.

1. **Non-contact mode**—the cantilever oscillates above the sample's surface and is affected by surface/tip forces (van der Waals) as it does so.
2. **Tapping Mode**—The AFM tip taps the sample surface during the closest point of approach of an oscillation cycle.



ADVANTAGES AND DISADVANTAGES

CONTACT MODE- Fast scanning, good for rough samples

But deforms soft samples

TAPPING MODE- good for biological samples

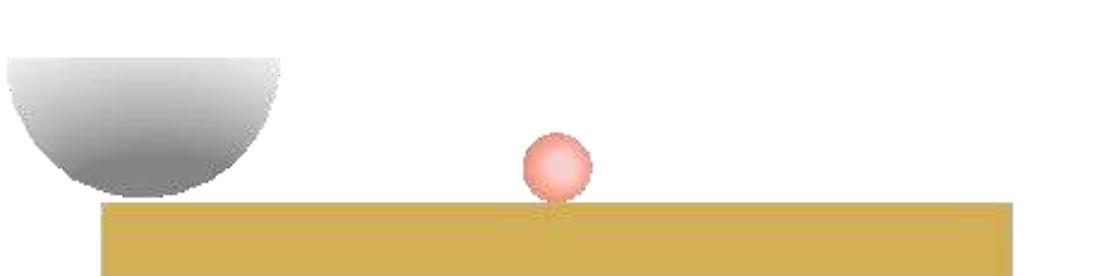
Slow scan speed and challenging in liquids

NON-CONTACT MODE-low force exerted on the sample

Low resolution contaminant layer can interfere usually need UHV system for good imaging

LIMITATIONS OF AFM

- Used to study variety of samples
- Does not require a conducting sample
- Does not reflect the true sample topography
- But represents the interaction between the tip and the surface called TIP CONVOLUTION



*Tip broadening – radius of curvature of the tip > size of the feature to be imaged

*As the tip scans the sides of the tip make contact before the apex and the microscope begins to respond to the feature

- **Advantages**

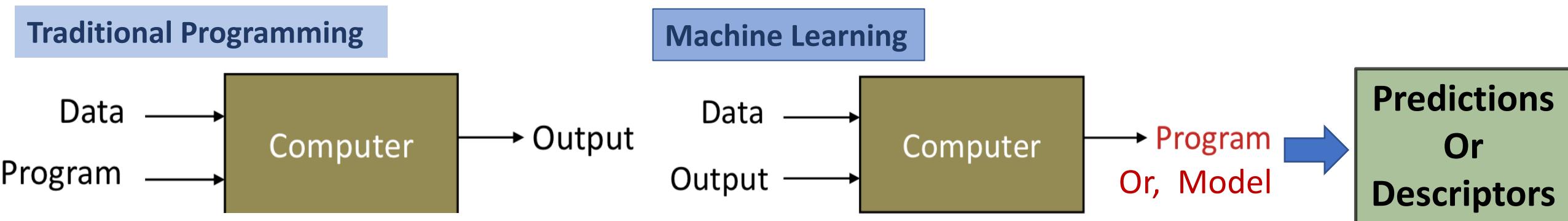
- The AFM has several advantages over the scanning electron microscope (SEM).
- Unlike the electron microscope which provides a two-dimensional projection or a two-dimensional image of a sample, the AFM provides a **true three-dimensional surface profile**.
- Additionally, samples viewed by AFM **do not** require any special treatments (such as metal/carbon coatings) that would irreversibly change or damage the sample.
- While an electron microscope needs an expensive **vacuum** environment for proper operation, most AFM modes can work perfectly **well** in ambient air or even a liquid environment.
- This makes it possible to study biological macromolecules and even living organisms.
- In principle, AFM can provide higher resolution than SEM. It has been shown to give true atomic resolution in ultra-high vacuum (UHV).

- **Disadvantages**

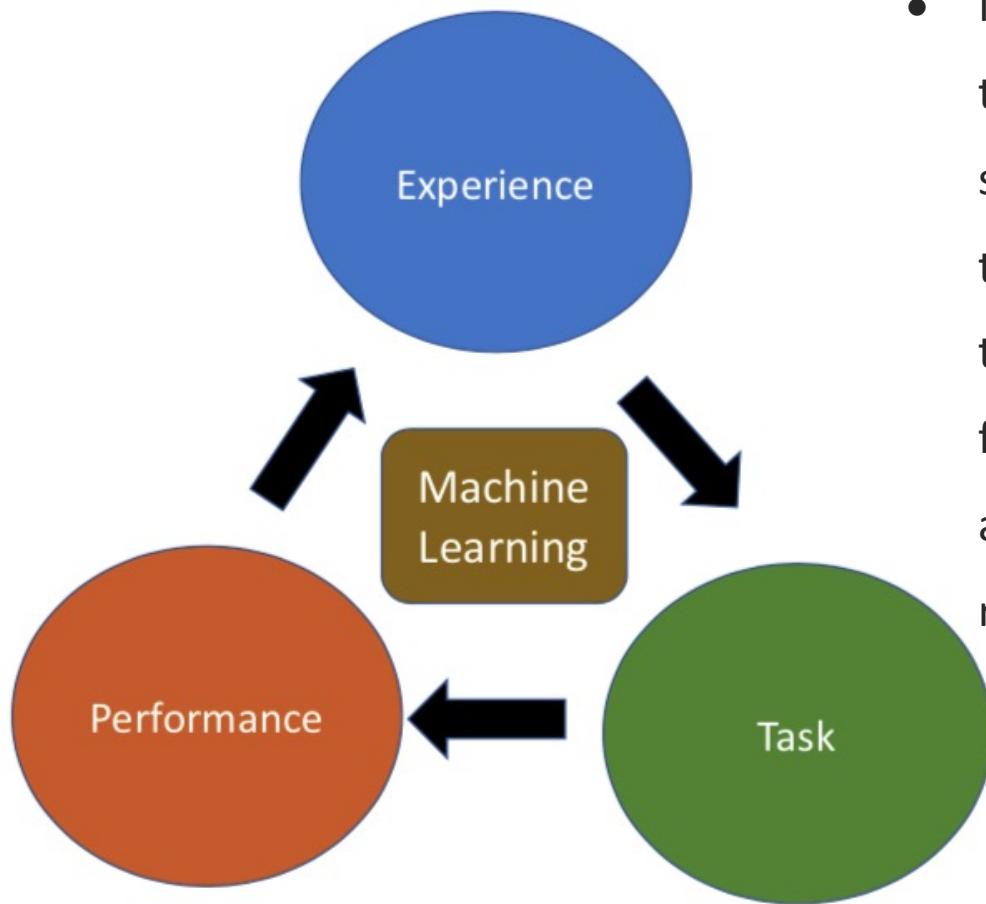
- A disadvantage of AFM compared with the **scanning electron microscope (SEM)** is the image size.
- The SEM can image an area on the order of **millimeters** by millimeters with a **depth of field** on the order of millimeters.
- The AFM can only image a maximum height on the order of micrometers and a maximum scanning area of around 150 by 150 micrometers.
- Another inconvenience is that at high resolution, the **quality of an image** is limited by the **radius of curvature** of the probe tip, and an incorrect choice of tip for the required resolution can lead to image artifacts.
- Slow scan and less scanner area
- Artefacts/Hystersis effects or cross-talk influences the image

Current computational and machine learning approach for as an electron microscopy image processing using Graphene

What is machine learning? (Ref: <https://mitsloan.mit.edu/ideas-made-to-matter/machine-learning-explained>)



- Machine learning (ML) is a subfield of artificial intelligence, which is broadly defined as the capability of a machine to imitate intelligent human behavior. Artificial intelligence (AI) systems are used to perform complex tasks in a way that is similar to how humans solve problems.
- The goal of AI is to create computer models that exhibit “intelligent behaviors” like humans, according to [Boris Katz](#), a principal research scientist and head of the InfoLab Group at CSAIL. This means machines that can recognize a visual scene, understand a text written in natural language, or perform an action in the physical world.
- Machine learning is one way to use AI. It was defined in the 1950s by AI pioneer [Arthur Samuel](#) as “the field of study that gives computers the ability to learn without explicitly being programmed.”



- Machine learning starts with data — numbers, photos, or text, like bank transactions, pictures of people, repair records, time series data from sensors, or sales reports. The data is gathered and prepared to be used as training data, or the information the machine learning model will be trained on. The more data, the better the program. Some data is held out from the training data to be used as evaluation data, which tests how accurate the machine learning model is when it is shown new data. The result is a model that can be used in the future with different sets of data.

Machine learning working principle has been shown. The algorithms are design to work in three steps.

1. The computer has been asked to perform a task
2. The task performance will be evaluated, and a reward will be given
3. With the reward the computer will gain experience and finally with the experience gain it will perform the task again

This cycle will go on a training data and computer will build a model. Finally, the model will be tested in a training set for prediction and validation.

Machine Learning in Materials Science

- **Supervised learning**
 - Prediction
 - Classification (discrete labels), Regression (real values)
- **Unsupervised learning**
 - Clustering
 - Probability distribution estimation
 - Finding association (in features)
 - Dimension reduction
- **Reinforcement learning**
 - Decision making (robot, chess machine)

Unsupervised Learning

Dataset: Only the inputs are known

Objective: Train a model to find existing patterns in the data to learn more about it.

Association

We want to discover rules that describes our data
e.g. material which is soluble in water, also soluble in kerosene.

Clustering

We want to discover the inherent categories in the data.
e.g. grouping of materials by their solubility.

Supervised Learning

Dataset: Has example inputs and outputs

Objective: Train a model to predict outputs from feature inputs.

Classification

The output variable is a category. e.g.
[spin up/spin down] or
[ferromagnetic/paramagnetic/diamagnetic]

Regression

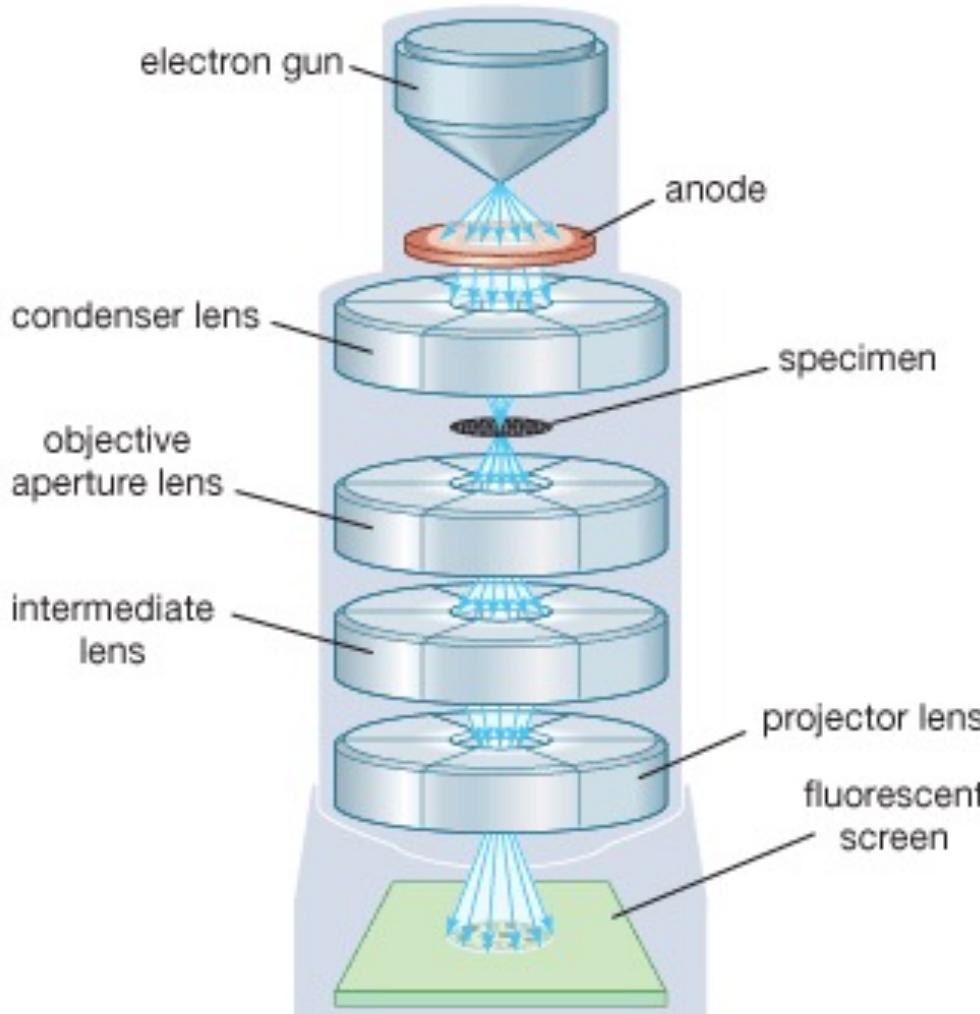
Attempts to determine the relationship between one dependent variable and a series of independent variables.

Ref: [1] Bishop CM. Pattern recognition and machine learning. New York: Springer; 2007.

- There are four types of machine learning that are commonly used in scientific fields
 - Unsupervised learning: In unsupervised learning, the agent learns patterns in the input, even when no explicit feedback is supplied. Clustering is a common example of an unsupervised task, which detects meaningful clusters among input data. For example, a regular office goer, Mr. Neogy, traveling from one area to the other in New York City, will develop a concept or percept of “good traffic days” and “bad traffic days” based on day to day experiences, without ever consulting motor vehicles department or traffic controllers for labelled examples of each.
 - Supervised learning: In this mode, the agent learns from a function that maps the input output pairs from some observed instances present in the data. In Mr. Neogy’s case, inputs are percepts about traffic conditions that he has developed over time and outputs are provided by him, where he gives directions to the cab-driver. Besides the inputs provided by Mr. Neogy, here the cab-driver can also alter the outcome based on let’s say if he passes a bus or a car or a pedestrian on the road and decides to take a different route or more time. Now, Mr. Neogy’s final outcome of reaching office on time or late is a function of states such as his own perceptions as well as the cab driver’s actions like braking, accelerating or stopping distance. The output is directly available from the agent’s percepts, the cab-driver is the environment and the final outcome can be changed if either the percept or environment changes.

- Semi-supervised learning: In this mode, we are given a few labelled instances and a large set of unlabeled ones. Let's assume, we are given a task of creating a model to predict what type of coffee a person drinks on a regular basis. We can gather some data (labelled examples) by interviewing people and / or by visiting multiple coffee shops, which would be identical to supervised learning. However, in reality, some of the people interviewed may not be truthful in their responses. Furthermore, the collected data may be inaccurate for other reasons, e.g., people not knowing specific coffee types and naming different coffee brands instead. Therefore, there is not only random noise in the data, but there are systematic inaccuracies present that can only be identified by utilizing unsupervised learning techniques. In other words, noise and lack of labelled instances create a continuum between supervised and unsupervised learning modes, which constitutes the domain of applicability of semi-supervised approaches.
- Reinforcement learning: This is another hybrid mode in which the agent learns from a series of past events or reinforcements (success or failure). Here, the model gets either rewards or penalties for the actions it performs, such as searches or trials, with a goal to maximize the total reward. For example, if Mr. Neogy reaches his office on time, that gives him an indication that he did something right along the way. It then falls on the agent to decide which of the actions prior to reinforcement had the most pronounced impact on the outcome.

What is electron microscopy? (Ref: <https://www.thermofisher.com/us/en/home/materials-science/learning-center/applications/sem-tem-difference.html>)

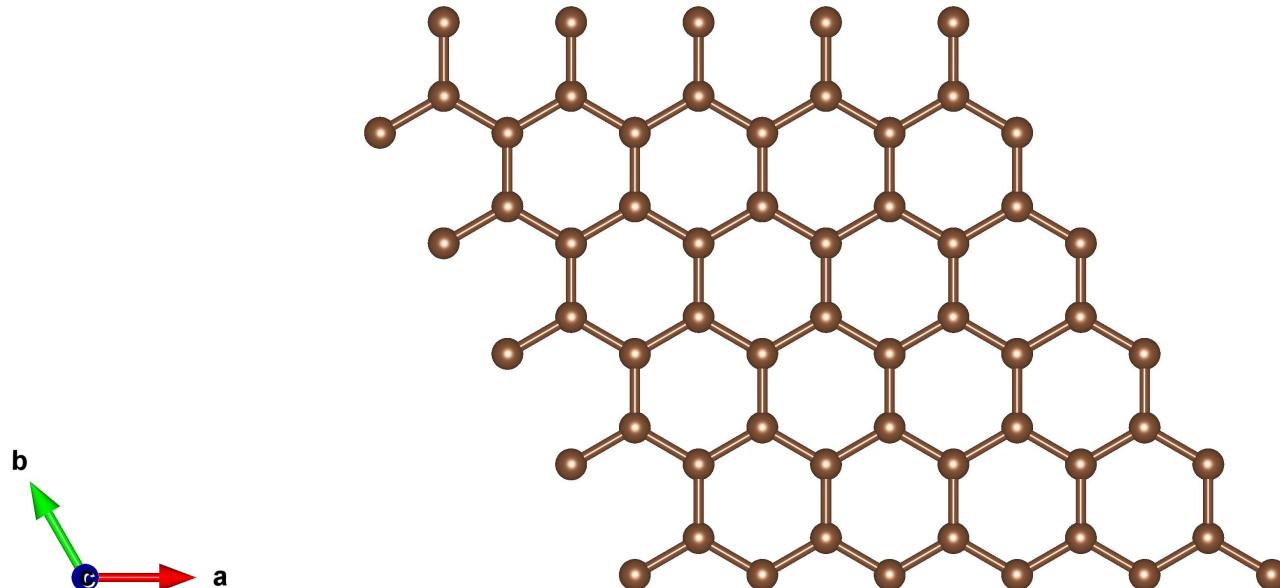


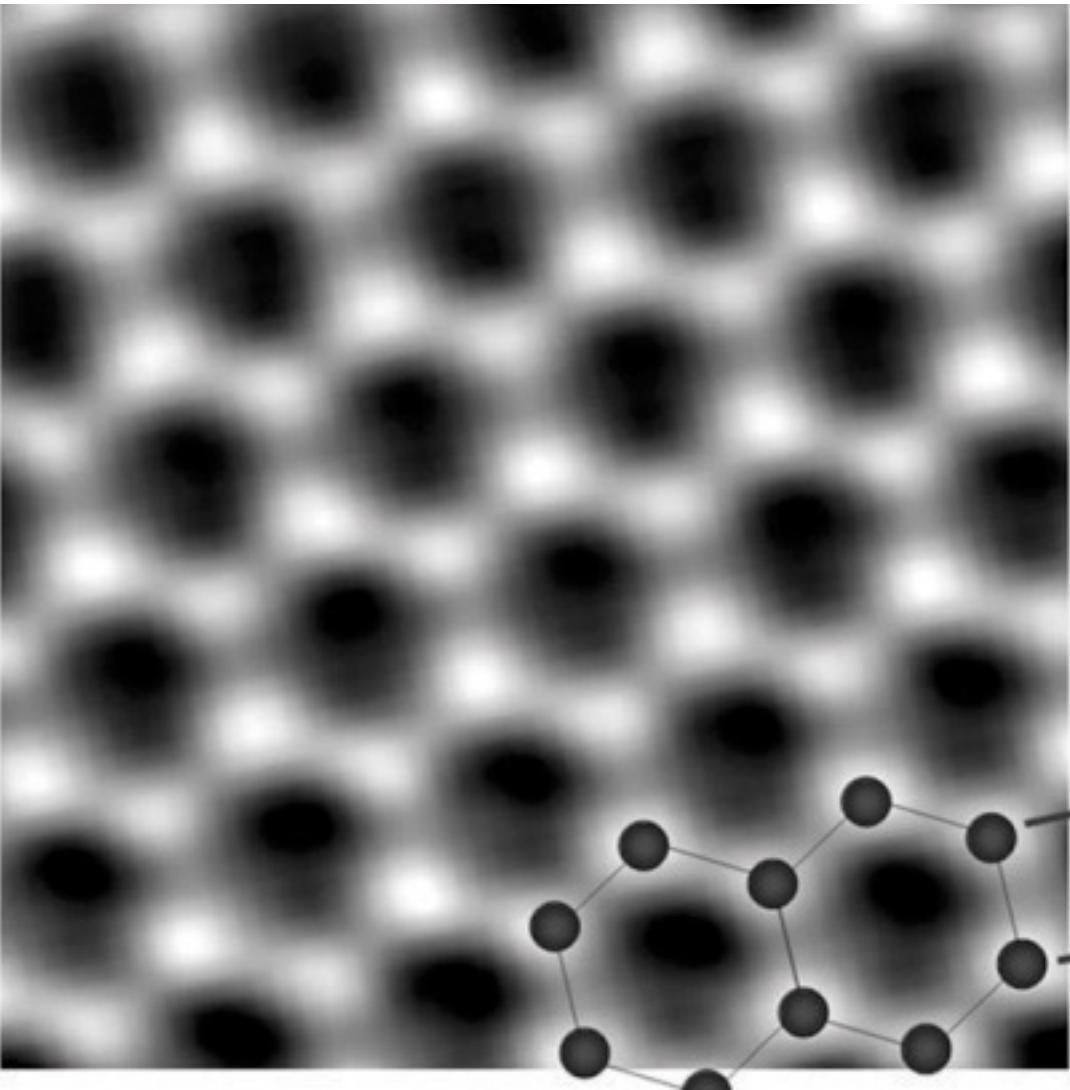
- Electron microscopes were developed in the 1930s to enable us to look more closely at objects than is possible with a light microscope. Scientists correctly predicted that a microscope that used electrons instead of visible light as the illumination source could view objects at far higher resolution than a light microscope. This is because the wavelength of visible light is what limits the resolution of light microscopes, and the wavelength of electrons is far smaller.
- Electron microscopes use a beam of electrons rather than visible light to illuminate the sample.

- Some electron microscopes can detect objects that are approximately one-twentieth of a nanometer (10^{-9} m) in size – they can be used to visualize objects as small as viruses, molecules or even individual atoms.
- Electron microscopes have emerged as a powerful tool for the characterization of a wide range of materials. Their versatility and extremely high spatial resolution render them a very valuable tool for many applications. The two main types of electron microscopes are the transmission electron microscope (TEM) and the scanning electron microscope (SEM).
- The main difference between SEM and TEM is that SEM creates an image by detecting reflected or knocked-off electrons, while TEM uses transmitted electrons (electrons that are passing through the sample) to create an image. As a result, TEM offers valuable information on the inner structure of the sample, such as crystal structure, morphology and stress state information, while SEM provides information on the sample's surface and its composition.
- For both techniques, electrons are used to acquire images of samples. Their main components are the same:
 - An electron source
 - A series of electromagnetic and electrostatic lenses to control the shape and trajectory of the electron beam
 - Electron apertures
- All of these components are housed inside a chamber that is under high vacuum.

What is a 2D material for example Graphene ?

Graphene is a single atomic layer of carbon atoms tightly packed in a two-dimensional honeycomb lattice. This novel material is atomically thin, chemically inert, consists of light atoms, and possesses a highly ordered structure. Graphene is electrically and thermally conductive, and is the strongest material ever measured. These remarkable properties make graphene the ideal support film for electron microscopy.





How electron microscopy can be used to take images of a 2D Graphene

- Now that we know about SEM, TEM and STEM, their working principles, we can use either of the techniques to image a 2D graphene

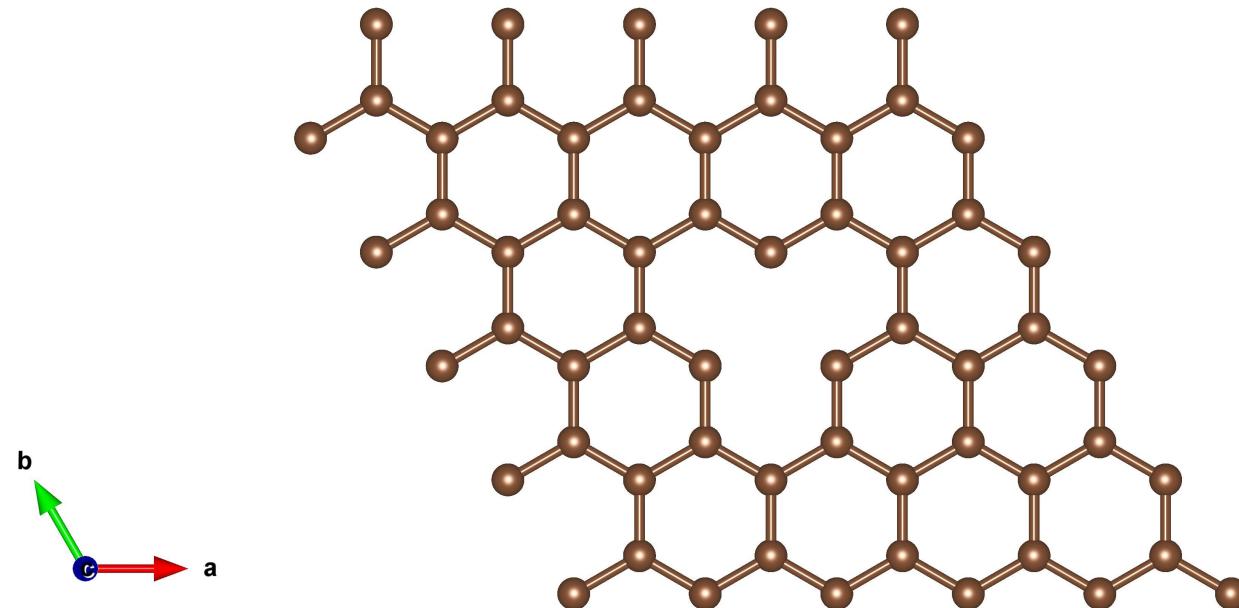
Electron Microscope Image of a 2D material Graphene

0.14 nm

What is the main challenge in electron microscopy of 2D Graphene?

Although the general structure of hexagonal rings of carbon can be seen by high-resolution microscopes, imaging the individual atoms and measuring their positions is not as straightforward.

The electron tip must scan the surface of the Graphene to take an electron microscope image. This way if the graphene surface is exposed to the electron beam for longer time, then defects will be formed in the Graphene.



How can machine learning help?

The machine learning models build from a previous large data set (taken from previous experiments) can help to guide on the (key points but not limited to)

- (a) Explore time of the beam to reduce defect formation
- (b) Where is focus for a clean high-resolution image
- (c) Improving signal-to-noise ratio, meaning increasing detections limits
- (d) Finite control over the experimental procedure to reduce the human error during performance of the experiment.

References

- Scanning Transmission Electron Microscopy Imaging and Analysis by Stephen J. Pennycook, Peter D. Nellist