
بسم الله الرحمن الرحيم

Subject: Nanotechnology & Nanostructures (Lecture # 11)

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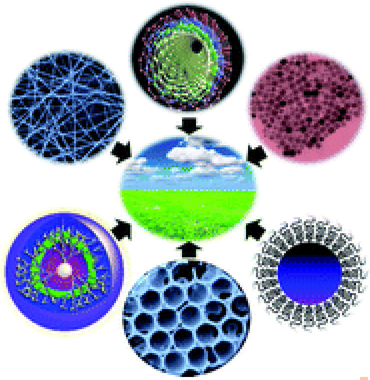
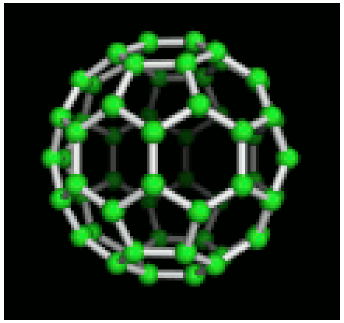
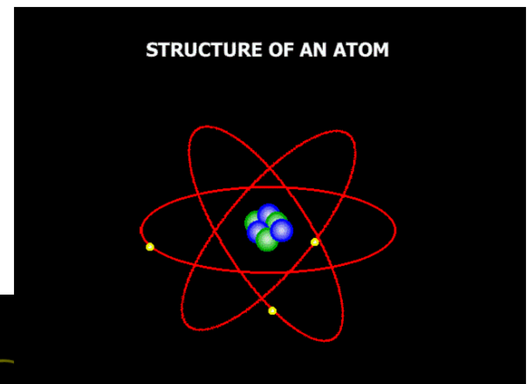


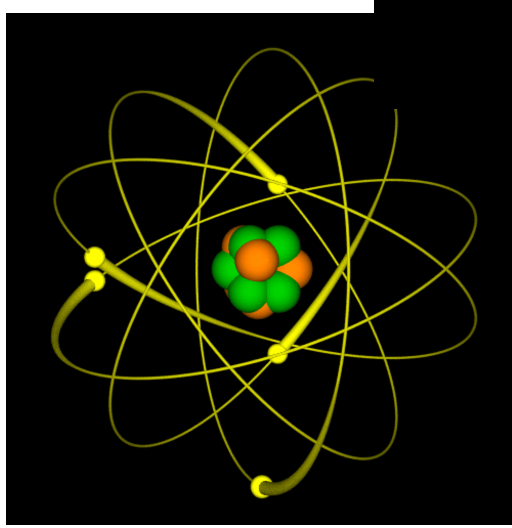


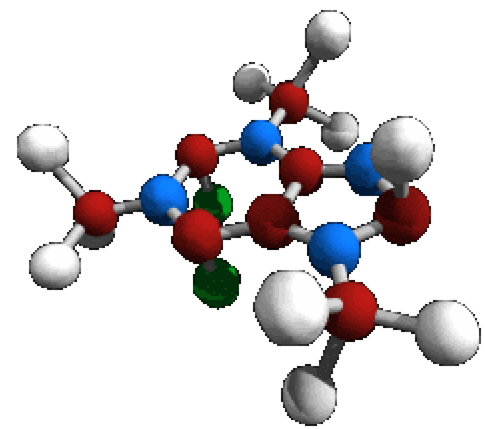
Properties of Nano materials

1. Mechanical Properties

Mechanical properties of solids depend on the microstructure, i.e. the chemical composition, the arrangement of the atoms (the atomic structure) and the size of a solid in one, two or three dimensions.







➢Grain size effect and Young's Modulus:

- The intrinsic elastic modulus (bond strength) of a nanostructured material is essentially the same as that of the bulk material having micrometer-sized grains unless the grain size becomes very small, less than 5 nm.

- Young's modulus is the factor relating stress and strain. It is the slope of the stress-strain curve in the linear region. The larger the value of Young's modulus, the less will be elastic the material.

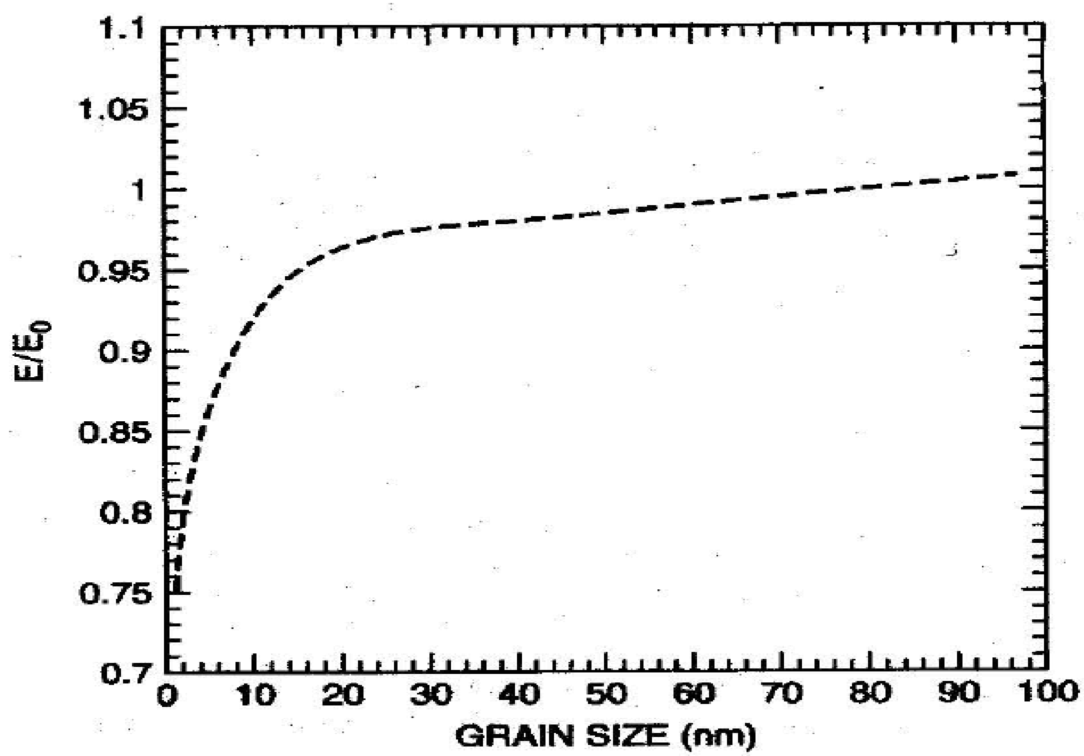


Figure is a plot of the ratio of Young's modulus E in nano-grained iron, to its value in conventional grain-sized iron E_O as a function of grain size. Below 20mn, Young's modulus begins to decrease from its value in conventional grain-sized materials.

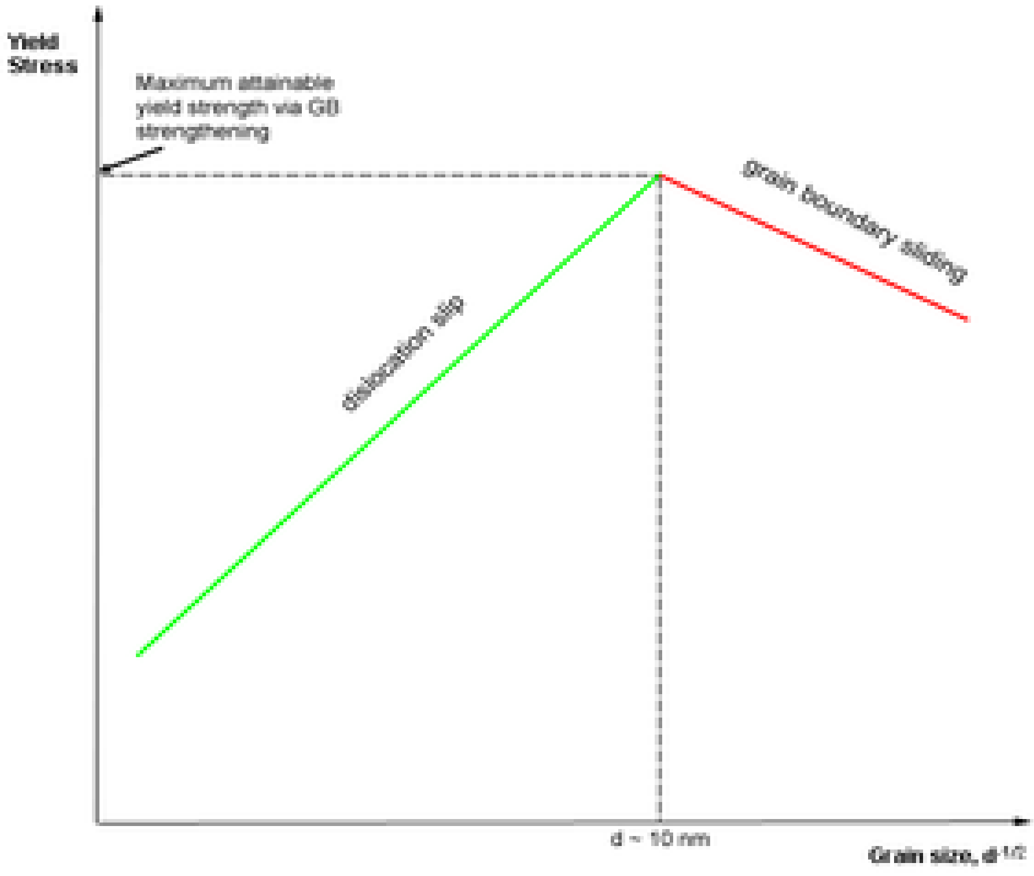
➢Grain size effect and Hall-Petch relation:

- The Hall-Petch relation predicts behavior accurately in metals with ordinary grain sizes (i.e. Few micrometers to few hundred micrometers).

- Metals typically follow the Hall-Petch relation when the average grain size is 100nm or larger, But Hall-Petch behaviour breaks down at smaller grain sizes.

- Indeed, an “Inverse Hall-Petch relationship” appears to exist at very small grain sizes, with yield strength actually decreasing as the grain size decreases.

Hall-Petch Strengthening Limit



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Hall-Petch Equation

The yield strength σ_y of a conventional grain-sized material is related to the grain size by the **Hall-Petch equation:**

$$\sigma_y = \sigma_0 + k/(d)^{1/2}$$

Where

σ_y = yield strength of metal

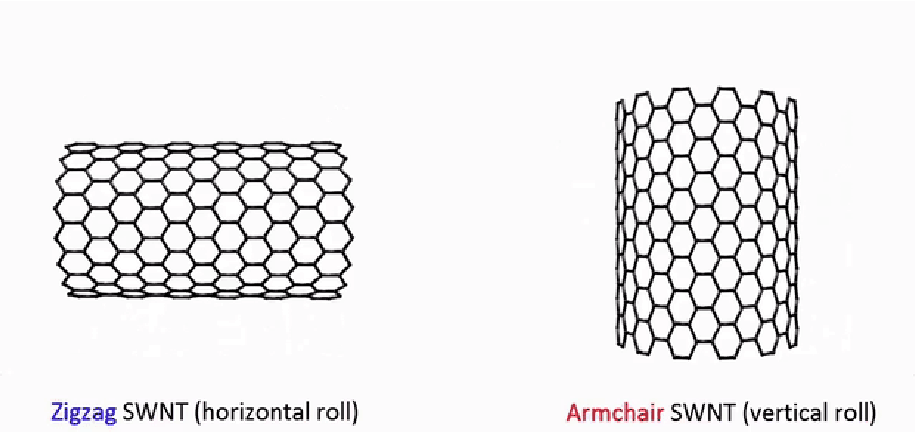
d = average grain diameter

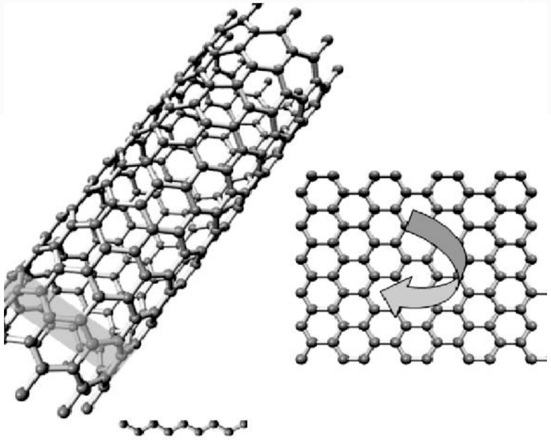
σ_0 and k = constant

- Hardness can also be described by a similar equation and the hardness H is just three times the strength σ.

➢Mechanical Properties of Carbon Nanotubes:

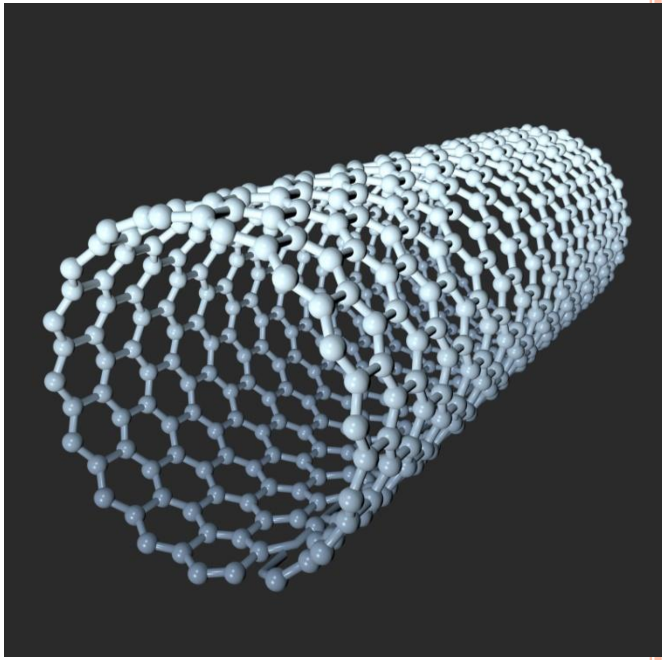
The carbon nanotube (CNT) is a rolled-up sheet of graphene and has three types depending upon the rolling direction such as armchair, zigzag and chiral.





❖The Young's modulus of steel is about 30,000 times that of rubber. Carbon nanotubes have Young's moduli ranging from 1.28 to 1.8TPa (1TPa = 10^7Pa).

❖Young's modulus of steel is 0.21 T Pa, which means that Young's modulus of carbon nanotubes is almost 10 times that of steel. This would imply that carbon nanotubes are very stiff and hard to bend.

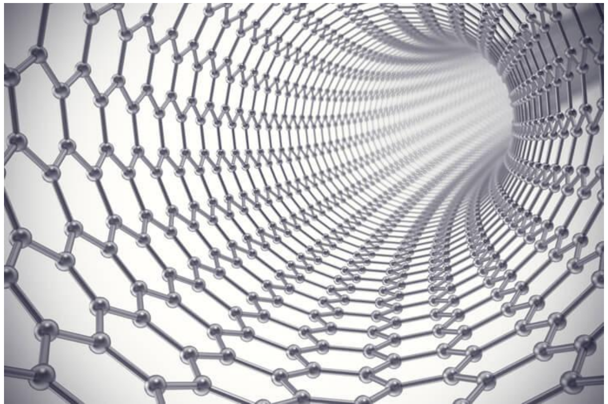


❖However, this is not quite true because they are so thin. When carbon nanotubes are bent, they are very resilient. They buckle like straws but do not break, and can be straightened back without any damage.

❖The reason behind that is bond nature between the carbon atoms. The electronic structure of carbon is $1s^2\ 2s^2\ 2p^2$ and when carbon atoms combine to form graphite, sp2 hybridization will occurs.

❖ In this process, one s-orbital and two p-orbitals combine to form three hybrid sp^2 -orbitals at 120° to each other within a plane. This in-plane bond is referred to as σ-bond (sigma–bond).

❖This is a strong covalent bond that binds the atoms in the plane, and results in the **high stiffness** and **high strength** of a CNT.



❖The remaining p-orbital is perpendicular to the plane of the σ-bonds. It contributes mainly to the interlayer interaction and is called the Π-bond (pi–bond).

❖These out-of planes, delocalized Π-bonds interact with the Π-bonds on the neighbouring layer.

❖This interlayer interaction of atom pairs on neighbouring layers is much weaker than a sigma bond.

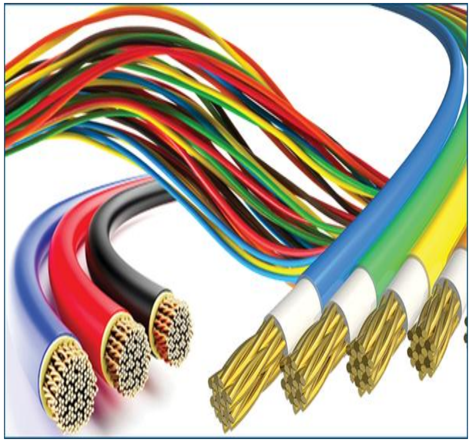
❖ Also Unlike bulk materials, the density of the defects in nanotubes is presumably less and therefore the strength is presumably significantly higher at the nanoscale.

❖Therefore Young's modulus is a measure of how stiff or flexible a material is. And Tensile strength is a measure of the amount of stress needed to pull a material apart.

❖ The tensile strength of carbon nanotubes is about 45 billion pascals. High-strength steel alloys break at about 2 billion pascals. Thus carbon nanotubes are about 20 times stronger than steel.

2. Electrical Properties

- In metallic state, conductivity of nanotubes is very high. These can carry upto million Ampere per cm^2.



- Copper wire fails to carry such a large amount of current because of the resistive heating, the copper wire melts.

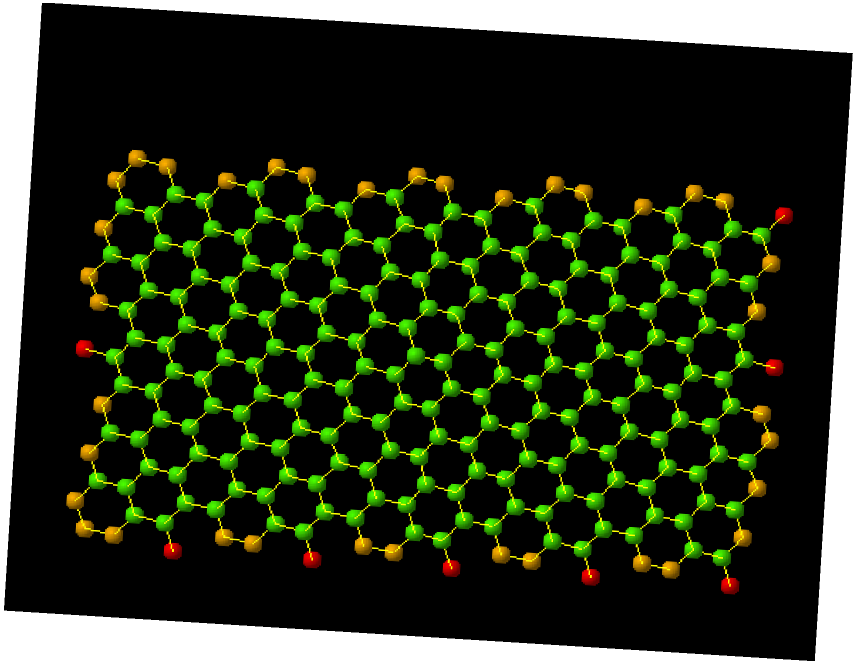
- Carbon nanotubes have the most interesting property that they are metallic or semiconducting depending on the diameter and chirality of the tube.

- **Chirality** refer to how the tubes are rolled. Synthesis generally results in a mixture of tubes two- third of which are semiconducting and one-third metallic.

•The electronic states of the Nanotubes do not form a single wide electronic energy band but instead split into one-dimensional sub-bands.

•These states can be modeled by a potential well having a depth equal to the length of the nanotube.

•Electron transport has been measured on individual single-walled carbon nanotubes.

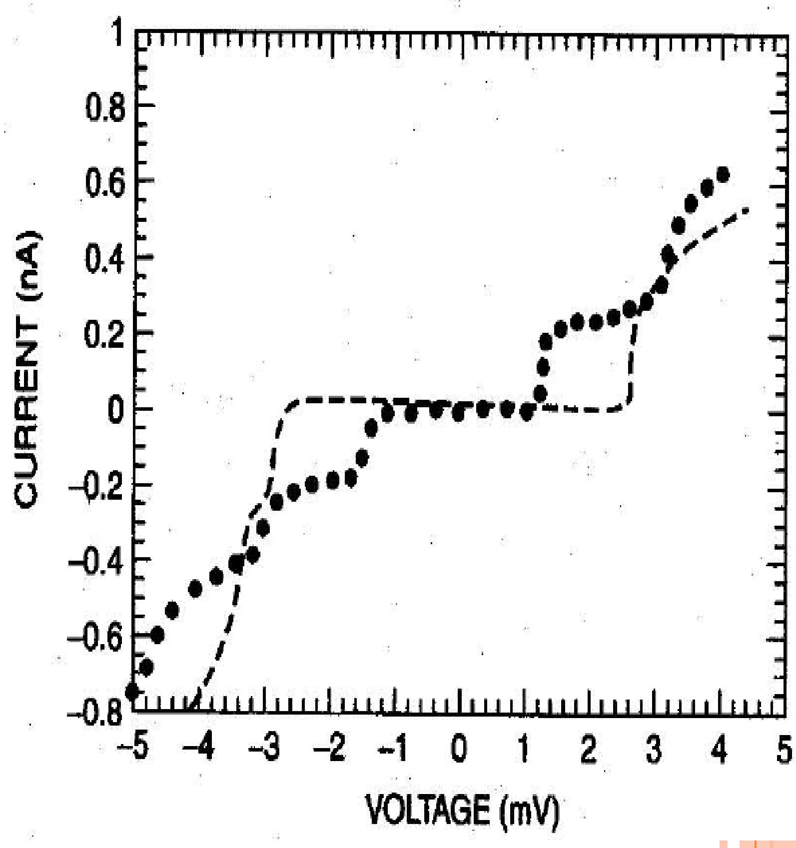


•The measurements at a milli kelvin (T=0.001 K) on a single metallic nanotube lying across two metal electrodes show step like features in the current- voltage measurements as shown in figure.

•The steps occur at voltages which depend on the voltage applied to a third electrode that is electrostatically coupled to the nanotube.

•This resembles a field effect transistor made from a carbon nanotube.

•The step like features in the curve are due to **single-electron tunneling** and **resonant tunneling** through single molecular orbitals. Single electron tunneling is a quantum mechanical effect in which an electron can penetrate a potential barrier higher than the kinetic energy of the electron.



THANK YOU