

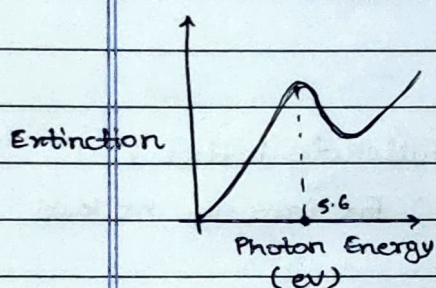
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## - Carbon nanotechnology

- Fullerene
- Carbon nanotubes
- Graphene (single sheets from graphitic structure)

(The general class of carbon molecules including graphene and all the tube and balloon structures it forms on curling up are known as fullerenes)

## - Optical spectrum of light coming from stars -



The peak at 5.6 eV is due to absorption from  $C_{60}$  present in interstellar dust.

## - Structure of $C_{60}$ fullerene.

- (named after Buckminster Fuller)  $\rightarrow$  (geodesic dome)
- 12 pentagonal } arranged symmetrically to  
20 hexagonal } form a molecular ball
- Diameter = 0.7 nm

$\nearrow$  resembles the structure of  $C_{60}$

## - Euler's Theorem $\{ V - E + F = 2 \}$

For  $C_{60}$  :  $F = 32$ ,  $V = 60$ ,  $E = 90$

(acc. to this theorem, any closed shell will be produced by 12 pentagons, irrespective of the number of hexagons.)



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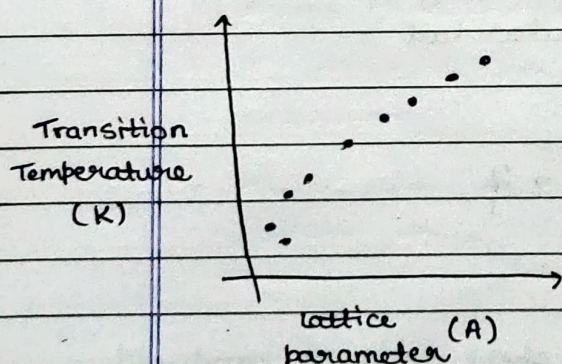
- Materials produced by assembling fullerene : Fullerite
  - The assemblies of pure fullerene molecules in condensed form as known as Fullerites.
  - Crystal structure of  $C_{60}$  is FCC
  - Separation b/w nearest-neighbour  $C_{60}$  is  $1\text{ nm}$ .
  - held by weak Van-der-Waals forces.
  - FCC crystal of  $C_{60}$  is an insulator.

(Fullerites are photosensitive, which makes it useful as a photoresist in lithographic processes.)

### - Fullerides

- (When other atoms are included in fullerite lattice)
- (Alkali metal atoms (ex. Na, K, Cs...) fit into the hollows left between the  $C_{60}$  cages)
- (have remarkable property of superconductivity)

- Plot of transition temperature of  $A_3C_{60}$ , where A is an alkali atom



as the radius of the dopant alkali atom increases, the cubic  $C_{60}$  lattice expands and the superconducting transition temperature goes up.

(The superconducting transition temperature increases with increasing size of the alkali atom)



(icosahedral)

## - Magic numbers in larger fullerenes.

•  $[60 + (R \times 6)]$  atoms  $R = 0, 2, 3, 4, \dots$ • for stable fullerene with  $n$  atoms,

$$\left\{ \text{number of hexagons} = \frac{n - 10}{2} \right\}$$

(There are especially stable numbers of atoms (special values of  $n$ ) when, the closed shell has a low-energy morphology. They are known as magic numbers)

•  $R = 0$  ( $C_{60}$ ), corresponds to first magic number.•  $C_{540}$  (magic number  $R = 80$ )

## - Other possible stable series

•  $C_{70}$  peaks: most prominent peak after  $C_{60}$ • structure of  $C_{70}$  (25 hexagonal & 12 pentagonal faces)

(including elliptical and tubular fullerenes - )

•  $70 + 30R$  ( $R = 0, 1, 2, 3$ )•  $84 + 36R$  ( $R = 0, 1, 2, 3, \dots$ )- CNT (length: few  $\mu m$   
diameter: as low as 1 nm)

• stable carbon structure

• rolled-up sheet of graphene sheet (1-atom thick)

• mainly made up of hexagonal rings.

• high aspect ratio:  $\frac{\text{length}}{\text{diameter}} > 1000$ Types

## ① Single-wall CNT

diameter: 1 nm

band gap: 0-2 eV

(Electrical conductivity can show metallic or semi-conductor behaviour?)

②

## Multi-walled CNT

interlayer distance: 3.4 Å

(a) Parchment model

(b) Russian doll





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## - Fabrication of CNT

(to produce SWNT, a small amount of cobalt, nickel or iron is used as a catalyst)

(no catalyst  $\rightarrow$  nested tubes / MWNT)

## - Discovery (Sumio Iijima)

diameter: 4-30 nm

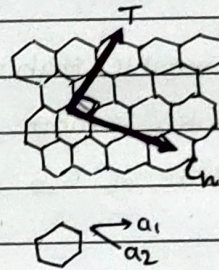
length: 1  $\mu$ m

no. of concentric walls: 2-7

## - T: axis vector about which the sheet is rolled.

$a_1, a_2$ : basis vector of 2D unit cell.

$C_n$ : circumferential vector, at right angles to T



## - Chirality

• (refers to how tubes are rolled w.r.t the direction of the T vector in graphite plane)

• (the choice of axis angle produces changes in electronic properties).

• The chirality of nanotube is specified by circumferential vector  $na_1 + ma_2$

## - Classifications

(n,n) Armchair: T  $\parallel$  C-C bond

(n,0) Zigzag: T not  $\parallel$  C-C bond

(n  $\neq$  m) Chiral: T not  $\parallel$  CC bond

: - nanotube has a helical / spiraling structure when viewed along its axis.

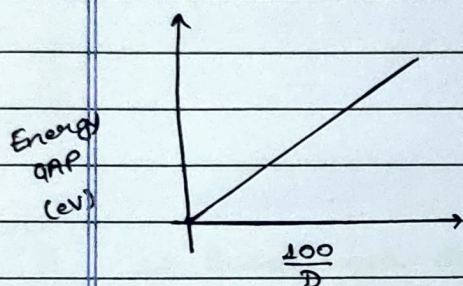


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- Synthesis of carbon NT =  $\frac{2}{3}$  semiconducting +  $\frac{1}{3}$  metallic

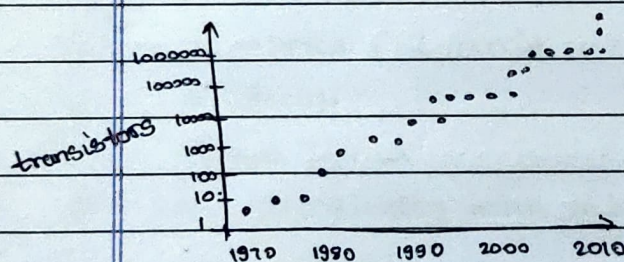
- all armchair (n,n) are conducting
- (n,m) tubes with [(n-m) = 3i] are almost metallic
- (n-m)  $\neq$  3i is semiconducting with bandgap  $\propto \frac{1}{\text{diameter (tube)}}$

- Electrical Properties



as the diameter of the semiconducting nanotube increases, the bandgap decreases.

- Moore's Law



exponential growth (doubling of components every 2 or 3 years) in ICs

- Graphene (single sheet of graphite, 2D honeycomb lattice arrangement of C atoms)

- ① High electrical current density
- ② high intrinsic mobility
- ③ high thermal conductivity
- ④ optical transparency
- ⑤ Strength
- ⑥ one of the world's thinnest material
- ⑦ toughest 2D material
- ⑧ Highest surface area
- ⑨ Density of graphene (0.77 mg/m<sup>2</sup>)