Carbon Nanotubes

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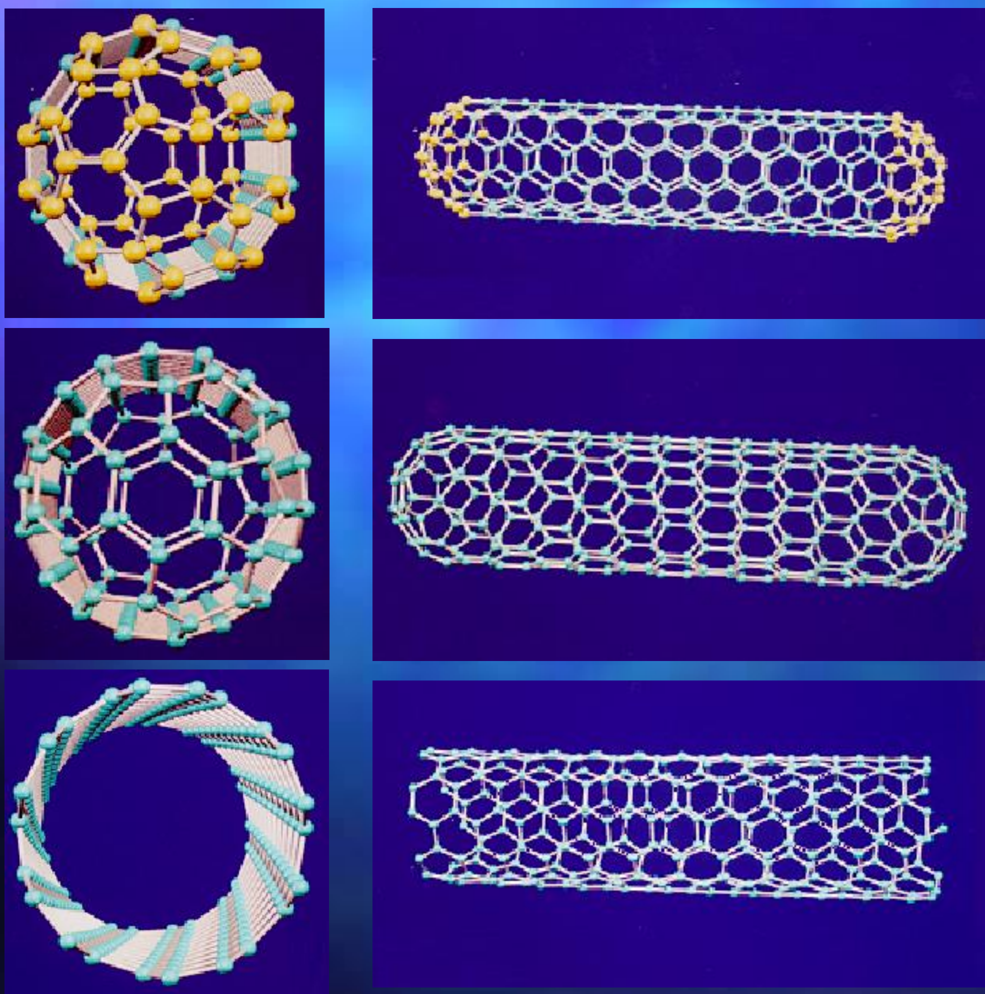


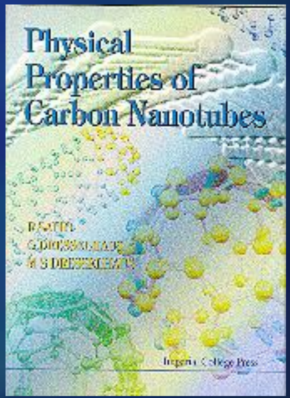
(5,5) Armchair Nanotube

(9,0) Zigzag Nanotube

(6,5) Chiral Nanotube

Solid State Properties of Carbon Nanotubes

- Structures and Symmetry
- Electronic and Phonon Properties
- Raman Intensities
- Transport Properties
- Magnetic Properties
- Applications



“Physical Properties of Carbon Nanotubes”,

by R. Saito, G. Dresselhaus and M.S. Dresselhaus,
Imperial College Press (1998) ISBN 1-86094-093-5

Chiral Vectors : *(n,m)*

- Chiral Vector (equator of nanotube): OA, C_h
- Translational Vector of 1D material: OB, T
- Unit Cell : OAB'B

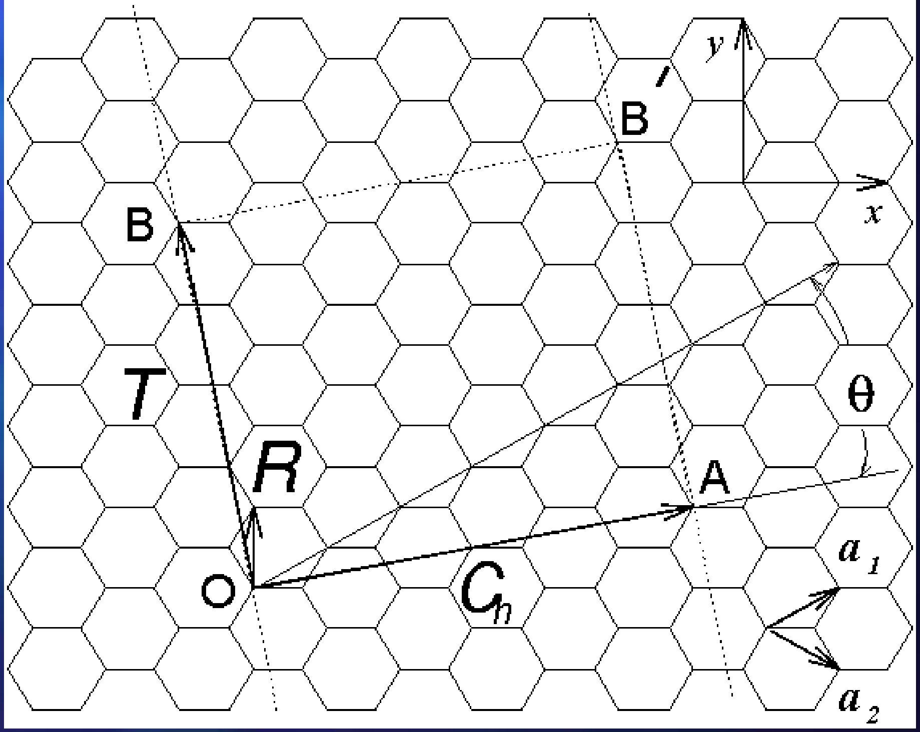
$$C_h = na_1 + ma_2 \equiv (n, m)$$

$$a_1, a_2 : \text{primitive lattice vectors}$$

$$T = t_1 a_1 + t_2 a_2 \equiv (t_1, t_2)$$

$$t_1 = \frac{(2m+n)}{d_R}, t_2 = -\frac{(2n+m)}{d_R}$$

$$d_R = \gcd(2n+m, 2m+n)$$



Symmetry

- Symmorphic (mirror symmetry)
  - Armchair Nanotube *(n,n), n=m*
  - Zigzag Nanotube *(n,0), m=0*
- Non-Symmorphic (axial chirality)
  - Zigzag Nanotube *(n,m), n≠m*

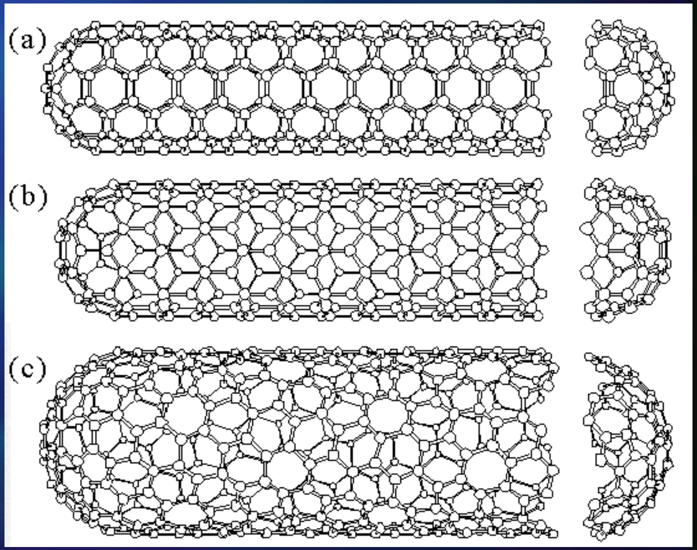


Fig: (a) (5,5) armchair,
(b) (9,0) zigzag, and
(c) (10,5) chiral nanotubes

Diameter and Chiral Angle

- Diameter : *d*

$$d = \frac{L}{\pi} = \frac{a\sqrt{n^2 + nm + m^2}}{\pi}$$

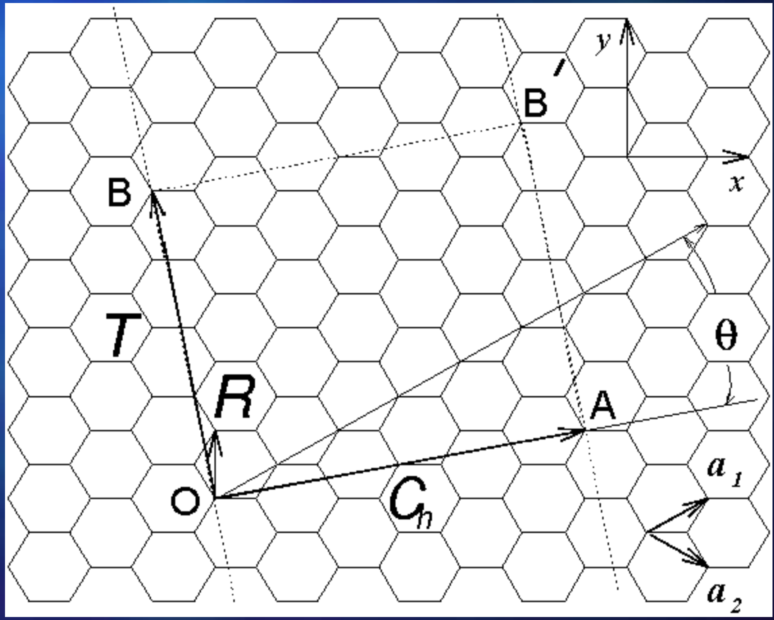
$$L = \left|C_h\right|$$

$$\text{Ex. } (10{,}10) \text{ armchair}$$

$$d = 13.7\,\text{Å} = 1.37\,\text{nm}$$

- Chiral Angle : θ
  - zigzag θ=0
  - armchair θ=π/6
  - chiral 0<θ<π/6

$$\theta = \tan^{-1}\frac{\sqrt{3}m}{2n+m},\ 0 \le \left|\theta\right| \le \frac{\pi}{6}$$



Reciprocal Lattice and Wave Vectors

- 1 Dimensional Wave Vectors
  - Nanotube axis direction

$$-\frac{\pi}{T} \leq k \leq \frac{\pi}{T}, \quad T : \text{translational vector}$$

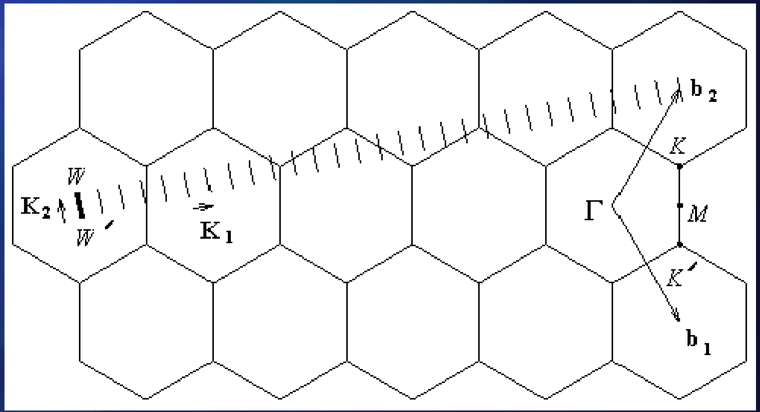
- Discrete in Circumferential Direction

$$C_h \cdot K_1 = 2\pi, \quad T \cdot K_2 = 2\pi$$

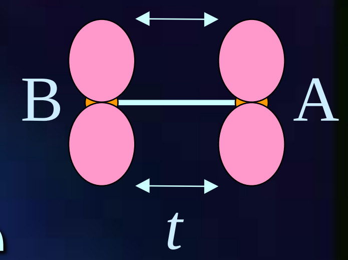
$$K_1 = \frac{1}{N}(-t_2 b_1 + t_1 b_2), K_2 = \frac{1}{N}(m b_1 - n b_2)$$

$$C_h = (4,2), T = (4,-5), N = 28$$

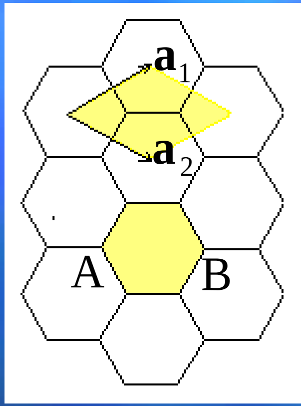
$$K_1 = (\tfrac{5}{28} b_1 + \tfrac{1}{7} b_2), K_2 = (\tfrac{1}{7} b_1 - \tfrac{1}{14} b_2)$$

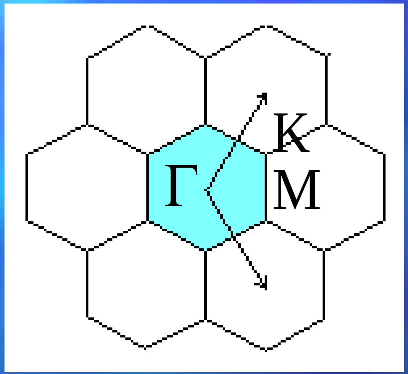


Electronic Properties of Graphene



- π band of graphite
  - Unit Cell, B. Z.

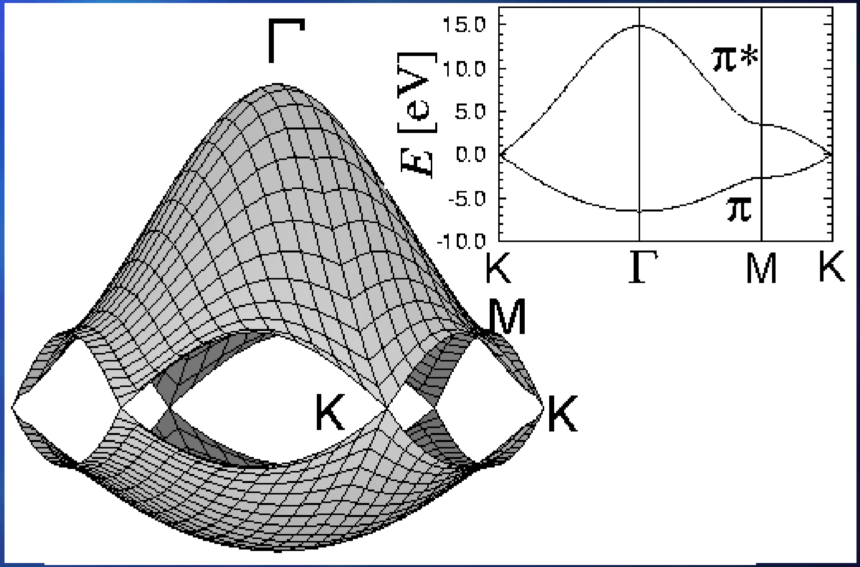




$$\mathbf{a}_1 = (\frac{\sqrt{3}}{2}, \frac{1}{2})a, \mathbf{a}_2 = (\frac{\sqrt{3}}{2}, -\frac{1}{2})a$$

$$\mathbf{b}_1 = (\frac{1}{2}, \frac{\sqrt{3}}{2})\frac{4\pi}{\sqrt{3}a}, \mathbf{b}_2 = (\frac{1}{2}, -\frac{\sqrt{3}}{2})\frac{4\pi}{\sqrt{3}a}$$

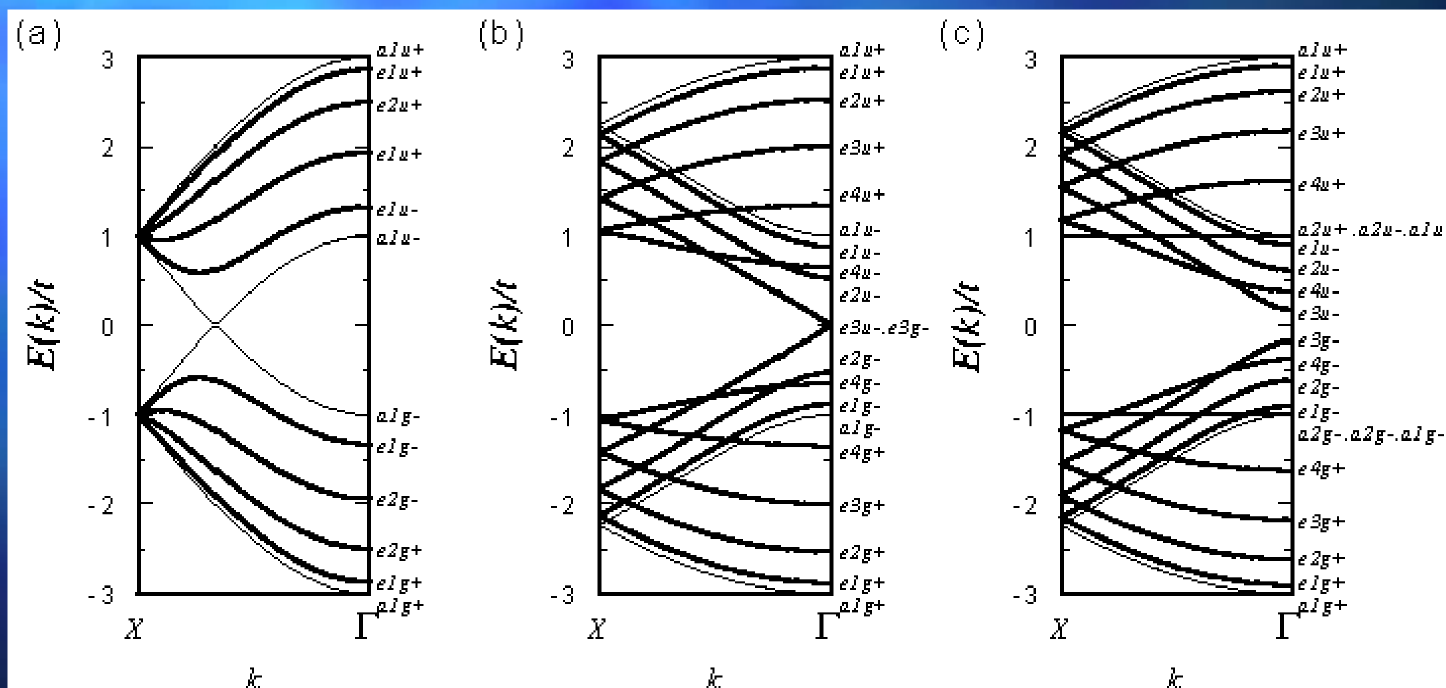
- Energy Band
  - Zero Gap Semiconductor



$$E_k = \pm t\sqrt{1 \pm 4\cos\frac{k_y a}{2}\cos\frac{\sqrt{3}k_x a}{2} + 4\cos^2\frac{k_y a}{2}}$$

Energy Bands of Nanotubes

- N one-dimensional bands



E_F

(5,5) (9,0) (10,0)

Metal or Semiconductor depending on chirality

- Density of States
- Rule for Metal Nanotube

$$n-m=\begin{cases}3p & \text{metal}\\ 3p\pm1 & \text{semiconductor}\end{cases}$$