Introduction of Nanomaterials

Introduction

A material with

- any external dimension in the nanoscale (size range from approximately $1\text{–}100\ \mathrm{nm}$).
- having internal structure or surface structure in the nanoscale.

At nanoscale, materials exhibit very unusual and very interesting properties. Examples: Graphene has very high young’s modulus and very high carrier mobility.

Nano object

An object with any external dimension is in the nanoscale.

Examples: carbon nanotube, bucky ball.

Nano structured material

A material where its internal or surface structure is in the nano scale.

Examples: $\mathrm{TiO_2}$ nanotube films.

Nano in nature

- Lotus leaves being superhydrophobic
- Gecko adhesive system

Nanoscience

Study of structures and materials on the nanoscale.

Nanotechnology

Development of materials and devices by exploiting the characteristics of particles on the nanoscale.

Applications

- Nanoscale transistors
  - Higher-performance
  - Improved energy efficiency
- Magnetic data storage
  - High data density and data capacity
  - Ultra compact
- Nanomedicine and drug delivery
- Energy storage

Preparation of nanomaterials

Top-down approach

Nanoscale dimensions are created using larger components, by externally controlled devices.

Examples: Lithography, Etching techniques.

Photolithography

Can be used to create nanoscale patterns in thin films or bulk substrates.

The steps:

1. Coat Si wafer with a photosensitive material.
   A material which changes its properties when exposed to electromagnetic radiation
2. Allow the radiation to pass through the mask on to photosensitive material.
3. Developer solution removes either reacted or unreacted material.
4. The silicon wafer is etched to transfer the pattern onto silicon wafer.
5. Photosensitive material is removed.

Bottom-up approach

Molecular components arrange themselves into more complex nano materials/objects.

Examples: Molecular self-assembly, Chemical vapour deposition

Graphene

Carbons arranged to a hexagonal network. 2D crystal based. Has 3 fold symmetry.

Unit Cell

- A rhombus with 120° .
- Lattice parameter is $2d\cos 30^\circ$ where d is the $\mathrm{C}-\mathrm{C}$ bond length.
- 2 atoms per unit cell.

> **Note**
>
> Single layer of graphene was discovered using scotch tape method and the discovery won a Nobel prize in 2010.

Synthesis

- Top-down approaches
  - Exfoliation (eg: Scotch tape method)
- Bottom-up approaches
  - Chemical vapor deposition

> **Note**
>
> Graphene has a band gap of 0.

Carbon Nanotubes

A rolled up sheet of graphene.

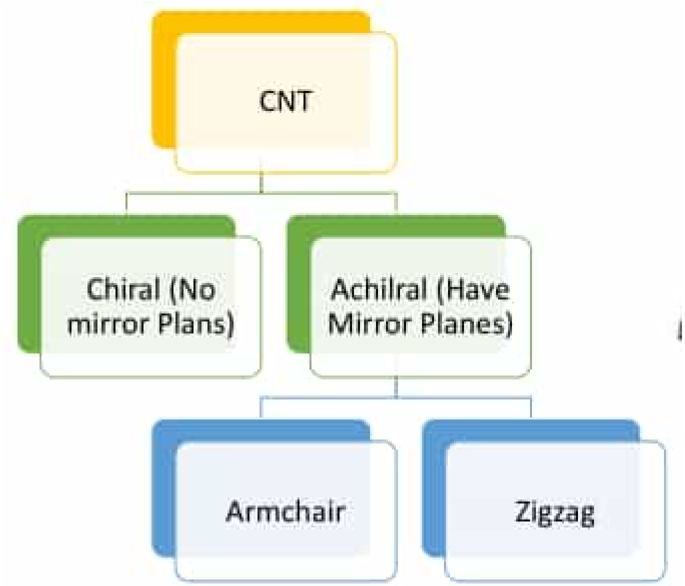
Classifications

Based on structure

1. Single wall carbon nanotubes (SWNT)
2. Multi-walled carbon nanotubes (MWNT)
   Similar to graphite but rolled up as a set of sheets.

Based on Chirality

Chirality means the way that graphene sheet is oriented with respect to the axis of carbon nanotube.

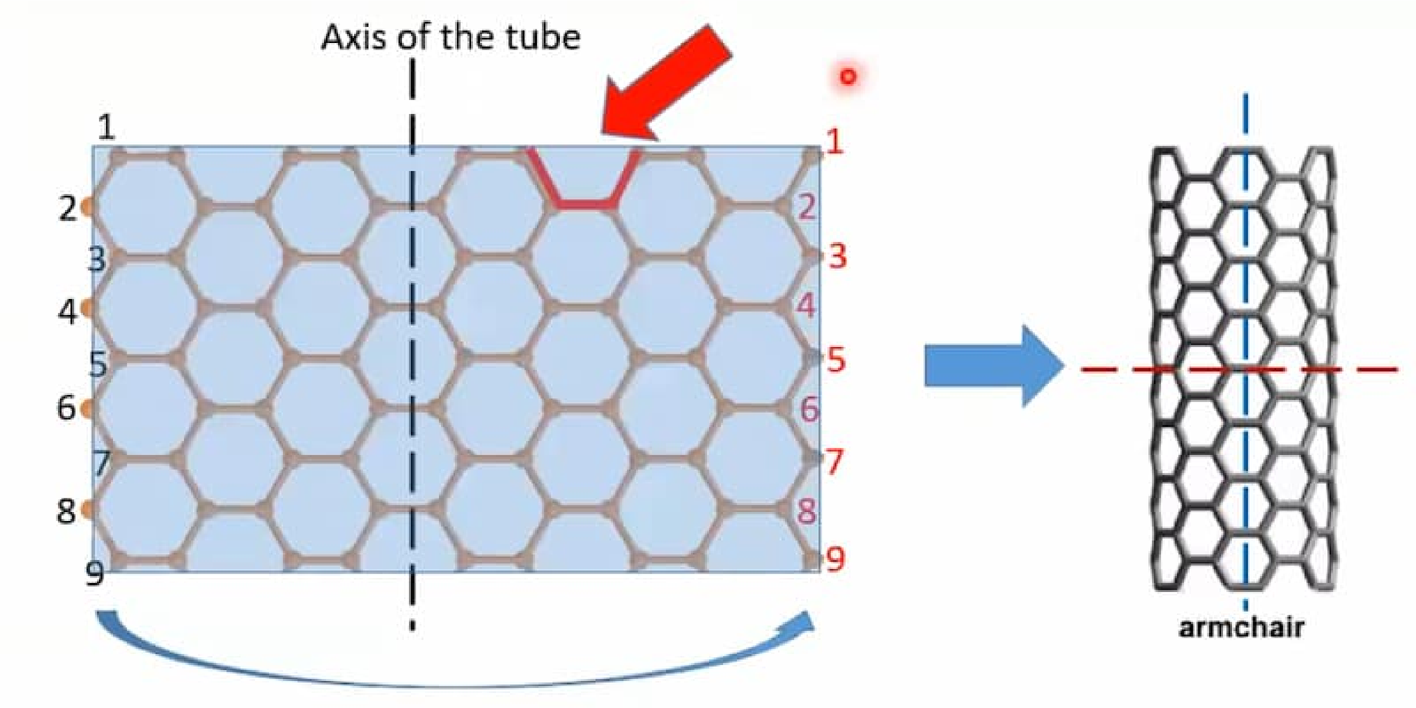


Achiral

Have mirror planes. Has 2 types.

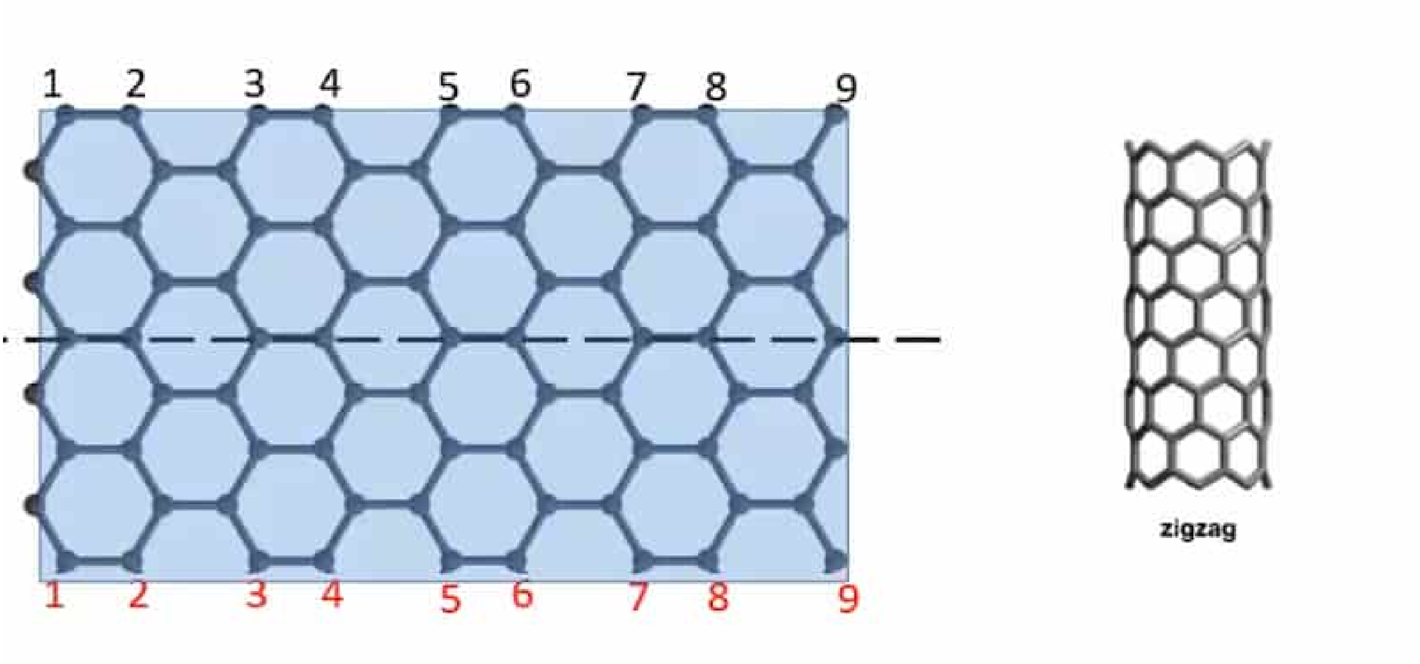
1. Armchair
2. Zigzag

Armchair



Circumference has a repeating armchair structure.

Zigzag



Circumference has a repeating zigzag structure.

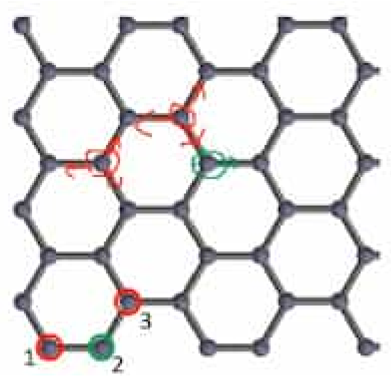
Chiral

No mirror planes. Definition for the chiral type is later explained.

Definitions

Equivalent Atoms

Equivalent atoms means the atoms having the same surrounding.



In graphene, next-near neighbours are equivalent atoms.

When a graphene sheet is rolled to create a CNT, only equivalent atoms can be connected.

Primitive Vectors

Vectors used to describe a unit cell.

For graphene, any 2 adjacent sides of the unit cell (rhombus) can be used as the primitive vectors.

Lattice Vectors

Any vector connecting 2 equivalent atoms. A lattice vector can be expressed in terms of primitive vectors.

Chiral Vector

The vector that constructs the circumference of a CNT. Also called as Circumferential vector.

(n,m) notation

If the chiral vector can be expressed as $na_1 + ma_2$ where a_1, a_2 are the primitive vectors, then the notation for the nanotube is (n, m)

- $n = 0 \vee m = 0$: zigzag tube
- $n = m$: armchair tube
- Otherwise: chiral tube

Chiral Angle

Angle between the chiral vector and nearest zigzag angle.

For a (n, m) tube where $n > 0$ and $n \geq m \geq 0$:

$$\theta = \tan^{-1}\left(\frac{\sqrt{3}m}{2n + m}\right)$$

- $\theta = 30^\circ$: armchair tube
- $\theta = 0^\circ$: zigzag tube
- $0^\circ < \theta < 30^\circ$: chiral tube

Chiral Vector Length

For a (n, m) tube, the chiral vector's length is given by:

$$|\mathrm{CH}| = a\sqrt{n^2 + m^2 + nm}$$

Here a is the bond length of C-C.

Diameter of CNT

The diameter can be expressed by:

$$D = \frac{|\mathrm{CH}|}{\pi} = \frac{a}{\pi}\sqrt{n^2 + m^2 + nm}$$

Properties

- Mechanical properties
  - High young’s modulus: depends on tube diameter, multi-walled or single-walled but not tube chirality.
  - Sustains higher strain
- Electrical properties
  - Depends on chirality and size
  - Exhibits superconductivity at $20\mathrm{K}$
  - Band structure changes with chirality
- Thermal properties
  - Conducts thermal energy only in the axial direction; radial direction is insulating

Chirality dependent electrical properties

For a (n, m) tube:

- If $n = m$, its armchair typed and is metallic (good conductors)
- If $n - m$ is a integer multiple of 3: small band gap semiconductors
- Else: large band gap semiconductors

Band gap decreases as the radius of the diameter increases.