Introduction of Nanomaterials

Introduction

A material with

- ullet any external dimension in the nanoscale (size range from approximately $1-100~\mathrm{nm}$).
- 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 nanoscale.

Examples: TiO_2 nanotube films.

Nano in nature

- Lotus leaves being super-hydrophobic
- Gecko adhesive system

Nano-science

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
- Nano-medicine 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. Add a mask and use an EM radiation.
- 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. Single sheet of graphite.

Unit Cell

- A rhombus with 120°.
- ullet Lattice parameter (side length of a unit cell) $a=2d\cos30\,^\circ$ where d is the ${
 m C-C}$ bond length.
- 2 atoms per unit cell.

(i) 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
 - o Chemical vapor deposition

Properties

- Band gap is 0
- ullet High tensile strength ($\sim 1100~\mathrm{GPa}$)
- ullet High young's modulus ($\sim 1~\mathrm{TPa}$)
- High charge carrier mobility (2)
- Highly transparent (97)

Carbon Nanotubes

A rolled up sheet of graphene.

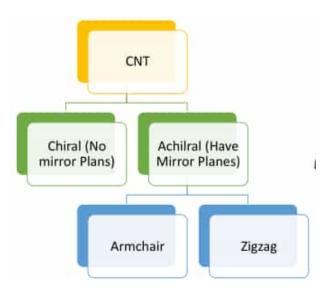
Classifications

Based on structure

- 1. Single wall carbon nanotubes (SWNT)
- 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.

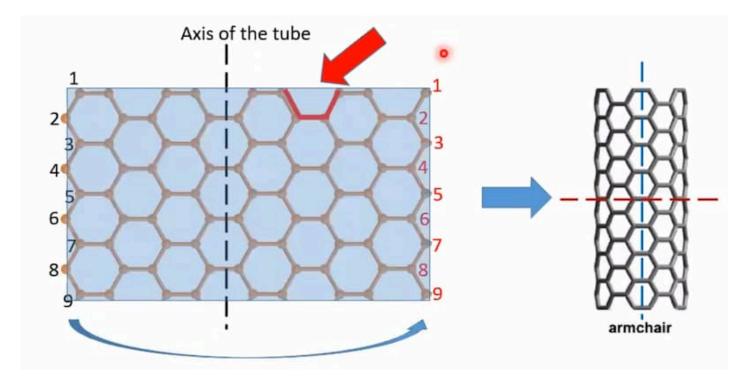


Achiral

Have mirror planes. Has 2 types.

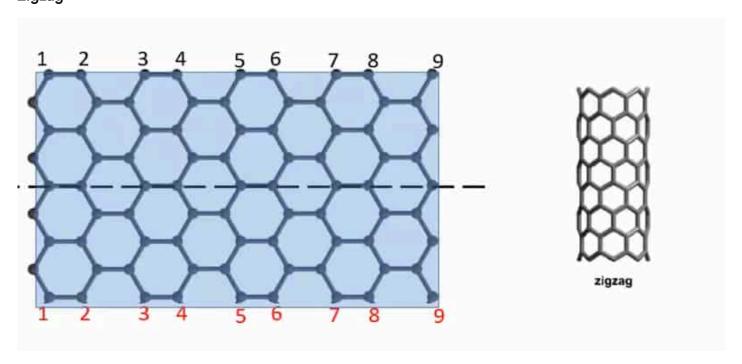
- 1. Armchair
- 2. Zigzag

Armchair



Circumference has a repeating armchair structure.

Zigzag



Circumference has a repeating zigzag structure.

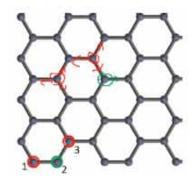
Chiral

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 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)

• $n=0 \lor m=0$: 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 $n\geq m\geq 0$:

$$heta= an^{-1}\left(rac{\sqrt{3}m}{2n+m}
ight)$$

 $oldsymbol{ heta}=30\,^{\circ}$: armchair tube

 $oldsymbol{ heta} = 0\,^\circ$: zigzag tube

• $0\degree < \theta < 30\degree$; 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:

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

Properties

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

Chirality dependent electrical properties

For a (n, m) tube:

- ullet 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.

Applications

- Conductive or reinforced plastic
- CNT based transistors
- Molecular electronics
- Energy storage devices
- Biomedical applications

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