MLL100

Experiment 4: To study the structure of Fullerene, Graphene and Nanotubes

1. Fullerene

1. (a) C_{60} is an Archimedean solid: Make a paper polyhedron model of C_{60} molecule from the template provided (sheet 1). Note that faces are regular polygons of two types: pentagons and hexagons. Thus, it is not a regular (or Platonic) solid. However, each vertex is still identical and all edges are of the same length. Such solids are named Archimedean solids. This particular one is called truncated icosahedron. Relate this model to a model of icosahedron.

[2]

1 (b) Euler's Polyhedron Formula satisfied: Count the number of vertices (V), edges (E) and faces (F) and verify the Euler's formula. [1]

V	E	F
$12 \times 5 = 60$	$12 \times 5 + 30 = 90$	$12 + 20 = 32$

$V - E + F = 60 - 90 + 32 = 2$

1 (c) No. of pentagons in any fullerene is always 12: C_{60} is the most prominent member of the family of closed cage-like carbon molecules. This is known as Buckminsterfullerene. There are other fullerenes such as C_{70}, C_{76}, C_{82}, C_{84} etc. All fullerene molecules have C atoms which are bonded to 3 other C atoms and their polyhedron consists only of hexagonal and pentagonal faces. Based on this information and Euler's polyhedron formula establish the interesting result that the number of pentagons in C_n for any n is always 12. [2].

Consider a fulleren C_n with n carbon atoms with P pentagons and H hexagons. We thus have

$V = n$ and $F = P + H$ ①

We can count the edges in two ways.

(a) Using vertices, since three edges meet at each vertex and an edge is shared between two vertices we have $E = \frac{3n}{2}$ ②

(b) Using faces, since pentagons have 5 and hexagons 6 edges and since each ~~face~~ edge is shared by two faces we have $E = \frac{5P + 6H}{2}$ ③

From ② and ③ we have $3n = 5P + 6H$ ④

Using Euler's relation we have

$V - E + F = 2 \Rightarrow n - \frac{3n}{2} + P + H = 2$ Using ① and ②.

$\Rightarrow -\frac{n}{2} + P + H = 2 \Rightarrow -n + 2P + 2H = 4$ (Contd.)

From prev. page

$-3n + 6P + 6H = 12 \Rightarrow -5P - \cancel{6H} + 6P + \cancel{6H} = 12$

$\Rightarrow \boxed{P = 12}$ independent of n.

2. Graphene

2 (a) Lattice of Graphene: A tiling of hexagons is provided in Sheet 2. Place an open circle representing a carbon atom at each vertex. Shade or fill a circle to represent a reference carbon atom. Now mark all other circles which are translationally equivalent to the reference atom so that their centres form a two-dimensional lattice of graphene. [2]

Centres of shaded black atoms form the lattice of graphene.

2 (b) No. of atoms in motif: How many atoms are there in the motif of graphene? [2]

There are two atoms in the motif as the shaded black and unshaded white atoms are translationally not equivalent.

2 (c) Unit cell: Outline a conventional cell of graphene. Measure its lattice parameter in mm for your paper drawing. [1+3]

Conventional cell $a = b$, $\gamma = 120°$

One cell is outlined in green.

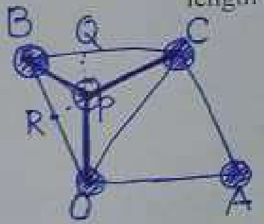
By measurement on the sheet $a = b \simeq 25$ mm.

2 (d) Is the unit cell primitive or nonprimitive? Give reason. [1+1]

Effective no. of lattice points in the unit cell

$= \frac{1}{4} \times 4 = 1 \Rightarrow$ Primitive Unit Cell

2 (d) Lattice Parameter: Find the relation between lattice parameter a in terms of C-C bond length d. Also measure a and d in mm on your pattern. [2+1]



$OP = PC = PB =$ C-C bond length $= d$

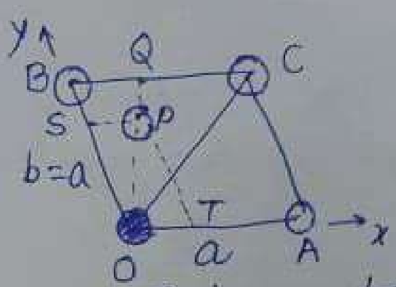
$OA = OB =$ lattice parameter $= a$

$PR \perp OB$ In isosceles $\triangle OPB$; $\angle OPB = 120° \Rightarrow \angle POR = 30°$

$\Rightarrow$ In right $\triangle POR$, $OR = \frac{OB}{2} = a/2$, $\frac{OR}{OP} = \cos 30° = \frac{\sqrt{3}}{2}$

$\Rightarrow a/2 = \sqrt{3}/2\, d \Rightarrow \boxed{a = \sqrt{3}d}$

2(e) Coordinates of atoms in the motif: Find the fractional coordinates of atoms in the motif in terms of your chosen crystal coordinate system. [4]



Atoms at O and P constitute a motif.

Coordinates of O : 0, 0

x-coordinate of P = OT = SP

y- " " P = OS

$\because$ P is centroid of equilateral $\triangle OBC$

$\therefore OP = \frac{2}{3} OQ = \frac{2}{3} \cdot OB \sin 60° = \frac{2}{3} \cdot a \frac{\sqrt{3}}{2} = \frac{a}{\sqrt{3}}$

(This result can be taken directly from above question 2(d).)

In $\triangle OSP$, $\frac{OP}{OS} = \cos\angle POS = \cos 30° = \sqrt{3}/2 \Rightarrow OS = 2/\sqrt{3}\, OP = \frac{2}{\sqrt{3}} \cdot \frac{a}{\sqrt{3}} = \frac{2}{3}a$.

$\frac{SP}{OP} = \tan 30° = 1/\sqrt{3}$, $SP = 1/\sqrt{3}\, OP = \frac{1}{\sqrt{3}} \cdot \frac{a}{\sqrt{3}} = a/3$. contd.

∴ Coordinates of P : SP, OS $= \frac{1}{3}a, \frac{2}{3}a$

Fractional coordinates of P $= \frac{1}{3}, \frac{2}{3}$

Note that

3 Nanotubes

3 (a) Wrapping or **Chiral vector and (n, m) designation of a nanotube**: On a fresh sheet representing graphene mark two primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ at 60° degrees. A lattice translation vector of graphene is given by

$$\mathbf{C} = n\,\mathbf{a}_1 + m\,\mathbf{a}_2$$

where n and m are integers. It is possible to wrap the graphene sheet into a nanotube such that the end points of **C** meet to define the circumference of the tube. Such a tube is designated an (n, m) tube and the corresponding vector **C** is called the chiral or wrapping vector of the tube. As an (n, m) tube is identical to (m, n) tube there is a convention to keep $n \geq m$. Mark the wrapping vectors of following nanotubes on your graphene Sheet 2:

(i) (8, 0)	(ii) (3, 3)	(iii) (5, 3)	[3]
O'L (red)	O'M (Blue)	O'N (Green)	

On the drawing →

Label the wrapping vectors with the type of the nanotube (chiral, zig-zag, or armchair) that will be produced on wrapping. [3]

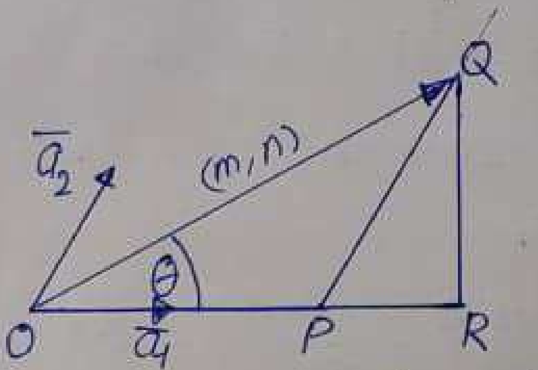
For armchair and zigzag, draw few connected C-C bonds to justify their name. [2]

3(b) Nanotube Models:

(i) Make a model of an armchair nanotube by wrapping a fresh sheet (Sheet 3) of graphene.
Determine its (n, m) designation. [2]

(ii) Make another model (Sheet 4) of a zig-zag tube.
Determine its (n, m) designation. [2]

3(c) Nanotube Diameter: Derive a formula for the length of the wrapping vector and hence the diameter D of an (n, m) nanotube in terms of n, m and d, the C-C bond length. [3]



$\bar{a}_1$ and $\bar{a}_2$ are the basis vectors with $|\bar{a}_1| = |\bar{a}_2| = a$ and angle $= 60°$.

$\overline{OQ}$ is the (n,m) wrapping vector.

$QP \parallel \bar{a}_2 \Rightarrow OP = na,\ PQ = ma$.

$\angle QPR = 60°$.

$QR \perp OR$. In $\triangle QPR$ $PR = PQ \cos 60° = \frac{ma}{2}$, $QR = PQ \sin 60° = ma\frac{\sqrt{3}}{2}$

In right $\triangle OQR$, $OQ^2 = OR^2 + QR^2$

$\Rightarrow OQ^2 = (OP + PR)^2 + QR^2$

$= \left(na + \frac{ma}{2}\right)^2 + \left(ma\frac{\sqrt{3}}{2}\right)^2$

$= n^2a^2 + nma^2 + \frac{m^2a^2}{4} + m^2a^2\frac{3}{4}$

$= n^2a^2 + m^2a^2 + nma^2 = (n^2 + m^2 + nm)a^2$ contd.

$\therefore$ Length of chiral (wrapping vector) (n, m)

$L_{nm} = OQ = (n^2 + m^2 + nm)^{1/2} a$

Diameter D_{nm} of tube $= \frac{L_{nm}}{\pi} = (n^2+m^2+nm)^{1/2} \cdot \frac{a}{\pi} = (n^2+m^2+nm)^{1/2} \frac{\sqrt{3}d}{\pi}$

3(d) Chiral angle: The angle θ which the chiral vector $\mathbf{C} = n\,\mathbf{a}_1 + m\,\mathbf{a}_2$ makes with the axis $\mathbf{a}_1$ is called the chiral angle. Derive a formula for θ in terms of n and m. Determine the chiral angles of the three vectors in 3(a) using your formula and check them by measurements on drawings of 3(a). [2]

From the figure for 3(c) the chiral angle θ is given by

$$\tan\theta = \frac{QR}{OR} = \frac{ma\frac{\sqrt{3}}{2}}{na + \frac{ma}{2}} = \frac{\sqrt{3}m}{2n+m}.$$

3(e) Verify the formulae derived for length of the wrapping vector and the chiral angle by actual measurements on the three wrapping vectors drawn in 3(a) [3]

For $(8,0)$ $L_{3,0}\cancel{D_{3,0}} = (8^2 + 0^2 + 3.0)^{1/2} a = 8a.$

(obvious in diagram).

$$\tan\theta = \frac{\sqrt{3}.0}{2.8+0} = 0 \Rightarrow \theta = 0$$

(obvious from figure).

For $(3, 3)$ $\overset{L_{3,3}}{\cancel{D_{3,3}}} = (3^2 + 3^2 + 3^2)^{1/2} a = 3\sqrt{3}\,a$

$a = 25$ mm $\quad L_{3,3} = 129.9$ mm.

Verified by measurement.

$$\tan\theta = \frac{\sqrt{3}.\,3}{2.3+3} = \frac{\sqrt{3}\,3}{9} = \frac{1}{\sqrt{3}} \quad \theta = 30^\circ$$

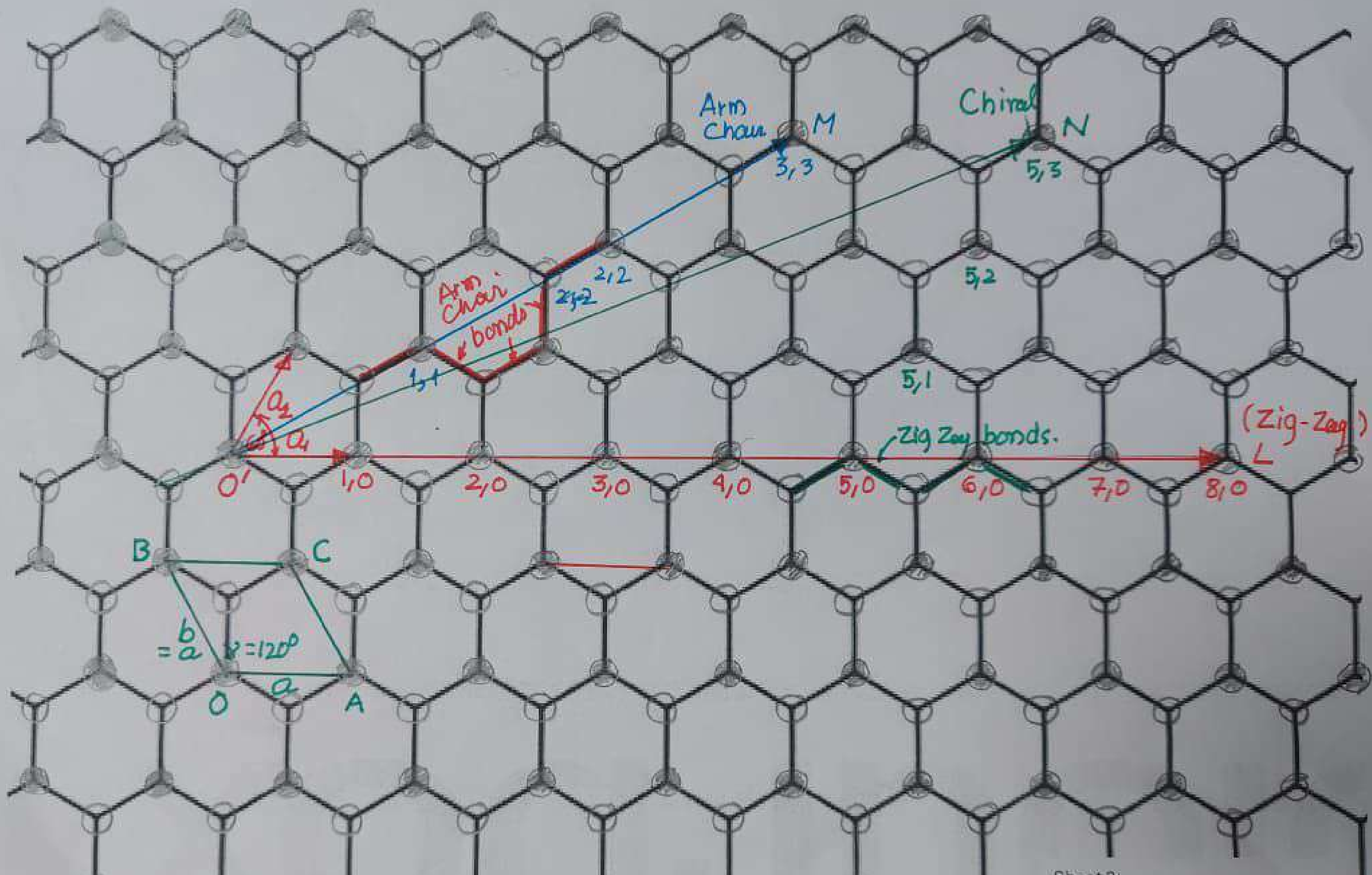
Obvious from figure.

For $(5,3)$ $L_{5,3} = (5^2 + 3^2 + 5.3)^{1/2} a = 7a$

$= 175$ mm. Measured 178 mm

$$\tan\theta = \cancel{\frac{\sqrt{3}.5}{2.3}} \frac{\sqrt{3}\,3}{2\times5+3} = \frac{3\sqrt{3}}{13} \quad \theta = 21.7^\circ.$$

$\theta_{measured} = 27^\circ$



Sheet 2:
Graphene and wrapping vectors
To be submitted