

17.5/18

Ayan
20/9/25

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Entry No: 2024ME10902

Lab Group No: 8

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MLL100 Materials Science

Experiment 7: To study the load-displacement behaviour of rubber and its contraction on heating

Reference:

Read pp. 246 – 249 in Material Science and Engineering book (5th. Edn.) by V. Raghavan.

There are two parts in this experiment:

- A. Load-displacement behavior of Rubber band at room temperature
- B. Behavior of rubber band after heating

A. Load-displacement behavior of Rubber band at room temperature:

2 Marks

Room temperature, $T: 24^{\circ}\text{C}$			Initial length of rubber band, $L_0 = 15.5$		
S. No.	Weight in the pan		Scale reading	Length of the rubber band, L	$\left(\frac{L}{L_0}\right) - \left(\frac{L_0}{L}\right)^2$
	Grams (g)	Newton (N)			
1	0	0	15.5 cm	15.5 cm	0
2	10	0.098	15.9 cm	15.9 cm	0.0549
3	20	0.196	16.3 cm	16.3 cm	0.14736
4	30	0.294	16.5 cm	16.5 cm	0.18906
5	40	0.392	16.9 cm	16.9 cm	0.24914
6	50	0.490	17.3 cm	17.3 cm	0.31497
7	60	0.588	17.8 cm	17.8 cm	0.39162
8	70	0.686	18.4 cm	18.4 cm	0.47747

(2)

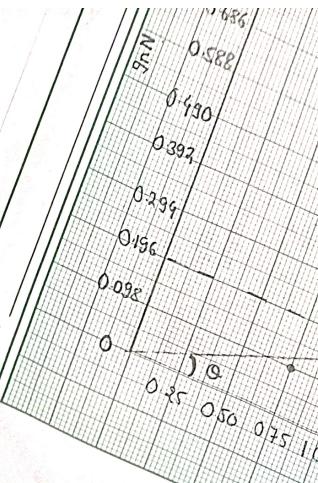
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B. Behaviour of Rubber band after heating: (2 marks)

Initial temperature of the heated rubber band,

$$T = 24^\circ C$$

Initial weight (pan weight + added weight in the pan),

$$F = 62.39 \text{ (} 50 + 12.3 \text{)}_\text{Pan}$$

Initial cursor reading,

$$R_1 = 729.95 \text{ mm}$$

Additional weight,

$$\Delta F_1 = 5g$$

Cursor reading,

$$R_2 = 722.05 \text{ mm}$$

Change in length (at initial temperature, T), $\Delta L_1 = (R_1 - R_2) =$

$$7.9 \text{ mm}$$

Increase in temperature,

$$\Delta T = 10$$

Cursor reading,

$$R_3 = 728.90 \text{ mm}$$

Change in length (due to increase in temperature, ΔT),

$$\Delta L_2 = (R_2 - R_3) = -3.85 \text{ mm}$$

Change in weight to bring the cursor reading back to R_2 ,

(i.e. length $L_0 + \Delta L_1$), $\Delta F_2 =$

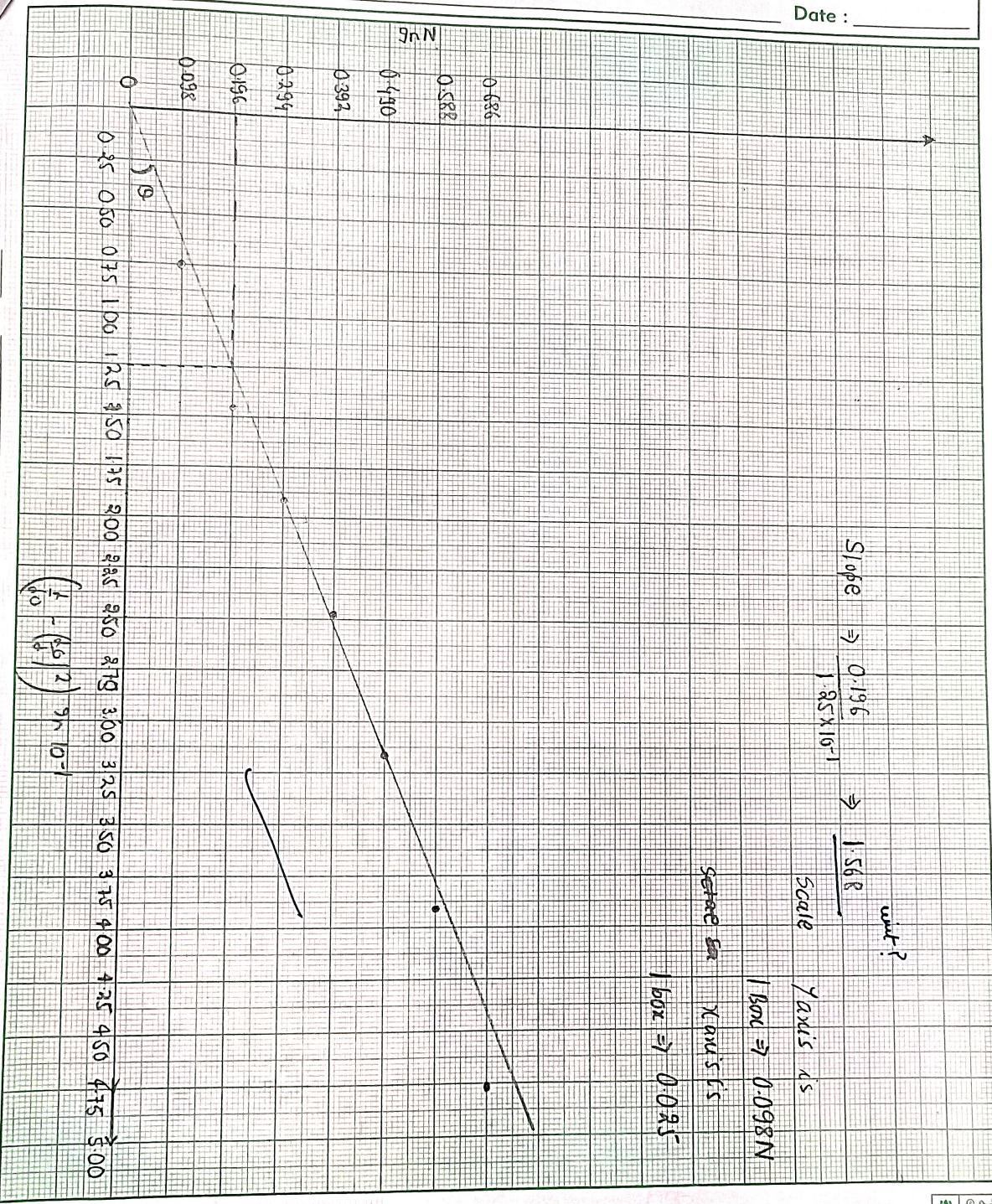
$$0.0245 \text{ N}$$

2

Topic : _____

Date : _____

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Session No. _____

(2 marks)

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1. Plot F (on y -axis) vs. $\left(\frac{L}{L_0}\right) - \left(\frac{L_0}{L}\right)^2$ on x -axis. Draw the best fit line *passing through the origin*. Using the slope of this line and the ‘equation of state’ of the elastomer (e.g., page 248 of your text book), calculate the number of cross-links in the rubber specimen. (6 marks)

$$F = \left(\frac{N_0 k T}{L_0} \right) \left(\frac{L}{L_0} - \frac{L_0}{L} \right)^2$$

so $\frac{N_0 k T}{L_0}$ = Slope $\Rightarrow 1.568$ unit?

$$N_0 k x T \Rightarrow 1.568 \times \frac{15.5}{100}$$

$$T \Rightarrow (273 + 24^\circ C) = 297 K$$

$$N_0 k \Rightarrow \left(\frac{1.568 \times 15.5}{100 \times 297} \right)$$

$$N_0 k = 8.183 \times 10^{-4}$$

$$N_0 \times (1.380649) \times 10^{-23} = 8.183 \times 10^{-4}$$

$N_0 \Rightarrow 5.92 \times 10^{19}$

2. Verify from your observation whether the ‘equation of state’ of an elastomer is a single valued and continuous function by evaluating the following product (see equation 10.14 of your book) (2 marks)

$$\frac{\Delta F_1}{\Delta L_1} \times \frac{\Delta L_2}{\Delta T} \times \frac{\Delta T}{\Delta F_2}$$

↪ putting Values from
prev table

$$\frac{(9.8 \times 5 \times 10^3) \times 3.85 \text{ mm}}{(7.9 \text{ mm})} \times \frac{10}{10} \times \frac{1}{0.0245 \text{ N}} \Rightarrow -0.974$$

$$\Rightarrow \frac{5 \text{ gm}}{7.9} \times \frac{3.85}{10} \times \frac{1}{0.0245} \Rightarrow -0.974$$

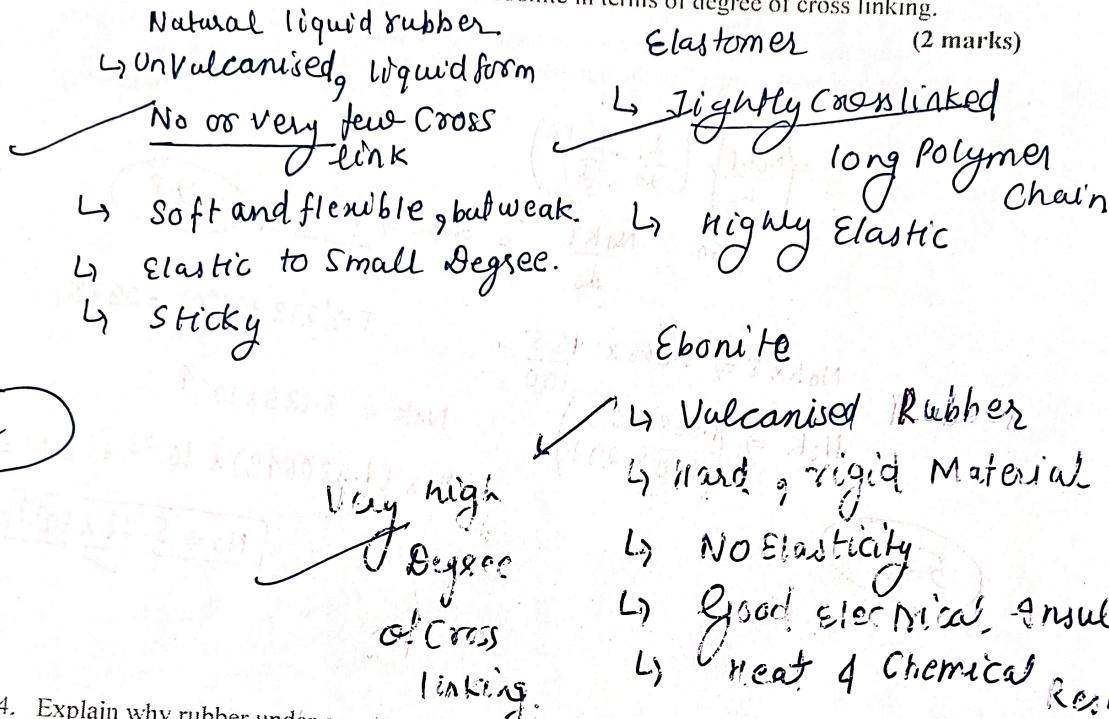
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3. Explain the difference between the mechanical behaviour of natural liquid rubber (as obtained from the tree), elastomer and ebonite in terms of degree of cross linking.



4. Explain why rubber under constant tension contracts on heating.

(4 marks)

$$G_1 = H - TS \quad \text{configurational entropy}$$

(4)

↳ when heated

$T \uparrow \text{se} \rightarrow$ minimize Entropy S to minimize G_1 . reducing Entropy

To increase Entropy, the Polymer chains recoil, reducing its length even under a constant pulling force

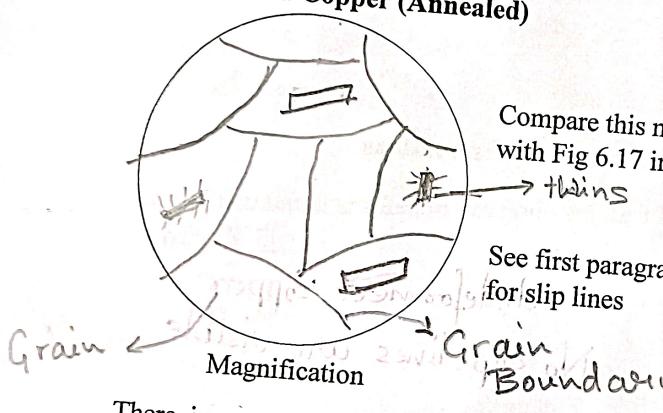
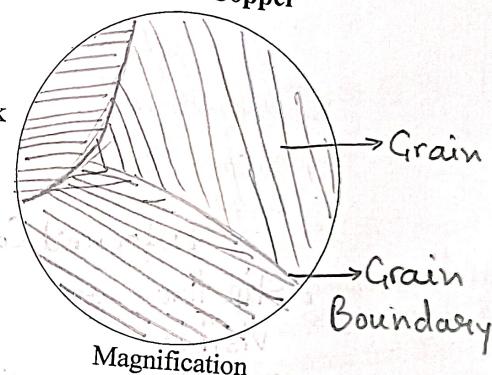
Heating increases Thermal motion, encouraging the polymer chains to adopt more disordered configuration, which lead to contradiction & decrease in length.

Reading reference:

Section 6.4 (pp. 137 – 143) of Chapter 6; Sections 7.3, 7.4, 7.5 (pp. 151 – 162) and 7.7.3 (pp. 165 – 169) of Chapter 7; Sections 11.2 (p. 264 – Slip lines) & 11.8 (p. 279 – ASTM grain size number) of Chapter 11 in Material Science and Engineering book (5th. Edtn.) by V. Raghavan.

I. Microstructure observation**[5 Marks]**

Sketch the observed microstructure indicating salient features. Do not try to exactly reproduce what you see in all details, just show all the salient feature and label them. Do not spend more than 10 mins on one sample.

Undeformed Copper (Annealed)**Deformed Copper**

There is a graduated reference line superimposed on the microstructure of **Undeformed Copper**. Total length of this line is 10 cm on the image plane. You should count the number of grain boundaries intersecting this line

12.5

No of grain boundaries intersecting as seen on the reference line

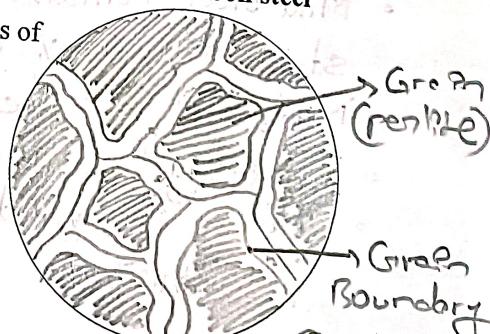
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Mild steel**Grain (Perlite)**

Rationalize the relative amounts of pearlite and ferrite in these two samples based on their composition and Fe-C diagram, Fig 7.11

Grain boundary
(Ferrite
α iron)

(25-30%) Perlite

Medium carbon steel

25-30% Ferrite α Iron

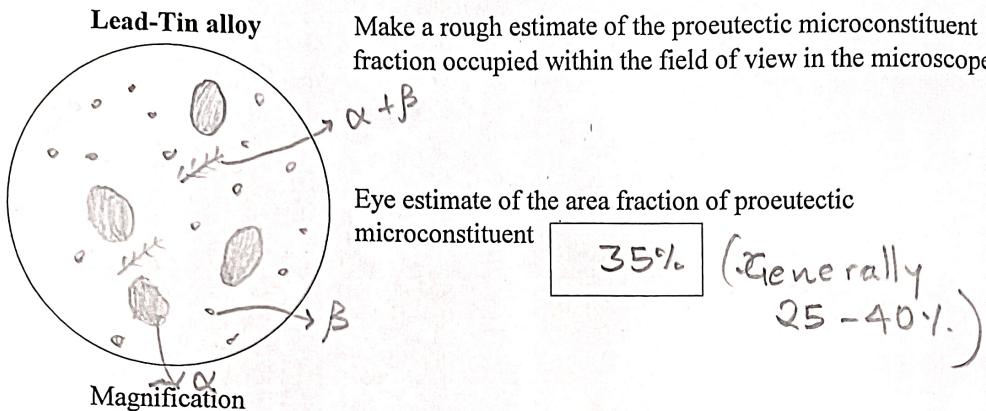
3

4

5

6

A



3) Using your estimate of sample, calculate the p. 279, paragraph af Marks]

II. Answer the following based on your microstructure observations

- 1) Compare and contrast the microstructural features observed in deformed and undeformed Copper [3 Marks]

Deformed Copper

- o Slip lines are visible.
- o Only lines are there inside grain boundaries

Undeformed Copper

- o No slip lines are visible
- o Rectangular shaped boxes known as twins are there (both bright and dark)

- 2) What is the difference between mild- and medium- carbon steels in terms of carbon concentrations? Compare and contrast the microstructures of mild and medium carbon steels. [3 Marks]

- o Mild steel contains 0-0.3% carbon whereas medium steel 0.4-0.5% carbon
- o Mild steel is softer due to low carbon concentration.
- o Percentage of ~~per~~ perlite is higher in mild steel.
- o Grains in mild steel is higher than grains in medium carbon steel

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- 3) Using your estimate of the no. of grain boundary intersections on the **Undeformed Copper** sample, calculate the average grain size in μm and also the ASTM grain size number. (see p. 279, paragraph after equation 11.22, of the textbook) [4 Marks]

$$M = 100 \times n = 12$$

$$L = 10 \text{ cm}$$

$$\text{Mean intercept} \approx d = \frac{L}{n} = \frac{10}{12} \approx \frac{1}{1.2} \text{ cm}$$

$$d^2 = \frac{1^2}{(0.00326)^2} \text{ cm}^2 = 9.4 \times 10^4$$

$$n \approx 2^{N-1} \Rightarrow N = [\log_2 n + 1]$$

~~$$N = 17.52$$~~

$$N = [17.5] = 17$$

$$\text{avg. grain size} = d = 0.00326 \text{ inch}$$

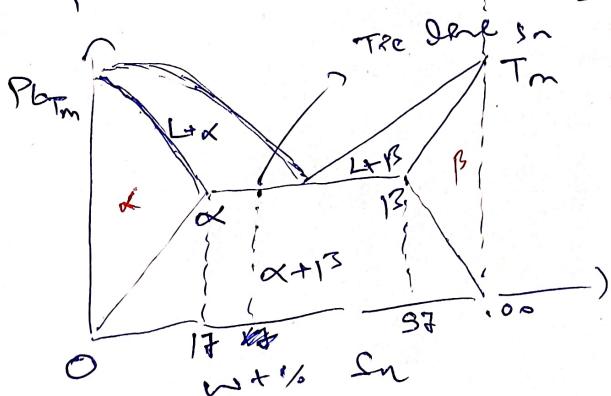
- 4) From your estimate of the area fraction of the proeutectic microconstituent and the knowledge that this phase is solid solution of tin in lead, make a rough estimate of the overall composition (wt. % Sn) of the alloy. (Assume area fraction = mass fraction and apply the lever rule). Make a neat sketch of the Pb-Sn phase diagram (Fig. 7.3 in your textbook) and indicate the Tie-line used for your calculation. [5 Marks]

$$\text{Area fraction } \alpha = 35\%$$

$$t_\alpha = \frac{C_E - C_\alpha}{C_E - C_\alpha} = \frac{62 - 46}{62 - 17} = \frac{35}{100}$$

$$\Rightarrow C_\alpha = 46.25\% \text{ by wt}$$

$$S_n(\%) = 53.75\%$$



MLL100: Introduction to Materials Science and Engineering – Lab
Session-Exp-09

Lab Group: 2B-7

Name and Entry no:

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20
20

Experiment 9: Tensile Test of Steel and Aluminium

Reading reference:

Section 11.1 (pp. 260 – 263) of Chapter 11 in Material Science and Engineering book (5th. Edtn.) by V. Raghavan.

Safety precautions:

- Handle the instrument and all related accessories safely and with utmost care.
- **Experimental Procedure:**
 - Tensile tests will be conducted on a Tensometer.
 - Plot the Engineering Stress (*y-axis*) vs Engineering Strain (*x-axis*) curve from your data. For comparison, plot both steel and aluminium on the same axis.
 - Measure all the required sample dimensions using Callipers.
 - Yield point in *Al* may be taken as 1/16 mm offset.

• **Observation and Calculations:**

[2 Marks]

S. No	Sample and Experiment details	Aluminium	Steel
1	Initial diameter (m)	9.35×10^{-3}	5.00×10^{-3}
2	Initial cross sectional area (m^2)	19.24×10^{-6}	19.63×10^{-6}
3	Gauge length (mm)	18 mm	18 mm
4	% Elongation (gauge section)	30%	45%
5	% Reduction in area (gauge section)	60%	78%
6	Load at yield point (N)	5020 N 3557	Upper 7090 N Lower 6150 N
7	Yield Strength ($M Pa(N/m^2)$)	272.87	Upper $361.65 N/m^2$ Lower 315.84
8	Load at maximum (N)	5900 N	8970 N
9	Tensile strength ($M Pa(N/m^2)$)	306.65	456.95
10	Young's modulus ($G Pa(N/m^2)$)	38.9	270
11	% Elongation (graph)	16.67 %	35.5 %

• Tensile test on Steel sample:

[2 Marks]

S. No.	Load, N	Elongation, mm	S. No.	Load, N	Elongation, mm
1	0	0	27	8920	5.2
2	5900	0.2	28	8930	5.4
3	7090	0.4	29	8890	5.6
4	6150	0.6	30	8820	5.8
5	6350	0.8	31	8830	6.0
6	6670	1.0	32	8780	6.2
7	7130	1.2	33	8690	6.4
8	7470	1.4	34	8580	6.6
9	7710	1.6	35	8400	6.8
10	7940	1.8	36	8190	7.0
11	8100	2.0	37	7980	7.2
12	8280	2.2	38	7690	7.4
13	8400	2.4	39	7270	7.6
14	8520	2.6	40	6810	7.8
15	8610	2.8	41	6250	8.0
16	8700	3.0			
17	8750	3.2			
18	8800	3.4			
19	8850	3.6			
20	8900	3.8			
21	8910	4.0			
22	8920	4.2			
23	8970	4.4			
24	8960	4.6			
25	8960	4.8			
26	8940	5.0			

• Tensile test on Aluminium sample:

[2 Marks]

S. No.	Load, N	Elongation, mm	S. No.	Load, N	Elongation, mm
1	0	0	14	5870	2.6
2	300	0.2	15	5900	2.8
3	1040	0.4	16	5870	3.0
4	2090	0.6	17	5830	3.2
5	3000	0.8	18	5750	3.4
6	3910	1.0	19	5570	3.6
7	5020	1.2	20	5380	3.8
8	5360	1.4	21	5110	4.0
9	5490	1.6	22	4870	4.2
10	5590	1.8	23	4600	4.4
11	5690	2.0	24	fractured (10)	4.5
12	5750	2.2			
13	5820	2.4			

• Answer the following questions
1a. Measure the

Load, N	Elongation, mm
270	5.2
540	5.4
518	5.6
580	5.8

[2 Marks]

Load, N	Elongation, mm
270	5.2
540	5.4
518	5.6
580	5.8

- Answer the following based on your experimental observations and understanding:

1a. Measure the work done in deforming Steel and Aluminium sample. (Work done is given by the area under the load-extension curve) [2 Marks]

1b. Find out the toughness for Steel and Aluminium [1 Marks]

1a) ≈ 180 boxes under the graph for Steel $\Rightarrow \text{Area} = 180 \times (0.4 \text{ mm}) \times (600 \text{ N})$
 ≈ 0 Work done in deforming Steel $= \cancel{24.72 \text{ J}} = 43.2 \text{ J}$ $\approx 24.72 \text{ J}$
 ≈ 87 boxes under the graph for Al $\Rightarrow \text{Area} = 87 \times (0.4 \text{ mm}) \times (600 \text{ N})$
 $\approx 20.88 \text{ J}$

b) Toughness $= \frac{\text{Work done}}{\text{Volume}}$ \therefore $\text{Toughness}_{\text{Al}} = \frac{43.2 \text{ J}}{(18 \text{ mm}) (\frac{2}{7}) (9.95 \text{ mm})^2} = 68.81 \times 10^3 \text{ J/mm}^3$ for Al
 $\text{Toughness}_{\text{Steel}} = \frac{43.2 \text{ J}}{(18 \text{ mm}) (\frac{2}{7}) (5 \text{ mm})^2} = 122.29 \times 10^3 \text{ J/mm}^3$ for Steel

2. Compare the % elongation as observed in rows (4) and (11) of your Table in page 1 and explain the discrepancy, if any. [3 Marks]

The row 4 only tells about plastic deformation as sample is broken/factured after unloading so it accounts only for plastic deformation.

Whereas row 11 considers both elastic & plastic deformation as it is measured while the sample is loaded.

This is why % elongation in row 11 is greater than % elongation in row 4.
 Elastic elongation becomes zero after breaking.

3. Compare the Young's moduli obtained by you with the standard values (210 GPa for steel & 70 GPa for aluminium). What could be the reason for discrepancy? [4 Marks]

- The experimentally obtained values differs from the standard values
- 1) There may be an issue in alignment of workpiece which may lead to non-uniform distribution of mass.
 - 2) There may be backlash error.
 - 3) Machine may not be accurate. Some errors in values as stress & elongation were changing very fast.
 - 4) The composition of steel or aluminium used in the experiment may not be identical to the standard composition leading to variation in Young's Modulus

(4)

4. Highlight the difference in the tensile behaviour of aluminium and carbon steel (Discuss in terms of Yield stress, UTS, ductility and Toughness) [4 Marks]

Carbon Steel

a) Yield Stress:

It is higher (250 - 400 MPa) than Al as steel resists plastic deformation more due to strong metallic bonding & presence of C.

b) Ultimate Tensile Strength (UTS):

It is higher (400 - 600 MPa) than Al

c) Ductility (Ability to deform plastically):

It is moderate to low

d) Toughness (Resistance to fracture):

It is high for Carbon Steel

Aluminium

a) Yield Stress:

It is lower (50 - 100 MPa) than Carbon Steel. Al's pure metallic bonding allows easier slip, hence lower yield stress.

b) UTS:

It is lower (100 - 150 MPa) than Carbon Steel as carbon atoms strengthen the crystal lattice. Steel's microstructure provided strong interatomic bonding, while Al has a more uniform & softer structure.

c) Ductility:

It is higher in Al as its atoms can move more easily, allowing greater plastic deformation. Carbon Steel's stronger lattice & impurities restrict atomic movement.

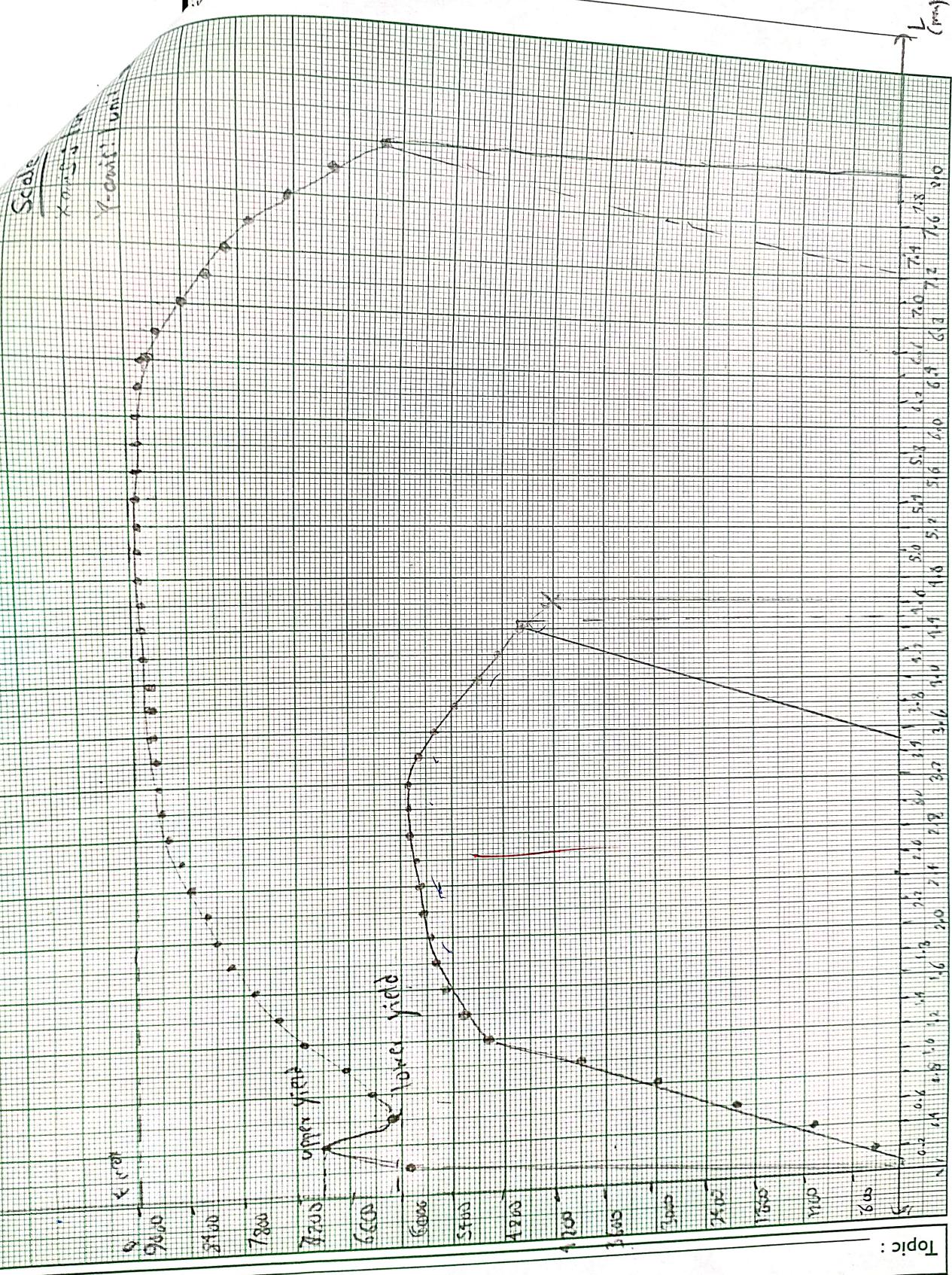
d) Toughness:

It is moderate in Al as steel combines strength with some ductility, enabling it to absorb large energy before fracture. Al, although ductile has lower strength, so total energy absorbed is less.

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Axis



In the standard values (210 GPa for reason for discrepancy? [4 Marks]

L-8C - 4845

(N)

(P)

MLL100: Introduction to Materials Science and Engineering – Lab Session-Exp-10

Lab Group: II B . 9_b

Name and Entry no: Aaditya 2024MS11124

Anurag Ghosh 2024BB10161

Amaan Afroz 2024TTU164

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Reading reference:

Creep Section (pp. 287 – 291) of Chapter 11 in Material Science and Engineering book (5th Edition.) by V. Raghavan.

Safety precautions:

- Handle the equipment and all related accessories safely and with utmost care.
- Conducting creep experiment on solder wire (Pb-based)
 - Experimental Procedure:
 - Measure the initial length (gauge length) of the solder wire.
 - Note down the temperature (i.e. room temperature) before starting the experiment and after completing the experiment.
 - Note down the load applied to the solder wire. Note down the initial time.
 - Measure all the required sample dimensions using Callipers or rulers.
 - Note down the time (minutes and sec) and elongation in the below Table in section c for every 1 mm elongation for the first 20 mm and subsequently for every 3 mm elongation till the solder wire breaks.
- Observation and Calculations: [2 marks]

S. No	Sample and Experiment details	
1	Initial length (i.e. Gauge length) (mm)	106.95645
2	Initial temperature (°C)	28
3	Final temperature (°C)	28
4	Applied load (in kg)	$1.25 + 0.6 \text{ kg}$ $= 1.85 \text{ kg}$
5	Time (sec) (start)	3:20:00
	(finish)	3:46:49

18.13
20.43 N

Creep experiment data:

[3 marks]

Answer the following based on your experimental observations and understanding:

1. How many stages of creep can you observe in your graph? Name them. [3 marks]

There are 3 stages of creep. 1 N

- ① Primary region: Creep rate is continuously decreasing over time.
 - ② Secondary region: Strain-rate is constant.
 - ③ Tertiary region: It is final accelerating phase leading to fracture.
Calculate the steady state creep rate (extension per unit length per unit time) from the

- ② Calculate the steady state creep rate (extension per unit length per unit time) from the

graph. [3 marks]

$$y_2 = 39.2 \text{ mm}$$

$$n_2 = 10 \text{ min}$$

$$y_1 = 24 \text{ mm}$$

$$n_1 = 6 \text{ min}$$

$$\therefore \text{Steady state creep rate} = \frac{y_2 - y_1}{L_0(n_2 - n_1)} = \frac{39.2 - 24}{X 10^{-6}} = 3.8 \text{ mm/min}$$

3. What would you observe if you had conducted this test on wire of either copper or iron? Give reason. [3 marks]

If test were conducted on copper/iron wire creep would be negligible because melting point of them copper & iron is too high compare to lead/tin. & Creep becomes significant only at temperatures 40% of T_m , & room temperature is much lower than this value for copper/iron

4. What is the effect of prior deformation on creep strength of a material? [3 marks]

Prior deformation introduces a high density of dislocation within the material, which act as barriers to further dislocation motion. As a result, the creep rate decreases & the creep strength of the material increases. However excessive prior deformation may also cause internal stress that may slightly reduce ductility.

5. What methods would you suggest for improving the creep strength of an aluminum alloy? [3 marks]

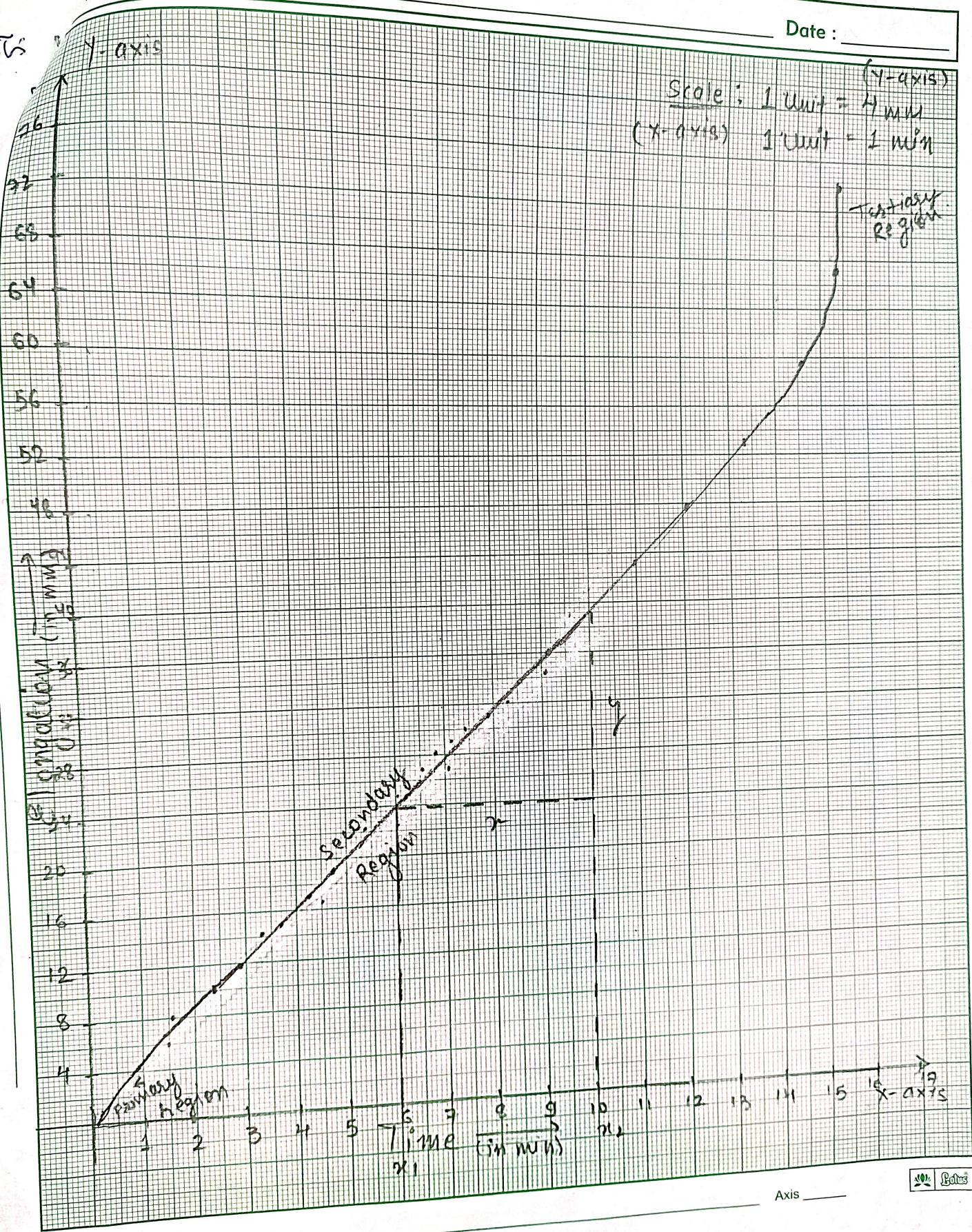
To improve the creep strength of all alloys, the following methods can be used.
Solid solution strengthening \rightarrow add alloying elements such as magnesium, silicon or copper to form a solid soln. that distorts the lattice and hinders dislocation movement.

Precipitation hardening from fine, stable precipitates thru heat treatment to obstruct dislocation motion at high temperature. This is most effective method for aluminium alloys.

Date : _____

Scale : 1 Unit = 4 mm (Y-axis)
(X-axis) 1 Unit = 1 min

Tertiary
Region



2024BB10818 \Rightarrow Vaibhav B. Sharma.

2024BB10981 \Rightarrow Aditya Gupta 2024TT10820 \Rightarrow Avneel Singh
2024MS10848 \Rightarrow Vanshika Saini 2024ME20824 \Rightarrow Bhoomi Soneri
2024AM10866 \Rightarrow Aayu Saini

MLL100: Introduction to Material Science and Engineering

Experiment 2: Two and Three-Dimensional Bravais Lattices

(A) Two-Dimensional Periodic Pattern

Crystals are nothing but three-dimensional periodic pattern of atoms. A periodic pattern can be described in terms of a lattice and a motif. We will look at a two-dimensional periodic patterns and identify its lattice and motif.

A1 Lattice: An infinite set of discrete points such that each has identical neighbours of other points is called a lattice. Any point of a periodic pattern can be selected as a reference lattice point. The set of all points exactly equivalent to this point constitutes the lattice of the pattern.

i) You are provided with a 2D pattern of footpath tiling outside Academic Complex East.. Place a sheet of tracing paper over the pattern. Choose any point of the pattern as a reference and mark your reference point with a dot. Now mark every translationally equivalent point of the pattern with a dot. These points constitute a finite portion of the infinite lattice. [2]

ii) Keeping the edges of the tracing paper parallel to the original directions, move the paper over the pattern so that the original dot now lies above some other feature. Note that the other dots give the positions of all points in the pattern which are equivalent to the new feature. Thus, the lattice of a pattern is the same whichever initial point is chosen as a reference point. Verify the above statement for different starting positions.

A2 Unit cell: A Lattice can be described by giving its unit cell which in 2D is a parallelogram and in 3D is a parallelepiped with lattice point at all corners. A *primitive unit cell* has lattice points at corners only. A *non-primitive unit cell* has extra lattice points apart from those at the corners. In 2D, a unit cell is defined by the edge lengths a and b and the included angle γ of the parallelogram. The quantities a , b and γ are known as the **lattice parameters**

[7]

i) Outline a primitive unit cell on the pattern. ABCD

ii) Measure a , b , γ and determine the area of the unit cell. $a = 2\sqrt{2}$, $b = 2\sqrt{2}$, $\gamma = 90^\circ$

iii) The choice of a unit cell is not unique. Outline a primitive unit cell of different shape and measure a , b , γ : $a = 2\sqrt{2}$, $b = \sqrt{2}$, $\gamma = 120^\circ$ \rightarrow EFGH

iv) How is the area of your second primitive unit cell related to that of your first choice? $\frac{1}{2}$ units²

v) Now outline a non-primitive unit cell. Label a , b and γ and find the area. $a = b = 2\sqrt{2}$, $\gamma = 135^\circ$

vi) How does the area of non-primitive cell relate to the area of the primitive cell? $\frac{1}{2}$ times

vii) What are the number of effective lattice points in non-primitive cells? 3

A3 Motif: A motif is the unit of the pattern associated with a lattice point. The choice of a motif is not unique. One way is to select the contents of a primitive unit cell as a motif. The whole pattern is always generated by repetition of a suitably selected motif at all the points of the lattice.

Determine the number of tiles that are contained in the motif? \rightarrow [1]

four

B. Three-Dimensional Crystals

B1 There are fourteen Bravais lattices. Each lattice has a conventional unit cell. Ball and stick models these unit cells are provided. Examine these models and identify them. [15]

B2. In the space below, draw a primitive cubic point of the edges of the unit cell. But there is no such lattice in

S. No.	Characteristic symmetry	Crystal system	Conventional Unit cell Parameters	Centering (P/I/F/S/R)	Bravais Lattice
1	None	Tetrahedral	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	P	ap
2	3 Two-fold	Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	P	op
3	1 □	Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	I	t F
4	3 0	orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	C	oc
5	3 Two-fold face centered	Orthorhombic face centered	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	if	of
6	1 △ 1 ◇	Trigonal Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	P	hp
7	3 4-fold ?	Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	I	cI
8	3 4-fold 3	Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	P	cp
9	3 Two-fold	Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	I	mp oI
10	3 4-fold	Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	F	cf
11	1 ■	Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	P	mp tp
12	2 3-fold hexagonal Rhombohedral	Hexagonal Rhombohedral	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$	R	tr
13	1 0	Monoclinic	$a \neq b \neq c$ $\alpha = \beta = 90^\circ, \gamma \neq 90^\circ$	C	mc
14	1 0	Monoclinic	$a \neq b \neq c$ $\alpha = \beta = 90^\circ, \gamma \neq 90^\circ$	P	mp

4, 3-fold

Trigonal crystal system

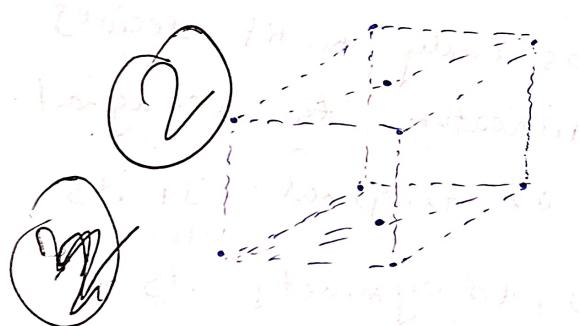
B2. In the space below, draw a primitive cubic (cP) unit cell. Add additional points at mid-point of the edges of the unit cell. We have thus created a unit cell of a possible "edge-centred lattice". But there is no such lattice in the list of Bravais lattices. Explain. [2]



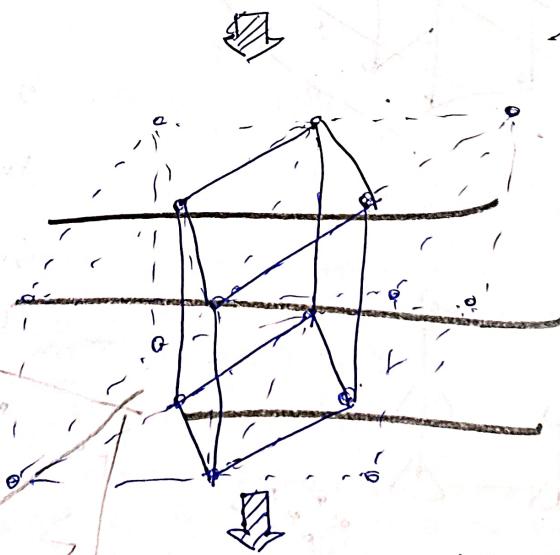
→ Possible "edge-centred lattice"
 $a=b=c$
 $\alpha=\beta=\gamma=90^\circ$

The surrounding of all the lattice points will not be same hence it will not exist.

B3. Draw a unit cell of primitive tetragonal (tP) lattice. Add additional lattice points on the centres of a pair of rectangular faces to convert it to a unit cell of an end-centred tetragonal (tS) lattice. But there is no tS lattice in the list of 14 Bravais lattice. Explain. [3]



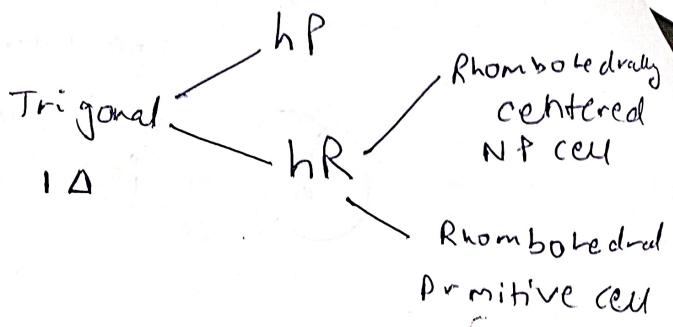
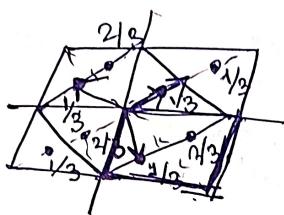
→ "end-centred lattice"
 $a=b \neq c$
 $\alpha=\beta=\gamma=90^\circ$



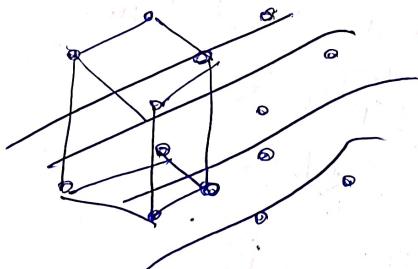
This forms another unit cell when we form new lattice joining the lattice its original symmetry is destroyed. Its ~~not~~ ^{now} 4 fold & now becomes 2 fold which is of orthorhombic.

This is due to addition of points at ends of faces' new characteristic is of orthorhombic.

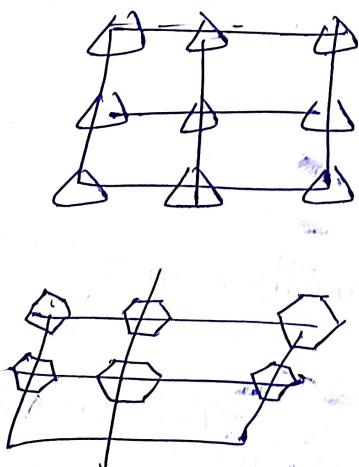
B4 The hexagonal rhombohedral (*hR*) lattice belonging to the trigonal crystal system is the only Bravais lattice which is associated with two conventional cells: a rhombohedrally centred hexagonal cell and a primitive rhombohedral cell. Draw a projection of 2×2 four hexagonal unit cells of an *hR* lattice showing the heights of the projected lattice points in terms of fractions of *c*. For one of the unit cell indicate the basis vectors \mathbf{a}_{H} and \mathbf{b}_{H} of the hexagonal cell. Superimpose on the diagram the three basis vectors \mathbf{a}_R , \mathbf{b}_R , \mathbf{c}_R of the rhombohedral cell of the *hR* lattice.



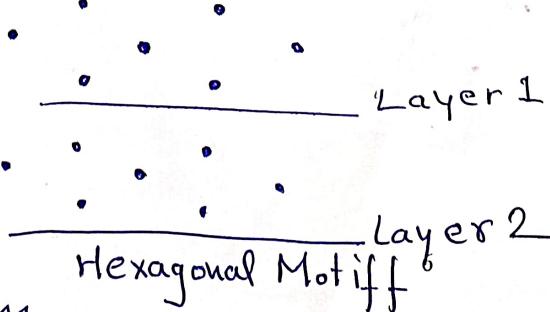
B5 Draw a projection of a primitive hexagonal unit cell. Associate a motif with the lattice points such that the crystal belongs to the trigonal system rather than hexagonal system.



Basically motif decides whether its hexagonal or trigonal - If its 3 fold symmetry its trigonal and if its 6 fold symm. its hexagonal



Trigonal System derived from Hexagonal



Layer 1
Layer 2
Hexagonal Motif

ystal system is the
ombohedrally
four
ion of 2×2 four
lattice points in
the lattice of the

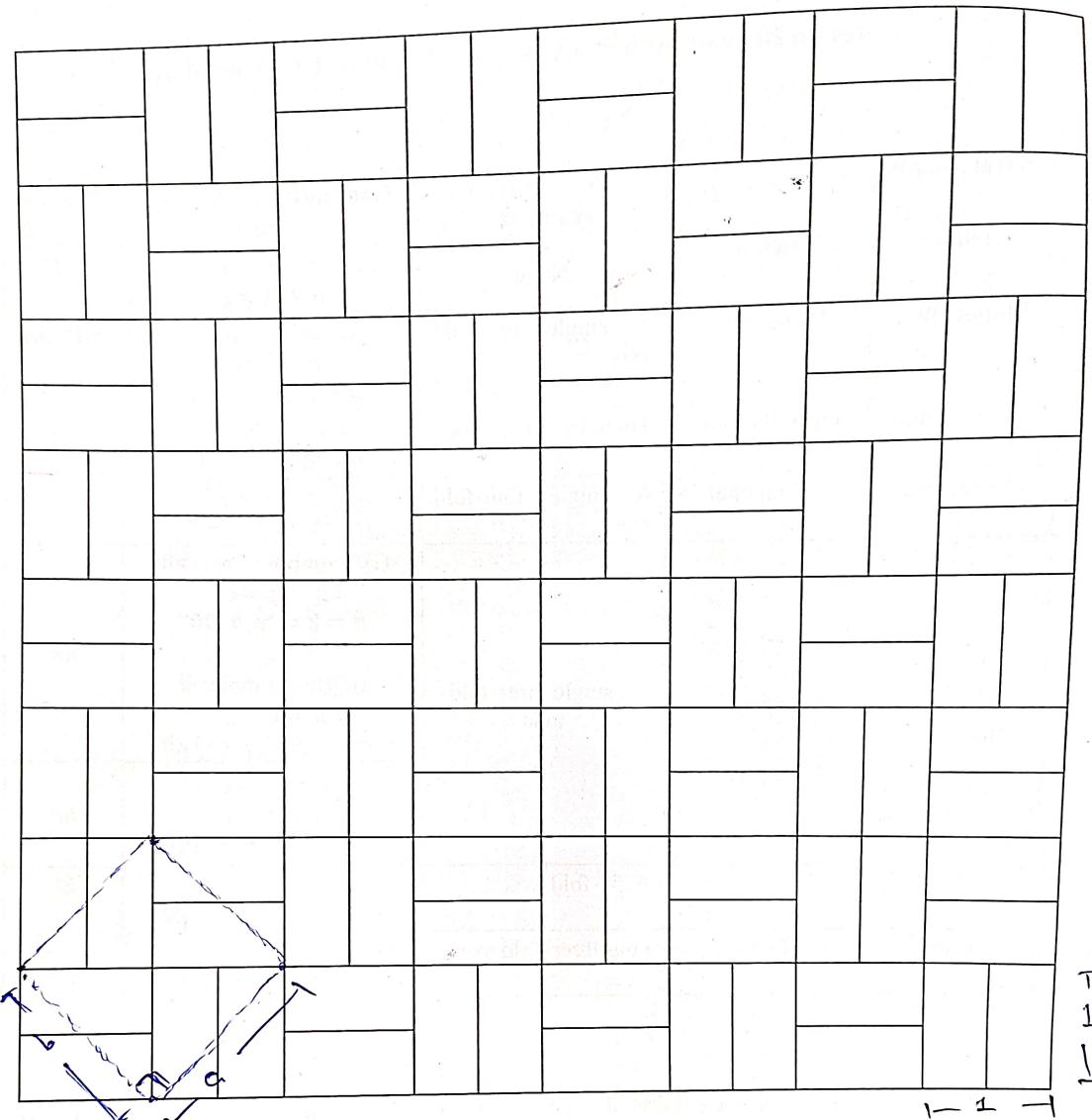
Notes on Bravais lattices and Crystal Systems (Experiment 2)

(Not to be submitted)

Crystal Family	Crystal system	Characteristic Symmetry	Conventional Unit Cell Shape	Bravais Lattices
Triclinic	Triclinic	None	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	aP
Monoclinic	Monoclinic	A single two-fold axis.	(i) Unique axis c $a \neq b \neq c$ $\alpha = \beta = 90^\circ \neq \gamma$	mP, mA
Orthorhombic	Orthorhombic	Three two-fold axes	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	oP, oI, oF, oC
Tetragonal	Tetragonal	A single four-fold axis	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	tP, tI
Hexagonal	Trigonal	A single three-fold axis	(i) Rhombohedral cell $a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$	hR
			(ii) Hexagonal cell $a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	
	Hexagonal	A six-fold axis	Hexagonal cell $a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	hP
Cubic	Cubic	Four three-fold axes	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	cP, cI, cF

NOTES:

1. The symbol for Bravais lattice consists of two letters: the first small letter represents the crystal family and second capital letter represents the centring of the conventional cell. Thus the first letters of the lattices of the different crystal families are:- Triclinic : a , Monoclinic : m , Orthorhombic : o , Tetragonal : t , Hexagonal : h , and Cubic : c . The letter a in the symbol for triclinic system stands for 'anorthic' meaning that no pair of the axes of the conventional cell are orthogonal. The centering symbols are: A : A-centered, B : B-centered, C : C-centred, S : (A , B , or C -centred), F : Face-centred, I : Body-centred, R : Rhombohedral centred.
2. The ' \neq ' sign should be interpreted as '*not required to be equal by the symmetry of the crystal system*'. They can sometimes be equal, these cases are known as '*accidental equality*'. Equivalently '=' stands for '*required to be equal by symmetry of the crystal system*'.
3. The lattice hR of the trigonal system has two alternative conventional cells associated with it: the rhombohedral cell or the hexagonal cell. The rhombohedral cell is primitive whereas the hexagonal cell is rhombohedrally centred. This is the only lattice for which two alternative conventional cells are associated. Irrespective of the choice of the cell the lattice is called hR .



Footpath Tiling Outside Academic Complex East

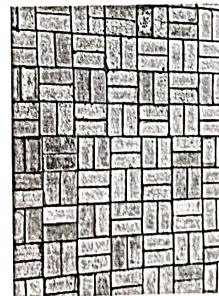
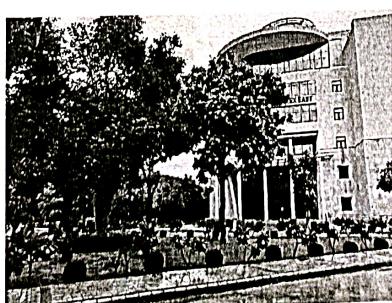


Photo: Kishore Kumar J.

MLL100: Introduction to Materials Science and Engineering – Lab Session

Student Names:

Shaurya

Sidnant Kumar

Om Jaiswal

Priyanshu P. Senapati,

SACHIN RAJ

Entry Nos:

2024MS11120

2024MS1093U

2024MS11158

2024MS10867

2024RTT10993

Group No:

24.5

25

Experiment 3: X-ray Diffraction Studies

Reading reference: Section 3.6 (pp.42-45) in Material Science and Engineering book (5th Edn.) by V. Raghavan.

(8 Marks)

Q1: Make a list of $h k l$ values for increasing values of $h^2 + k^2 + l^2$ (note that for some values of $h^2 + k^2 + l^2$ there is no corresponding $h k l$ whereas for some there are more than one set of $h k l$ values). Then using the extinction rules for cubic crystals (Table 3.3 of pg. 44 in your textbook) indicate the reflections that are present in SC, BCC, FCC and DC crystals by their corresponding $h^2 + k^2 + l^2$ values. The first three rows have been filled as an example.

8

$h^2 + k^2 + l^2$	$h k l$	$h^2 + k^2 + l^2$ value for allowed reflection			
		SC	BCC	FCC	DC
1	100	1			
2	110	2	2		
3	111	3		3	3
4	200	4	4	4	-
5	210	5			
6	211	6	6	-	-
7	220				
8	220	8	8	8	8
9	300/221	9	-	-	-
10	310	10	10	-	-
11	311	11	-	11	11
12	222	12	12	12	-
13	320	13	-	-	-
14	321	14	14	-	-
15	-				
16	400	16	16	16	16
17	410/322	17	-	-	-
18	411/330	18	18	-	-
19	331	19	-	19	19
20	420	20	20	20	-
21	421	21	-	-	-
22	232	22	22	-	-

1

Attendance. Tuesday Buffer.

<u>Slno</u>	<u>Name</u>	<u>Entry no.</u>	<u>Group no.</u>
1.	Mahima chotiya	2024 ME11187	2A 10 / 2A
2.	Shawrya	2024 MS11120	2
3.	Sidhant Kumar	2024 NS10934	2
4.	Anubhav Kr. Verma	2024 ME10360	2, (2A)
5.	Krish Bansal	2024 ME10360	1, (2A)
6.	Rishi Jain	2024 ME10360	2, (2A)
7.	Airudh Bohra	2024 AM10977	5 (2A)
8.	Pratiksh Kumar	2024 AM11185	5 (2A)
9.	Jessica	2024 AM10056	5 (2A)
10.	Divya Yadav	2024 TT10282	5 (2A)
11.	Satyam Kumar	2024 NS10421	9 (2A)
12.	Manish Kumar	2022 ME12036	6 (2A)
13.	Himanshu Jeph	2024 ME20350	6 (2A)
14.	Arje Saurabh	2022 CS11610	6 (2A)
15.	Radha Gupta	2024 ME20461	10 (2A)
16.	Vipul Meena	2024 ME10754	1 (2A)
17.	Soham Soham Gupta	2024 AM10632	1 (2A)
18.	SHUBH PATEL	2024 AM10423	9 9 (2A)
19.	Divyanka Meena	2024 ME10888	11 11 (2A)
20.	Manish Girish Rane	2024 ME10315	05 (2A)
21.	Gaurav Agarwal	2024 AM10593	12 (2A)
22.	Nysa Jindal	2024 ME20837	12 (2A)
23.	Apurva	2024 UME2 0149	08 (2A)
24.	Naina Mittal	2024 ME20416	3 (2A)
25.	Nancy Tripathi	2022 ES11204	3 (2A)
26.	Kunal Bisht	2022 ES11861	

27.	Rhythm Shah	2022ES11791	3 (2A)
28.	Ninit Jain	2022ES11200	3 (2A)
29.	Robert Agarwal	2022ES11233	4 (2A)
30.	Harsh Mittal	2022ES11796	4 (2A)
31.	Ashlesha Ratnaparkhi	2022CH11486	4 (1B)
32.	Shreya Khare	2022CH11440	7 (2A)
33.	Subhang Ladher	2022CH11430	
34.	Aditya Deshmukh	2022CH11439	
35.	Sanchit Vijay	2022CH11428	
36.	Siddhesh Ray	2022CH11025	4 (4A)

Q2: X-ray diffraction pattern from a cubic crystal system (12 marks)

Set No:

You are provided with an x-ray diffraction pattern from a cubic crystal (SC/BCC/FCC/DC). You should index the peaks and determine the Bravais lattice. Place the indices determined by you next to the peaks on the diffraction pattern.

Determine the lattice parameter, a , using the data for the highest diffraction angle. Use the value of $\lambda = 1.54 \text{ \AA}$.

Peaks	$2\theta_i$	θ_i	$\sin^2(\theta_i)$	$\frac{\sin^2(\theta_i)}{\sin^2(0_1)}$	Clear Fraction	$h^2 + k^2 + l^2$	hkl
1	38.57	19.29	0.1091	1	2	2	(110)
2	45.71	22.85	0.1808	1.8	4	4	(200)
3	66.43	33.21	0.2999	2.9	6	6	(211)
4	80.00	40.00	0.4132	4.1	8	8	(220)
5	84.28	42.14	0.4802	4.8	10	10	(310)
6	101.43	50.71	0.599	5.9	12	12	(222)
7	114.28	57.14	0.7056	7.05	14	14	(321)
8	119.29	59.64	0.7845	7.84	16	16	(400)
9							
10							

The diffraction pattern is for BCC lattice.

Lattice parameter a

$$(h, k, l) = (4, 0, 0)$$

$$\lambda = 2d_{hkl} \sin \theta \Rightarrow 1.54 = \frac{2 \times a}{\sqrt{4^2 + 0^2 + 0^2}} \times 0.8628$$

$$\Rightarrow a \approx 3.5 \text{ \AA}$$

Q2: X-ray diffraction pattern from a cubic crystal system
Set No: b
 You are provided with an x-ray diffraction pattern from a cubic crystal system.
 You should index the peaks and determine the Bravais lattice. Place the indices determined by you next to the peaks on the diffraction pattern.
 Determine the lattice parameter a using the data for the highest diffraction angle. Use the value of $\lambda = 1.54 \text{ \AA}$.

Peaks	$2\theta_i$
1	38.18
2	44.6
3	6
4	

(12 marks)

ystal (SC/BCC/FCC)
; the indices determin

Q2: X-ray diffraction pattern from a cubic crystal system

(12 marks)

Set No: **B**

12

You are provided with an x-ray diffraction pattern from a cubic crystal (SC/BCC/FCC/DC). You should index the peaks and determine the Bravais lattice. Place the indices determined by you next to the peaks on the diffraction pattern.

Determine the lattice parameter, a , using the data for the highest diffraction angle. Use the value of $\lambda = 1.54 \text{ \AA}$.

Peaks	$2\theta_i$	θ_i	$\sin^2(\theta_i)$	$\frac{\sin^2(\theta_i)}{\sin^2(\theta_1)}$	Clear Fraction	$h^2 + k^2 + l^2$	hkl
1	38.18	19.09	0.107	1	3	3	(111)
2	44.48	22.24	0.143	1.336	4	4	(200)
3	65.45	32.72	0.292	2.728	8	8	(220)
4	78.74	39.37	0.402	3.757	11	11	(311)
5	82.94	41.47	0.438	4.093	12	12	(222)
6	90.72	49.86	0.584	5.457	16	16	(400)
7	112.31	56.15	0.690	6.449	19	19	(331)
8	117.2	58.6	0.728	6.804	20	20	(420)
9							
10							

✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓ ✓

5 + 4
= 9

The diffraction pattern is for FCC lattice.

Lattice Parameter (a)

$$(hkl) = (420)$$

$$\lambda = 2d_{hkl} \sin \theta = \frac{2a}{\sqrt{h^2+k^2+l^2}} \sin \theta = 2$$

$$\Rightarrow 1.54 = 2 \times \frac{a}{\sqrt{16+4+0}} \sin(58.6^\circ) \Rightarrow a = 5.8 \text{ \AA}$$

$$\Rightarrow a = 4.03 \text{ \AA}$$

4.5

Q3: Mr. Prasad will demonstrate an XRD experiment in today's lab. Please observe and complete the following questions: (5 marks)

- (i) What is the target and its characteristic radiation in the machine?

Target - copper ✓ Characteristic Radiation - copper-K α ✓

1

- (ii) What is the scan rate for the samples used?

10°/minute ✓

1

1200

(iii) Draw the XRD pattern schematic observed (Intensity vs 2 θ) from the experiment.

Intensity ↑

60.00

50.00

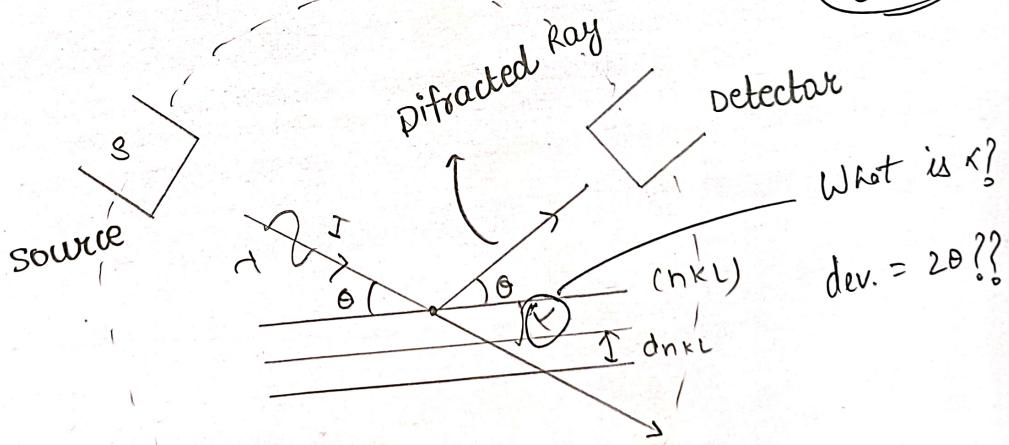
2 θ

70.00

2

- (iv) Draw a schematic of the essential features of an XRD highlighting X-rays from the tube on a crystal and detector measuring the intensity of diffracted X-rays. Highlight the incident and diffracted rays.

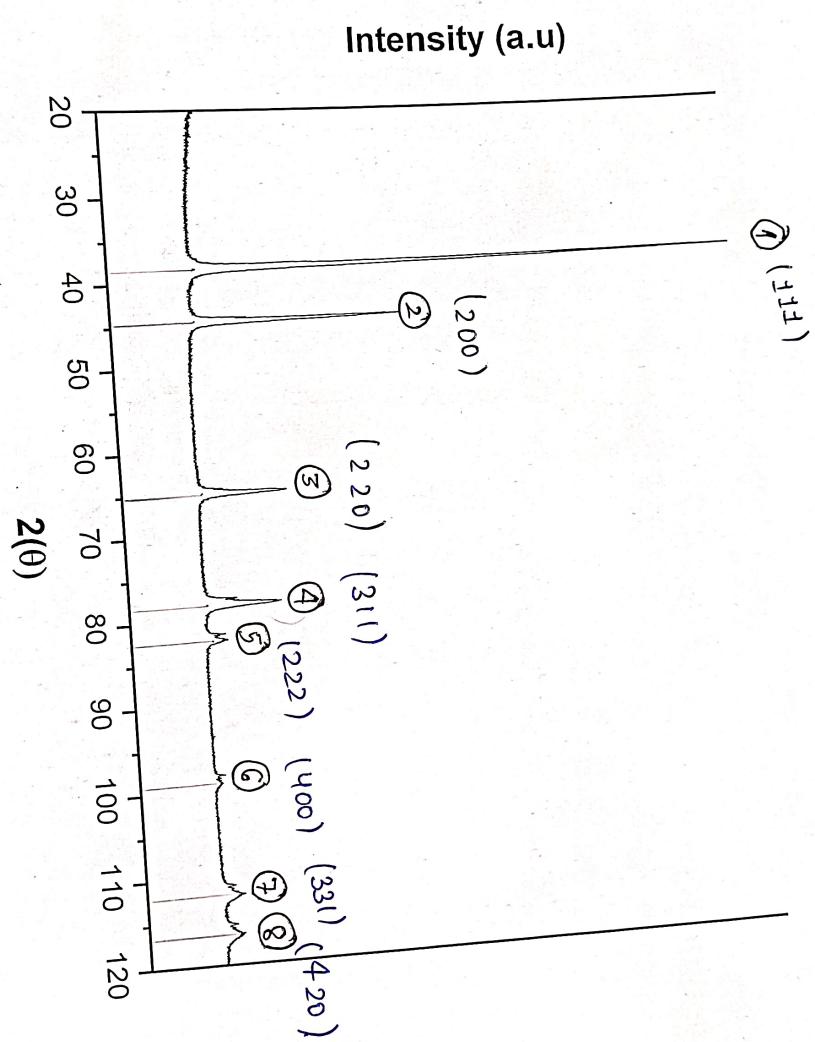
0.5



$$\lambda_{CuK\alpha} = 1.54 \text{ \AA}$$

$$\lambda = 2d_{nkl} \frac{\sin \theta}{3}$$

$$= \frac{2a}{\sqrt{h^2 + k^2 + l^2}} \sin \theta$$



B

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]

$$\begin{aligned} V &= 12 \times 5 = 60 \\ F &= 20H + 12P = 32 \\ E &= 30 + 12 \times 5 \\ &= 90 \end{aligned}$$

$$\begin{array}{c} V \\ E \\ 90 \\ F \\ 32 \end{array}$$

$$F + V - E = 2$$

1

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].

$F = P + H$ only, $P \rightarrow$ number of pentagonal faces
 $H \rightarrow$ number of hexagonal faces

$$E = \frac{\text{total no. of edges}}{2} \quad [\text{shared by } 2]$$

$$= \frac{5P + 6H}{2}$$

Let no. of vertices be x

$$\Rightarrow \text{No. of edges} = \frac{3x}{2} \quad \left\{ \begin{array}{l} \text{each carbon has an edge with 3 others} \\ \text{and each edge is shared twice} \end{array} \right\}$$

Using Euler's polyhedron formula:

$$F + V - E = 2$$

$$P + H + x - \frac{3x}{2} = 2$$

$$\Rightarrow P + H - \frac{x}{2} = 2$$

$$\Rightarrow P + H - \frac{5P + 6H}{6} = 2$$

$$\Rightarrow \frac{P}{6} = 2 \Rightarrow P = 12$$

\Rightarrow There are always 12 pentagonal faces and ^{only} no. of hexagonal faces change.

$$\frac{3x}{2} = \frac{5P + 6H}{2}$$

$$\Rightarrow x = \frac{5P + 6H}{3}$$

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

[2]

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

2

2

[2]

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

$$a = b = c = 26 \text{ mm}$$

$$d = 15 \text{ mm} \quad [1+3]$$

4

$$\gamma = 120^\circ$$

$$a = s_1 = s_2 = 2 \times d \cdot \cos 30^\circ$$

$$a = s_1 = s_2 = 25.5 \text{ mm}$$

$$= 2 \times \frac{\sqrt{3}}{2} \times 15 = 25.5 \text{ mm}$$

2 (d) Is the unit cell primitive or nonprimitive? Give reason.

[1+1]

→ Primitive

2

→ This is primitive because there are no lattice points apart from corners.

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.

$$d = 15 \text{ mm}$$

$$\Rightarrow a = \sqrt{3}d$$

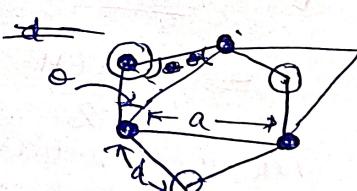
[2+1]

3

$$a = 2 \cdot d \cdot \cos \theta$$

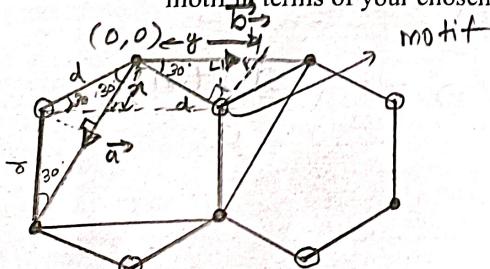
$$= 2 \cdot 15 \cdot \cos 30^\circ = 2 \times \frac{\sqrt{3}}{2} \times 15$$

$$= 25.5 \text{ mm}$$



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]



$$x = d \cos 30^\circ$$

$$x = \frac{\sqrt{3}d}{2}$$

$$2x \cos 30^\circ = d$$

$$\sqrt{3}x = d$$

$$\sqrt{3}x = \frac{d}{\sqrt{3}}$$

$$x = \frac{a}{3}$$

$$y = \frac{d \cos 30^\circ}{\sqrt{3}} = \frac{d}{\cos 30^\circ}$$

$$y = \frac{a}{\sqrt{3}} \times \frac{2}{\sqrt{3}}$$

$$y = \frac{2a}{3}$$

Hence, coordinates of motif in (\vec{a}, \vec{b}) form
 $= \left(\frac{a}{3}, \frac{2a}{3} \right)$

3 (a) Wrapping or Chiral vector and (n, m) q representing graphene motif two primitive vectors where n and m are integers. As an example, the end points of graphene is given by vectors (n, m) tube and $3N_z$

Graphene?
Sheet 2. Place an open circle to represent a reference point equivalent to the reference graphene.

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 \mathbf{C} meet to define the circumference of the tube. Such a tube is designated an (n, m) tube and the corresponding vector \mathbf{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:

8 (i) $(8, 0)$

Zigzag

(ii) $(3, 3)$

armchair

(iii) $(5, 3)$

chiral

[3]

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

Armchair $= (n, m)$

Zigzag $= (n, 0)$

[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.

~~$(3, 3)$~~ $= (n, m)$

[2]

- (ii) Make another model (Sheet 4) of a zig-zag tube.

Determine its (n, m) designation.

~~$(0, 0)$~~ $= (n, m)$

$(11, 0) = (n, m)$ [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.

$$|\mathbf{C}_H| = \bar{\alpha}_1 n + \bar{\alpha}_2 m$$

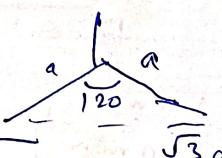
so, $|\bar{\alpha}_1| = |\bar{\alpha}_2| = d\sqrt{3}$

$$\therefore |\mathbf{C}_H| = \sqrt{(d\sqrt{3})^2 n^2 + (d\sqrt{3})^2 m^2 + 2nm \bar{\alpha}_1 \bar{\alpha}_2}$$

$$= \sqrt{3}d \sqrt{n^2 + m^2 + nm}$$

$$D_{\pi} = C_H$$

$$D = \frac{\sqrt{3}d}{\pi} \sqrt{n^2 + m^2 + nm}$$



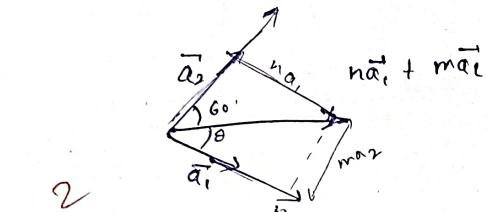
[3]

3

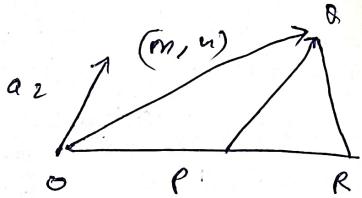
3(d) Chiral angle: The angle θ which the chiral vector $C = n \vec{a}_1 + m \vec{a}_2$ makes with the axis \vec{a}_1 is called the chiral angle. Derive a formula for θ in terms of n and m . Determine the chiral angles of the three vectors in 3(a) using your formula and check them by measurements on drawings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

$$\cos \theta = \frac{\vec{a}_1 \cdot (n \vec{a}_1 + m \vec{a}_2)}{(\vec{a}_1) |n \vec{a}_1 + m \vec{a}_2|} [2]$$

$$(|\vec{a}_1| = |\vec{a}_2| = a)$$



$$\cos \theta = \frac{n a^2 + m a^2}{2a}$$



$$\tan \theta = \frac{ma \sqrt{3}/2}{na + ma/2} = \frac{(0R + 1R)^2 + (0R)^2}{(na + ma/2)^2 + (\frac{ma \sqrt{3}}{2})^2}$$

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]

(3,0)

$$L_{3,0} = (3^2 + 0^2 + 3 \cdot 0)^{1/2} a = 8a$$

$$\tan \theta = \frac{\sqrt{3} \cdot 0}{2 \cdot 8 + 0} = 0 \Rightarrow \boxed{\theta = 0}$$

verified from figure

(3,3)

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

$$\tan \theta = \frac{\sqrt{3} \cdot 3}{2 \cdot 3 + 3} = \frac{\sqrt{3} \cdot 3}{3a} = \frac{1}{\sqrt{3}} \quad \boxed{\theta = 30^\circ}$$

3

$$a = 25.5 \text{ mm}$$

$$L_{3,3} = 130 \text{ mm}$$

verified from figure

(5,3)

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

$$\tan \theta = \frac{\sqrt{3} \cdot 3}{2 \cdot 5 + 3} = \frac{3\sqrt{3}}{13} \Rightarrow \boxed{\theta = 21.7^\circ}$$

figure $\theta = 26^\circ$

$$L_{5,3} = 175 \text{ mm}$$

$$\text{measured} = 177 \text{ mm}$$

verified

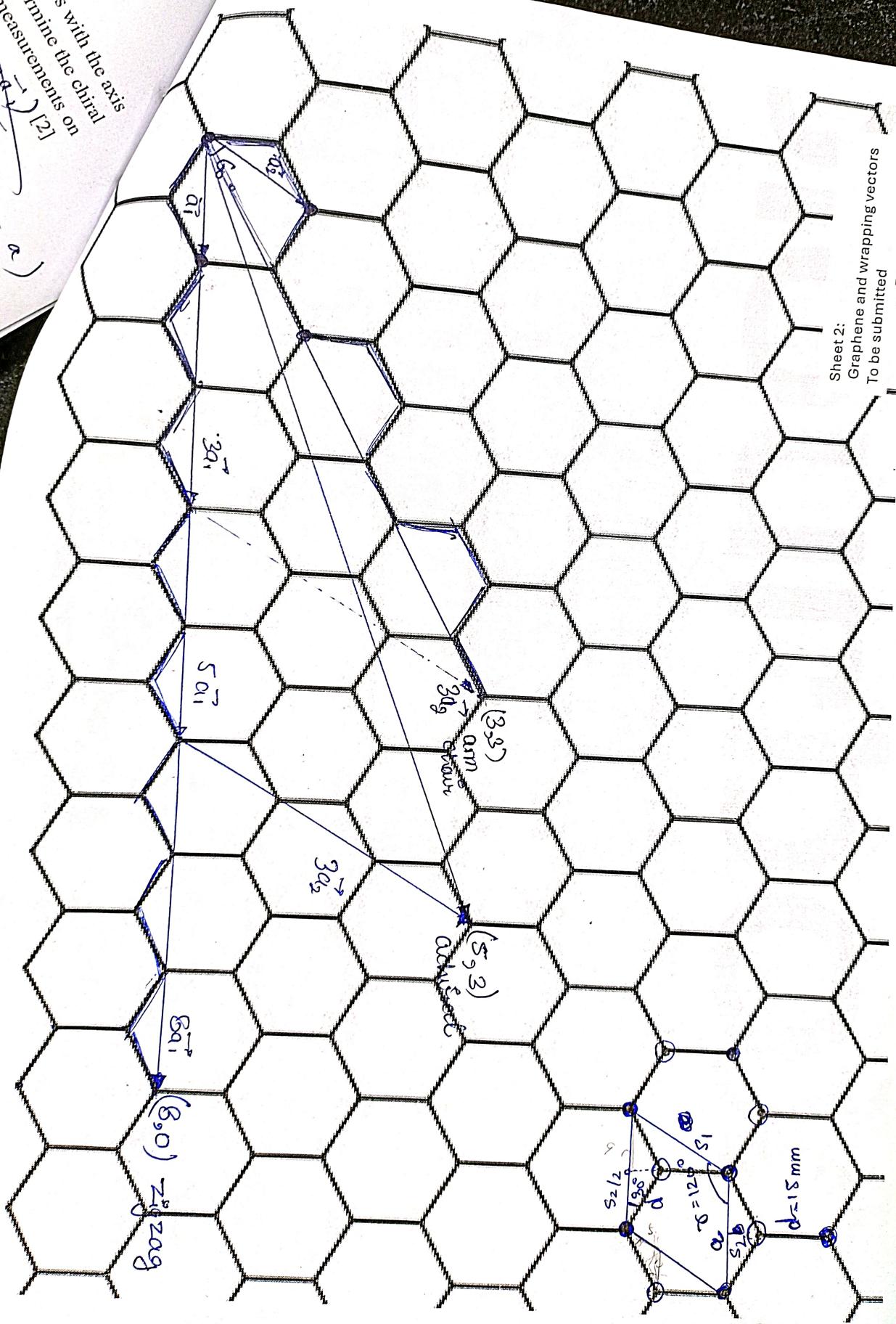
human error

4

$a_1 + m a_2$ makes with the axis
of n and m . Determine [2]

($n \cdot \bar{a}_1 + m \bar{a}_2$) $= (\bar{a}_1 + a)$

check them by θ .



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MLL100: Introduction to Materials Science and Engineering – Lab Session

Student Name:

Entry No:

Lab Group No: 04

Experiment 6 : To study the models depicting defects in 3D crystalline Structures and 2D graphene

Important instruction:

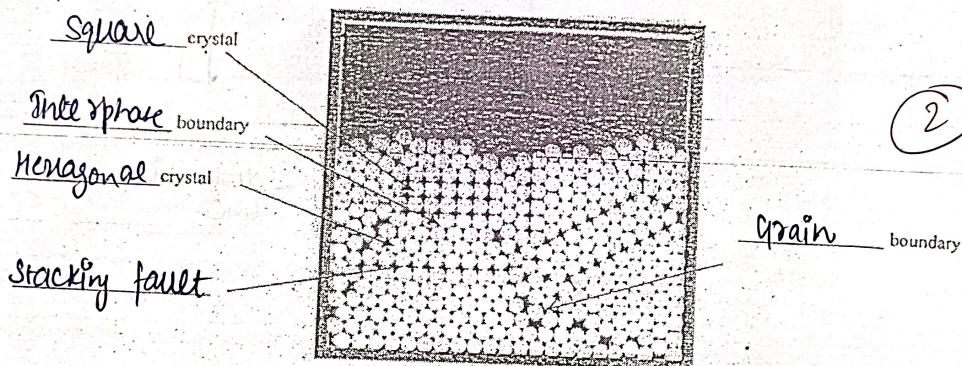
All models used for this experiment are fragile. Do not play with them. You are requested to handle them with extreme care. Do not pull or push on the models while passing it to others.

17
17

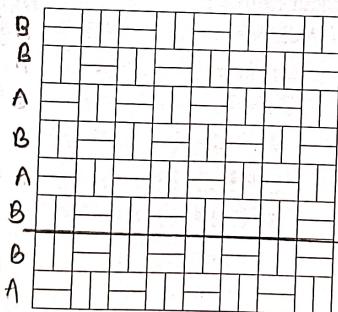
1. Ball bearing model: Identify the defects in them

[2 Marks]

Balls represent hard sphere atoms. By shaking the model you can get the balls in different configurations and see vacancies, grain boundaries, stacking faults and free surface. You can also generate three different phases: square crystals, hexagonal crystal and amorphous phases. By gentle tapping of the model, it is also possible to get the entire model into a single crystal. The following figure depicts one such configuration of balls generated in this model. Here vacancies are not seen but you will find that it gets generated very easily in the actual model. Complete all the labels in the figure giving brief justification.



2. Recall that an error was found in drawing of the 99C footpath tiling provided to you Experiment 2 on Two and Three-Dimensional Bravais Lattices. On careful observation it turns out that there is a boundary that separates two otherwise perfect regions of the tiling. Draw this boundary and characterise it, in analogy to defects in 3D crystals, as a dislocation, grain boundary or stacking fault. Give reasons.

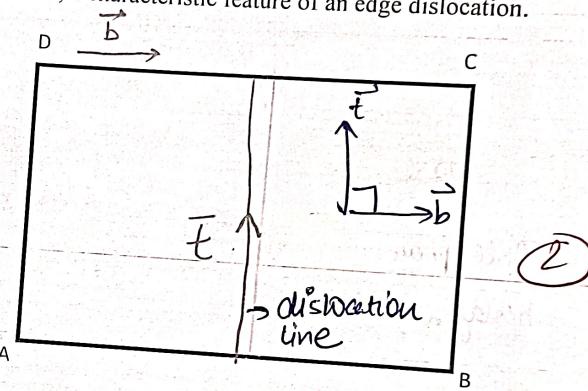
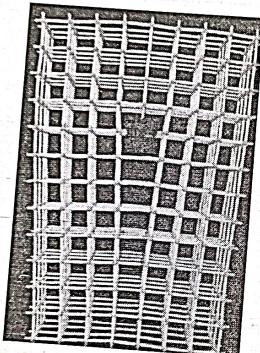


Stacking fault is present in these tiles, if we consider the 1st row is A and 2nd is B, the pattern is ABAB which is disrupted at boundary with continuous BB.
This yields to a stacking point

3. Model 1 (Edge dislocation): Identify the related characteristics [2 Marks]

You are provided with a model of an edge dislocation, in that:

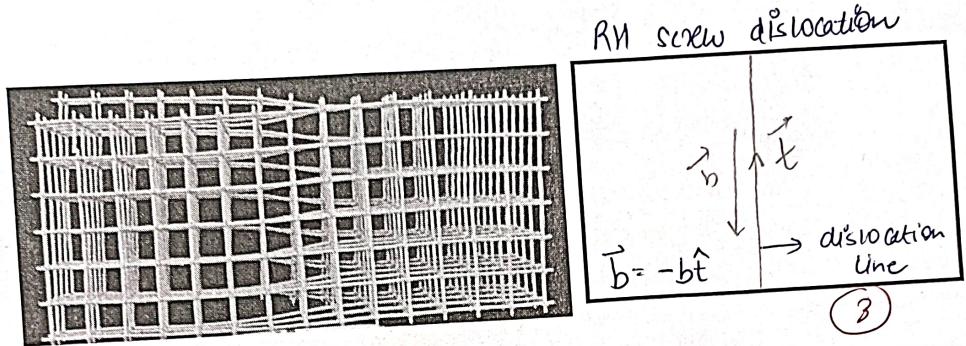
- Locate the extra half plane and the dislocation line by putting a pencil along it.
- Select a positive sense of the vector \vec{t} (unit vector tangent to the dislocation line) either going into the model or coming out of it.
- Select a starting point and follow a Burgers circuit (Right Hand Finish to Start Rule) around the dislocation. Notice that the circuit fails to close due to the presence of the dislocation. The vector from the finish to start point is the Burgers vector \vec{b} of the dislocation.
- Identify the slip plane of the model. The rectangle ABCD, represents the slip plane of the model with AB on the front side. Sketch the dislocation line, the line vector \vec{t} and Burgers vector \vec{b} in the diagram.
- Notice that \vec{t} and \vec{b} are perpendicular, a characteristic feature of an edge dislocation.



4. Model 2 (Screw dislocation): Identify the related characteristics [3 Marks]

You are provided with a model of a screw dislocation, in that:

- Locate the dislocation line by putting a pencil along it. Note that planes perpendicular to the dislocation line acquire a screw character. Is it a left-handed (LH) or right-handed (RH) screw dislocation?
- Select a positive sense of the line vector \vec{t} (unit vector tangent to the dislocation line) either going into the model or coming out of it.
- Select a starting point and follow a Burgers circuit (Right Hand Finish to Start Rule) around the dislocation line. Notice that the circuit fails to close due to the presence of the dislocation. The vector from the finish to start point is the Burgers vector \vec{b} of the dislocation.
- A rectangle, representing the slip plane of the model, is shown below. Sketch the dislocation line, the line vector \vec{t} and Burgers vector \vec{b} in that diagram.
- Notice that \vec{t} and \vec{b} are parallel (or anti-parallel), a characteristic feature of a screw dislocation.



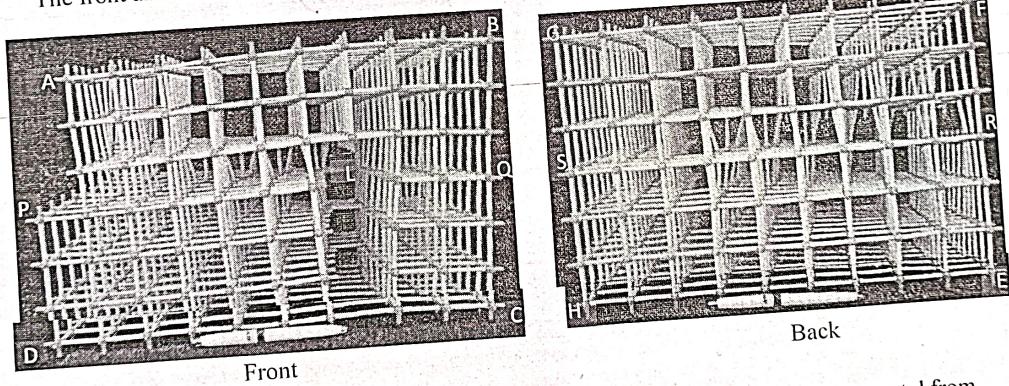
5. Model 3 (Mixed dislocation): Identify the related characteristics [4 Marks]

Two properties of a dislocation:

(A) A dislocation cannot end abruptly inside a crystal.

(B) The Burgers vector of a dislocation remains constant.

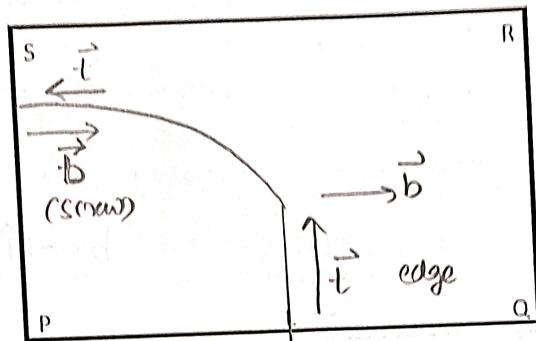
The front and the back views of this model containing dislocations are shown below:



(a) Note that an extra half plane (and hence an edge dislocation) enters into the crystal from the front face at a point marked L. However, unlike Model 1, no half plane or dislocation comes out from the back face. Look at the model carefully to resolve this apparent contradiction to the property (A).

(b) Select a starting point and follow a Burgers circuit (Right Hand Finish to Start Rule) around both the end point of the dislocation line and convince yourself that the Burgers vector \vec{b} is the same (property (B)). For this you need to select \vec{t} vectors at the two ends which are consistent with each other, i.e., if it goes into the model at one end it should come out of it at the other end.

(c) Identify the slip plane of the model. A rectangle, representing the slip plane PQRS of the dislocation in this model, is shown below. Sketch the dislocation line, and choose your line vector \vec{t} . Indicate the edge and screw segments of the dislocation line.



(1)

6. Ask your TA to show and explain a low angle symmetric tilt boundary [2 Marks]

(2)

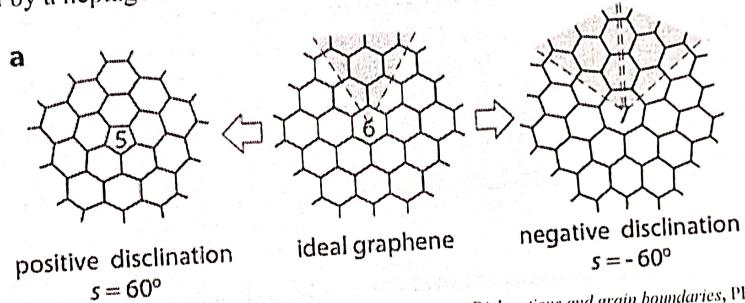
Note your observations:

Along the grain boundary there is a symmetry. There is an array of edge dislocation & along the grain boundary & it is in the region of ~~000~~ angles hence it is a low angle symmetric tilt boundary.

$\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}$ symmetry line (about this line grain boundary region exists) [2 marks]

6. Disclinations in Graphene:

As you have seen, graphene is a two-dimensional crystal with 3-coordinated carbon atoms located at the corners of hexagonal rings. There are two kinds of disclination defects which are possible in the structure. In one case, positive disclination ($s=+60^\circ$), a hexagonal ring is replaced by a pentagon. In the other case, the negative disclination ($s=-60^\circ$), the hexagonal ring is replaced by a heptagon. In both the cases the carbon atoms are still 3-coordinated.



(2)

[From Oleg V. Yazyev and Steven G. Louie, *Topological defects in graphene: Dislocations and grain boundaries*, PHYSICAL REVIEW B 81, 195420, 2010]

From one of the patterns of graphene cut out a 60° sector. Although the sector boundary is shown as cutting the bonds perpendicularly, it may be easier to take these boundaries along the C-C bonds. Preserve this sector for the next model. Carefully rejoin the cut edges to create a $+60^\circ$ disclination. Note that flat graphene acquires a curvature. This curvature is like that of a cone (funnel)

From another sheet of hexagonal ring make a cut and insert the 60° sector removed from the previous model. You have now created a -60° disclination. Note that the surface now acquires a curvature. The shape of curvature is that of a saddle.

Group - ②

Shawrya
Sachin
Priyanshu

Sidhant

MLL100 Sem 1 2025-2026

Om

Experiment 5

56
56

To study the arrangement of atoms & voids in close packed crystals

Reading:

Section 5.3 (pp.88-97) in Material Science and Engineering book (5th. Edn.) by V. Raghavan.

1. Show your stella octangula and cuboctahedron models to lab instructor and get his/her signature.
2. Stacking sequence in closed packed structures:

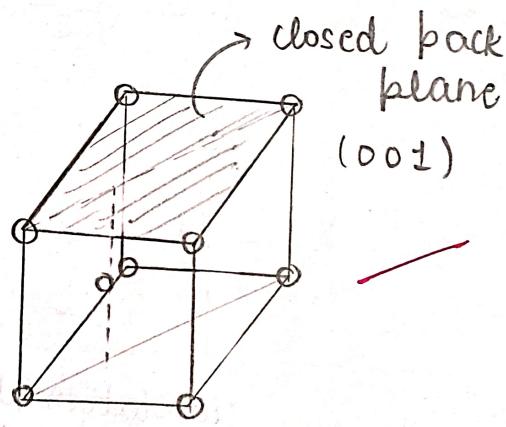
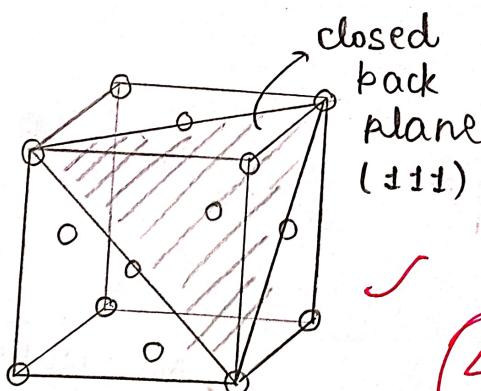
Two important structures in which many metals crystallize are cubic close packed (CCP) and hexagonal close packed (HCP). Examples of CCP structure are γ -Fe, Cu, Ni, Ag, Au, Pt etc. Examples of HCP structure are α -Ti, Zn, Mg, Cd, Zn, Be etc. These structures can be described in terms of stacking of spherical atoms in close packed layers. The stacking sequence is described by letters A, B, C etc. Each letter describes a single layer of atoms in which each atom touches 6 other atoms. In sequence of letters such as ..ABAB.. the layers represented by adjacent letters are touching, while layers represented by the same letter are vertically (perpendicular to the plane of the layer) above each other. Further, the layers represented by different letters are shifted horizontally (in the plane of the layer). Examine unit cells of CCP and HCP structure and look for close-packed planes and determine their stacking sequence.

CCP: ABC ABC

HCP: AB AB AB

3. Arrange three or more close-packed layers in CCP and HCP. Note that there are see-through holes in HCP but not in CCP structure. Try to identify the 3D unit cells in these layers. Sketch the unit cells and indicate the close packed planes for both structures. For clarity, you can draw the neighbouring atoms as separate.

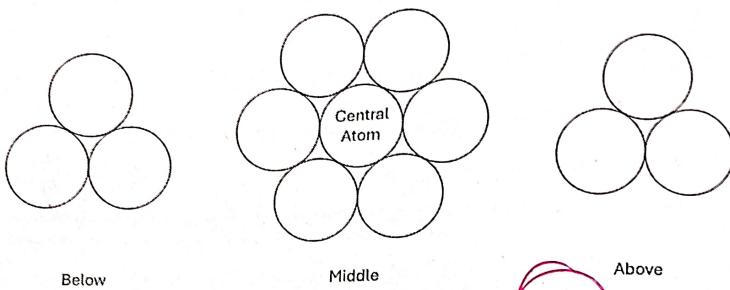
(4)



Exp 5. 1/4

4. Coordination number and coordination polyhedra:

The number of nearest neighbours of a given atom in a structure is called its coordination number and the polyhedron defined by the centres of the neighbouring atoms is called the coordination polyhedron. Using the ball models pieces provided (shown below) assemble the coordination polyhedron for the CCP and HCP structure.



Fill the following table based on your observations:

	Coordination Polyhedron			Name
	V (CN)	E	F	
CCP	12	24	T: 8 F: 8 S: 6	cuboctahedral / stella octangula
HCP	12	24	T: 14 F: 8 S: 6	cuboctahedral (twisted)

V: No. of vertices; E: No. of edges; F: Number of faces; T: Triangles, S: Squares; CN: Coordination Number.

CCP \rightarrow cuboctahedral

HCP \rightarrow twisted cuboctahedral

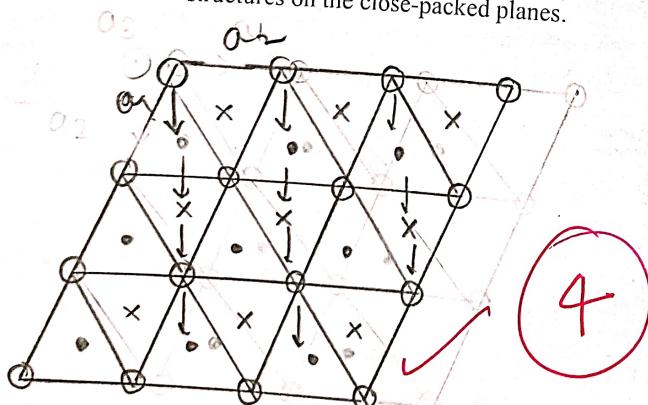
only

~~both~~ cuboctahedral

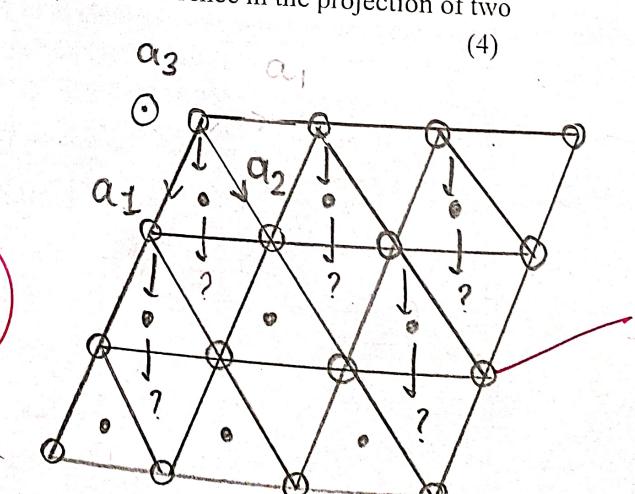
~~stella octangula~~

5. Description of CCP and HCP structure in terms of lattice and motif

Convince yourself that all atoms in the ABCABC sequence (CCP) are translationally equivalent and hence are located on lattice points. In contrast, in ABAB sequence atoms on A plane are not equivalent to that on B plane. Show this difference in the projection of two structures on the close-packed planes.



O \rightarrow A
● \rightarrow B
x \rightarrow C
Translational symmetry



O \rightarrow A
● \rightarrow B
No Translational Symmetry
Exp 5. 2/5

Reason \rightarrow 2 atom motif. in triangular lattice.

Fill the following table.

(6)

Crystal Structure	Bravais Lattice	Basis or Motif	
		No. of atoms in motif	Coordinates of atoms in the motif*
CCP	cF	1	$\langle 0,0,0 \rangle$
HCP	hP	2	$\langle 0,0,0 \rangle$ & $\langle \frac{2}{3}, \frac{1}{3}, \frac{1}{2} \rangle$

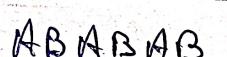
* Note that the coordinates you give for atoms in the motif of HCP should correspond to the axes you show.

6. Voids in closed-packed structures:

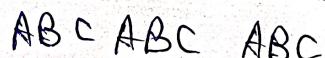
In both CCP and HCP structures the entire space can be divided into an assemblage of tetrahedra and octahedra such that they share faces, edges and corners and no space is left unoccupied (a 3D tiling of space by tetrahedra and octahedra) and center of every atom is located at the vertices of these polyhedra. The polyhedra themselves represent the tetrahedral and octahedral voids present in these structures. These can be occupied by other atoms in interstitial solid solutions. Try to stack two layers of wooden models of tetrahedra and octahedra and observe the structure formed.

A. Give the crystal structure and stacking sequence in which you find the following arrangement of voids

i. Tetrahedra on tetrahedra and octahedra on octahedra: (2)



ii. Tetrahedra on octahedra and octahedra on tetrahedra:



B. Fill the following table based on your observations:

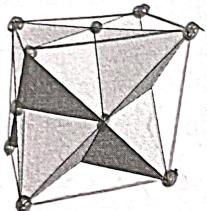
(6)

Crystal Structure	No. of TH voids around a central sphere	No. of OH voids around a central sphere	No. of spheres around a TH void	No. of spheres around a OH void	Effective no. of TH voids per sphere	Effective no. of OH voids per sphere
CCP	8	6	4	6	2	1
HCP	8	6	9	6	2	1

TH: tetrahedral; OH: Octahedral

Exp 5. 3/5

- (2B)
7. The model of *Stella Octangula* that you made in Experiment 1 can be related to the unit cell and voids in one of the two structures, CCP or HCP? Describe this relationship.



As we can see, *Stella octangula* compares to CCP unit cell in the manner shown. Joining these we can get octahedral voids forming in between.

8. Close Packed planes and directions:

Close packed planes act as slip planes and close packed directions as slip direction during plastic deformation of close-packed crystals. We will study this later in the course.

Identify the close-packed planes and close-packed directions in a unit cell of CCP and HCP: (6)

Crystal Structure	No. of distinct (differently oriented) close-packed planes	No. of distinct (differently oriented, not counting sense) close-packed directions	No. of close packed direction in one close-packed plane*
CCP	4	6	3
HCP	1	3	3

* Consider a direction with opposite sense the same.

9. Some Important Crystal Structure:

(12)

Crystal Structure	Examples of elements or compounds having the structure	Bravais lattice	Motif (No. of atoms and coordinates)	Coordination No. (No. of nearest neighbours)	Distance of nearest neighbours in terms of lattice parameter, a	Packing fraction (assuming nearest neighbours in contact)*
Monatomic BCC	Na	cL	1, <0,0,0>	8	$\frac{\sqrt{3}a}{2}$	68%

(12)

CCP	Cu	cF	$1, (0,0,0)$	12	$\frac{a\sqrt{2}}{2}$	74%
HCP	Zn	hP	$2, (0,0,0)$ $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$	12	$\frac{a}{2}$	74%
Diamond Cubic	Si	cP	$2, (0,0,0)$ $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$	4	$\frac{\sqrt{3}a}{4}$	34%

Show the calculation of PE

[8]

1) spheres in BCC = 2

$$2R = a \quad 4R = \sqrt{3}a \quad R = \frac{\sqrt{3}a}{4}$$

(8)

$$\text{P.E.} = \frac{\rho \times \frac{4}{3} \pi \frac{(\sqrt{3}a)^3}{64} \times 16^8}{a^3} \times 100 = \frac{\sqrt{3}\pi}{8} = 68\%$$

2. spheres in CCP = 4

$$2R = a/\sqrt{2} \quad R = a/2\sqrt{2}$$

$$\text{P.E.} = \frac{4 \times \frac{4}{3} \pi \times \frac{a^3}{16\sqrt{2}}}{a^3} \times 100 = \frac{\pi}{3\sqrt{2}} = 74\%$$

3. spheres in hcp = 2 $2R = a \Rightarrow R = a/2$

$$\text{P.E.} = \frac{4 \times \frac{4}{3} \pi \times \frac{a^3}{8}}{\frac{3\sqrt{3}a^3}{2}} \times 100 = 74\%$$

Exp 5. 5/5

4. Diamond Cubic no. of atoms per cell = 8

$$2R = \sqrt{3}a/4 \quad R = \sqrt{3}a/8$$

$$P.E. = \frac{8 \times \frac{4}{3} \times \pi \times \frac{8\sqrt{3}a^3}{512} \times 16}{a^3} \times 100 = \frac{\pi \sqrt{3}}{16} \times 100$$
$$= 34\%$$