MLL100 Sem 1 2025-2026

Experiment 5

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.

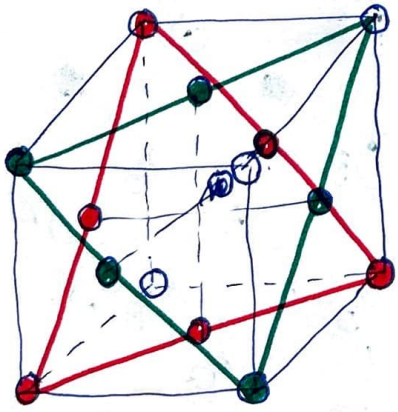
1. Show your stella octangula and cuboctahedron models to lab instructor and get his/her signature. (2)

2. **Stacking sequence in closed packed structures:**

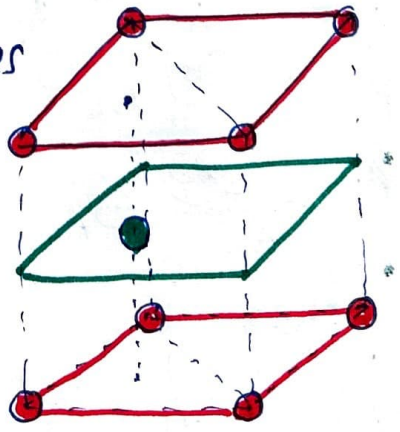
Two important structures in which many metals crystallize are cubic close packed (CCP) and hexagonal close packed (HCP). Examples of CCP structure are γ-Fe, Cu, Ni, Ag, Au, Pt etc. Examples of HCP structure are α-Ti, Zn, Mg, Cd, Zn, Be etc. These structures can be described in terms of stacking of spherical 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: ..ABCABC.. **HCP:** ..ABAB.. **(2)**

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)



CP planes in red and green

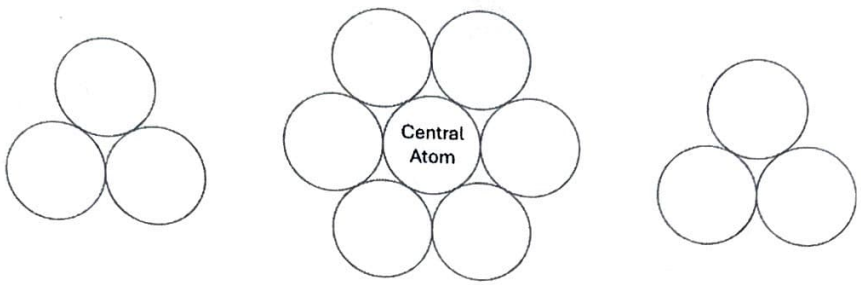


CCP: Close-packed plane ⊥ to the body diagonal

HCP: Close-Packed Planes ⊥ to the c-axis.

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 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: (4)

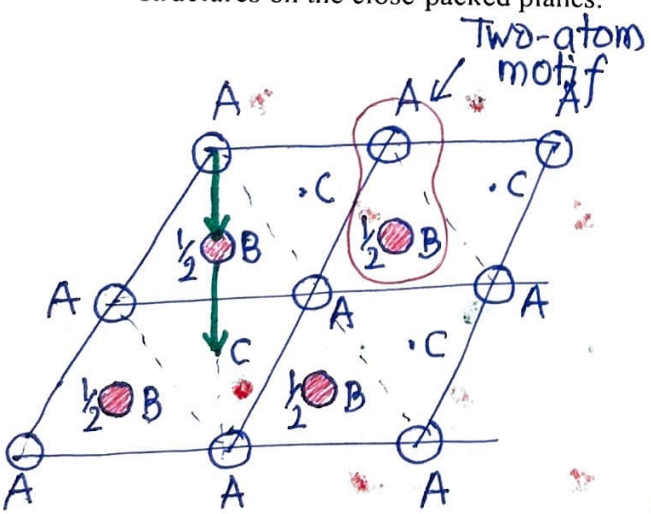
	Coordination Polyhedron			
	V (CN)	E	F	Name
CCP	12	24	T: 8 S: 6	Cuboctahedron
HCP	12	24	T: 8 S: 6	Twisted Cuboctahedron

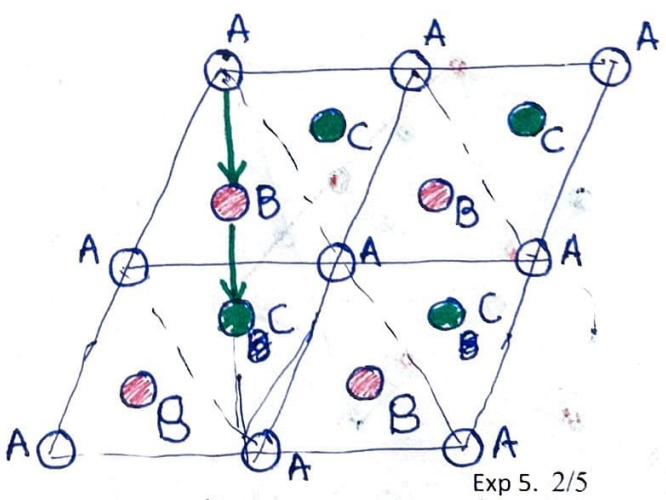
V: No. of vertices; E: No. of edges; F: Number of faces; T: Triangles, S: Squares; CN: Coordination Number.

Which of these coordination polyhedron you made in experiment 1?

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. (4)





A has neighbour B at a vector shown in green. At the same vector from B we have no neighbour ⇒ A & B not equivalent.

In ABC C sites are also filled. All sites equivalent ⇒ All lattice Points ⇒ Single atom motif.

Fill the following table. (6)

Crystal Structure	*Bravais Lattice*	*Basis or Motif*	
		No. of atoms in motif	**Coordinates of atoms in the motif***
CCP	~~cP~~ cF	1	000
HCP	hP	2	000, $\frac{2}{3}\frac{1}{3}\frac{1}{2}$

In the diagram on p2

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

$\frac{1}{3}\frac{2}{3}\frac{1}{2}$ also possible

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 **(2)**

i. Tetrahedra on tetrahedra and octahedra on octahedra:

HCP : .. ABAB..

ii. Tetrahedra on octahedra and octahedra on tetrahedra:

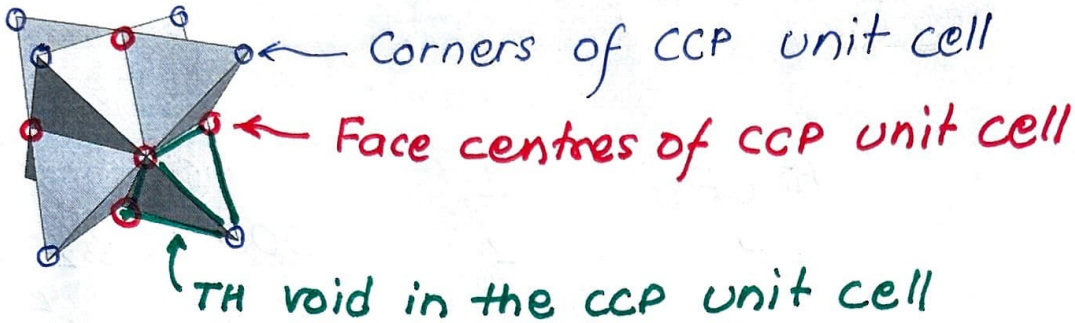
CCP : ... ABCABC...

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	4	6	2	1

TH: tetrahedral; OH: Octahedral

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.



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 (⊥ to Body dig)	6 (along face-diag)	3
HCP	1 (⊥ to c)	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	α-Fe Cr	cI	1 0,0,0	8	$\frac{\sqrt{3}a}{2}$	

CCP	Au, Ag, Pt, γ-Fe	CF	1 0,0,0	12	$a/\sqrt{2}$	
HCP	Mg, Be, Ti	hP	2 000 $\frac{2}{3}\frac{1}{3}\frac{1}{2}$	12	a	
Diamond Cubic	C, Si Ge	CF	2 000 $\frac{1}{4}\frac{1}{4}\frac{1}{4}$	4	$\frac{\sqrt{3}a}{4}$	

Show the calculation of PE [8]