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 (5^{th}. Edn.) by V. Raghavan.

1. Stacking sequence in closed packed structures: **(2)**

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: **HCP:**

2. 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.

3. Description of CCP and HCP structure in terms of lattice and motif **(3)**

Crystal Structure	***Bravais Lattice***	***Basis or Motif***	
		No. of atoms in motif	**Coordinates of atoms**
CCP			
HCP			

4. 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. Note: TH and OH refers to Tetrahedral and Octahedral.

A. Try to stack two layers of wooden models of tetrahedra and octahedra and observe the structure formed.

B. Give the crystal structure and stacking sequence in which you find the follwing arrangement of voids **(2)**

   i. Tetrahedra on tetrahedra and octahedra on octahedra:

   ii. Tetrahedra on octahedra and octahedra on tetrahedra:

C. Fill the following table based on your observations: **(3)**

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						
HCP						

5. Some Important Crystal Structure: **(6)**

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						
CCP						
HCP						

Diamond Cubic						
CsCl*						
NaCl*						

*For packing efficiency of CsCl and NaCl, you also need the radius ratio of two types of ions R_{Cs}/R_{Cl} and R_{Na}/R_{cl}.. Find the packing efficiency in terms of these ratios.

Attach separate sheets showing the calculation of PE [5]

6. 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.

A. Identify the close-packed planes and close-packed directions in a unit cell of CCP and HCP: **(3)**

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			
HCP			

B. In a neat sketch of unit cell of CCP, draw one close packed plane and show all close-packed directions lying in it. Give the Miller indices of the plane and directions. Do the same in a HCP unit cell. **[2(1+3)=8]**

C. (a) Give Miller indices for all close packed planes in CCP. Give the single Miller indices for the family. **(4 marks)**

(b) Repeat the above for HCP **(4 marks)**