

## CHEM 281 LAB: SOLID STATE STRUCTURE OF METALS

**Objective:** The purpose of this experiment is to extend our understanding and familiarity of the three dimensional structures of solids. We will use models and the Institute for Chemical Education (ICE) Solid-State Model Kits which are designed for creating a variety of common and important solid state structures.

**Amorphous solids:** Solids that do not possess any long-range order, so they do not typically form well-defined faces nor do they fracture evenly. Glass is an example of an amorphous solid. Amorphous solids have very interesting properties in their own right that differ from those of crystalline materials. We will not consider their structures in this laboratory exercise.

### Classification of crystalline materials

The forces which stabilize the crystal may be ionic (electrostatic) forces, covalent bonds, metallic bonds, London dispersion forces, hydrogen bonds, or a combination of these. The properties of the crystal will change depending upon what types of bonding is involved in holding the atoms, molecules or ions in the lattice. The fundamental types of crystalline solid are based upon the types of forces that hold them together are:

<b>Metallic Solids</b>	Metal cations held together by a sea of electrons
<b>Ionic Solids</b>	Cations and anions held together by predominantly electrostatic attractions
<b>Network Solids</b>	Atoms bonded together covalently throughout the solid (also known as <i>covalent crystal</i> or <i>covalent network</i> ).
<b>Molecular Solids</b>	Collections of individual molecules; each lattice point in the crystal is a molecule

Often crystals held together by more than one type of force and thus may have intermediate properties.

### Structure of Metals

The structures of pure metals are crystalline (**crystal lattice**) with regular arrangement of metal atoms that are identical perfect spheres. For cubic system, they form four basic structures: simple cubic (*SC*), body-centered cubic (*BCC*), hexagonal closest-packed (*HCP*), and cubic closest-packed (*CCP*).

### Crystal lattice

The structures of pure metals are crystalline (**crystal lattice**) with regular arrangement of metal atoms that are identical perfect spheres.

**Coordination number (CN):** The number of nearest neighboring metal atoms (four, six, eight to twelve) which each atom is surrounded in the crystal lattice.

### Crystal Packing

#### Unit cell:

Wallpaper has regular repeating design that extends from one edge to the other. Crystals have a similar repeating unit called unit cell that extends in 3-D from one edge of the solid to the other. Unit cell has, three edges,  $a$ ,  $b$ ,  $c$  and their angles,  $\alpha$ ,  $\beta$ ,  $\gamma$ .

**Filling efficiency:** Is the percent ratio of volume filled by the metals to the total unit cell volume.

**Cubic crystal system** ( $a = b = c$  and these angles,  $\alpha = \beta = \gamma = 90^\circ$ .  
For the cubic crystals, there are four basic unit cells.

**Cubic Crystal Structures**

	<i>Stacking Pattern</i>	<i>Structure (Unit cell)</i>	<i>Coordination Number</i>	<i>Filling efficiency</i>
<b>Open-packed</b> A on top of A B in spaces of A layers	AAAAAAA... ABABABAB...	simple cubic (SC) body-centered cubic (BCC)	6 8	52% 68%
<b>Close-packed</b> Between the spaces of layer below	ABABABAB... ABCABCABC..	hexagonal closest-packed (HCP) cubic closest-packed (CCP-FCC)	12 12	74% 74%

**Part of the Atom in the Unit Cell**

The part of the atom in the unit cell is counted according to the following locations

corner = 1/8	edge = 1/4	face = 1/2	body = 1
--------------	------------	------------	----------

**Number of Atoms in the Cubic Unit Cell**

SC = 1 (8 corners)	FCC = 4 (8 corners, 6 faces)
BCC = 2 (8 corners, 1 body)	Other unit cells?

**Interstitial Sites and Holes:** The remaining unoccupied space in any sphere packing scheme of unit cell is found as void space. This void space occurs between the spheres and gives rise to so-called holes. Holes

**Holes:** The easiest way to determine the type of hole is by looking at how the atoms surround the ion in the hole.

**Hexagonal (HCP) and cubic close packing (CCP-FCC):**

**Octahedral hole:** Space in an octahedral hole is surrounded by six other metals oriented octahedral.

**Octahedral hole:** Space in a tetrahedral hole is surrounded by four other metals oriented tetrahedrally.

**Bravais Lattice:** A Bravais Lattice is a three dimensional lattice. A Bravais Lattice tiles space without any gaps or holes. There are 14 ways in which seven crystal systems this can be accomplished. Basic types of Bravais unit cells P (primitive), I (body centered), F (face centered), C (centered on  $c$  axis) and R/P (rhombohedral/primitive)

**Seven Crystal Systems**

<b>Crystal Systems</b>	<b>Unit cell Constraints</b>	<b>Fourteen Bravais Lattices</b>
1. Cubic	$a = b = c, \alpha = \beta = \gamma = 90^\circ$	P, I, F (3)
2. Tetragonal	$a = b \neq c, \alpha = \beta = \gamma = 90^\circ$	P, I (2)
3. Orthorhombic	$a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$	P, C, I, F (4)
4. Trigonal	$a = b = c, \alpha = \beta = \gamma \neq 90^\circ$	R/P (1)
5. Monoclinic	$a \neq b \neq c, \beta \neq \alpha = \gamma = 90^\circ$	P, C (2)
6. Hexagonal	$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$	P (1)
7. Triclinic	$a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90^\circ$	P (1)

**LAB Activity: Chapter 3 Metallic Structure**

**1. Classify the crystalline materials given to you as, Metallic Solids, Ionic Solids Network Solids and Molecular Solids. How they differ in following properties?**

<b>Material</b>	<b>Type of crystalline materials</b>	<b>Mechanical properties</b>	<b>Electrical Conductivity</b>	<b>Water Solubility</b>	<b>Intermolecular Force</b>

**2. Using the materials given to you build following cubic staking patterns and Identify the units cells they created. Draw a picture of your model.**

**a) Open-packed A on top of AAAAAAAAA.**

**b) Open-packed A on top of B in spaces of B layers:ABABABABAB.**

**c) Close-packed A between the spaces of B layer: ABABABABAB.**

**d) x Close-packed A between the spaces of layer B and B on C but A and C are displaced:**

3. Draw following unit cells and show interstitial sites and identify them as octahedral, cubic and tetrahedral holes.

- a) Simple cube (SC):
- b) Body-centered cubic (BCC):
- c) Cubic closest-packed (CCP):
- d) Hexagonal closest-packed (HCP):

4. Coordination number of atoms and the holes (interstitial sites) in following unit cells:

- a) Simple cube (SC):
- b) Body-centered cubic (BCC):
- c) Cubic closest-packed (CCP):
- d) Hexagonal closest-packed (HCP):

5. Draw a simple cubic unit (cubic crystal system) and label the origin, axes and angles

6. How unit cell axes and angles different for following crystal systems?

Crystal system	Axes and angles
Tetragonal	
Orthorhombic	
Trigonal	
Monoclinic	
Hexagonal	
Triclinic	
Cubic	

7. Draw diagram to show how a part of the Atom could be following locations of cubic unit cell.

- a) corner
- b) edge
- c) face
- d) body

8. Identify the fourteen Bravais Lattice (unit cells) given and classify them into seven crystal systems

Crystal Systems	Unit cell Constraints	Fourteen Bravais Lattices
9.	$a = b = c, \alpha = \beta = \gamma = 90^\circ$	P, I, F (3)
10	$a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$	P, I (2)
11	$a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$	P, C, I, F (4)
12	$a = b = c, \alpha = \beta = \gamma \neq 90^\circ$	R/P (1)
13	$a \neq b \neq c, \beta \neq \alpha = \gamma = 90^\circ$	P, C (2)
14	$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$	P (1)
15	$a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90^\circ$	P (1)