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## Theory: Solid State Chemistry Simplified

### What is Solid State?

The solid state is one of the three fundamental states of matter where particles (atoms, molecules, ions) are tightly packed in a fixed, orderly arrangement. Solids have a definite shape, volume, and high density compared to liquids and gases.

### 1. Characteristics of Solids

- Incompressible: Very little space between particles.
- Rigid: Particles arranged closely and strongly bonded.
- Fixed shape and volume.
- High melting and boiling points depending on bonding.

### 2. Classification of Solids

Solid materials are classified based on bonding and structure into:

- **Crystalline solids:** Particles arranged in a highly ordered geometric pattern called a crystal lattice. Examples: NaCl, diamond.
- **Amorphous solids:** No long-range order, particles arranged randomly. Examples: Glass, rubber.

Further types of crystalline solids based on bonding:

Type	Bonding/Forces	Properties	Examples
Ionic	Ionic bonds	Hard, brittle, high melting point	NaCl, KBr, MgO
Molecular	Van der Waals, H-bonding	Soft, low melting point, non-conducting	Ice, Dry ice (CO <sub>2</sub> )
Metallic	Metallic bonds	Conduct electricity, malleable	Fe, Cu, Al
Covalent Network	Covalent bonds	Very hard, high melting point	Diamond, Quartz

### 3. Crystal Lattice and Unit Cell

- The **crystal lattice** is the 3D arrangement of particles.
- The **unit cell** is the smallest repeating unit showing the full symmetry.
- Types of unit cells based on lattice points: Simple cubic (SC), Body-centered cubic (BCC), Face-centered cubic (FCC).

### 4. Packing in Solids

- Efficiency of space covered by atoms (packing efficiency).
- FCC and Hexagonal close packed (HCP) have the highest packing efficiency (74%).

- BCC: Packing efficiency ~68%, SC ~52%.

## 5. Density of Unit Cell

$$\text{Density} = \frac{\text{Mass of atoms in unit cell}}{\text{Volume of unit cell}}$$

Used to relate microscopic structure to macroscopic measurable density.

## 6. Defects in Solids

- **Point defects:** Vacancy (missing atom), Interstitial (extra atom between lattice points), Substitutional (impurity atom replaces host).
- Defects affect electrical and mechanical properties.
- Schottky and Frenkel defects are common in ionic solids.

## 7. Electrical Properties of Solids

- Conductors, Insulators, and Semiconductors based on band theory.
- Band gap energy determines conductivity.
- Semiconductor doping: n-type and p-type materials.

## 8. Magnetic Properties

- Paramagnetism, Diamagnetism, Ferromagnetism based on electron spin and alignment.

## 9. X-ray Diffraction (XRD)

- Used to study crystal structure by diffraction of X-rays through crystals.
  - Provides information about lattice parameters and arrangement.
  - Bragg's law:  $n\lambda = 2d\sin \theta$  relates wavelength  $\lambda$ , lattice spacing  $d$ , and angle  $\theta$ .
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## Examples

### Example 1: Packing Efficiency of FCC

FCC unit cell has 4 atoms (8 corners  $\times$  1/8 + 6 faces  $\times$  1/2). The packing efficiency is 74%, meaning 74% volume is occupied by atoms.

### Example 2: Vacancy Defect Effect on Density

Vacancy defects reduce density since some atoms are missing from lattice sites.

### Example 3: Calculating Density of BCC Iron

Given cell edge and atomic mass, calculate volume and mass in unit cell; then density by formula.

### Example 4: Band Theory Application

Intrinsic semiconductors have energy gap ~1.1 eV (silicon), doping reduces gap and increases conductivity, used in electronic devices.

### **Example 5: Bragg's Law Calculation**

For X-rays with  $\lambda = 1.54\text{\AA}$  diffracted at  $\theta = 30^\circ$ , calculate spacing  $d$ :

$$d = \frac{n\lambda}{2\sin \theta} = \frac{1 \times 1.54}{2 \times 0.5} = 1.54 \text{\AA}$$

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### **Practice Questions**

#### **Basic Level (Board Exam)**

1. Define solid state in chemistry.
2. What is a crystalline solid?
3. Differentiate between crystalline and amorphous solids.
4. Name the types of bonding in solids.
5. What is a unit cell?
6. What is packing efficiency?
7. Define vacancy defect.
8. Mention two properties of ionic solids.
9. What is a semiconductor?
10. State Bragg's law.

#### **Moderate Level (Bridging Board & JEE)**

11. Calculate the number of atoms in a FCC unit cell.
12. Find the packing efficiency of a simple cubic lattice.
13. Derive the expression for density of a cubic unit cell.
14. What happens to density in the presence of vacancy defects?
15. Explain doping in semiconductors.
16. Describe the differences between n-type and p-type semiconductors.
17. What types of solids conduct electricity? Give reasons.
18. Calculate the edge length of a BCC unit cell if the atomic radius is 140 pm.
19. Explain how X-ray diffraction helps in studying crystal structure.
20. Write the formula relating density, molar mass, and unit cell volume.

#### **Advanced Level (JEE Main/Advanced, MCQs included)**

21. (MCQ) The coordination number in an FCC lattice is:

- o (A) 6

- (B) 8
- (C) 12
- (D) 10

22. (MCQ) The number of atoms present in a BCC unit cell is:

- (A) 1
- (B) 2
- (C) 4
- (D) 8

23. Calculate the radius of an atom in FCC lattice if the edge length is 4 Å.

24. (MCQ) Schottky defect can be observed in which of the following solids?

- (A) NaCl
- (B) KCl
- (C) ZnS
- (D) Silicon

25. Calculate Bragg angle for the first order diffraction for a plane with spacing  $d = 2$  Å using X-rays of wavelength 1.54 Å.

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### Answers and Detailed Explanations

1. Solid state is the state of matter where particles have a fixed, ordered arrangement, giving solids fixed shape and volume.
2. Crystalline solids have particles arranged in a regular repeating pattern.
3. Crystalline solids have order and sharp melting points; amorphous solids lack this order and melt over a range.
4. Bonding in solids includes ionic, covalent, metallic, and molecular (Van der Waals/H-bond).
5. Unit cell is the smallest 3D building block of a crystal lattice showing symmetry.
6. Packing efficiency is the fraction of space filled by particles in a unit cell.
7. Vacancy defect is when an atom is missing from its lattice site.
8. Ionic solids are hard, have high melting points, and do not conduct electricity in solid state.
9. Semiconductors have moderately filled energy bands; conductivity increases with temperature or doping.
10. Bragg's law:  $n\lambda = 2d \sin \theta$ ; explains X-ray diffraction.
11. FCC has 4 atoms/cell (8 corners  $\times 1/8 + 6$  faces  $\times 1/2$ ).

- 12.** Packing efficiency of SC = 52%.
- 13.** Density formula  $\rho = \frac{Z \times M}{N_A \times a^3}$ , where  $Z$ = atoms/unit cell,  $M$ molar mass,  $N_A$ Avogadro's number,  $a$ edge length.
- 14.** Vacancy defects decrease density as mass per unit volume decreases.
- 15.** Doping introduces impurities to alter electrical conductivity of semiconductors.
- 16.** n-type adds electrons, p-type creates holes as charge carriers.
- 17.** Metals conduct due to free electrons; ionic solids do not conduct in solid form as ions are fixed.
- 18.** For BCC,  $a = \frac{4r}{\sqrt{3}} = \frac{4 \times 140}{1.732} \approx 323.2 \text{ pm}$ .
- 19.** XRD reveals lattice spacing by measuring angles at which X-rays are diffracted.
- 20.**  $\rho = \frac{Z \times M}{N_A \times a^3}$ , connecting atomic scale to macroscopic density.
- 21.** (C) 12 – FCC atoms touch along face diagonal with 12 nearest neighbors.
- 22.** (B) 2 atoms in BCC unit cell.
- 23.** In FCC,  $a = 2\sqrt{2}r \Rightarrow r = \frac{a}{2\sqrt{2}} = \frac{4}{2 \times 1.414} = 1.414 \text{ \AA}$ .
- 24.** (A) NaCl shows Schottky defects (vacancy of cations and anions).
- 25.** Using Bragg's law for  $n = 1$ ,

$$\sin \theta = \frac{\lambda}{2d} = \frac{1.54}{4} = 0.385 \Rightarrow \theta = 22.6^\circ$$


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