Lecture 2: Crystal Structures

1. Introduction to Crystal Structure

In materials science, a **crystal structure** describes the orderly, repeating arrangement of atoms, ions, or molecules in a solid material. Most metals, ceramics, and some polymers have a crystalline structure.

A crystal structure is defined by:

- **Lattice:** A three-dimensional geometric arrangement of points
- **Basis:** One or more atoms associated with each lattice point

Crystal structure = Lattice + Basis

Understanding crystal structures helps us explain mechanical, electrical, thermal, and magnetic properties of materials.

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2. Atomic Arrangement in Solids

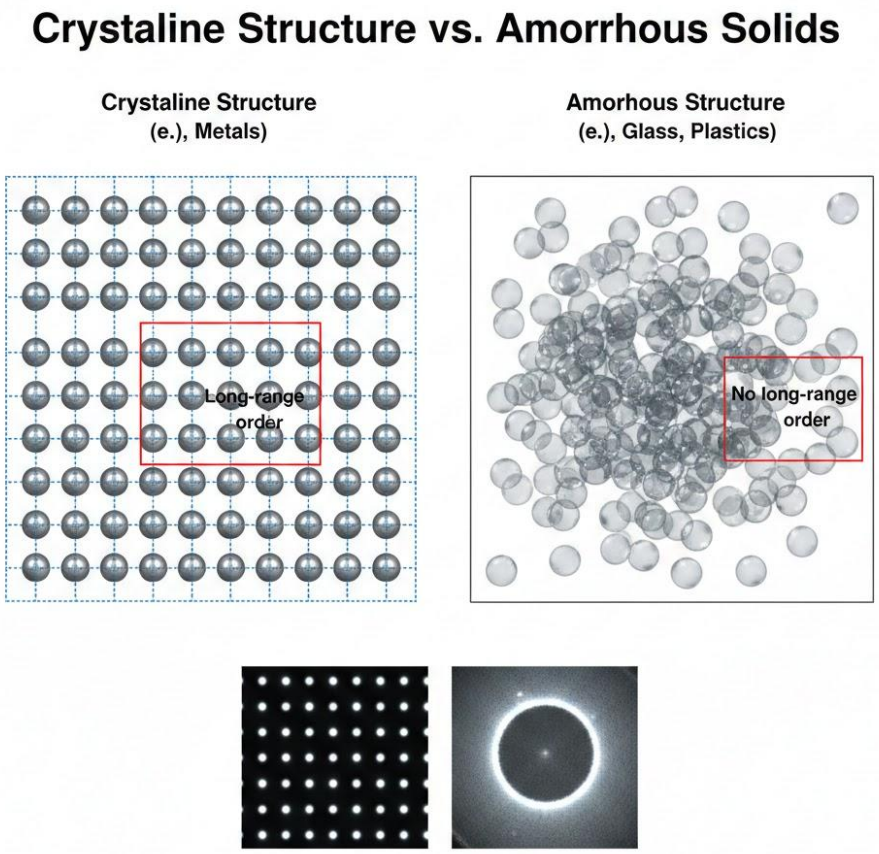
Atoms in solids can be arranged in two main ways:

2.1 Crystalline Solids

- Atoms are arranged in a **regular, repeating pattern**
- Have a definite melting point
- Examples: Iron, Copper, Aluminum

2.2 Amorphous Solids

- Atoms are arranged **randomly**
- No sharp melting point
- Examples: Glass, plastics



Unit Cell

The **unit cell** is the smallest repeating volume that represents the entire crystal structure.

3. Types of Crystal Structures (Based on Unit Cell Geometry)

Before studying each structure in detail, it is important to know the **main types of crystal structures** commonly discussed in materials science, especially for metals.

The most important crystal structures for first-year engineering students are:

3.1 Simple Cubic (SC)

- Atoms are located **only at the corners** of the cube
- Very rare in metals
- Atoms per unit cell = 1
- Coordination number = 6

Example: Polonium (rare case)

3.2 Body-Centered Cubic (BCC)

- Atoms at the corners and **one atom at the center** of the cube
- Common in many engineering metals

3.3 Face-Centered Cubic (FCC)

- Atoms at the corners and **atoms at the centers of all faces**
- Very dense packing

3.4 Hexagonal Close-Packed (HCP)

- Atoms arranged in a **hexagonal prism**
- Close-packed structure similar to FCC

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4. Body-Centered Cubic (BCC) Structure

3.1 Description

The **BCC structure** consists of:

- 8 atoms at the corners of a cube
- 1 atom at the center of the cube

3.2 Atoms per Unit Cell (BCC)

- Corner atoms: $8 \times \frac{1}{8} = 1$
- Center atom: $\frac{1}{1} = 1$

Total atoms per unit cell = 2

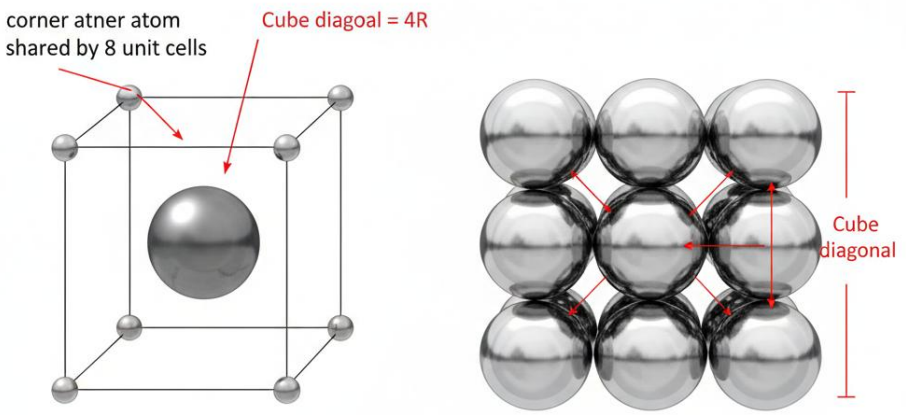
3.3 Coordination Number

- **Coordination number = 8**

3.4 Examples of BCC Metals

- Iron (α-Fe)
- Chromium
- Tungsten

2.1 Body-Centered Cubic (BBC) Structure



Corner-sharing view Space-filling view

4. Face-Centered Cubic (FCC) Structure

4.1 Description

The **FCC structure** consists of:

- 8 atoms at the corners
- 6 atoms at the centers of each face

4.2 Atoms per Unit Cell (FCC)

- Corner atoms: $8 \times \frac{1}{8} = 1$
- Face atoms: $6 \times \frac{1}{2} = 3$

Total atoms per unit cell = 4

4.3 Coordination Number

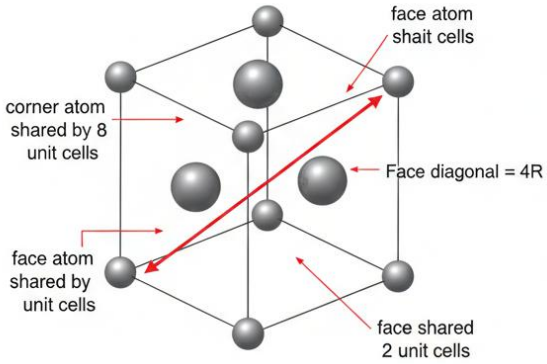
- **Coordination number = 12**

4.4 Examples of FCC Metals

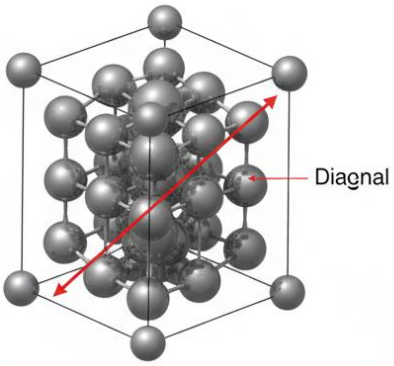
- Aluminum
- Copper
- Gold
- Silver

2.2 Face-Centered Cubic (FCC) Structure

Corner-sharing view



Space-filling view



Key Properties

- Atoms per unit cell (N) = 4
- Atoms per Number (CN) 12
- Coordination Number (CN 12
- Atomic Packing Factor APF = 0.74
- Common Metals: Al, Cu, Au, Ag, Pb, Ni

Lattice Constant (a) Calculation

- Along face diagoal: $(4R^2 = a^2 + a^2$
  $16R^2 = 2a^2$
  $a^2 = 8a^2$
  $a = (44)\sqrt{2}$

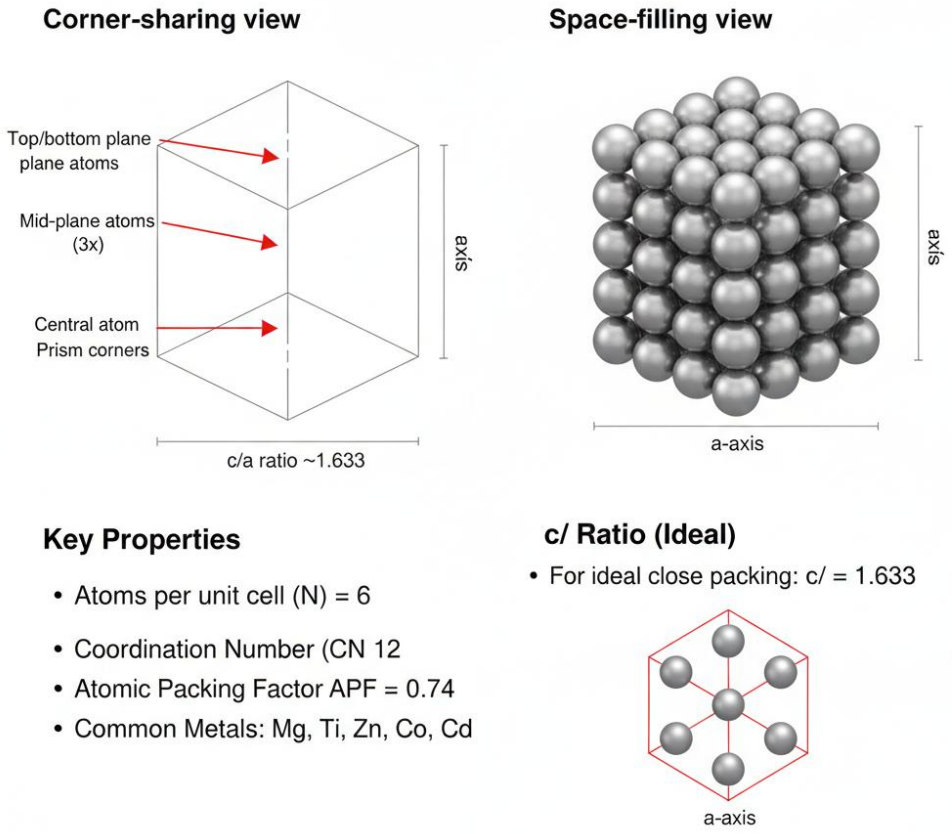
5. Hexagonal Close-Packed (HCP) Structure

5.1 Description

The HCP structure is a bit more complex than the cubic structures. It consists of three layers of atoms. The top and bottom layers have 6 atoms arranged in a regular hexagon with one atom in the center. The middle layer has 3 atoms nestled in the depressions of the layer below.

Take a look:

2.3 Hexoganal Close-Packed (HCP) Structure



5.2 Coordination Number

- **Coordination number = 12**

5.3 Atoms per Unit Cell

- 12 corner atoms (6 top, 6 bottom) contribute 1/6 each to the unit cell (12 * 1/6 = 2 atoms).

- 2 face-centered atoms (1 top, 1 bottom) contribute 1/2 each (2 * 1/2 = 1 atom).
- 3 internal atoms contribute 1 each (3 * 1 = 3 atoms).
- Total: **6 atoms** per unit cell.

5.4 Examples of HCP Metals

- Magnesium
- Zinc
- Titanium

5.5 Layer Arrangement (HCP)

- Stacking sequence: **ABABAB**

6. Atomic Packing Factor (APF)

6.1 Definition

The **Atomic Packing Factor (APF)** is the fraction of the unit cell volume that is occupied by atoms.

$$APF = \frac{Volume\ of\ atoms\ in\ unit\ cell}{Volume\ of\ unit\ cell}$$

Where:

- Volume of atoms in unit cell = (Number of atoms per unit cell) * (Volume of one atom)
- Volume of one atom (assuming spherical atoms) = $\frac{4}{3}\pi R^3$ (where R is the atomic radius)

7. APF Calculations

7.1 APF for BCC Structure

Given:

- **Number of atoms per unit cell (N):** 2

- **Relationship between atomic radius (R) and lattice parameter (a):** For BCC, atoms touch along the body diagonal.
  - Body diagonal = $a\sqrt{3}$
  - Body diagonal = 4R
  - Therefore, $a\sqrt{3}$ = 4R $\longrightarrow \boldsymbol{a = \frac{4R}{\sqrt{3}}}$
- **Volume of unit cell:** $\boldsymbol{a^3 = \left(\frac{4R}{\sqrt{3}}\right)^3 = \frac{64R^3}{3\sqrt{3}}}$
- **Volume of atoms in unit cell:** $\boldsymbol{2 \times \frac{4}{3}\pi R^3 = \frac{8}{3}\pi R^3}$

Now, let's calculate APF

$$\text{APF}_{\text{BCC}} = \frac{\frac{8}{3}\pi R^3}{\frac{64R^3}{3\sqrt{3}}} = \frac{8\pi}{64/\sqrt{3}} = \frac{8\pi\sqrt{3}}{64} = \frac{\pi\sqrt{3}}{8} \approx 0.68$$

7.2 APF for FCC Structure

Given:

- **Number of atoms per unit cell (N):** 4
- **Relationship between atomic radius (R) and lattice parameter (a):** For BCC, atoms touch along the body diagonal.
  - Body diagonal = $a\sqrt{2}$
  - Body diagonal = 4R
  - Therefore, $a\sqrt{2}$ = 4R $\longrightarrow \boldsymbol{a = \frac{4R}{\sqrt{2}}} \longrightarrow \boldsymbol{a = 2R\sqrt{2}}$
- **Volume of unit cell:** $\boldsymbol{a^3 = \left(2R\sqrt{2}\right)^3 = 16R^3\sqrt{2}}$
- **Volume of atoms in unit cell:** $\boldsymbol{4 \times \frac{4}{3}\pi R^3 = \frac{16}{3}\pi R^3}$

Now, let's calculate APF

$$APF_{BCC} = \frac{\frac{16}{3}\pi R^3}{16R^3\sqrt{2}} = \frac{16\pi}{48\sqrt{2}} = \frac{\pi}{3\sqrt{2}} \approx 0.74$$

7.3 APF for HCP Structure

$APF_{HCP} = 0.74$

8. Solved Numerical Problems

Problem 1: Number of Atoms in BCC

Question:
Calculate the number of atoms per unit cell in a BCC structure.

Solution:

- Corner atoms: (8 \times 1/8 = 1)
- Center atom: (1 \times 1 = 1)

Answer: 2 atoms

Problem 2: APF of FCC Structure

Question:
What is the atomic packing factor of an FCC crystal?

Solution:

$$APF = \frac{Volume\ of\ atoms}{Volume\ of\ unit\ cell} = 0.74$$

Answer: 0.74 (74%)

Problem 3: Comparison Question

Question:
Which structure is more densely packed: BCC or FCC?

Solution:

- APF of BCC = 0.68
- APF of FCC = 0.74

Answer: FCC is more densely packed

Problem 4: Determining Lattice Parameter for BCC Iron

Question: Iron (α-Fe) has a BCC crystal structure, an atomic radius of 0.124 nm, and an atomic weight of 55.85 g/mol. Calculate its lattice parameter 'a'.

Understanding the Law/Formula:

For a BCC structure, the atoms touch along the body diagonal. The relationship between the atomic radius (R) and the lattice parameter (a) is given by:

$$\boldsymbol{a = \frac{4R}{\sqrt{3}}}$$

Solution:

We are given:

- Atomic radius (R) = 0.124 nm

Using the formula for BCC:

$$a = \frac{4 \times 0.124\ nm}{\sqrt{3}}$$

$$a = \frac{0.496\ nm}{1.732}$$

$$a \approx 0.286\ nm$$

Answer: The lattice parameter 'a' for BCC iron is approximately 0.286 nm.

9. Summary Table

Structure	Atoms/Unit Cell	Coordination No.	APF
BCC	2	8	0.68
FCC	4	12	0.74
HCP	6	12	0.74

10. References

1. *Engineering Materials: An Introduction to Their Properties and Applications*
2. *Materials Science*
3. *Engineering Metallurgy*
4. *Materials for the Engineering Technician*
5. الخواص الكهربائية والمغناطيسية للمواد
6. مبادئ علم المعادن

Questions

1. How many atoms are present in one BCC unit cell?
2. Define a unit cell.
3. Write the formula for Atomic Packing Factor (APF).
4. A metal has a BCC crystal structure. What is its atomic packing factor?
5. Why is the FCC structure more ductile than the BCC structure?
6. Give two examples of metals with HCP structure.