Crystal Structure

If atoms bonded together in a regular 3-D pattern they form a CRYSTAL.- Long range order

Each type of atom has a preferred arrangement depending on temperature and pressure (most stable configuration).

These patterns known as SPACE LATTICES.

Each repeating unit or building block is known as the UNIT CELL.

Define UNIT CELL then can define location of all atoms in crystals.

There are 7 types of CRYSTAL SYSTEMs (Tab 3.2, C. p40) and 14 standard UNIT CELLS.

Unit Cells

Table 3.2 The 14 Crystal (Bravais) Lattices

<table>
<thead>
<tr>
<th>Simple cubic</th>
<th>Body-centered cubic</th>
<th>Face-centered cubic</th>
<th>Simple tetragonal</th>
<th>Body-centered tetragonal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple orthorhombic</td>
<td>Body-centered orthorhombic</td>
<td>Base-centered orthorhombic</td>
<td>Face-centered orthorhombic</td>
<td>Rhombohedral</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>Simple monoclinic</td>
<td>Base-centered monoclinic</td>
<td>Triclinic</td>
<td></td>
</tr>
</tbody>
</table>
Metallic Crystal Structures

Most metals crystallize into one of three densely packed structures.

- **BODY CENTERED CUBIC** – BCC
- **FACE CENTERED CUBIC** – FCC
- **HEXAGONAL CLOSE PACKED** - HCP

**BCC Structure**

Atoms at cube corners and one in cube center.

Lattice Constant for BCC: \( a = \frac{4r}{\sqrt[3]{3}} \)

Atoms/unit cell: \( 1 + 8 \times \frac{1}{8} = 2 \)

Atomic Packing Factor (APF): \( \sqrt{3} \pi / 8 \approx 0.68 \)

Typical metals: \( \alpha \)-Fe, Cr, Mo, W
FCC Structure

Atoms at cube corners and one in each face center.

Lattice Constant for FCC: \( a = 2\sqrt{2}r \)

Atoms/unit cell: \( 6 \times \frac{1}{2} + 8 \times \frac{1}{8} = 4 \)

Atomic Packing Factor (APF): \( \frac{\pi}{3\sqrt{2}} \approx 0.74 \)

Typical metals: Al, Ni, Cu, Ag, Pt, Au

HCP Structure

Top and bottom hexagonal planes and an extra plane in middle.

Lattice Constant for HCP: \( a = 2r, \frac{c}{a} = 1.633 \)

Atoms/unit cell: \( 12 \times \frac{1}{6} + 2 \times \frac{1}{2} + 3 = 6 \)

Atomic Packing Factor (APF): \( \frac{\pi}{3\sqrt{2}} \approx 0.74 \)

Typical metals: Be, Mg, Zn
Semiconductor Crystal Structures

MOST semiconductors crystallize into diamond cubic or Zinc blende structures.

Diamond Cubic

The structure is built on an FCC Bravais lattice.

It accommodates tetrahedral bonding.

Atoms/unit cell:

\[ 4 + 6 \times \frac{1}{2} + 8 \times \frac{1}{8} = 8 \]

APF: 0.34

Typical semiconductors: Si, Ge
Zinc Blende

The arrangement is basically the same with Diamond Cubic.

However, the successive atoms in the crystal are from DIFFERENT chemical elements.

Typical semiconductors: GaAs, InP, ZnS, ZnSe