Chapter 3: The structure of crystalline solids

Outline

- Instruction
- Fundamental concepts
- Unit cells
- Metallic crystal structure
- Density and polymorphism
- Crystal systems

Fundamental concepts

- Crystalline materials: atoms are situated in a repeating or periodic array over large atomic distances
- Crystalline structure: how atoms, ions, or molecules are arranged spatially
- Lattice: a three-dimensional array of points coinciding with atom position

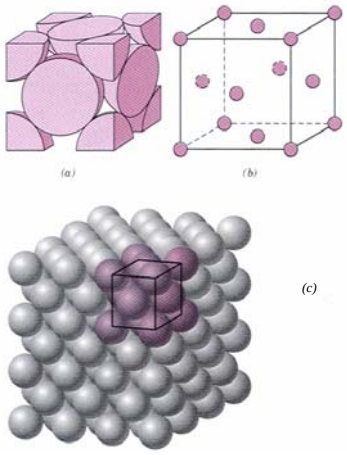
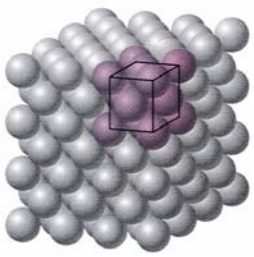


Fig 3.1 (a) a hard sphere unit cell (b) a reduced-sphere unit cell, (c) an aggregate of many atoms

Unit cells

- Small repeating units in a crystal
- Basic structural unit or building block of the crystal structure
- Not unique
- A highest level of geometrical symmetry



Metallic crystal structure

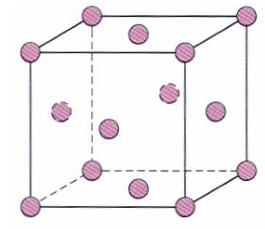
- Features of metallic crystal structure
  - non-directional in nature
  - no restriction on the number and position of nearest-neighbor atoms
  - close-packed: low energy
  - common type: face-centered cubic (FCC), body-centered cubic (BCC), hexagonal closed-packed (HCP)

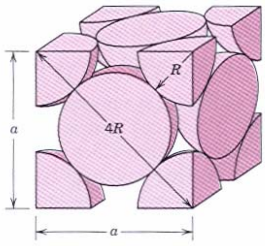
The FCC crystal structure

- Total atoms per unit cell=4
  - 8x1/8 atoms at corner+6x1/2 face-centered atoms=4
- The relation between cubic edge a and the radius R

$$a = 2\sqrt{2}R$$

- Coordination number=12
  - the number of nearest-neighbor or touching atoms
- Atomic packing factor (APF)
  - APF=volume of atoms in a unit cell/total unit cell volume

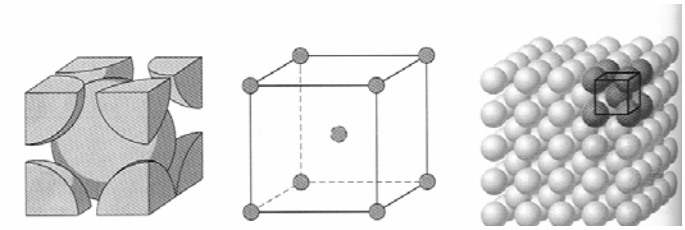




The BCC crystal structure

- Total atoms per unit cell

- Coordination number

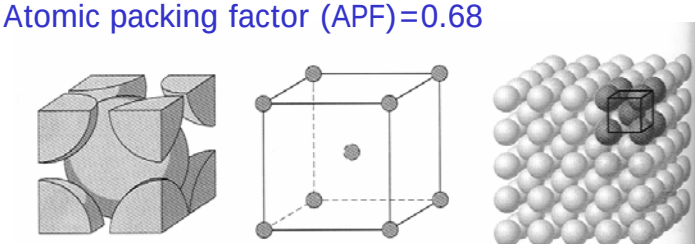


The BCC crystal structure

- The relation between cubic edge a and the radius R

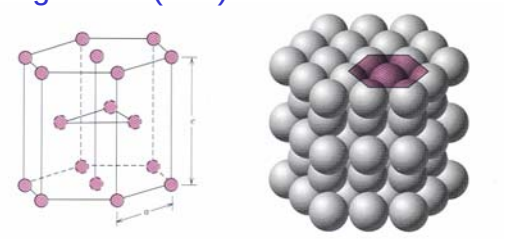
$$a = \frac{4R}{\sqrt{3}}$$

- Atomic packing factor (APF)=0.68



The HCP crystal structure

- Total atoms per unit cell=6
- Coordination number=12
- Atomic packing factor (APF)=0.74



Density and polymorphism

Density computation

$$\rho = \frac{nA}{V_C N_A}$$

Where n=number of atoms associated with each unit cell, A= atomic weight, Vc=volume of the unit cell, N_A=Avogadro's number (6.023x 10^{23} atoms/mol)

Polymorphism: a phenomenon that material has more than one crystal structure

Crystal systems

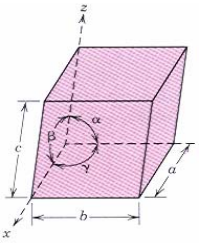
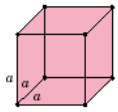
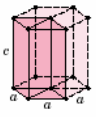
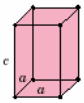
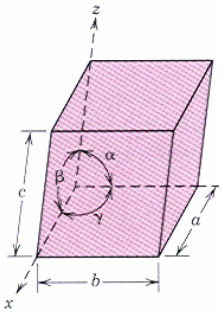
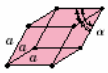
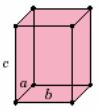
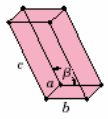
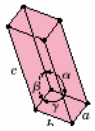


Table 3.2 Lattice Parameter Relationships and Figures Showing Unit Cell Geometries for the Seven Crystal Systems

Crystal System	*Axial Relationships*	*Interaxial Angles*	*Unit Cell Geometry*
Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90°$	
Hexagonal	$a = b \neq c$	$\alpha = \beta = 90°, \gamma = 120°$	
Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	

Crystal systems



Rhombohedral	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	
Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	
Monoclinic	$a \neq b \neq c$	$\alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	

Crystal Systems

Cubic:
Lead ore

Rhombic:
Topaz

Hexagonal:
Emerald

Tetragonal:
idocrase

Monoclinic:
Gypsum

Triclinic:
Axinite