SCIENCE AND ENGINEERING MATERIALS

Crystal Structure

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Chapter Description

- Learning Objectives
  - Describe crystalline and non-crystalline materials
  - Define and draw unit cells for crystal structure of:
    - Simple cubic (SC)
    - Face-centered cubic (FCC)
    - Body-centered cubic (BCC)
    - Hexagonal close-packed (HCP)
  - Demonstrate and derive the relationships between unit cell edge length and atomic radius for FCC and BCC crystal structures
  - Solve and compute the densities for metals with FCC and BCC crystal structures

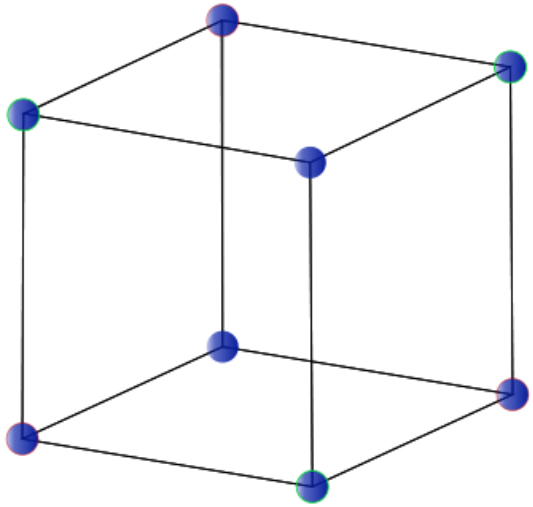
Crystalline and Amorphous Structure

- Most of engineering materials are crystalline – atoms are arranged in a regular and repeating manner
- Metals are crystalline
- Minerals such as celestite ($SrSo_4$), amethyst (SiO_2), alloys and some ceramic materials are also crystalline
- Amorphous – without form, or non-crystalline such as polymers, glasses and some metals

Simple Cubic (SC)

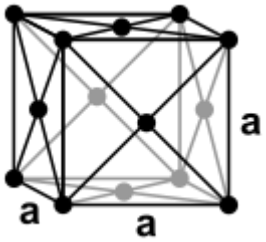
- Rare arrangement due to poor packing
- Example: Po

Source: Brilee89; Wikimedia



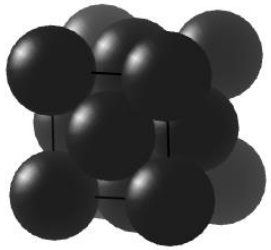
Source: DaniFeri; Wikimedia

Face-centered Cubic (FCC)



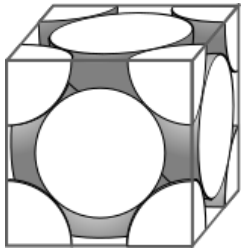
Source: Daniel Mayer and DrBob; Wikimedia

Atomic-site unit cell



Source: Brilee89; Wikimedia

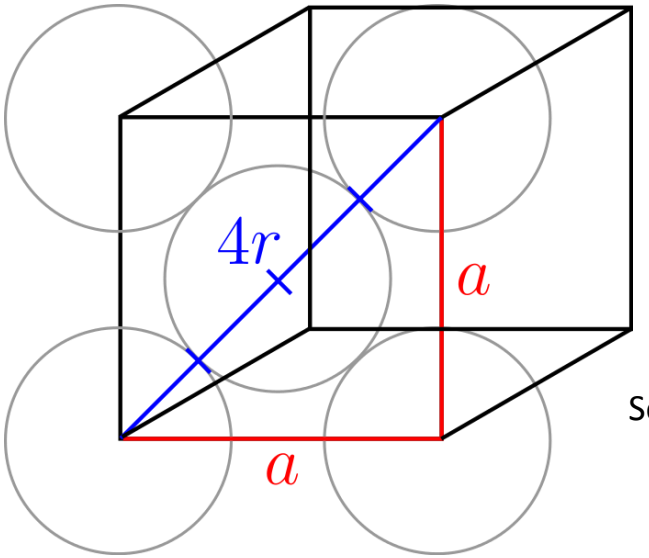
Hard-sphere unit cell



Source: Cdang; Wikimedia

Isolated unit cell

Face-centered Cubic (FCC)



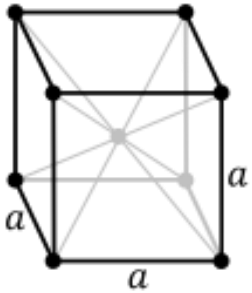
Source: Johannes Schneider; Wikimedia

- From above depiction, correlation between lattice constant *a*, and atomic radius *R* can be represented by:

$$\sqrt{2}a = 4R$$

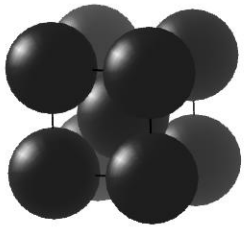
- Most of common metals posses FCC arrangement due to denser packing
- Example: γ-Fe, Ni, Al, Ag, Cu, Pt, A

Body-centered Cubic (BCC)



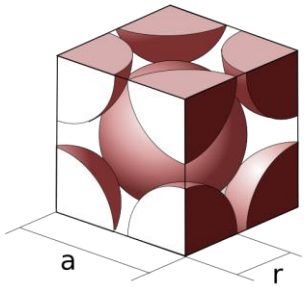
Source: Daniel Mayer and DrBob; Wikimedia

Atomic-site unit cell



Source: Brilee89; Wikimedia

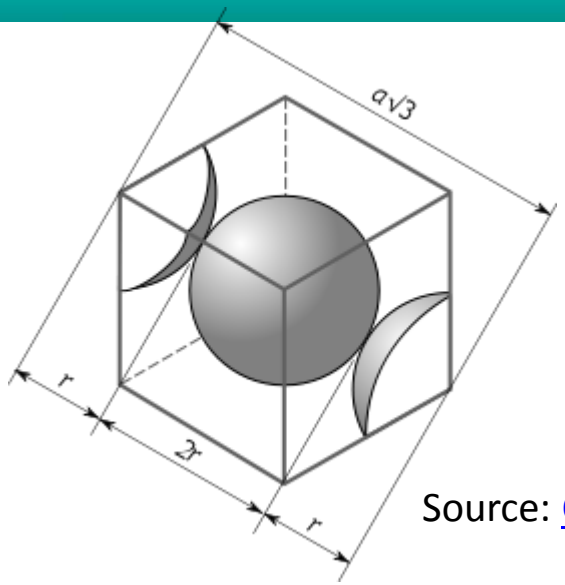
Hard-sphere unit cell



Source: Cdang and Samuel Dupré; Wikimedia

Isolated unit cell

Body-centered Cubic (BCC)



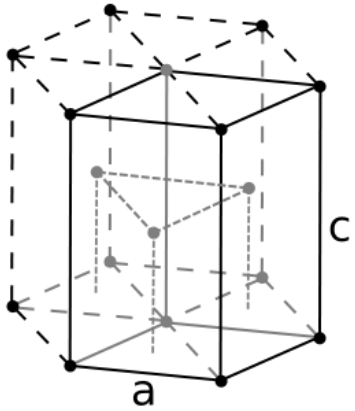
Source: Cdang; Wikimedia

- Based on above illustration, correlation between lattice constant *a*, and atomic radius *R* of BCC can be represented by:

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

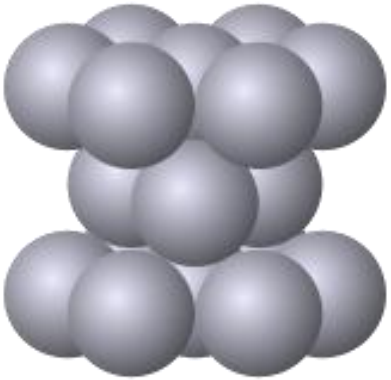
- Typical metals with BCC arrangement: α-Fe, V, Cr, Mo, W

Hexagonal Close-packed (HCP)



Source: Dornelf; Wikimedia

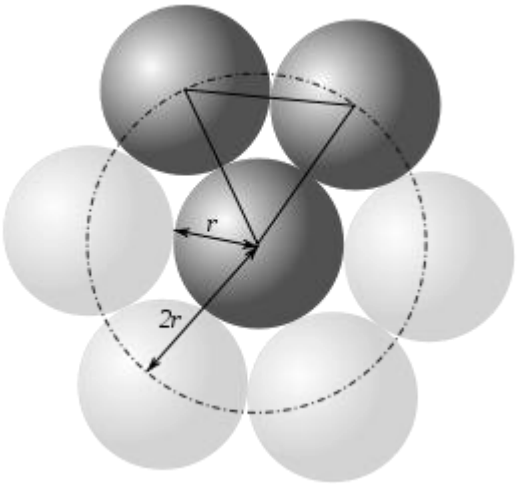
Atomic-site unit cell



Source: ARTE; Wikimedia

Hard-sphere unit cell

Hexagonal Close-packed (HCP)



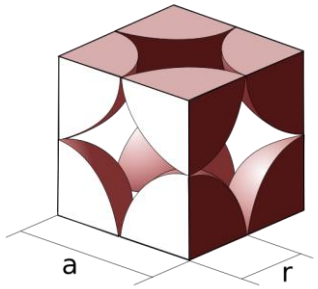
Source: Christophe Dang Ngoc Chan; Wikimedia

- Based on above, the relationship between edge length and atomic radius of HCP is:

  $a = 2r$

- Metals with HCP arrangement: Be, Mg, α-Ti, Zn, Zr

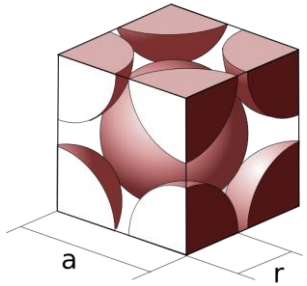
Atoms in Unit Cell



SC Unit cell contains:
8 Corners x 1/8

= 1 atom/unit cell

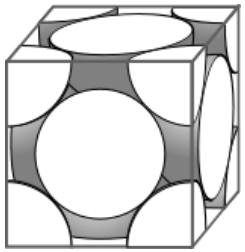
Source: Cdang, Samuel Dupré and Daniele Pugliesi; Wikimedia



BCC Unit cell contains:
1+ 8 Corners x 1/8

= 2 atom/unit cell

Source: Cdang, Samuel Dupré and Daniele Pugliesi; Wikimedia



FCC Unit cell contains: **= 4 atom/unit cell**
(6 Face x ½)+ (8 corners x1/8)

Source: Cdang; Wikimedia

Atomic Packing Factor (APF)

- APF relates to the fraction of unit-cell volume occupied by atoms

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

*assume hard spheres

APF for the BCC and FCC unit cell can be calculated, with the assumption that the atoms to be hard spheres.

Theoretical Density (ρ)

$$\text{Density} = \rho = \frac{\text{Mass of Atoms in Unit Cell}}{\text{Total Volume of Unit Cell}}$$

$$\rho = \frac{n A}{V_C N_A}$$

where n = number of atoms/unit cell

A = atomic weight

V_C = Volume of unit cell (a^3 for cubic)

N_A = Avogadro's number (6.022×10^{23} atoms/mol)

Conclusion of The Chapter

- Atoms in crystalline material are positioned accordingly in and ordered and repeated patterns, while non-crystalline materials (amorphous) are positioned in random and disoriented manner.
- There are three common arrangement of crystal structure unit cell in metals which are:
  - Body-centered cubic (BCC)
  - Face-centered cubic (FCC)
  - Hexagonal close-packed (HCP)

References

[1] Callister, Jr. W. D. Fundamentals of Materials Science & Engineering, Wiley, Third Edition.

[2] Shackelford, J. F. Introduction to Materials Science for Engineers, Pearson, Prentice Hall, 1231276190

[3] Smith, W. F. & Hashemi, J. Foundations of Materials Science & Engineering, McGraw Hill, 0071256903

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