MSE200
Lecture 3 (CHAPTER 3.1-3.5)
Crystal Structures and Crystal Geometry
Instructor: Yuntian Zhu

Objectives/Outcomes:

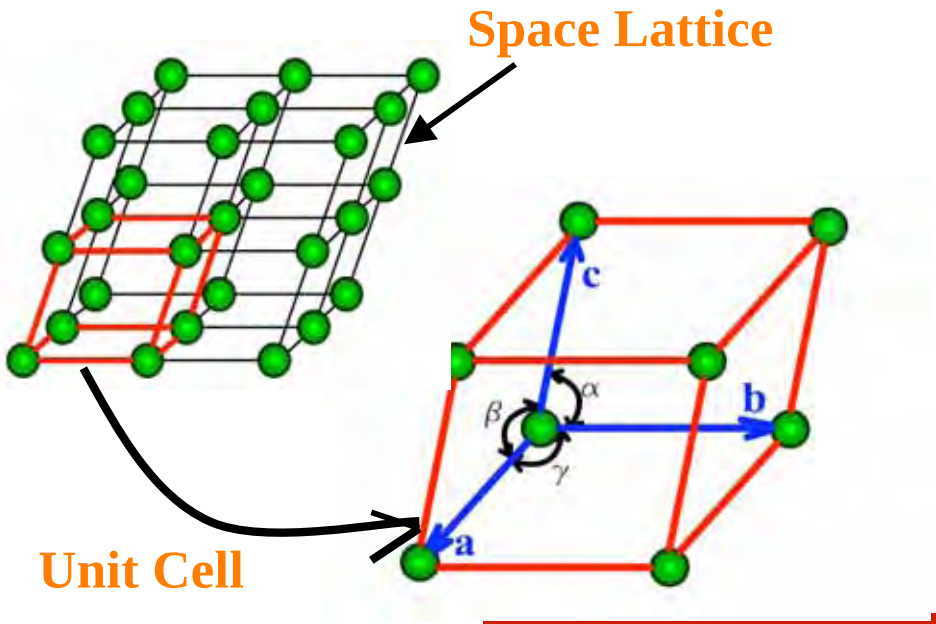
- Describe crystal lattices and the unit cell.
- Describe the principal metallic crystal structures: the body-centered cubic, the face-centered cubic, and the hexagonal close-packed structures.
- Determine directions in the cubic system.

The Space Lattice and Unit Cells

- **Atoms, arranged in repetitive 3-D pattern in long range order give rise to *crystal structure***
- **Why do we care?**
- **An imaginary network of lines, with points at intersections, representing the arrangement of atoms is called *space lattice*.**

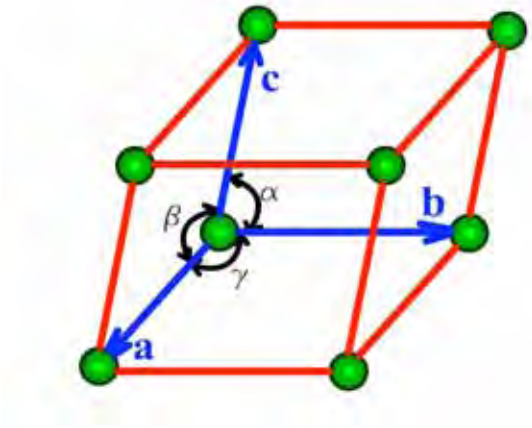
- **Unit cell.**

- **Amorphous materials**



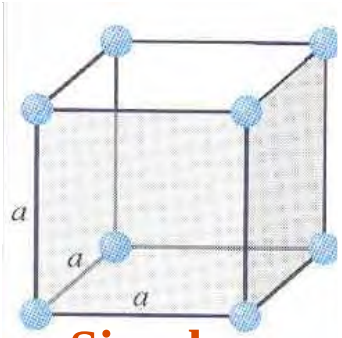
Crystal Systems and Bravais Lattice (Fig. 3.2)

- **Only 7 different types of unit cells are necessary to create all point lattices.**
- **According to Bravais: 14 standard unit cells.**

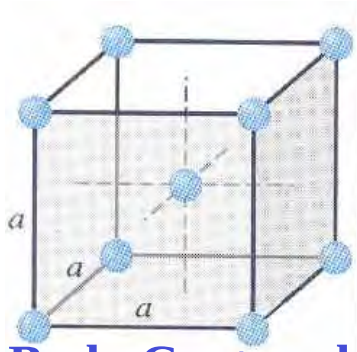


Types of Unit Cells

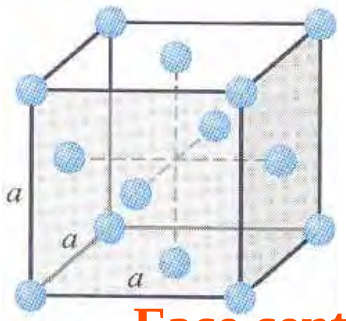
- **Type 1: Cubic Unit Cell**
  - **a = b = c**
  - **α = β = γ = 90⁰**



Simple



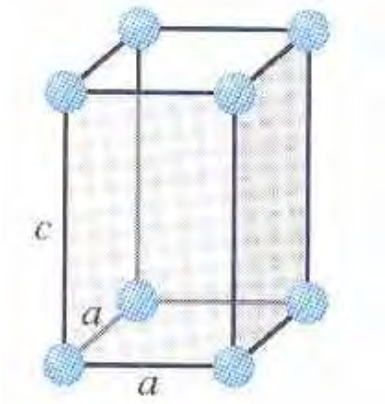
Body Centered (bcc)



Face centered (fcc)

Figure 3.2

- **Type 2: Tetragonal**
  - **a =b ≠ c**
  - **α = β = γ = 90⁰**



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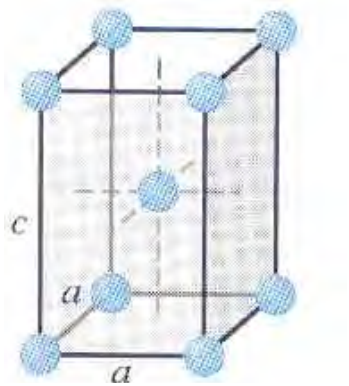
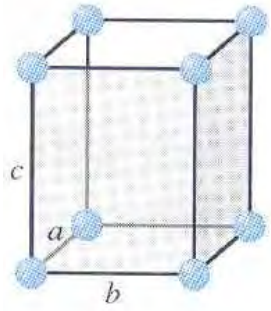


Body Centered

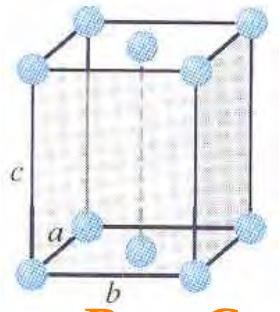
Adapted from C. Moffatt, G.W. Pearsall, & J. Wulff, "The Structure and Properties of Materials," vol. I, Structure, Wiley, 1954, p.47)

Types of Unit Cells (Cont..)

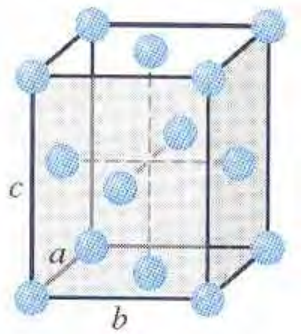
- **Type 3: Orthorhombic**
  - **$a \neq b \neq c$**
  - **$\alpha = \beta = \gamma = 90^0$**



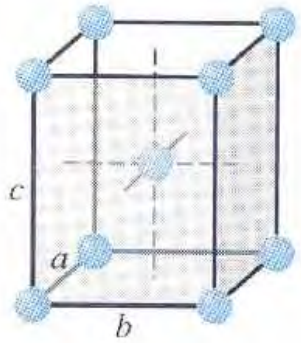
Simple



Base Centered



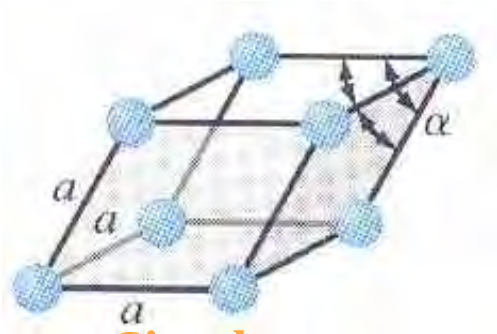
Face Centered



Body Centered

- **Type 4: Rhombohedral**
  - **$a = b = c$**
  - **$\alpha = \beta = \gamma \neq 90^0$**

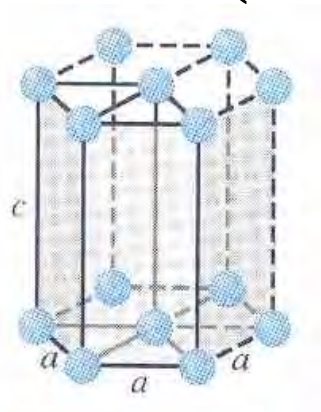
Figure 3.2



Simple

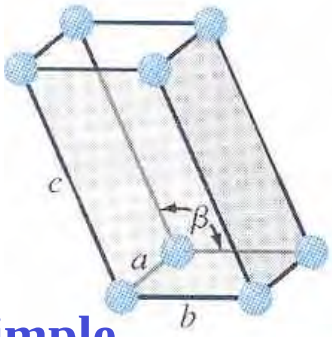
Types of Unit Cells (Cont..)

- **Type 5: Hexagonal**
  - **a = b ≠ c**
  - **α = β = 90⁰**
  - **γ = 120⁰**

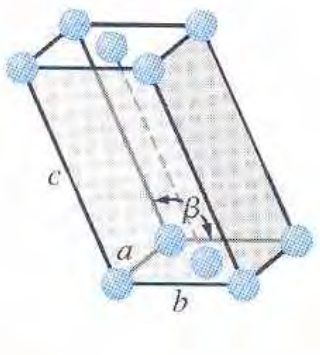


Simple

- **Type 6: Monoclinic**
  - **a ≠ b ≠ c**
  - **α = γ = 90⁰ ≠ β**

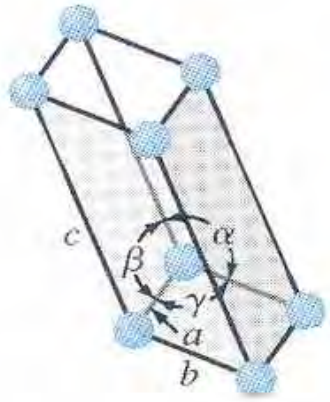


Simple



Base Centered

- **Type 7: Triclinic**
  - **a ≠ b ≠ c**
  - **α ≠ β ≠ γ ≠ 90⁰**

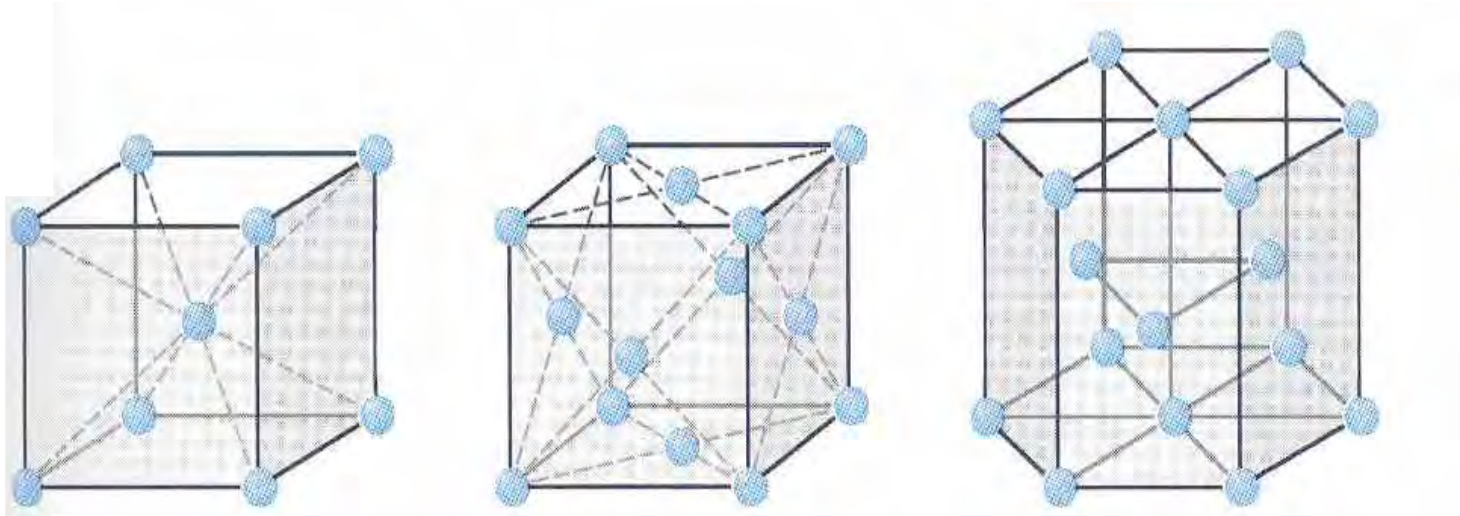


Simple

Figure 3.2

Principal Metallic Crystal Structures

- **90% of the metals have either Body Centered Cubic (BCC), Face Centered Cubic (FCC) or Hexagonal Close Packed (HCP) crystal structure.**
- **HCP is denser version of simple hexagonal crystal structure.**



BCC Structure **FCC Structure** **HCP Structure**

Figure 3.3

Body Centered Cubic (BCC) Crystal Structure

- **Represented as one atom at each corner of cube and one at the center of cube.**
- ***coordination number*:**
- **Examples :-**
  - **Chromium (a=0.289 nm)**
  - **Iron (a=0.287 nm)**
  - **Sodium (a=0.429 nm)**

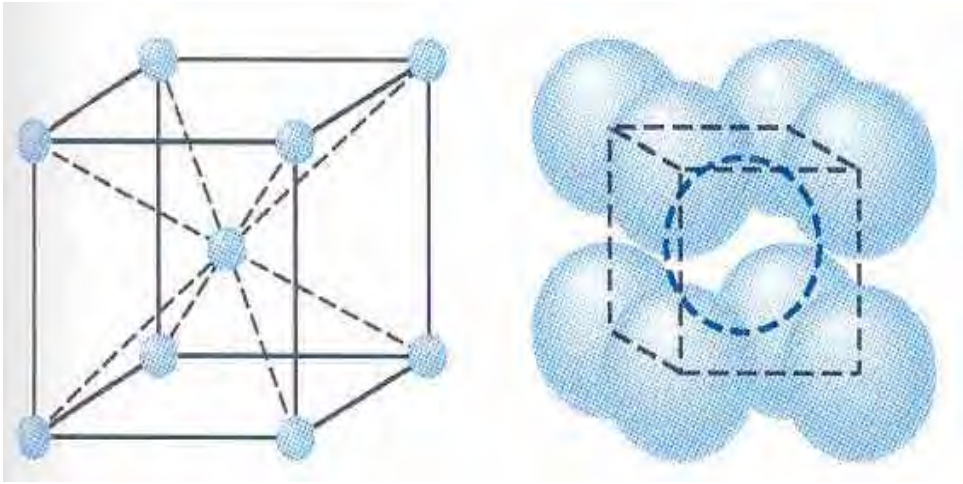
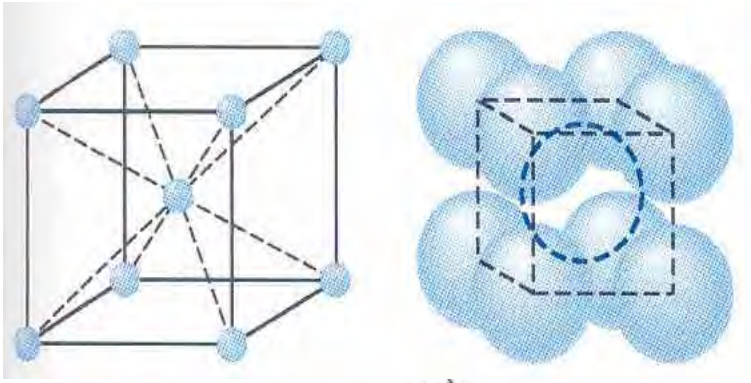


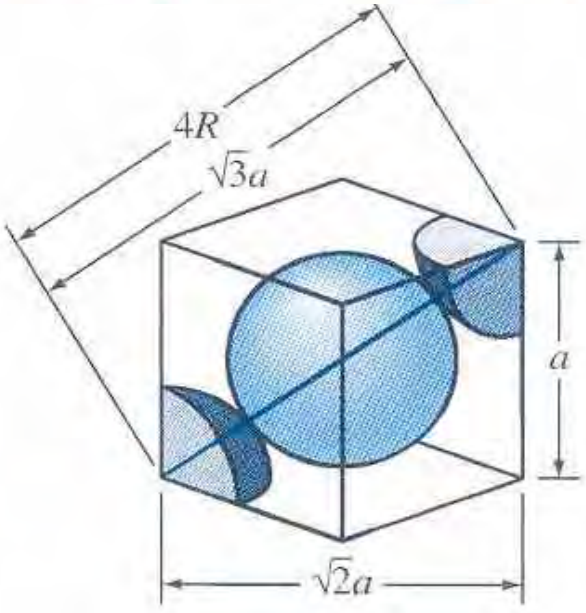
Figure 3.4 a&b

BCC Crystal Structure (Cont..)

- **# of atoms in the unit cell**



- **Atoms contact each other at cube diagonal**



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

Example 3.1

Packing factor:

Face Centered Cubic (FCC) Crystal Structure

- **FCC structure: 1 atom at each corner and face center**

- **Coordination number:**
- **Atomic Packing Factor:**
- **Examples :-**
  - **Aluminum (a = 0.405)**
  - **Gold (a = 0.408)**

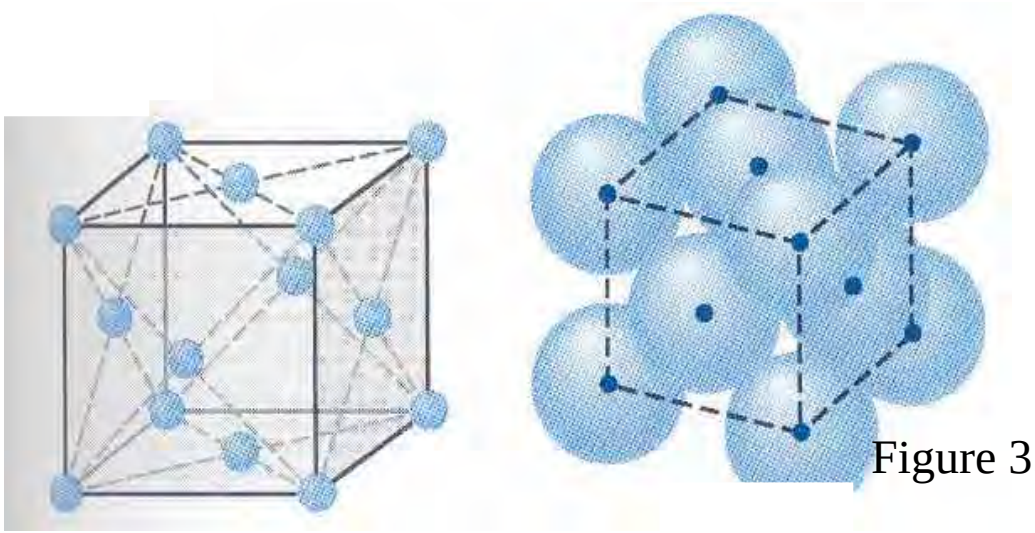
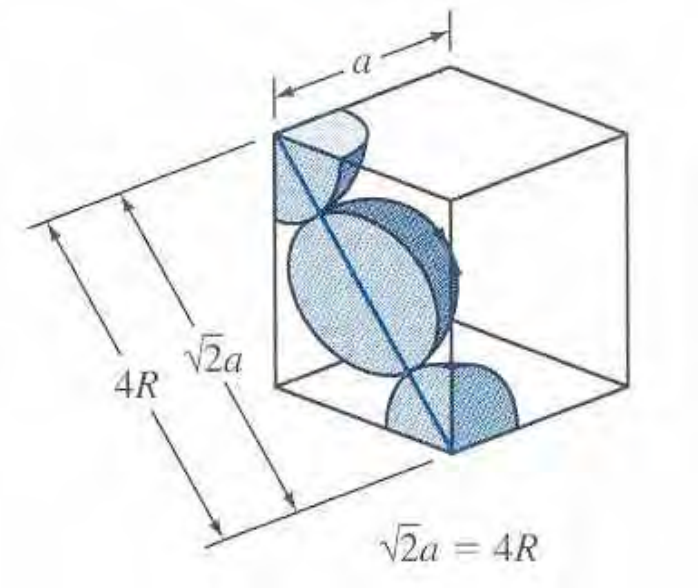


Figure 3.6 a&b

FCC Crystal Structure (Cont..)

- **# of atoms in a unit cell**

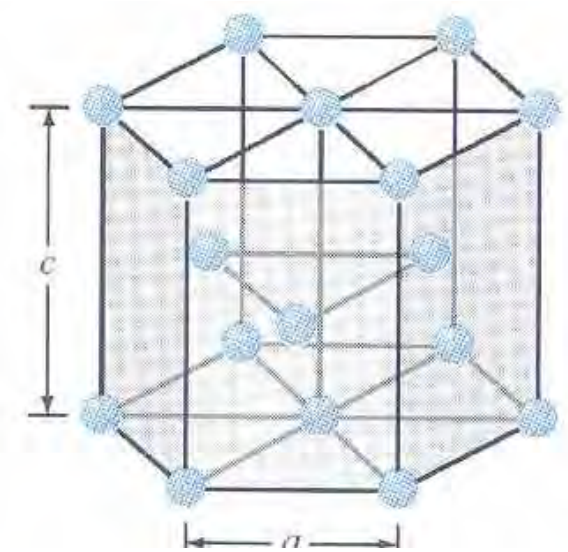


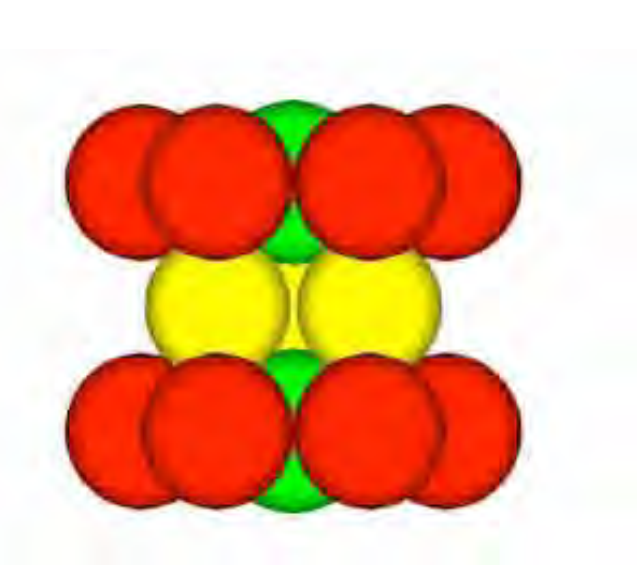
Lattice constant

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

Hexagonal Close-Packed Structure

- **The HCP structure is represented as an atom at each of 12 corners of a hexagonal prism, 2 atoms at top and bottom face and 3 atoms in between top and bottom face.**
- **The coordination number is 12, packing factor = 0.74.**



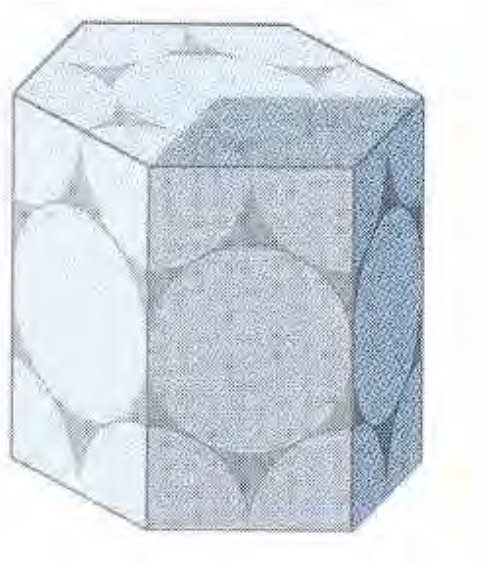


HCP Crystal Structure (Cont..)

- **# of atoms in each HCP unit cell:**

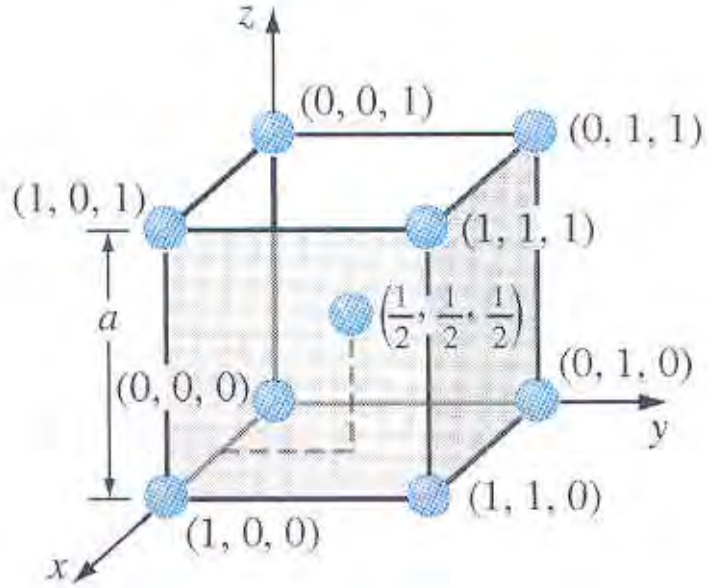
- **Examples:-**
  - **Zinc (a = 0.2665 nm, c/a = 1.85)**
  - **Cobalt (a = 0.2507 nm, c/a = 1.62)**

- **Ideal c/a ratio is 1.633.**



Atom Positions in Cubic Unit Cells

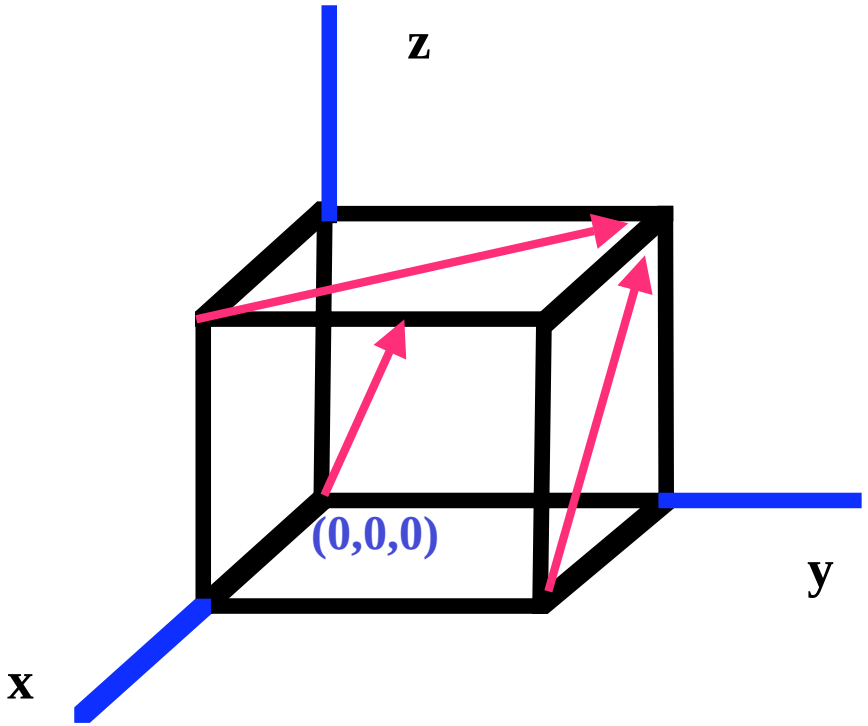
- **In a cubic unit cell**
  - ➢



- **Atom positions are located using unit distances along the axes.**

Figure 3.10 b

Find Direction Indices



Example 3.4

Homework

- Example Problems: 3.1, 3.2, 3.4, 3.5, 3.6,
- Regular Problems, Chapter 3: 6, 7,8, 9, 10, 11, 12, 13, 14, 15, 16, 18, 20, 21, 22, 31, 32, 33, 34,36,
- Reading assignment for the next class: 3.6-3.11