Crystal Structures

Remember the seven systems are:

- Cubic (isometric)
- Tetragonal
- Orthorhombic
- Trigonal (rhombohedral)
- Hexagonal
- Monoclinic and
- Triclinic

Coordination Number

It is The number of lattice points closest to a given point

Or

(number of nearest-neighbors of each point).

- Because of lattice periodicity, **all lattice points have the same** number of nearest neighbors or **coordination number**.

Examples

1. **Simple Cubic (SC)** coordination number **= 6**
2. **Body-Centered Cubic** coordination number **= 8**
3. **Face-Centered Cubic** coordination number **= 12**

Number of atoms per unit cell

Arrangement of lattice points in the unit cell & No. of Lattice points / cell

		Position of lattice points	Effective number of Lattice points / cell
1	P	8 Corners	= 8 x (1/8) = 1
2	I	8 Corners + 1 body centre	= 1 (for corners) + 1 (BC)
3	F	8 Corners + 6 face centres	= 1 (for corners) + 6 x (1/2) = 4
4	B/	8 corners + 2 centres of opposite faces	= 1 (for corners) + 2x(1/2) = 2

Closed-packed structures

(or, what does stacking fruit have to do with solid state physics?)

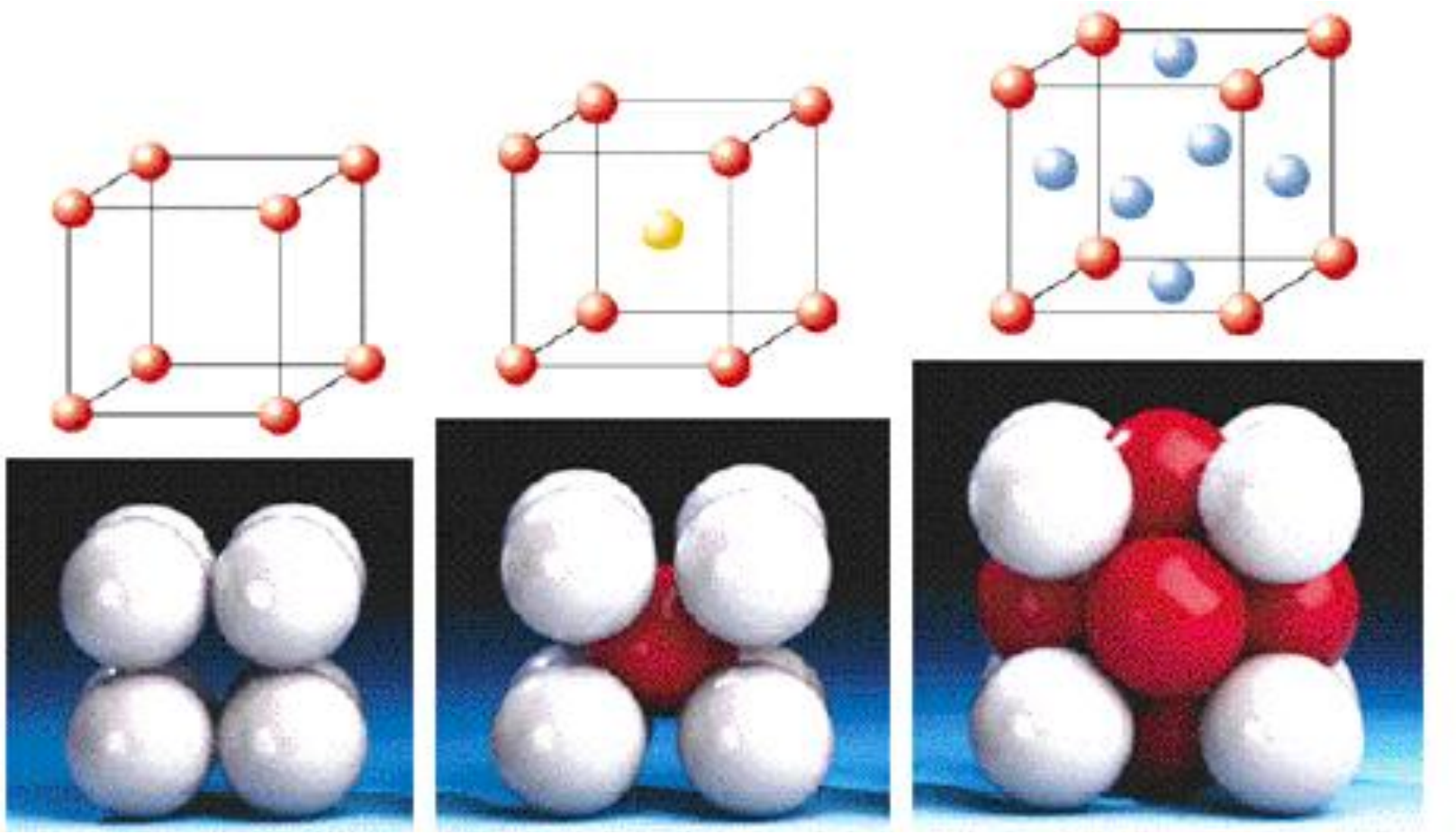
The Atomic Packing Factor (APF) ≡ **volume of the atoms within the unit cell divided by the volume of the unit cell.**

$$\text{APF} = \frac{\text{Volume of Atoms in Unit Cell}}{\text{Volume of Unit Cell}}$$

- When calculating the APF, the volume of the atoms in the unit cell is calculated *AS IF each atom was a hard sphere*, centered on the lattice point & large enough to just touch the nearest-neighbor sphere.

1- CUBIC CRYSTAL SYSTEMS

3 Common Unit Cells with



(a) Simple Cubic (SC)

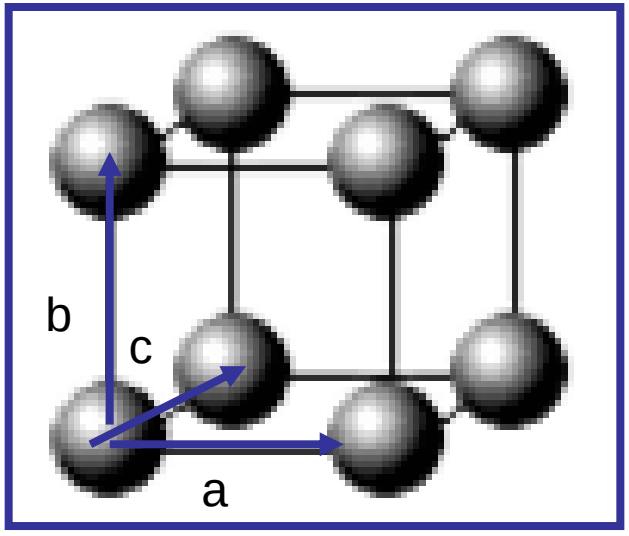
(b) Body Centered Cubic (BCC)

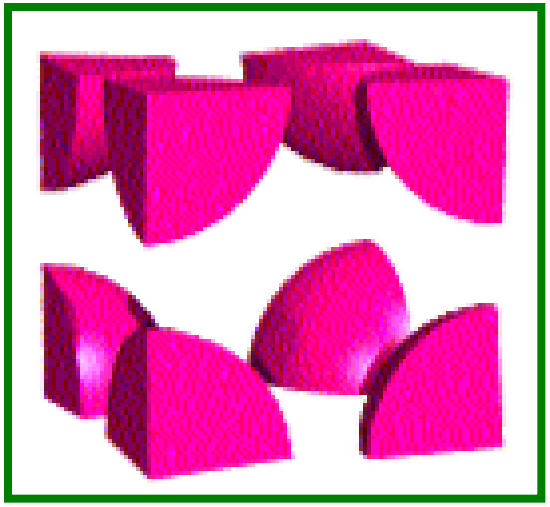
(c) Face Centered Cubic (FCC)

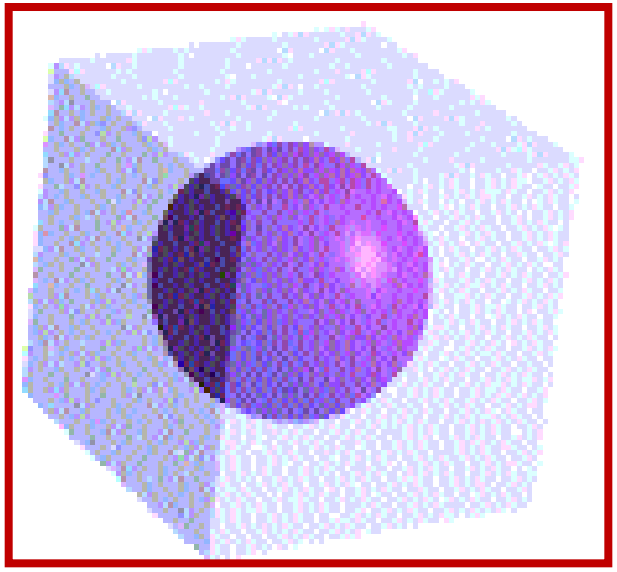
a- Simple Cubic (SC) Lattice

- The SC Lattice has one lattice point in its unit cell, so it's unit cell is a primitive cell.
- In the unit cell on the left, the atoms at the corners are cut because only a portion (in this case 1/8) "belongs" to that cell. The rest of the atom "belongs" to neighboring cells.

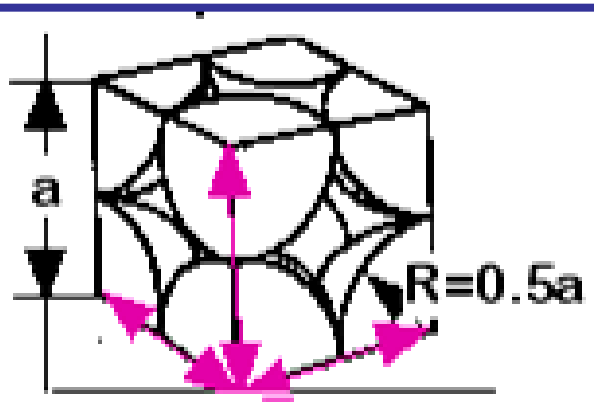
Coordinatination Number of the SC Lattice = 6.







Atomic Packing Factor



close-packed directions

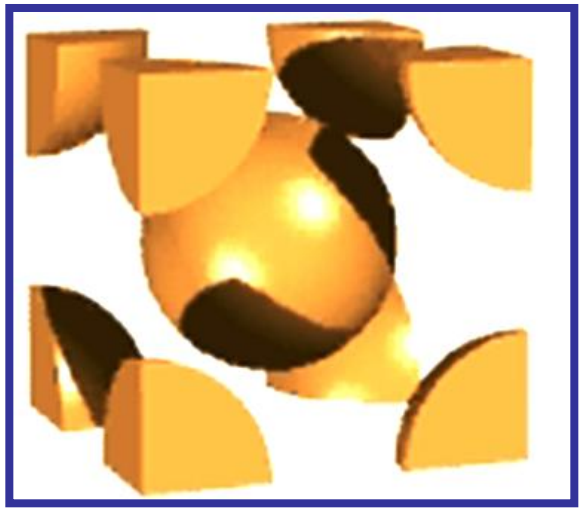
contains 8 x 1/8 = 1atom/unit cell

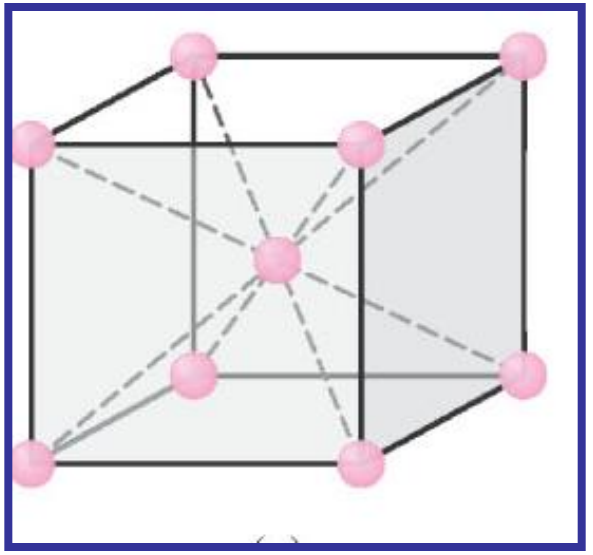
APF = 0.52 for simple cubic

$$APF = \frac{\left(\frac{\text{atom}}{\text{unit cell}}\right)\left(\frac{\text{volume}}{\text{atom}}\right)}{\frac{\text{volume}}{\text{unit cell}}} = \frac{1\left(\frac{4}{3}\pi (0.5a)^3\right)}{a^3}$$

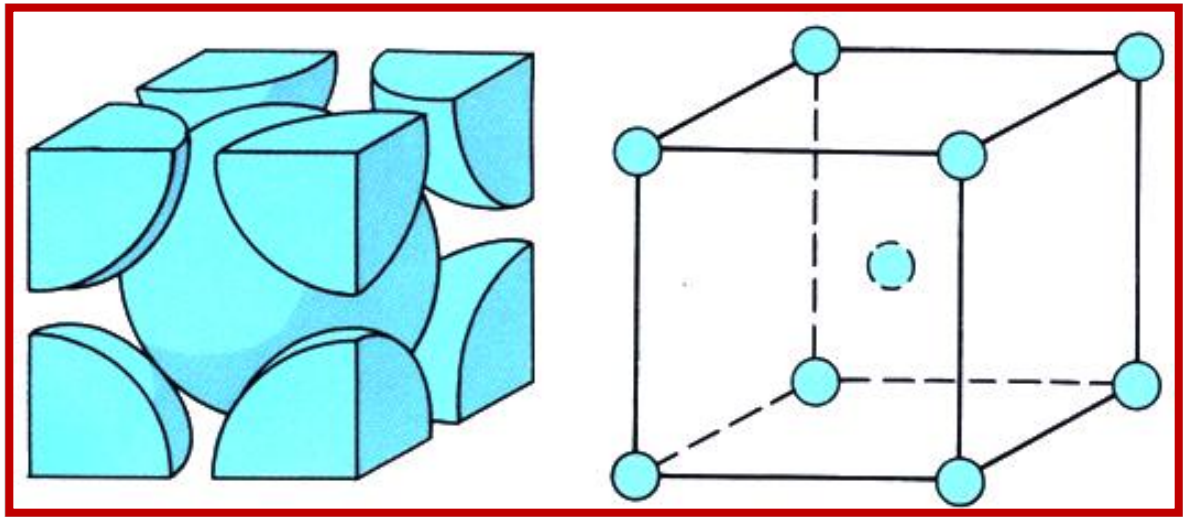
b- Body Centered Cubic (BCC) Lattice

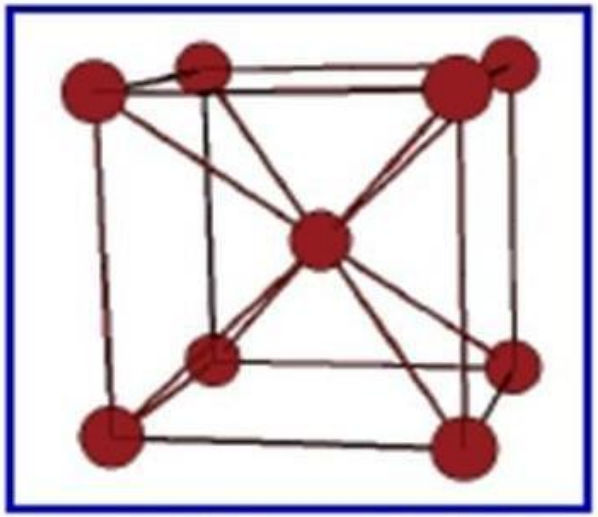
- The BCC Lattice has two lattice points per unit cell so the BCC unit cell is a non-primitive cell.
- Every BCC lattice point has 8 nearest-neighbors. So (in the hard sphere model) each atom is in contact with its neighbors only along the body-diagonal directions.
- Many metals (Fe,Li,Na..etc), including the alkalis and several transition elements have the BCC structure.



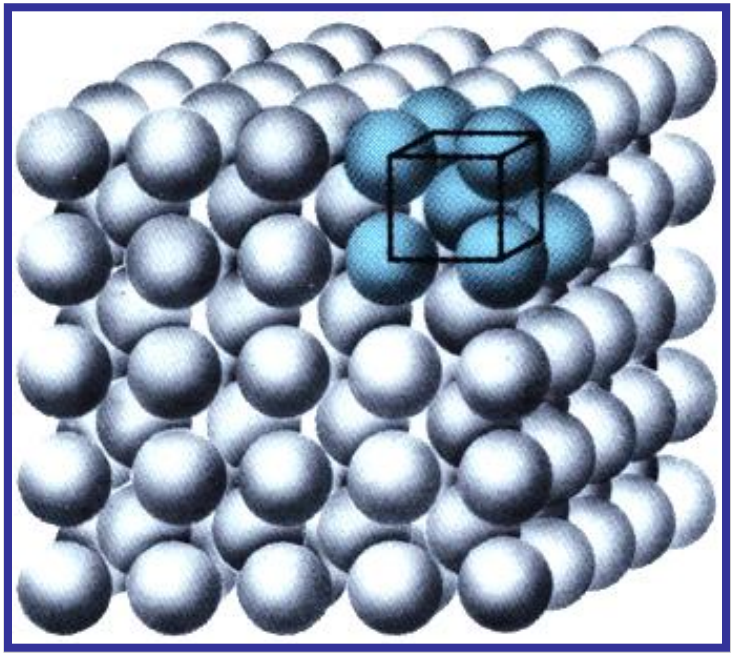


Body Centered Cubic (BCC) Structure

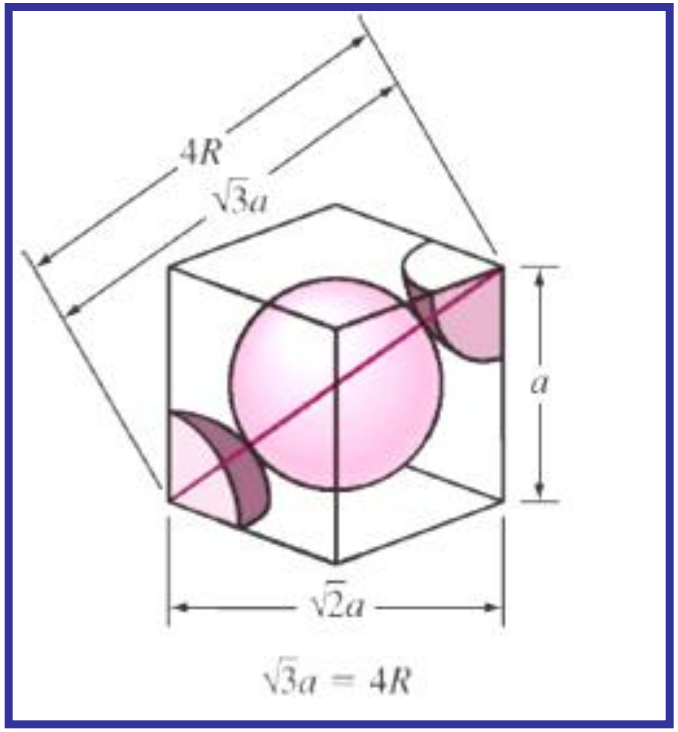




Body Centered Cubic
and related structures



Atomic Packing Factor



$$APF = \frac{\text{atom}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \cdot \frac{\text{volume}}{\text{unit cell}}$$

$$APF = \frac{2 \left(\frac{4}{3} \pi (0.433a)^3 \right)}{a^3}$$

$$APF_{BCC} = \frac{V_{atoms}}{V_{unitcell}} = 0.68$$

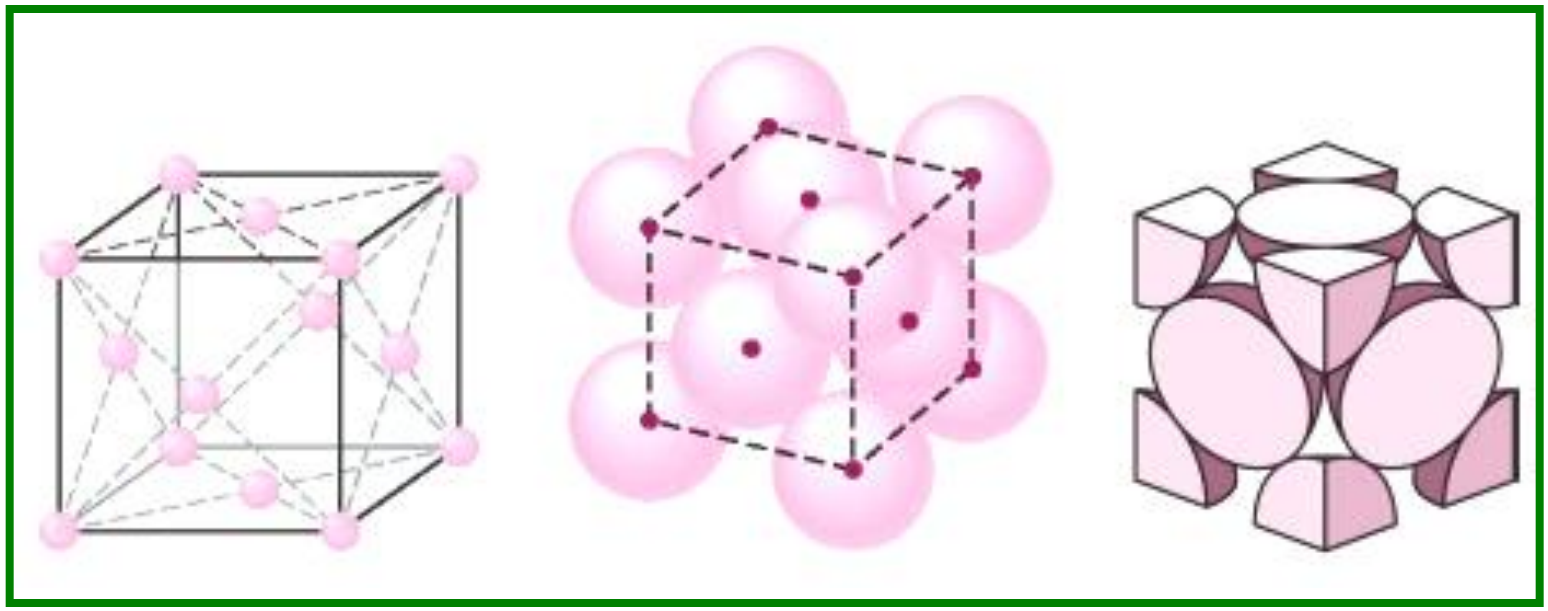
Elements That Form Solids with the BCC Structure

Table 4.2
ELEMENTS WITH THE MONATOMIC BODY-CENTERED CUBIC CRYSTAL STRUCTURE

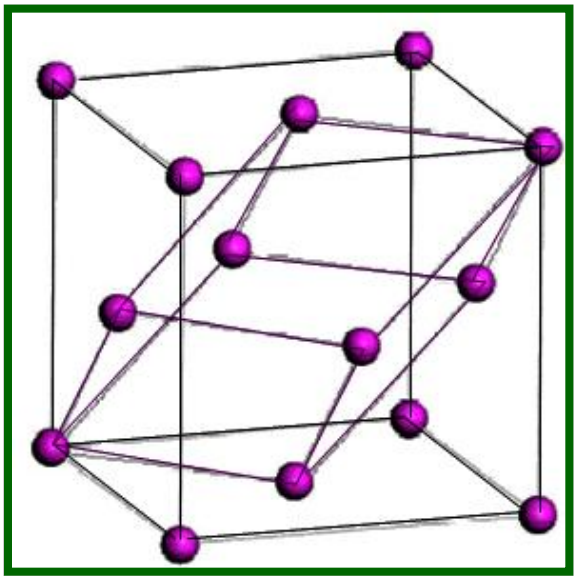
ELEMENT	*a* (Å)	ELEMENT	*a* (Å)	ELEMENT	*a* (Å)
Ba	5.02	Li	3.49 (78 K)	Ta	3.31
Cr	2.88	Mo	3.15	Tl	3.88
Cs	6.05 (78 K)	Na	4.23 (5 K)	V	3.02
Fe	2.87	Nb	3.30	W	3.16
K	5.23 (5 K)	Rb	5.59 (5 K)		

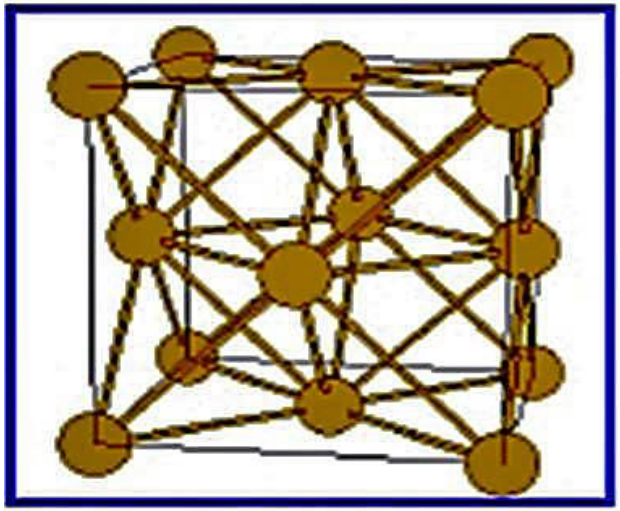
c- Face Centered Cubic (FCC) Lattice

- In the **FCC Lattice** there are atoms at the corners of the unit cell and at the center of each face.
- The FCC unit cell has 4 atoms so it is a non-primitive cell.
- Every **FCC Lattice** point has 12 nearest-neighbors.
- **Many common metals** (**Cu,Ni,Pb..**etc) crystallize in the **FCC structure.**

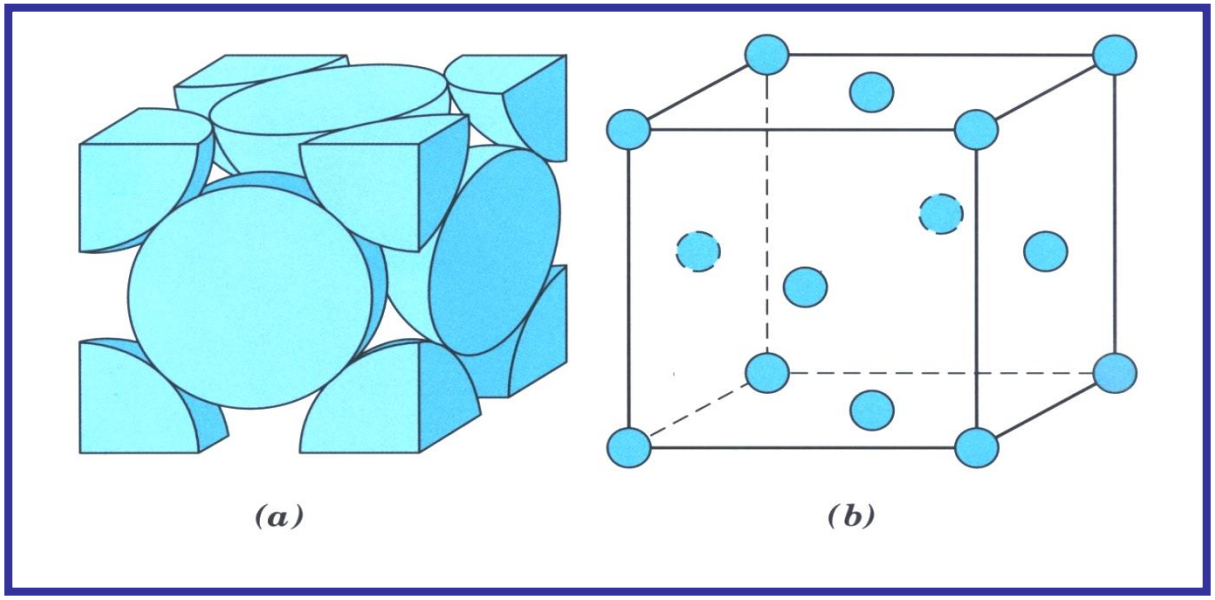


Face Centered Cubic (FCC) Structure

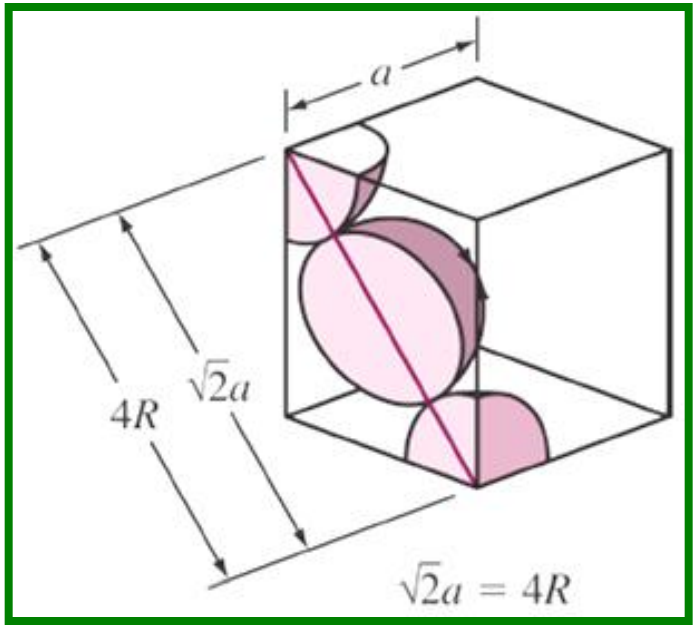




A1 (fcc) Structure



Face Centered Cubic (FCC) Lattice
Atomic Packing Factor



$$APF = \frac{\text{atom}}{\text{unit cell}} \cdot \frac{\text{volume}}{\text{atom}} \cdot \frac{\text{volume}}{\text{unit cell}}$$

$$APF = \frac{4 \cdot \frac{4}{3}\pi (0.353a)^3}{a^3}$$

APF in this case = 0.74

Elements That Form Solids with the FCC Structure

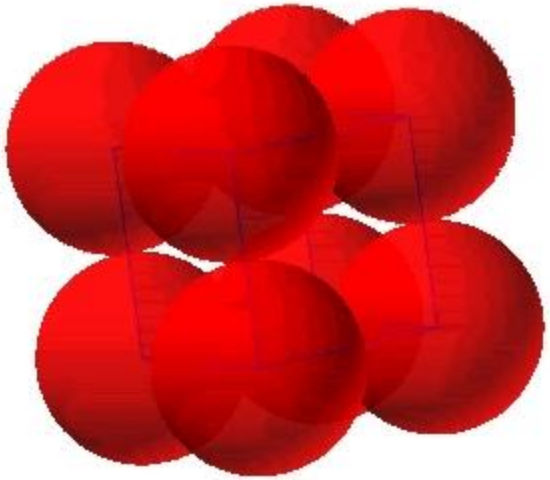
ELEMENTS WITH THE MONATOMIC FACE-CENTERED CUBIC CRYSTAL STRUCTURE

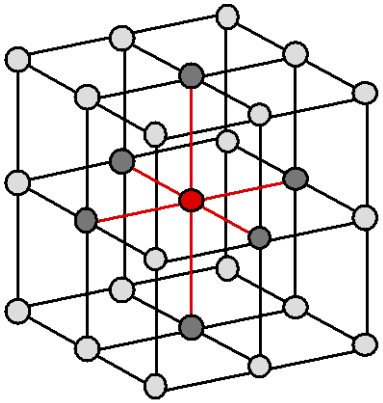
ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ar	5.26 (4.2 K)	Ir	3.84	Pt	3.92
Ag	4.09	Kr	5.72 (58 K)	δ-Pu	4.64
Al	4.05	La	5.30	Rh	3.80
Au	4.08	Ne	4.43 (4.2 K)	Sc	4.54
Ca	5.58	Ni	3.52	Sr	6.08
Ce	5.16	Pb	4.95	Th	5.08
β-Co	3.55	Pd	3.89	Xe (58 K)	6.20
Cu	3.61	Pr	5.16	Yb	5.49

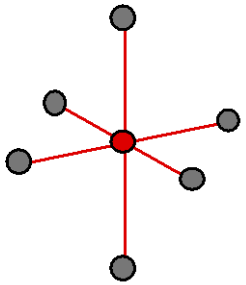
Data in Tables 4.1 to 4.7 are from R. W. G. Wyckoff, *Crystal Structures*, 2nd ed., Interscience, New York, 1963. In most cases, the data are taken at about room temperature and normal atmospheric pressure. For elements that exist in many forms the stable room temperature form (or forms) is given. For more detailed information, more precise lattice constants, and references, the Wyckoff work should be consulted.

Simple Cubic Structure (SC)

- Rare due to low packing density (only Po – Polonium -- has this structure)
- Close-packed directions are *cube edges.*







- Coordination No. = 6

(# nearest neighbors)
for each atom as seen

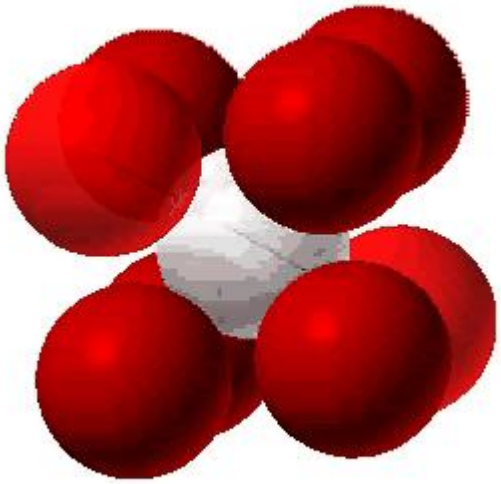
(Courtesy P.M. Anderson)

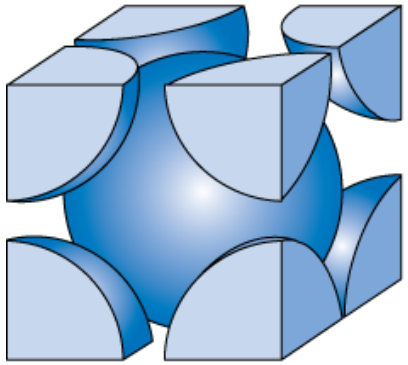
Body Centered Cubic Structure (BCC)

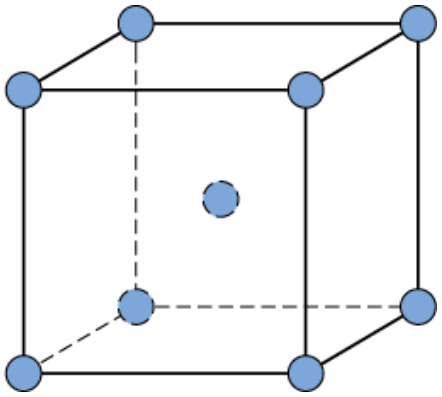
- Atoms touch each other along *cube diagonals within a unit cell*.

--Note: All atoms are identical; the center atom is shaded differently only for ease of viewing.

ex: Cr, W, Fe (α), Tantalum, Molybdenum







Adapted from Fig. 3.2, *Callister 7e.*

- Coordination # = 8

2 atoms/unit cell: (1 center) + (8 corners x 1/8)

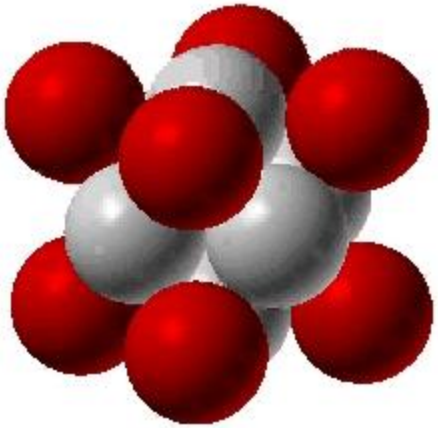
(Courtesy P.M. Anderson)

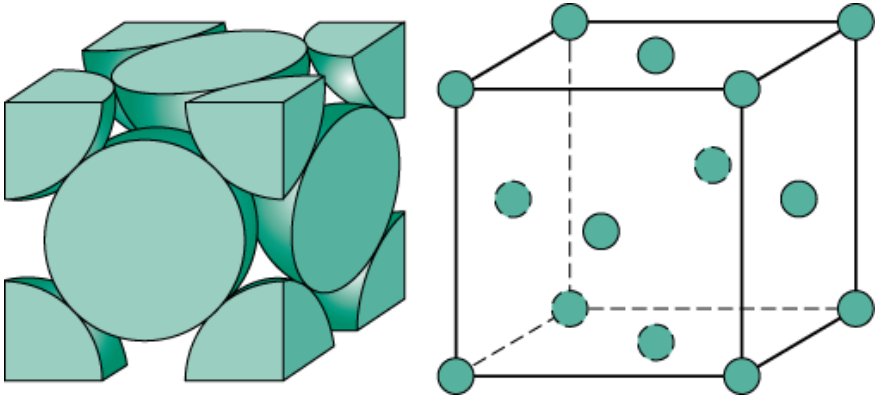
Face Centered Cubic Structure (FCC)

- Atoms touch each other along *face diagonals*.
  --Note: All atoms are identical; the face-centered atoms are shaded differently only for ease of viewing.

ex: Al, Cu, Au, Pb, Ni, Pt, Ag

- Coordination # = 12





Adapted from Fig. 3.1, *Callister 7e.*

4 atoms/unit cell: (6 face x ½) + (8 corners x 1/8)

(Courtesy P.M. Anderson)