1

Metallic and Ionic Solids

2

Types of Solids

Table 13.6

TYPE	EXAMPLE	FORCE
Ionic	NaCl, CaF_2, ZnS	Ion-ion
Metallic	Na, Fe	Metallic
Molecular	Ice, I_2	Dipole Ind. dipole
Network	Diamond Graphite	Extended covalent

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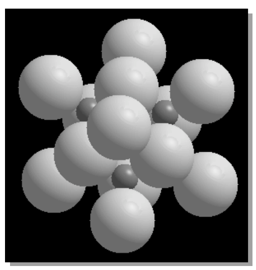
Properties of Solids

1. Molecules, atoms or ions locked into a CRYSTAL LATTICE
2. Particles are CLOSE together
3. STRONG IM forces
4. Highly ordered, rigid, incompressible

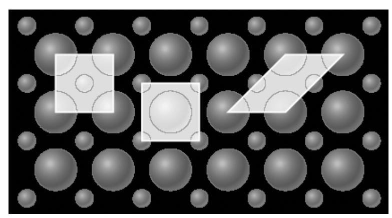


ZnS, zinc sulfide

4

Crystal Lattices

- Regular 3-D arrangements of equivalent LATTICE POINTS in space.
- Lattice points define UNIT CELLS
  - smallest repeating internal unit that has the symmetry characteristic of the solid.



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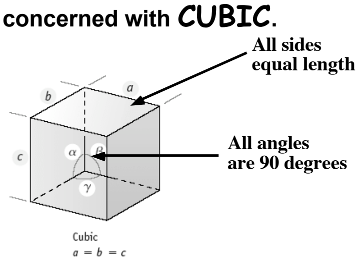
Cubic Unit Cells

There are 7 basic crystal systems, but we are only concerned with CUBIC.



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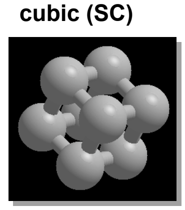
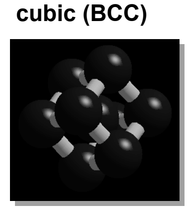
Cubic Unit Cells of Metals

Figure 13.27

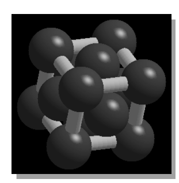
Simple cubic (SC)



Body-centered cubic (BCC)



Face-centered cubic (FCC)



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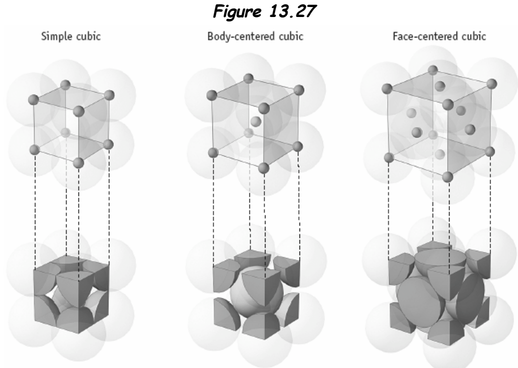
Cubic Unit Cells of Metals

Figure 13.27



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Units Cells for Metals

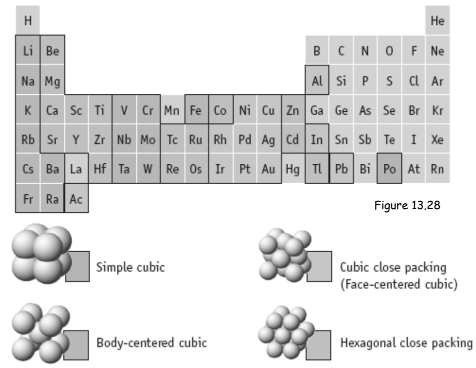

Figure 13.28

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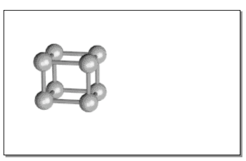
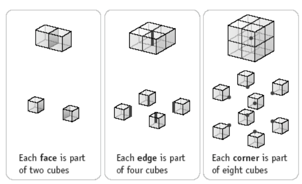
Simple Cubic Unit Cell

Figure 13.26





- E atom is at a corner of a unit cell and is shared among 8 unit cells.
- Each edge is shared with 4 cells
- Each face is part of two cells.

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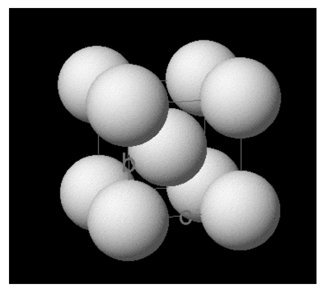
Body-Centered Cubic Unit Cell



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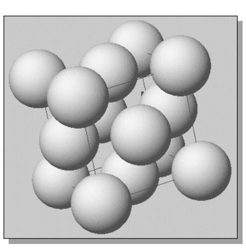
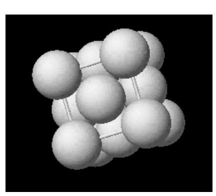
Face Centered Cubic Unit Cell

Atom at each cube corner plus atom in each cube face.





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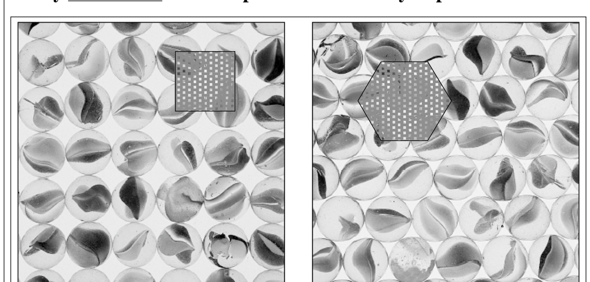
Atom Packing in Unit Cells

Assume atoms are hard spheres and that crystals are built by PACKING of these spheres as efficiently as possible.



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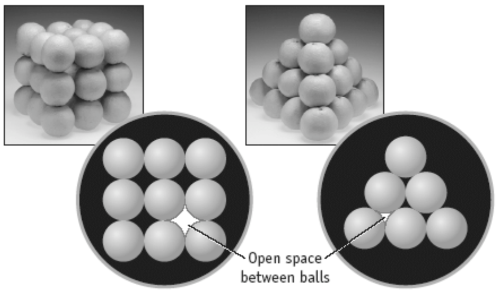
Atom Packing in Unit Cells

Assume atoms are hard spheres and that crystals are built by PACKING of these spheres as efficiently as possible.



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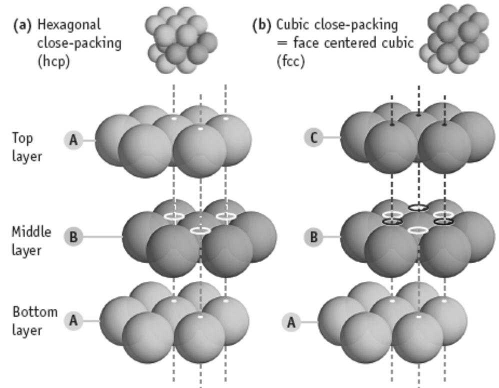

Atom Packing in Unit Cells

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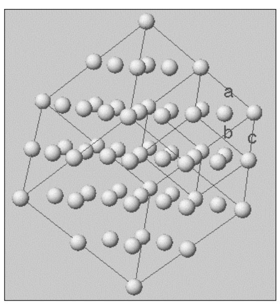
Crystal Lattices— Packing of Atoms or Ions

- **FCC is more efficient than either BC or SC.**
- **Leads to layers of atoms.**



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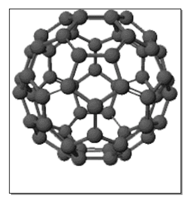
Crystal Lattices— Packing of Atoms or Ions



Packing of C_{60} molecules. They are arranged at the lattice points of a FCC lattice.

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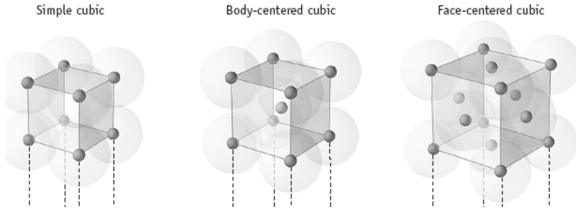
Number of Atoms per Unit Cell

Unit Cell Type	Net Number Atoms
SC	1
BCC	2
FCC	4



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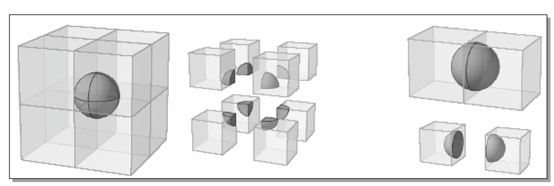
Atom Sharing at Cube Faces and Corners



Atom shared in corner --> 1/8 inside each unit cell

Atom shared in face --> 1/2 inside each unit cell

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Simple Ionic Compounds

Lattices of many simple ionic solids are built by taking a SC or FCC lattice of ions of one type and placing ions of opposite charge in the holes in the lattice.

<u>EXAMPLE:</u> CsCl has a SC lattice of Cs^+ ions with Cl^- in the center.

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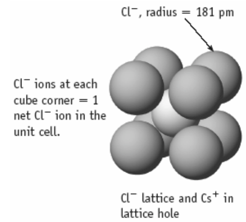
Simple Ionic Compounds



CsCl unit cell has a SC lattice of Cl^- ions with Cs^+ in the center.

1 unit cell has 1 Cs^+ ion plus

(8 corners)(1/8 Cl^- per corner) = 1 net Cl^- ion.

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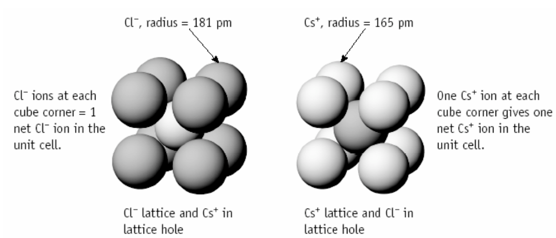
Two Views of CsCl Unit Cell

- **Lattice can be SC lattice of Cl^- with Cs^+ in hole**
- ***OR* SC lattice of Cs^+ with Cl^- in hole**
- **Either arrangement leads to formula of 1 Cs^+ and 1 Cl^- per unit cell**



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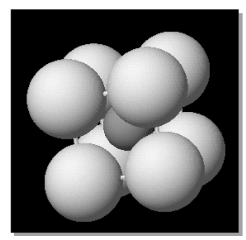
Simple Ionic Compounds

Salts with formula MX can have SC structure — but not salts with formula MX_2 or M_2X



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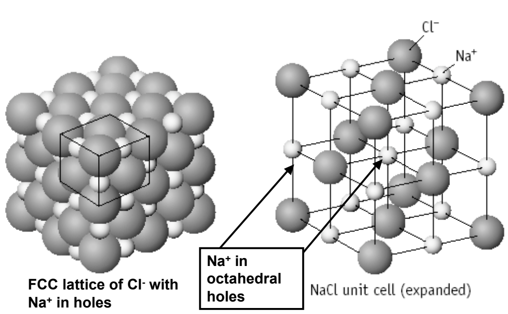
NaCl Construction



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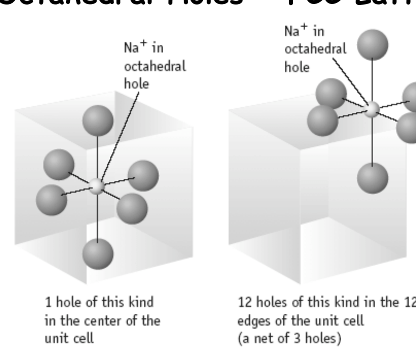
Octahedral Holes - FCC Lattice



Octahedral holes in a face-centered lattice

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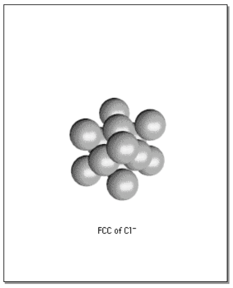
The Sodium Chloride Lattice



Na^+ ions are in OCTAHEDRAL holes in a face-centered cubic lattice of Cl^- ions.

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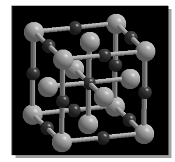
The Sodium Chloride Lattice

Many common salts have FCC arrangements of anions with cations in OCTAHEDRAL HOLES — e.g., salts such as CA = NaCl

- FCC lattice of anions ----> 4 A^-/unit cell
- C^+ in octahedral holes ---> 1 C^+ at center
  + [12 edges • 1/4 C^+ per edge]
  = 4 C^+ per unit cell



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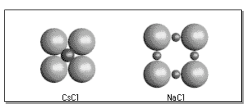
Comparing NaCl and CsCl



- Even though their formulas have one cation and one anion, the lattices of CsCl and NaCl are different.
- The different lattices arise from the fact that a Cs^+ ion is much larger than a Na^+ ion.

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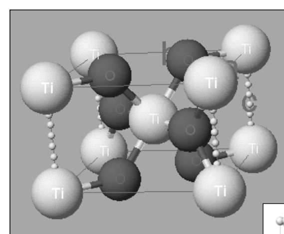
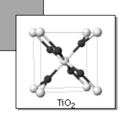
Common Ionic Solids





Titanium dioxide, TiO_2

There are 2 net Ti^{4+} ions and 4 net O^{2-} ions per unit cell.

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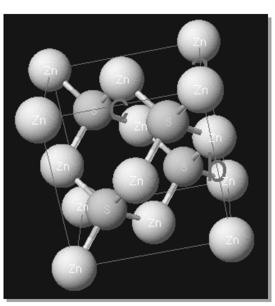
Common Ionic Solids



- Zinc sulfide, ZnS
- The S^{2-} ions are in TETRAHEDRAL holes in the Zn^{2+} FCC lattice.
- This gives 4 net Zn^{2+} ions and 4 net S^{2-} ions.

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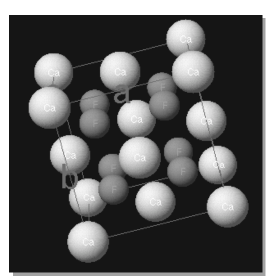
Common Ionic Solids



- Fluorite or CaF_2
- FCC lattice of Ca^{2+} ions
- This gives 4 net Ca^{2+} ions.
- F^- ions in all 8 tetrahedral holes.
- This gives 8 net F^- ions.

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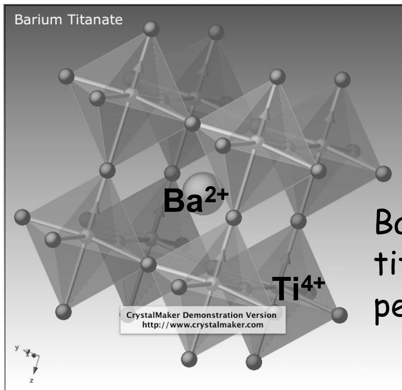

$BaTiO_3$

Barium titanate, a perovskite

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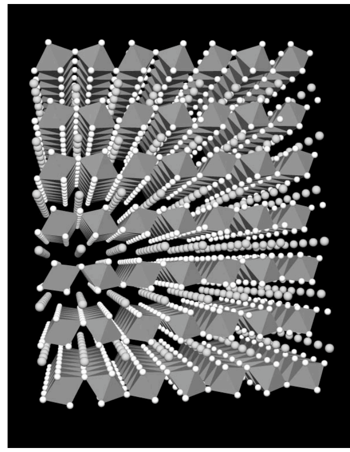

Common Ionic Solids

Magnesium silicate, $MgSiO_3$

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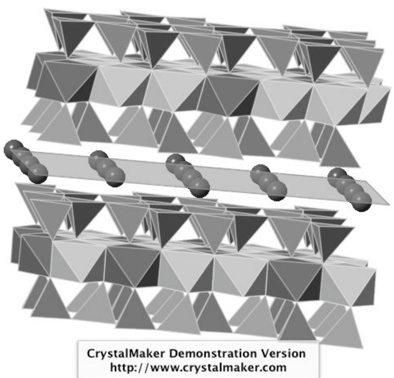

Biotite

- Layers of linked octahedra of MgO_6 and FeO_6.
- Layers of linked SiO_4 tetrahedra.
- K ions between layers

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Finding the Lattice Type

PROBLEM Al has density = 2.699 g/cm^3 and Al radius = 143 pm. Verify that Al is FCC.

SOLUTION

1. Calc. unit cell volume

V = (cell edge)^3

Edge distance comes from face diagonal.

Diagonal distance = √2 • edge

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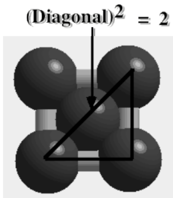
Finding the Lattice Type

PROBLEM Al has density = 2.699 g/cm^3 and Al radius = 143 pm. Verify that Al is FCC.

SOLUTION

V = (cell edge)^3 and face diagonal = √2 • edge

$(\text{Diagonal})^2 = 2\,(\text{edge})^2$



Therefore,
Diag = √2 • (edge)

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Finding the Lattice Type

PROBLEM Al has density = 2.699 g/cm^3 and Al radius = 143 pm. Verify that Al is FCC.

SOLUTION

Here diagonal = 4 • radius of Al = 572 pm

Therefore, edge = 572 pm / √2 = 404 pm

In centimeters, edge = 4.04×10^{-8} cm

So, V of unit cell = $(4.04 \times 10^{-8}\text{ cm})^3$

V = 6.62×10^{-23} cm^3

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Finding the Lattice Type

PROBLEM Al has density = 2.699 g/cm³ and Al radius = 143 pm. Verify that Al is FCC.

SOLUTION

2. Use V and density to calc. mass of unit cell from DENS = MASS / VOL

Mass = density • volume

= $(6.62 \times 10^{-23}\ cm^3)(2.699\ g/cm^3)$

= 1.79×10^{-22} g/unit cell

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Finding the Lattice Type

PROBLEM Al has density = 2.699 g/cm³ and Al radius = 143 pm. Verify that Al is FCC.

SOLUTION

3. Calculate number of Al per unit cell from mass of unit cell.

$$\text{Mass 1 Al atom} = \frac{26.98\ g}{mol} \cdot \frac{1\ mol}{6.022 \times 10^{23}\ atoms}$$

1 atom = 4.480×10^{-23} g, so

$$\frac{1.79 \times 10^{-22}\ g}{\text{unit cell}} \cdot \frac{1\ \text{atom}}{4.480 \times 10^{-23}\ g} = 3.99\ \text{Al atoms/unit cell}$$

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Number of Atoms per Unit Cell

How can there be 4 atoms in a unit cell?

1. Each corner Al is 1/8 inside the unit cell.

   8 corners (1/8 Al per corner) = 1 net Al

2. Each face Al is 1/2 inside the cell

   6 faces (1/2 per face) = 3 net Al's