# *ORGANIZATION of PARTICLES* (Crystal Packing)

Models of Particle Organization
- Describe how the particles are arranged in physical space
- Based on a *unit cell* (the simplest structure that is repeated in the crystal).
- Can be applied to *any* group of particles but is mostly in reference to metals
- Helps explains differences in properties such as hardness and density
- Describes relative arrangement of layers
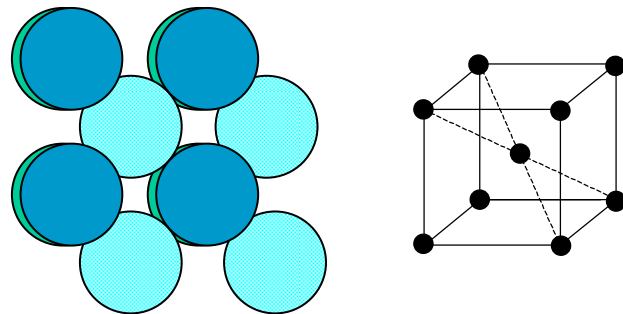
Simple Cubic Packing

- Particles are arranged in straight, neat layers
- Each layer oriented directly <u>above</u> lower layers.
- Leaves larges spaces between particles - found more in ionic crystals than metals
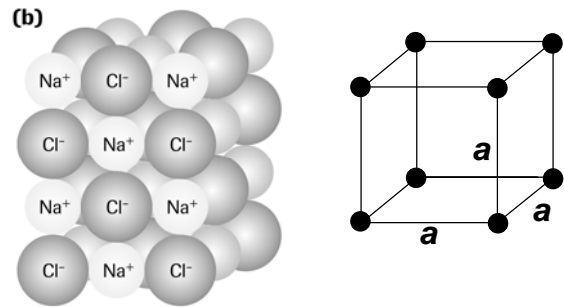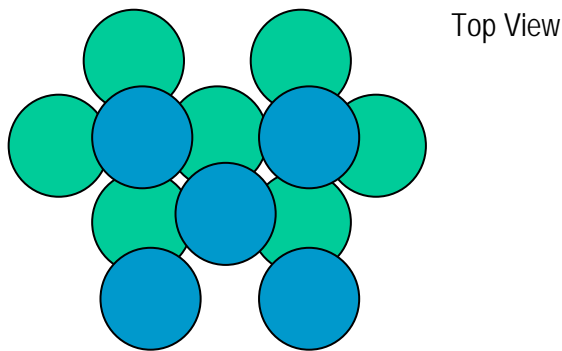
Body Centered Cubic Packing

Top View

- Organized, linear layers
- Each layer off-set from the above layers
- Arrangement is more compact.

Face-Centered Cubic Packing

- Layers are altered to bring particles closer
- Layers are stacked so particles fit in gaps (like body-centered)
- More compact than body-centered.

Top View

Metallic Bonding in the Solid State:

Metallic atoms have low electronegativities; therefore the electrons are delocalized over all the atoms. We can think of the structure of a metal as an arrangement of positive cores in a sea of electrons.

Metallic Sea of Electrons
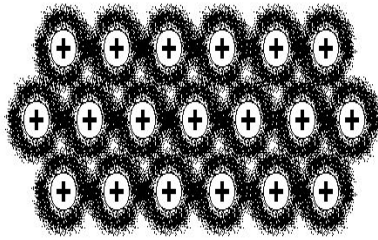
Electrons are not bonded to any particular atom
and are free to move about in the solid.

To maximize the bonding in a metal it makes sense to pack as many atoms around each other as possible, maximize the number of nearest neighbours (called the "coordination number") and minimize the volume.

Close packed layers of atoms.

If we treat the atoms as spheres and consider all the atoms in the solid to be of equal size (as is the case for elemental metals), the most efficient form of packing is the close packed layer. This is illustrated below where it is clear that close-packing of spheres is more efficient than, for example, square packing.

Below on the left is a square packed array compared to the more densely packed close packed array.
Within the square packed layer the coordination # of each atom is 4, in the close packed layer it is 6.
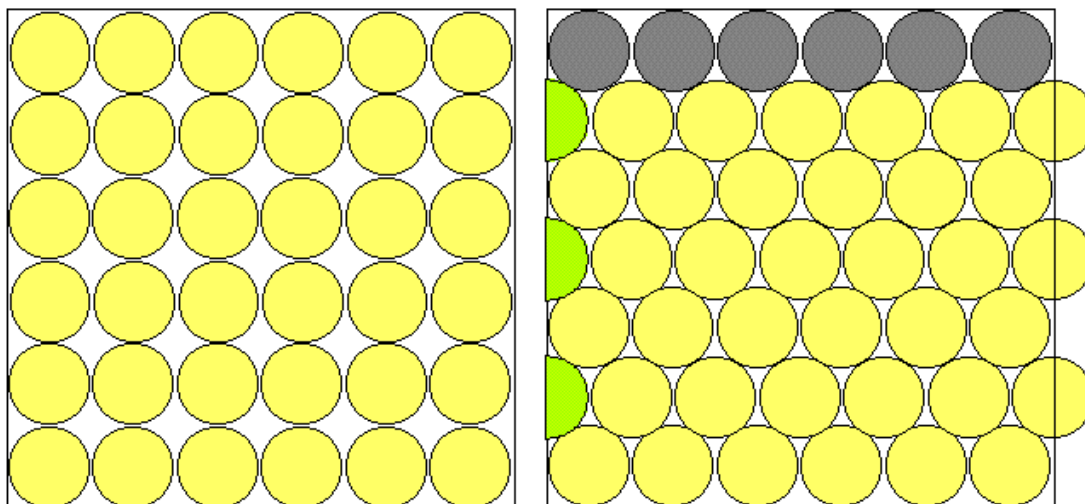
Close Packed Crystal Structures.

To build our 3-dimensional metal structures we now need to stack the close packed layers on top of each other. There are several ways of doing this. The most efficient space saving way is to have the spheres in one layer fit into the "holes" of the layer below.

If we call the first layer "A", then the second layer ("B") is positioned as shown on the left of the diagram below. The third layer can then be added in two ways. In the first way the third layer fits into the holes of the B layer such that the atoms lie above those in layer A. By repeating this arrangement one obtains **ABABAB... stacking or <u>hexagonal close packing</u>**.

1. # <u>Hexagonal Close Packing</u>. **(HCP)**
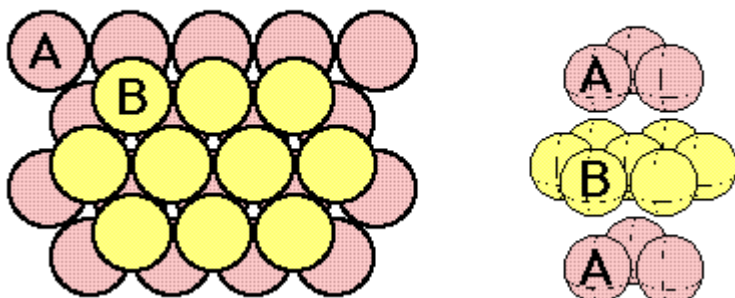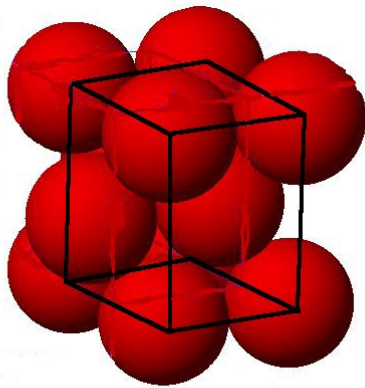
A more extended side view of the packing is shown below:
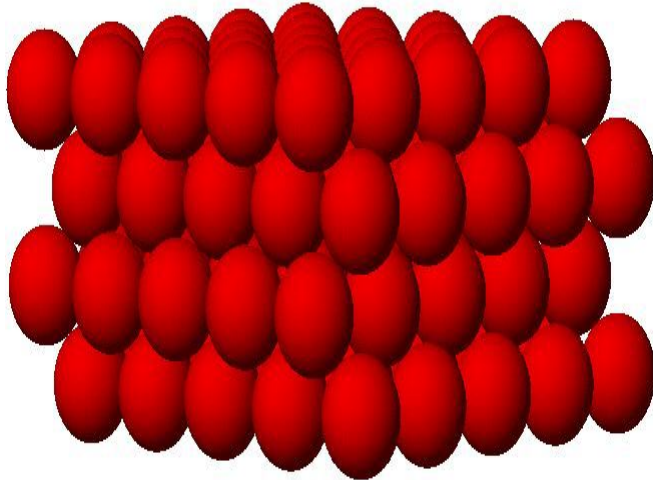
The {ABAB... } type stacking of close packed layers is called Hexagonal Close Packing (hcp) because the smallest lattice repeat is a **Primitive Hexagonal** unit cell.

In the primitive hexagonal cell we have 1 atom at each of the corners of the cell (each is "worth" 1/8) and 1 atom within the cell giving us 2 atoms/unit cell.
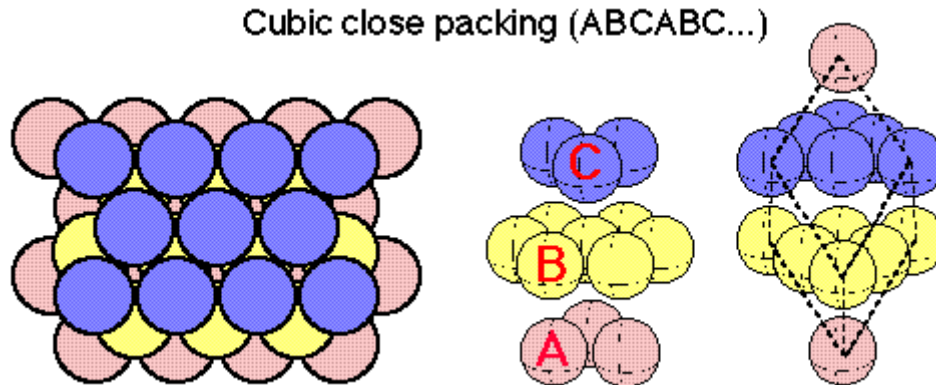
The coordination number of the atoms in this structure is 12. They have 6 nearest neighbours in the same close packed layer, 3 in the layer above and 3 in the layer below.

This is one of the most efficient methods of packing spheres (the other that is equally efficient is cubic close packing, see below). In both cases the spheres fill 74% of the available space.

HCP is a very common type of structure for elemental metals. Examples include Be, Mg, Ti, Zr, etc.

2. Cubic Close Packing (CCP)

While for the HCP structure the third close packed layer was positioned above the first , an alternate method of stacking is to place the third layer such that it lies in an unique position, in this way an "ABCABC..." close packed layer sequence can be created, see below. This method of stacking is call **Cubic Close Packing** (ccp)

Cubic close packing (ABCABC...)

The reason this is called cubic close packing is because the smallest unit cell that can describe this arrangement is **face centered cubic**. Two sides of the unit cell are apparent in the figure below.
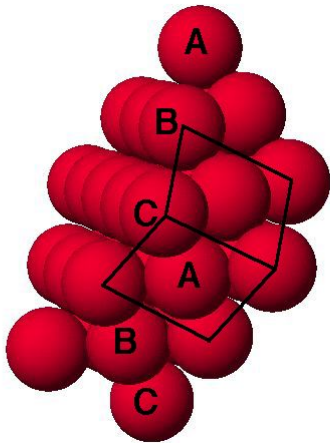
By reorienting the structure the entire face centered cubic cell and its contents are apparent.
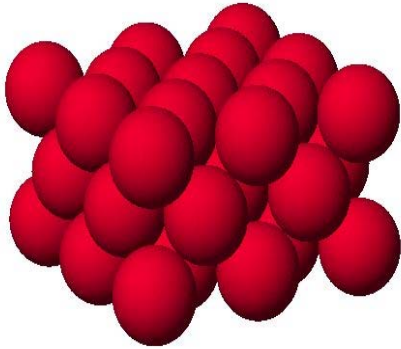
Because the ccp structure is still close packed it is as efficient in its packing as the hcp structure (74%), and the coordination number of the atoms is still 12.

How many atoms are there in the fcc unit cell ?
8 at the corners (8x1/8 = 1), 6 in the faces (6x1/2=3), giving a total of 4 per unit cell.
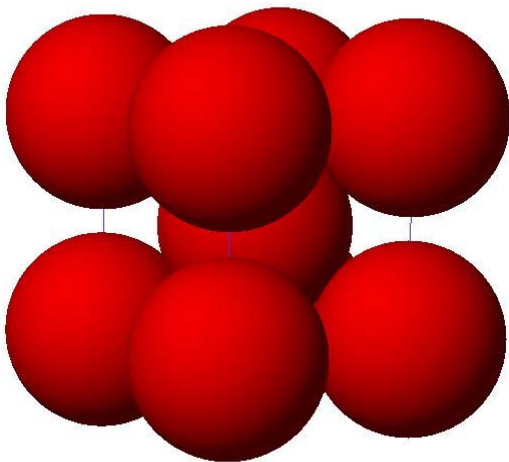
Again there are many examples of ccp (fcc) (ABCABC) metal structures, e.g. Al, Ni, Cu, Ag, Pt.

Other common types of metal structures
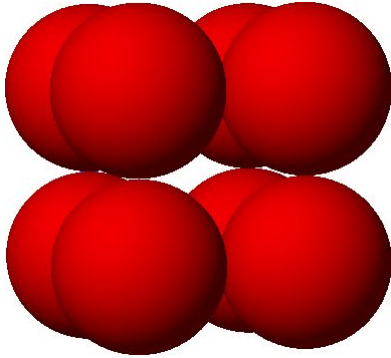
3. Body Centered Cubic (BCC)

Not close packed - atoms at corners and body center of cube. # atoms/unit cell = 2.
Coordination number = 8; less efficient packing (68%). The atoms are only in contact along the body diagonal.

Examples of BCC structures include one form of Fe, V, Cr, Mo, W.
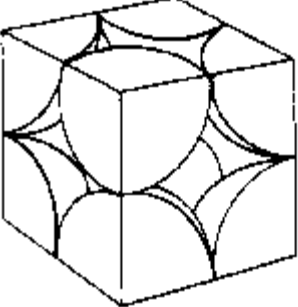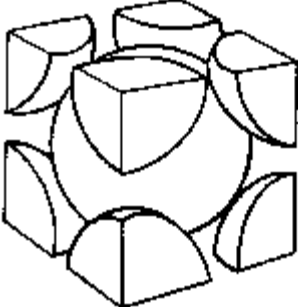
4. <u>Simple Cubic</u>

Again not close packed - primitive or simple cubic cell with atoms only at the corners. # atoms/unit cell = 1.
Coordination number = 6; least efficient method of packing (52%)
The atoms are in contact along the cell edge.
A very rare packing arrangement for metals, one example is a form of Polonium (Po)

Summary of Packing types for Metallic Structures.

Type of Packing	Packing Efficiency	Coordination Number
Simple cubic (sc)	52%	6
Body-centered cubic (bcc)	68%	8
Hexagonal close-packed (hcp)	74%	12
Cubic close-packed (ccp or fcc)	74%	12