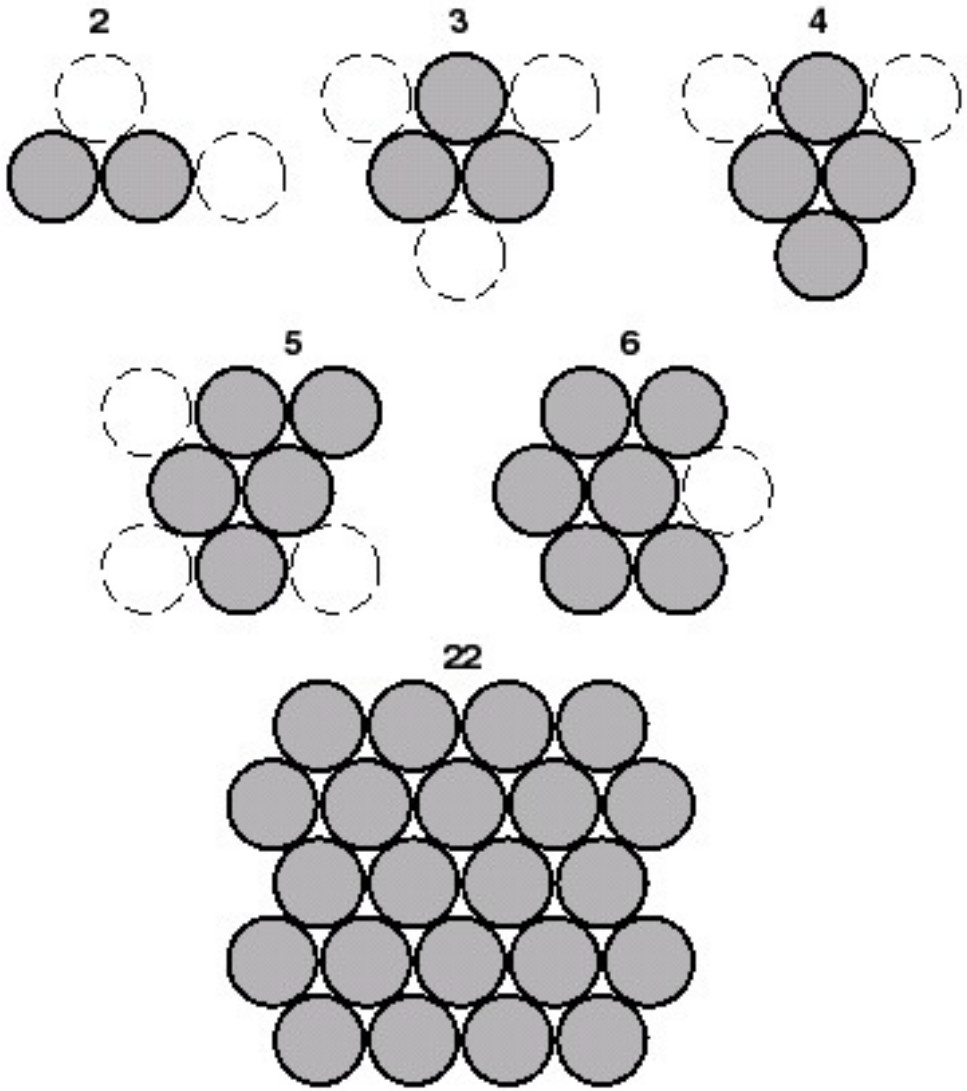
N&BM 03-06: Building Crystals by Packing Atoms (1)



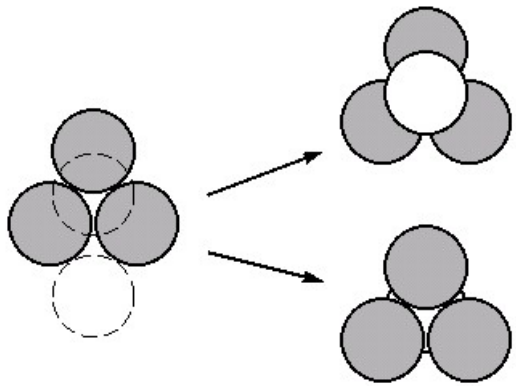
To build a metal crystal, think of the atoms as spheres with a well-defined radius (billiard balls) and mutual attraction.

Build the structure with the lowest possible energy.

That means: Make each sphere touch as many other spheres as possible.

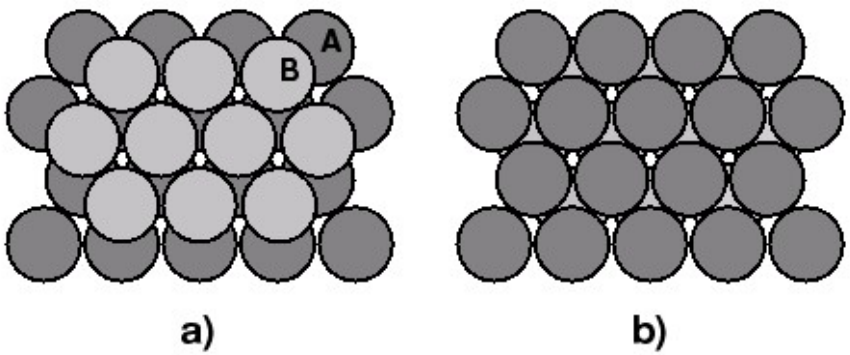
In 2D, the best configuration is a hexagonal array.

N&BM 03-07: Building Crystals by Packing Atoms (2)



What if we allow for packing in 3D ?

The best place for the fourth atom is on top or at the bottom of the first three. In either case, the four atoms form a tetrahedron.

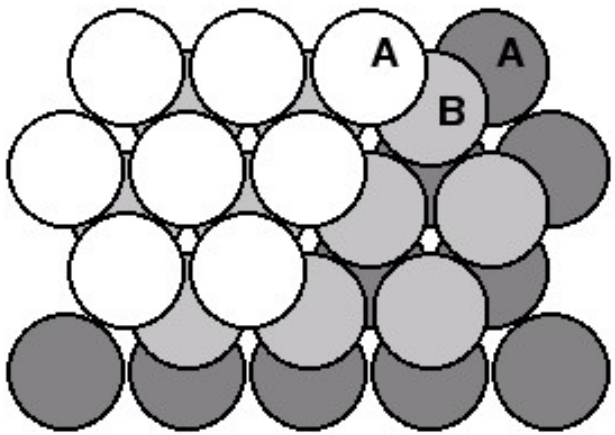


For a larger number of atoms, the best arrangement is two hexagonal layers stacked on top of each other: B on top of A, or A on top of B.

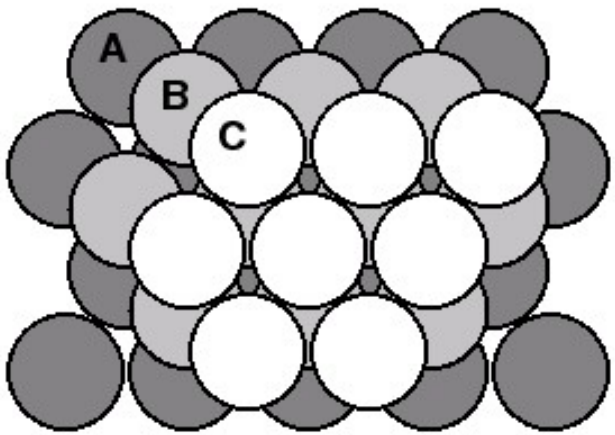
N&BM 03-08: Building Crystals by Packing Atoms (3)

What about **three layers** ?

If you have two stacked layers AB, then there are two different ways of putting on the third layer !



ABABAB



ABCABC

The layers can repeat themselves as ABABAB .. or ABCABC ..

N&BM 03-09: Building Crystals by Packing Atoms (4)

Both types of stacking achieve **close-packing**, and we will call the resulting structures **close-packed**.

Close-packing maximizes the number of nearest neighbors for an atom. In both cases this is **12 nearest neighbors**.

The two structures have special names:

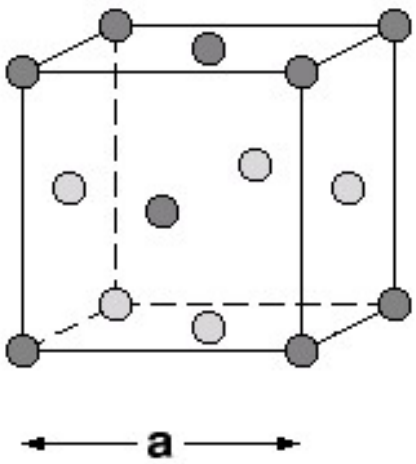
ABABAB	<=>	hexagonal close-packed
ABCABC	<=>	cubic close-packed

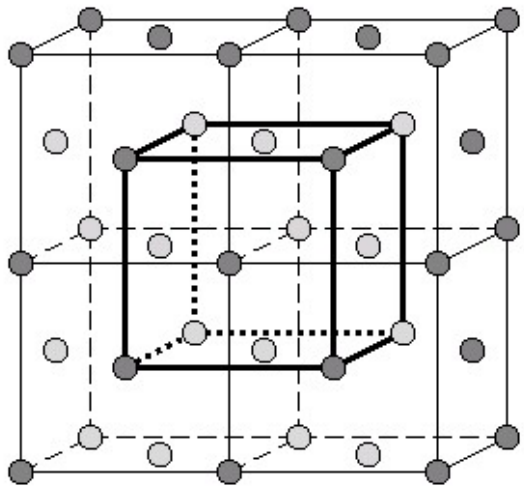
The first name should be evident. The second name will become clear shortly.

N&BM 03-10: Structure of Metals (1)

1. Face-centered Cubic Structure (FCC)

Examples of materials having this structures are: Al, Cu, Ni, Pd, Ag, Au.





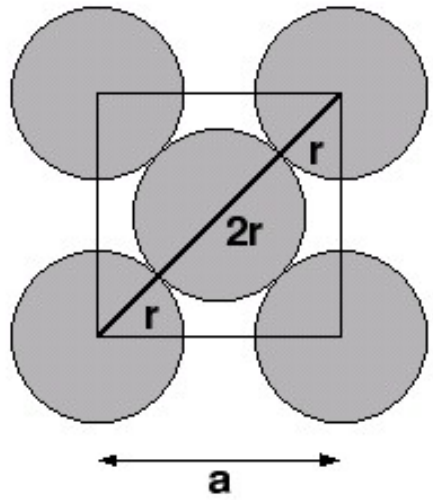
Note:
All atoms are the same. Different colors are used for clarity.
All atoms are equivalent: Corners and centers of the faces of the **unit cell**, in this case the unit cube, are interchangeable.
The size, or length of the unit cube is called **lattice constant a**.

N&BM 03-11: Structure of Metals (2)

Properties of the FCC structure:

1) The number of nearest neighbors, also know as the **coordination number**, is equal to 12 (see the big cube before).

2) Atoms touch along the face diagonal of the unit cube:



Therefore one has:

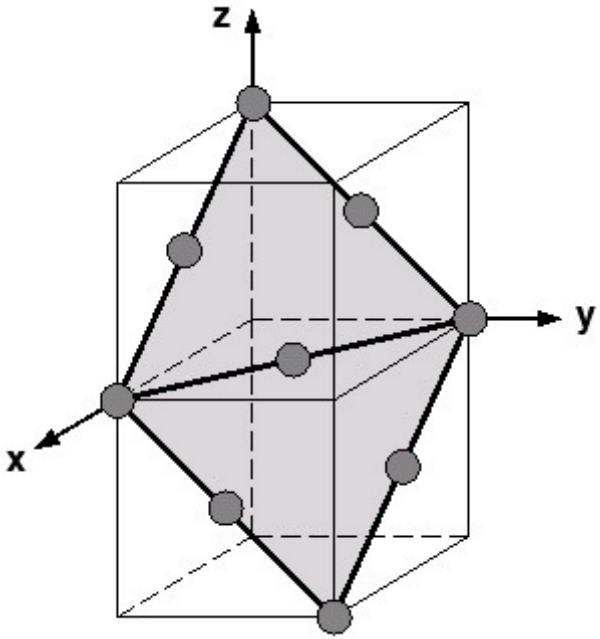
$$a = 2\sqrt{2} \times r$$

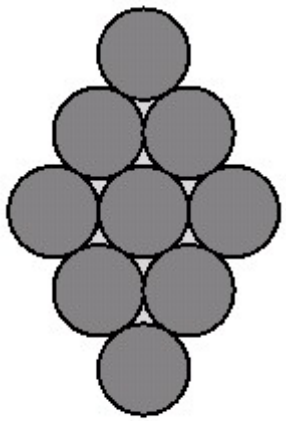
3) The **atomic packing factor APF** is defined as the fraction of the cube volume occupied by atoms:

$$APF = \frac{\frac{4}{3}\pi r^3 \times 4}{a^3} \quad \text{or} \quad APF(\text{FCC}) = \frac{\pi}{3\sqrt{2}} = 0.74$$

N&BM 03-12: Structure of Metals (3)

But what about close-packing ?





Consider two FCC cubes cut along a diagonal plane as shown:

The atoms on this plane form a hexagonal array !

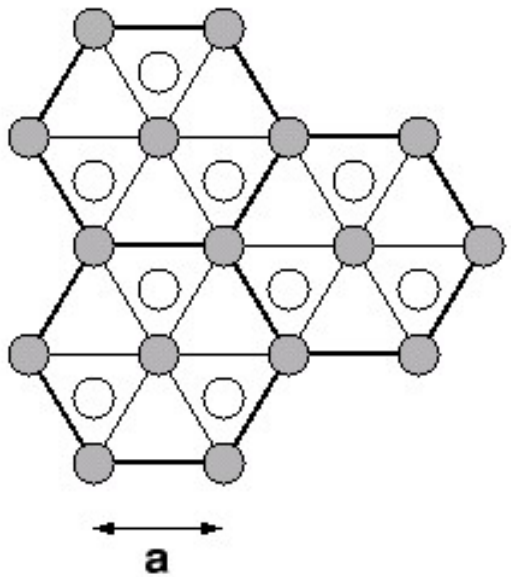
We may conclude:

face-centered cubic = cubic close-packed

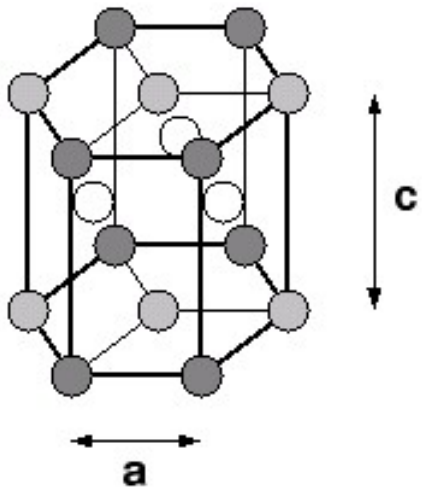
Convince yourself that these kinds of planes are stacked ABCABC.

2. Hexagonal Close-packed Structure (HCP)

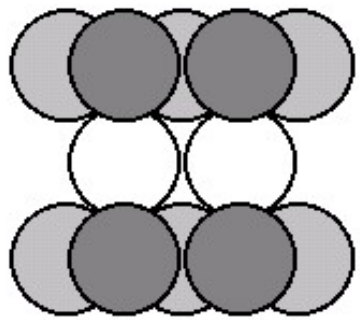
Examples of materials having this structures are: Be, Mg, Ti, Co, Zn, Zr.



Top view (3 unit cells)



Perspective view



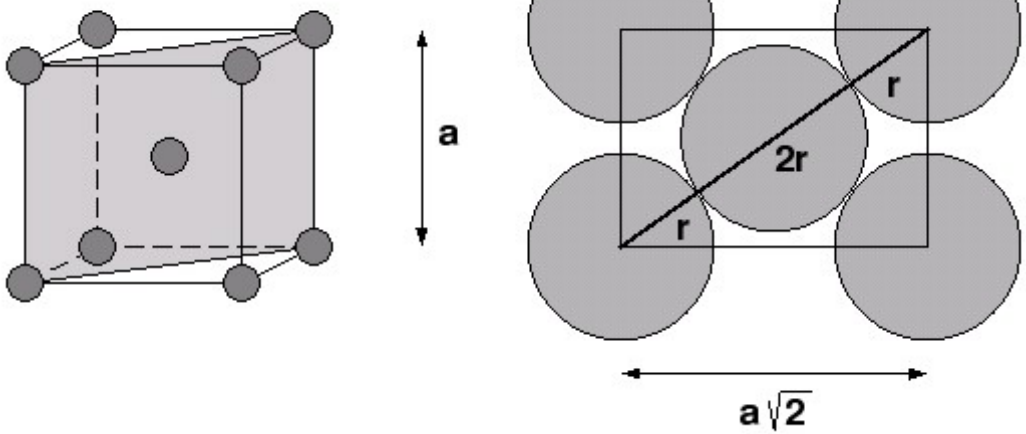
Side view

This structure is non-cubic: It requires two dimensions, a and c, to characterize the unit cell.

The coordination number is 12 and the *APF* (HCP) is 0.74, as for FCC.

3. Body-centered Cubic Structure (BCC)

Examples of materials having this structures are: Li, Na, K, Fe, Cr, Mo, W.



The number of nearest neighbors is 8.

Atoms touch along the body diagonal of the cube. Hence

$$a = 2\sqrt{3} \times r$$

From this follows:

$$APF = \frac{\frac{4}{3}\pi r^3 \times 2}{a^3} = 0.68$$

N&BM 03-15: Structure of Metals (6)

Summary of the properties of metal crystals:

Crystal	Coord. Number	APF
FCC	12	0.74
HCP	12	0.74
BCC	8	0.68

A lower coordination number for BCC goes along with a lower APF.

If the goal is close packing, why is there a difference between FCC and HCP, and why is there BCC ?