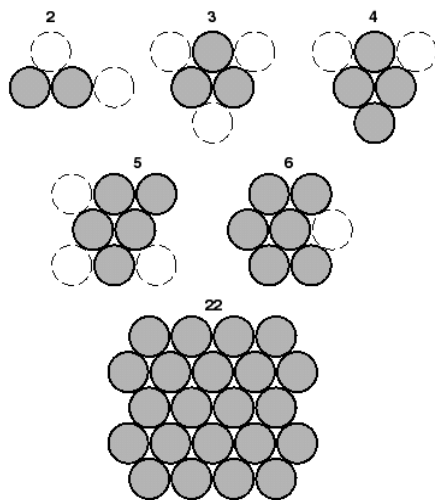


## N&BM 03-06: Building Crystals by Packing Atoms (1)



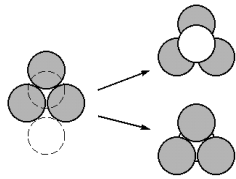
To build a metal crystal, think of the atoms as spheres with a well-defined radius (billiard balls) and mutual attraction.

Build the structure with the lowest possible energy.

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

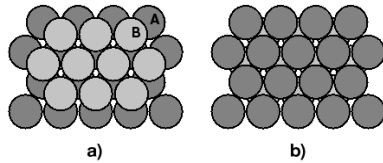
In 2D, the best configuration is a hexagonal array.

## 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.



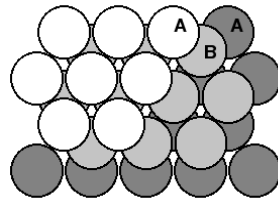
For a larger number of atoms, the best arrangement is two hexagonal layers stacked on top of each other: B on top of A, or A on top of B.

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

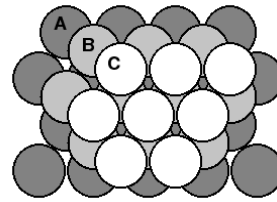


What about **three layers** ?

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:

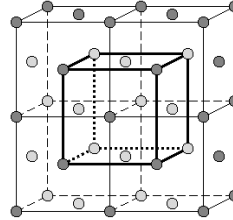
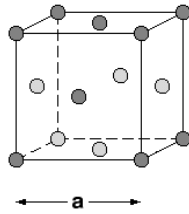
ABABAB	<=>	hexagonal close-packed
ABCABC	<=>	cubic close-packed

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)

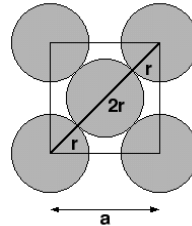
Properties of the FCC structure:

1) The number of nearest neighbors, also known 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:

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

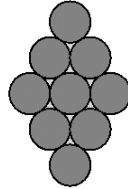
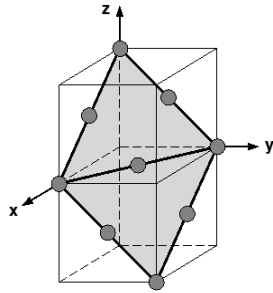


3) The **atomic packing factor APF** is defined as the fraction of the cube volume occupied by atoms:

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

## 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:

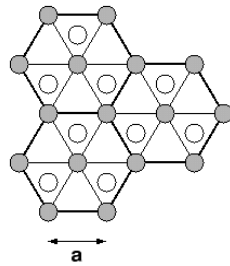
face-centered cubic = cubic close-packed

Convince yourself that these kinds of planes are stacked ABCABC.

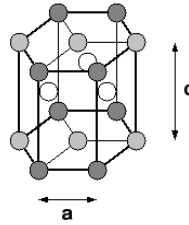
## N&BM 03-13: Structure of Metals (4)

### 2. Hexagonal Close-packed Structure (HCP)

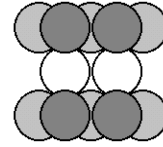
Examples of materials having this structures are: Be, Mg, Ti, Co, Zn, Zr.



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.

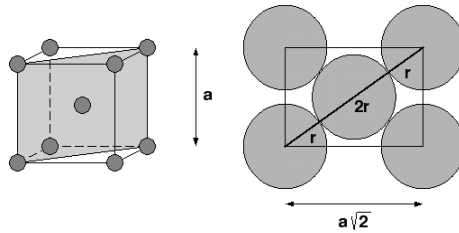
The coordination number is 12 and the  $APF$  (HCP) is 0.74, as for FCC.



## N&BM 03-14: Structure of Metals (5)

### 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:

<b>Crystal</b>	<b>Coord. Number</b>	<b>APF</b>
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 ?