Chapter 8 The structures and properties of metals and alloys

8.1 The metallic bond and the general properties of metals

8.1.1 The “free-electron” model of the metallic bond

The Schrödinger equation for the “free electrons” is

$$\nabla^2\psi + [8\pi^2 m]/h^2]E\psi=0$$

V=0

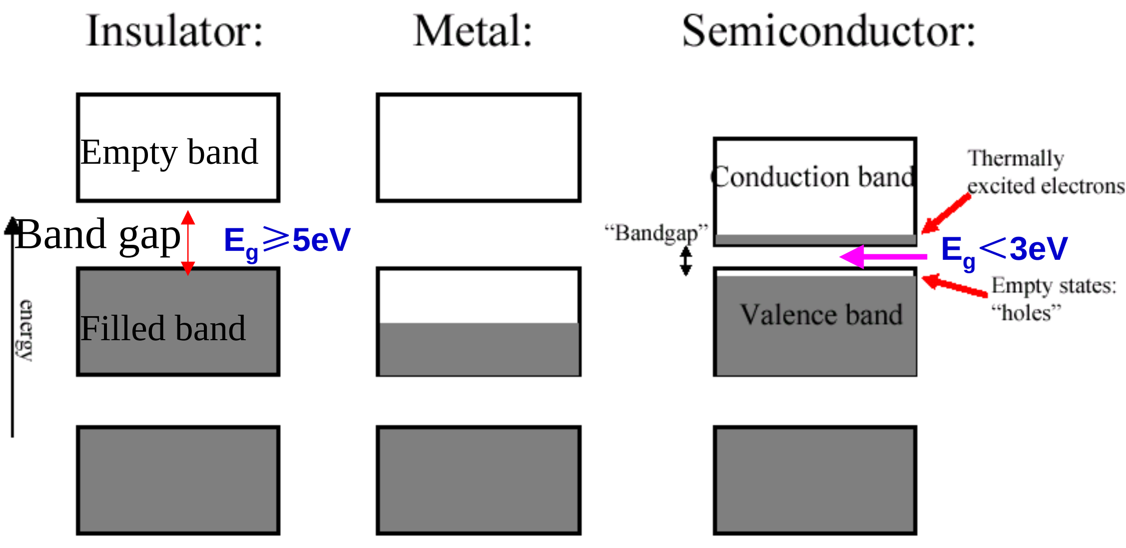
$E_F = 5.04*10^{-19}$ J or 3.15eV (for Na)

Experimental value 3.2 eV

8.1.2 The band theory of solids

Considering the electrons in metals moving in a periodic potential field of the metal atoms, the Schrodinger equation is

$$(-h^2/[8\pi^2 m]\ \nabla^2 + V)\ \psi = E\psi$$



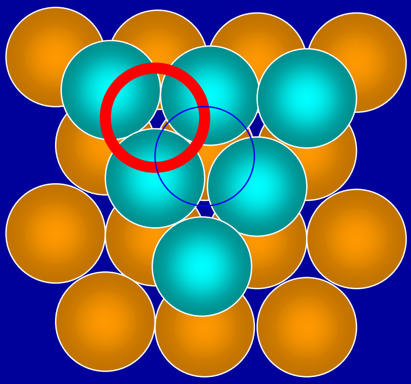
Partially filled bands ---- conduction bands

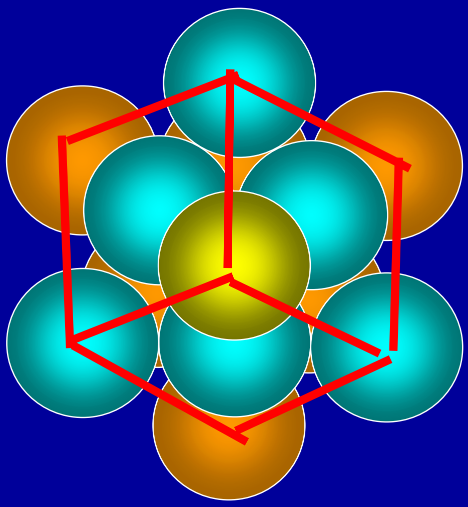
8.2 Close packing of spheres and the structure of pure metals

8.2.1 packing of indentical spheres

1. Cubic close packing ccp, ABCABC

Type A1





ccp or *fcc*

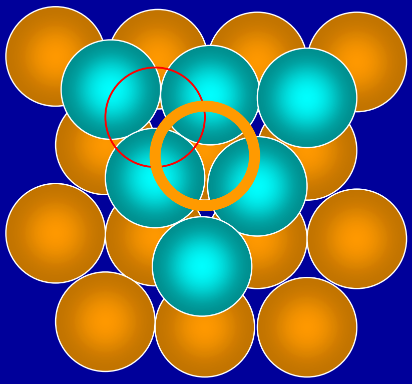
Cubic close packing, faced centered cubic

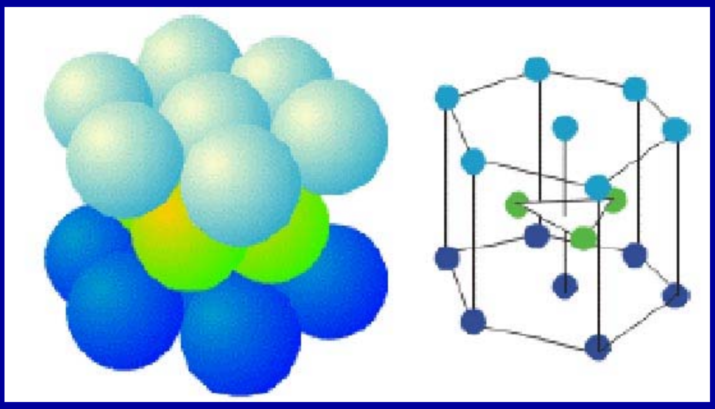
---

2. Hexagonal close packing hcp ABAB

Type A3

(The two most common close-packed structure)





hcp

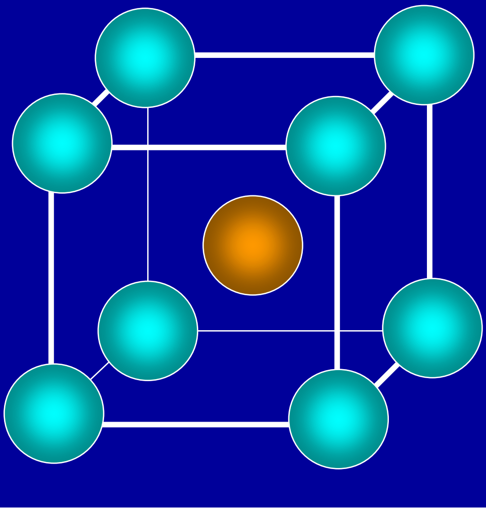
hexagonal close packing

3. Other types of close-packed structure:

ABAC…..

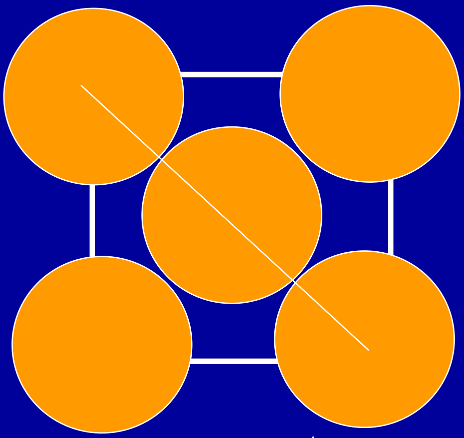
ABABCBCAC……..

4. Body-centred cubic packing (bcp or bcc) A2



8.2.2 Packing density

ccp packing---fcc



a=(4R)/√2 = 2√2R

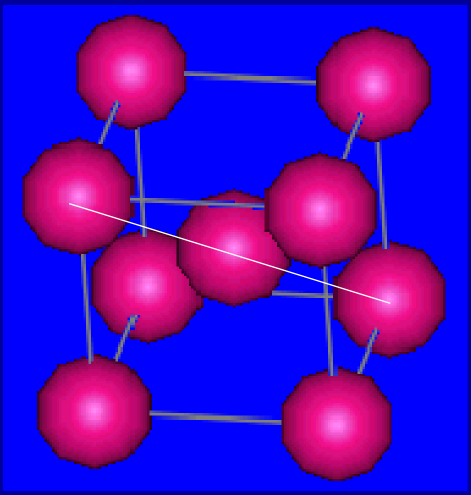
The volume of the unit cell : $V_{\text{unit cell}} = a^3 = 16\sqrt{2}R^3$

The total volume of the four spheres in the unit cell: $V_{\text{sphere}} = 4 (4/3) \pi R^3$

Packing coefficient = $V_{\text{sphere}} / V_{\text{unit cell}} = ((16/3) \pi R^3) / (16\sqrt{2}R^3) = 0.7405$

Close packing of identical spheres gives the same packing density. (74.05%)

Body-centred cubic packing (bcp or bcc)



$\sqrt{3}a=4r$

packing coefficient =

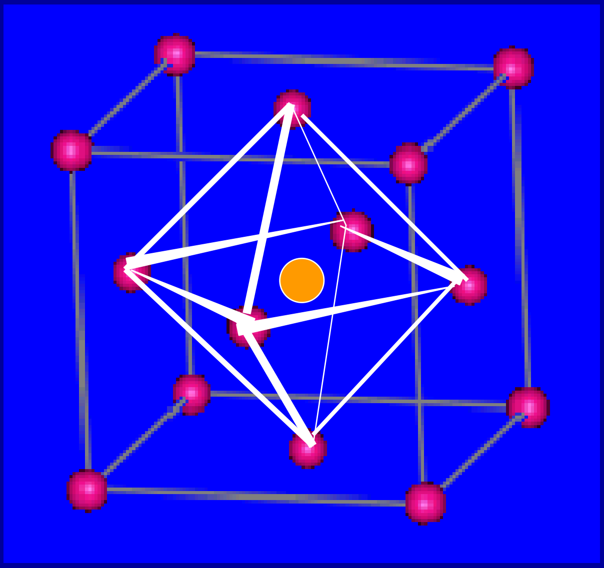
$$\frac{2 \times (4/3)\pi r^3}{a^3}$$

=68%

Is not a close-packed structure. The packing coefficient is 0.6802

8.2.3 Interstices

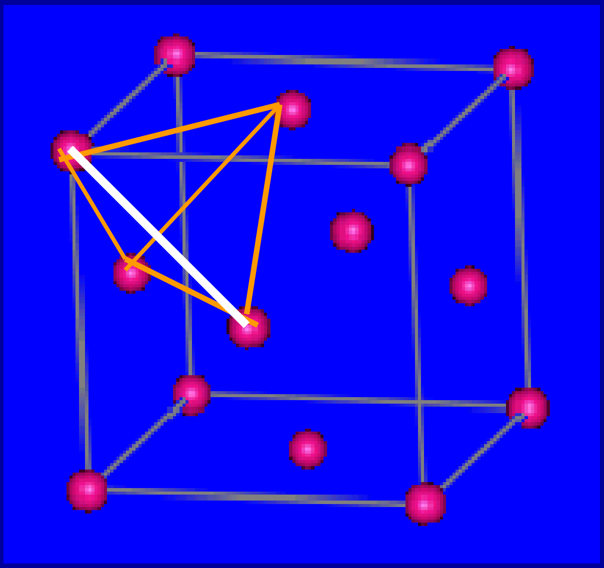
octahedral holes



$\sqrt{2}R-R = 0.414\ R$

For a close-packed structure formed from N spheres of radius R, the hole size is 0.414R.

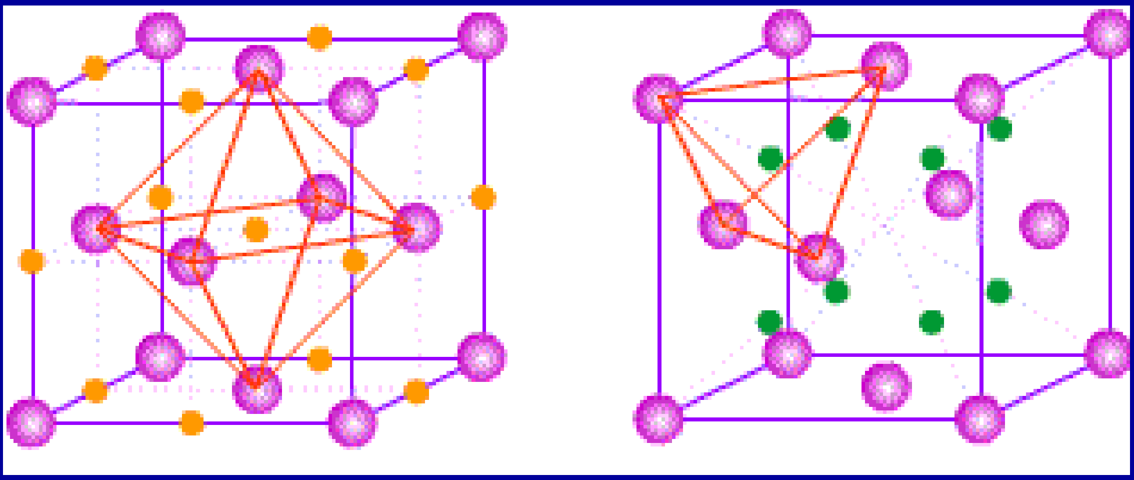
tetrahedral holes



For a close-packed structure formed from N spheres of radius R, the hole size is 0.225R.

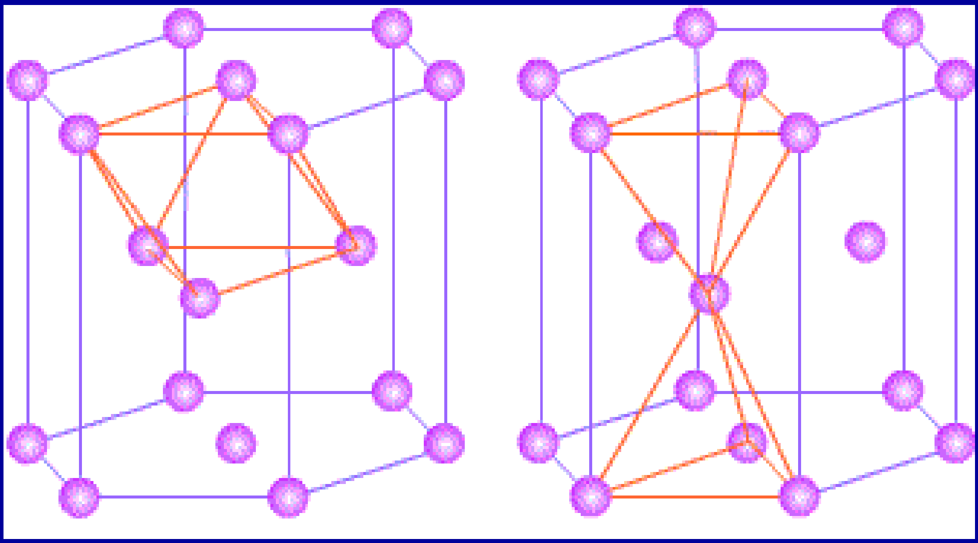
---

ccp (fcc) structure

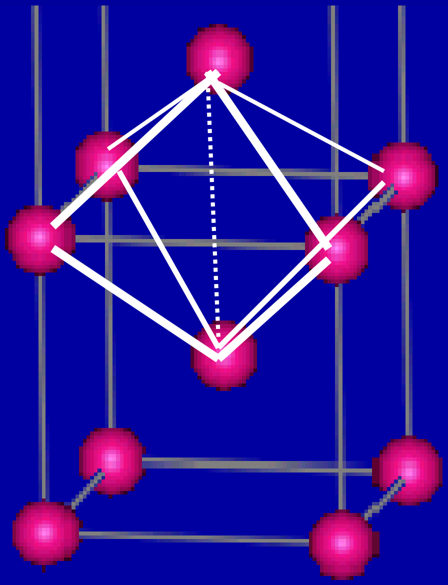


It contains N octahedral holes and 2N tetrahedral holes

hcp structure



Interstices in bcp structure



There are 3 octahedral holes.

The holes are not regular octahedra but are compressed.

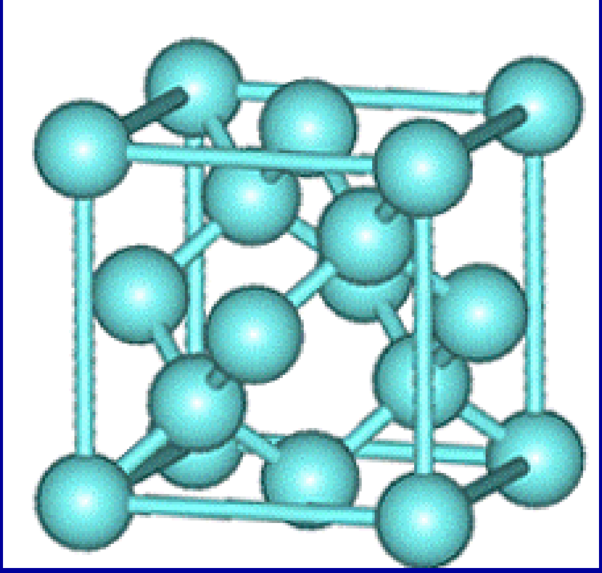
r/R = 0.154

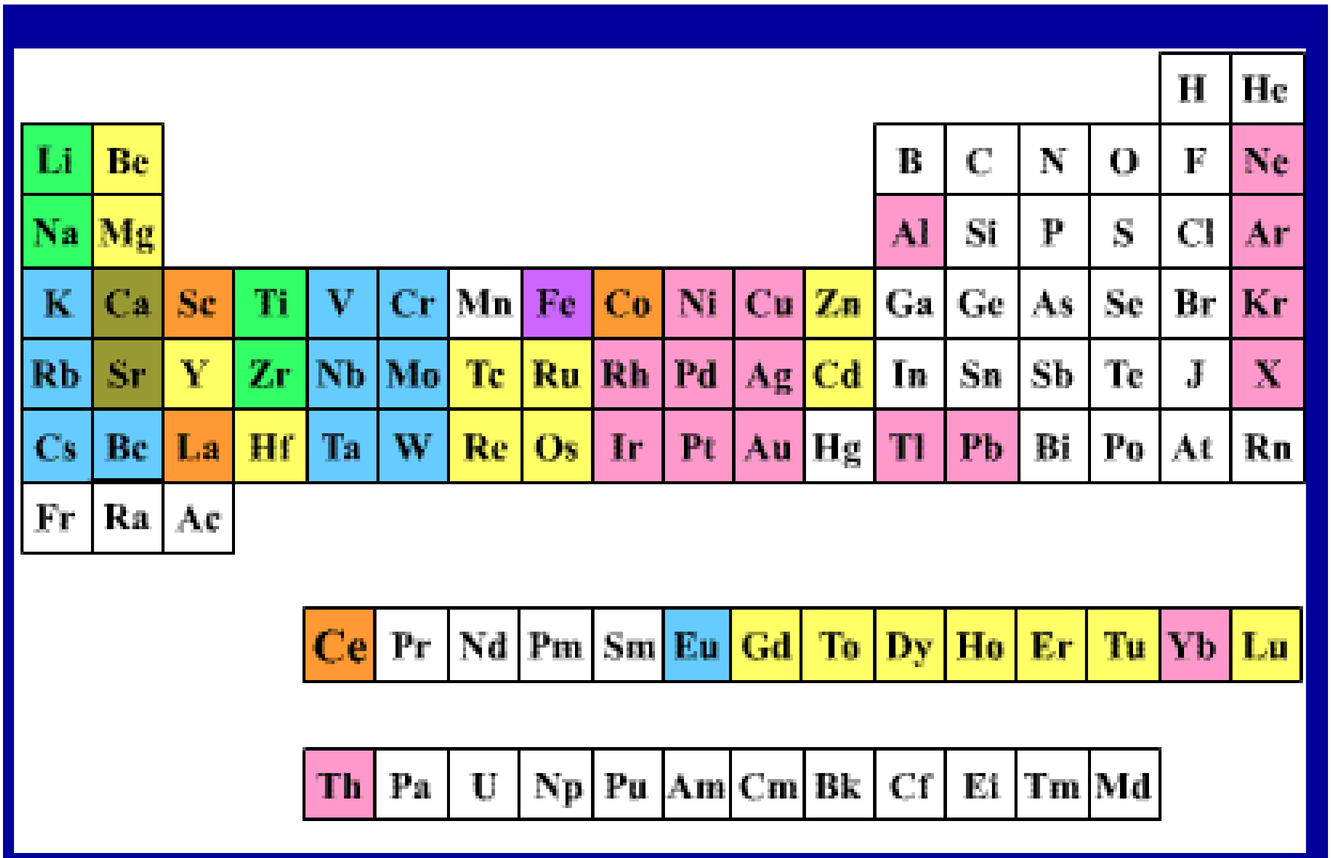
There are 6 tetrahedral holes and 12 trigonal holes.

8.2.4 A structural survey of pure metals

A1, A2, A3

A4 (The diamond structure)





																H	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	J	X
Cs	Be	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															
				Ce	Pr	Nd	Pm	Sm	Eu	Gd	To	Dy	Ho	Er	Tu	Yb	Lu
				Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Ei	Tm	Md		

bcp fcc hcp

The number of electrons in the s and p orbital affects the type of structure:

When the average number of s and p electrons for each atoms

is small, type A2 is preferred Na [Ne]$3s^1$

is large A1 is preferred Al $3s^23p^1$

is intermediate value, A3 is preferred Mg $3s^2$

8.2.5 Atomic radii of metals

(1) Within a family, the atomic radius increases as the atomic number increases.

(2) Within the same period, the atomic radius decreases as the atomic number increases

(3) For transition metals within the same period, the atomic radius first decreases steadily and then increase slightly.

(4) “lanthanide contraction” effect

8.3 The structures and properties of alloys

Alloy is the product of two and more metal.

Alloys may be divided into three major categories:

Metallic solid solution

Metallic compounds

Metallic interstitial compounds

8.3.1 The structure of metallic solid solutions

- The structure of a bimetallic solid solution is usually similar to the metals except that fraction of the atoms of one metal is statistically substituted by the atoms of another metal.
- The tendency to form a solid solution depends on :

(1) The positions in the periodic table and the similarity in chemical as well as physical properties.

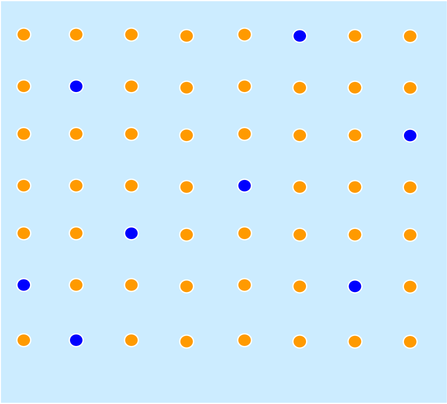
(2) the similarity in atomic radii

(3) the structural type of the pure metals.

ccp: Cu, Ag, Au, Ni, β-Co, γ-Fe, Pt, Ir, Rh, Pd

bcp: α-Fe, V, Cr

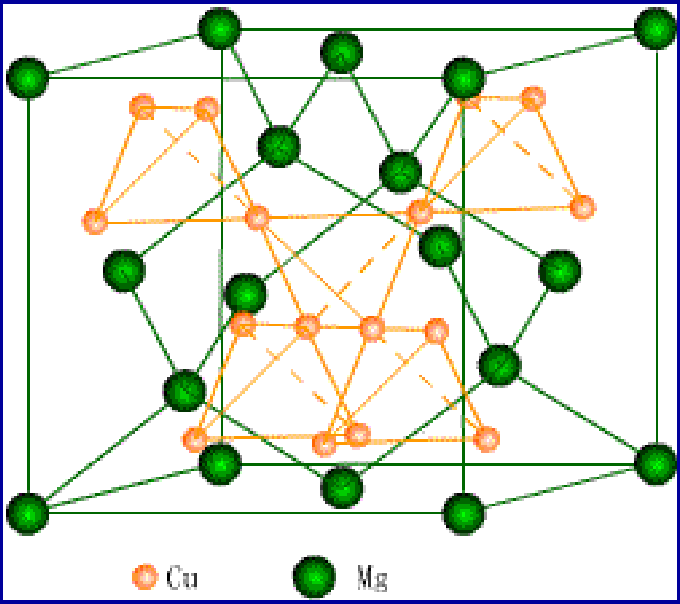
bcp: Mo, W



8.3.2 The structure of metallic compounds

The stoichiometric phase

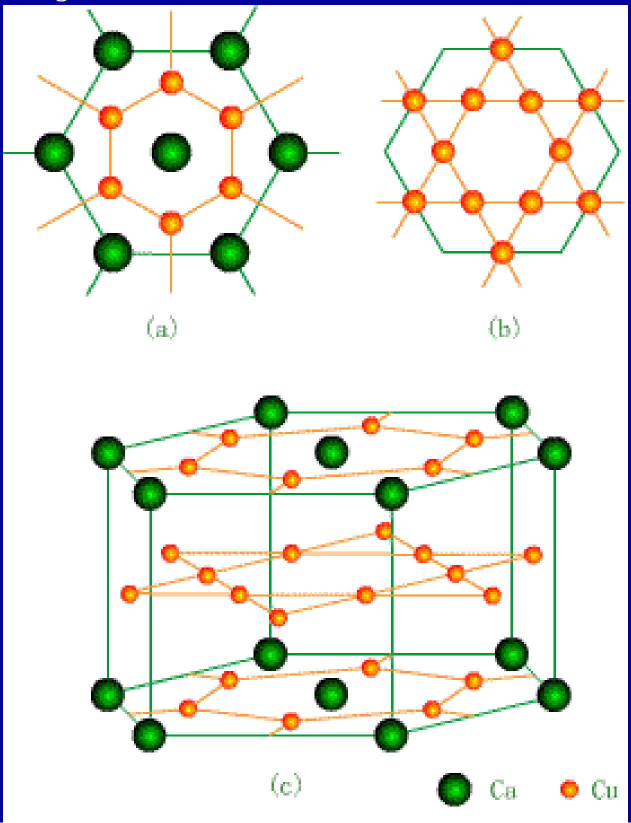
1. The structure of the alloy $MgCu_2$



---

2. The structure of the alloy $CaCu_5$

Many alloys which act as reservoirs for hydrogen such as LaNi5, LaCo5 and CeCo5 have the same structure as CaCu5.



8.3.3 The structure of interstitial metallic compounds

The term interstitial compound is given to compounds of metals with B, C, N, etc..

•The salient characteristics of interstitial compounds are:

(1) Most interstitial compounds adopt the NaCl structure irrespective of the original structure of the pure metals.

(2) These compounds are very hard and melt at very high temperatures.

(3) They have good conductivity metallic cluster and all other properties of alloys.

- The structure and properties of steel

Steel is an alloy system consisting of iron and carbon and is a basic industrial material.

Iron that contains less than 0.02% C is known as pure iron, with more than 2.0% C pig iron or cast iron, and with intermediate concentration between these two limits steel.

Pure iron: A2 (bcp) structure α-Fe (room temperature)

A1 (fcc) structure γ -Fe (910°C)

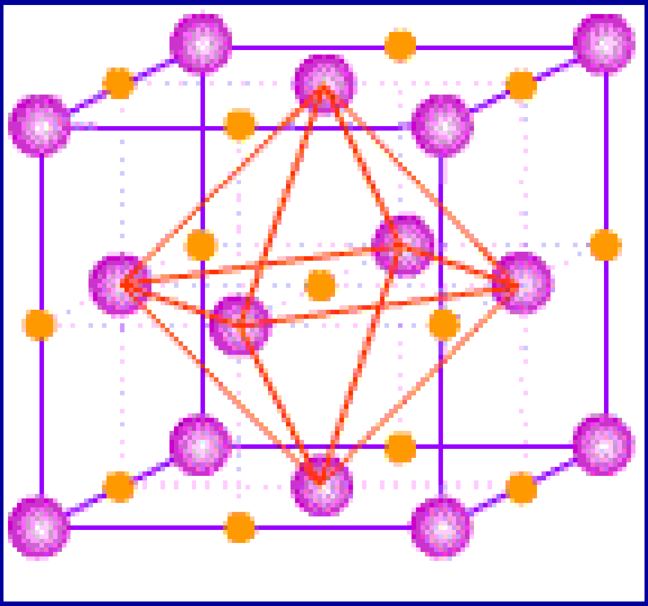
(bcp) structure δ-Fe (1390 °C)

melting point 1535 °C

Iron is ferromagnetic below 760 °C and non-ferromagnetic above this temperature.

a. Austenite: an interstitial solid solution of C in γ-Fe (about 0.8% by weight)

The C atoms are distributed randomly at the octahedral positions . There is one C atom in every six or seven fcc unit cells.

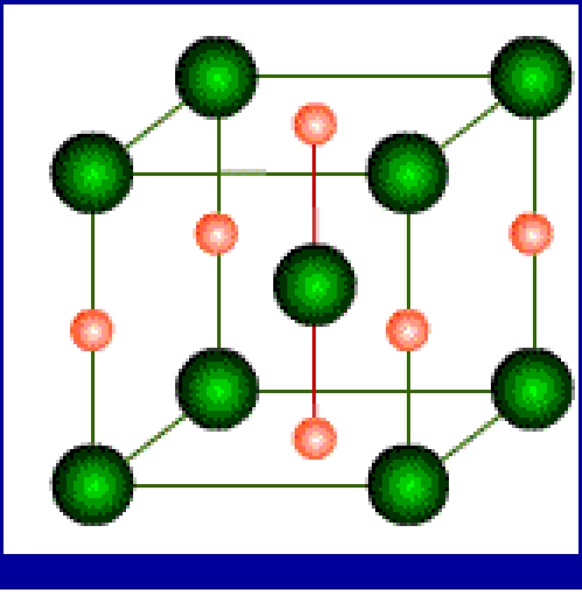


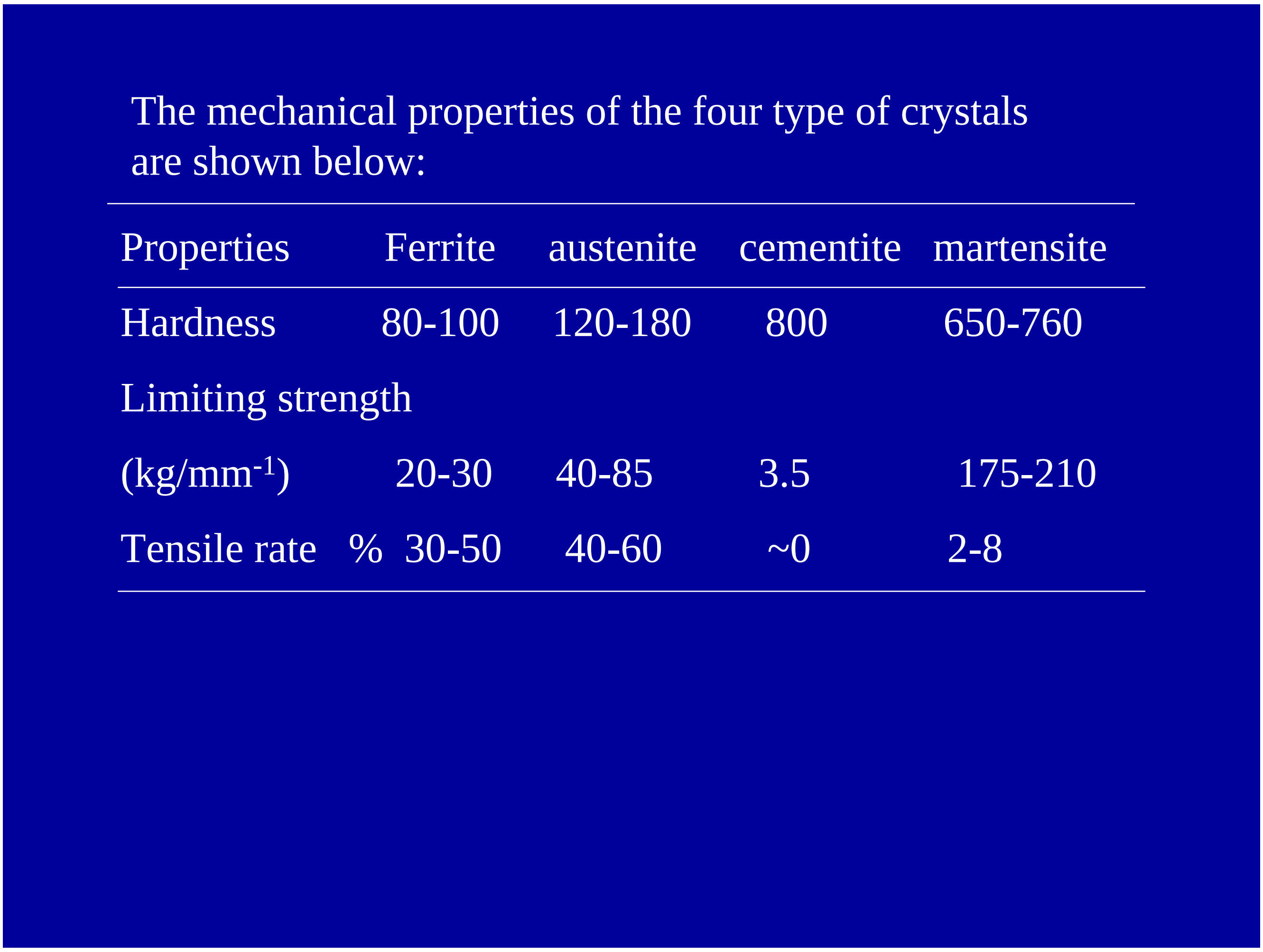
---

b. Ferrite: a solid solution of C in α-Fe. Since the size of the octahedral holes in is very small in α-Fe, the solubility is very low (the highest solubility is 0.02%)

c. Cementite: Fe_3C (6.67%)

d. Martensite: a supersaturated solid solution of C in in α-Fe.





The mechanical properties of the four type of crystals are shown below:

Properties	Ferrite	austenite	cementite	martensite
Hardness	80-100	120-180	800	650-760
Limiting strength (kg/mm^{-1})	20-30	40-85	3.5	175-210
Tensile rate %	30-50	40-60	~0	2-8