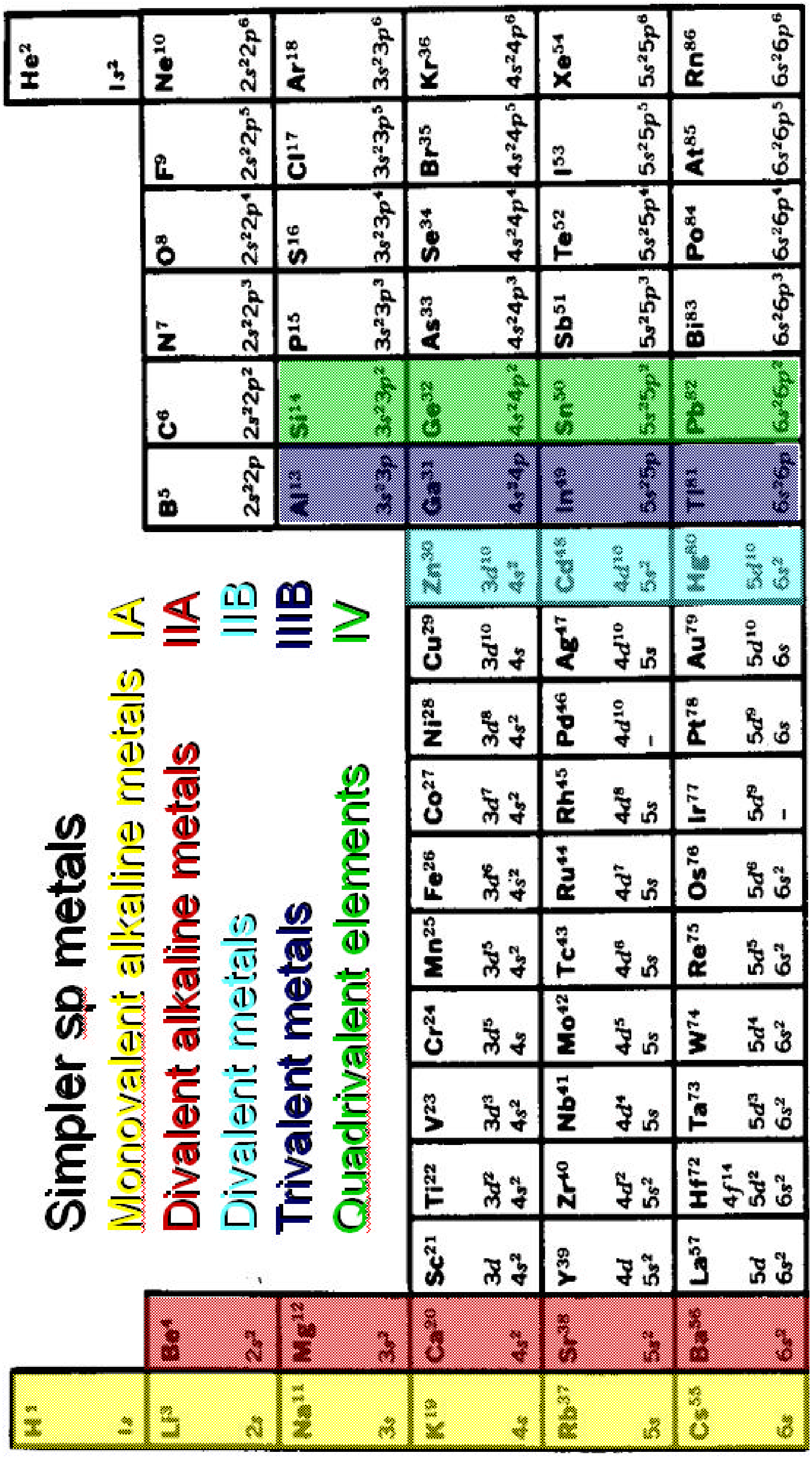
Band structure of various metals



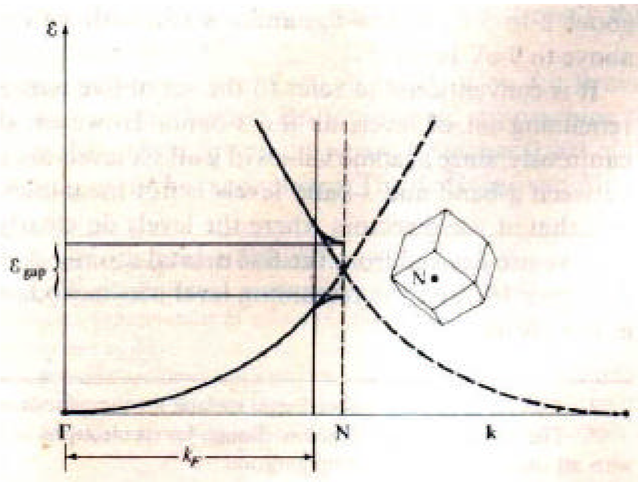
From the lecture notes of Prof. R. Cywinski (Univ. of Leeds)

(1) Monovalent metals (NFE model good)

THE MONOVALENT METALS

ALKALI METALS (BODY-CENTERED CUBIC)[a]		NOBLE METALS (FACE-CENTERED CUBIC)	
Li:	$1s^2 2s^1$		—
Na:	$[Ne]3s^1$		—
K:	$[Ar]4s^1$	Cu:	$[Ar]3d^{10}4s^1$
Rb:	$[Kr]5s^1$	Ag:	$[Kr]4d^{10}5s^1$
Cs:	$[Xe]6s^1$	Au:	$[Xe]4f^{14}5d^{10}6s^1$

Alkali metals (Li, Na, K, Rb, Cs)



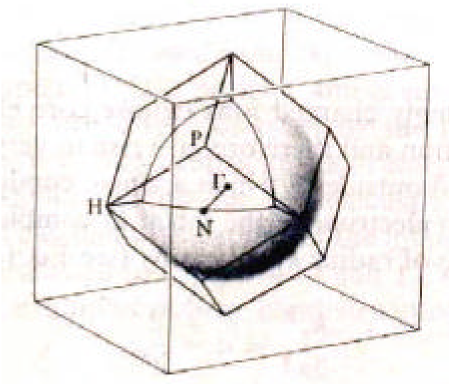
$$\begin{cases} k_F = (3\pi^2 n)^{1/3}, \\ n = 2/a^3 \end{cases}$$

$\rightarrow k_F = (3/4\pi)^{1/3}(2\pi/a)$

$\Gamma N = (2\pi/a)[(1/2)^2 + (1/2)^2]^{1/2}$

$\therefore k_F = 0.877\,\Gamma N$

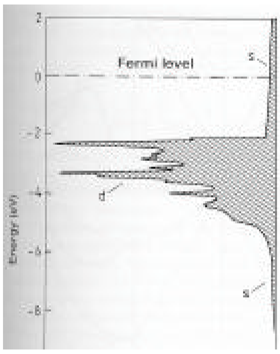
First BZ (of a bcc lattice) and the Fermi sphere

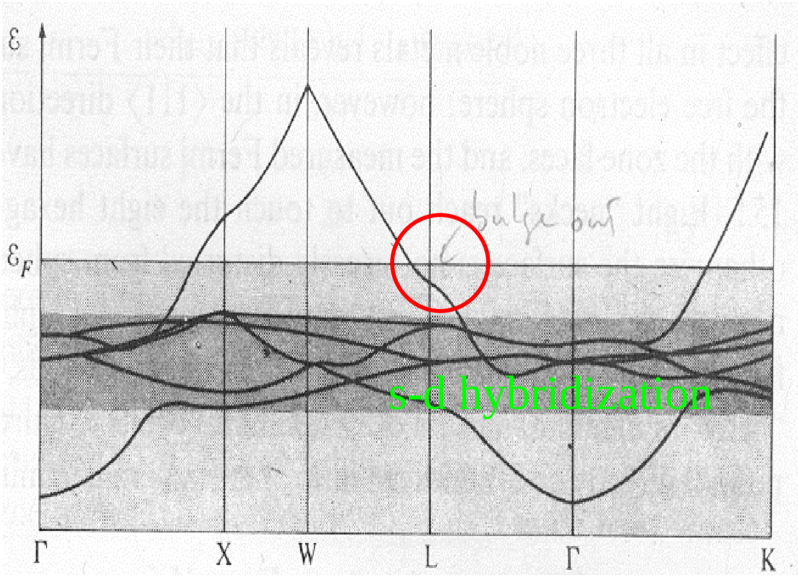


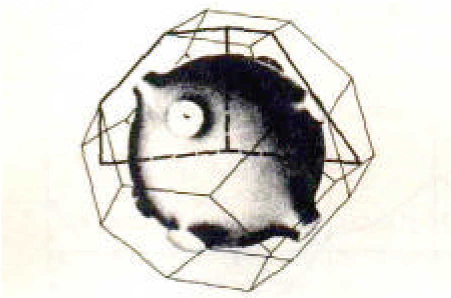
$4\pi/a$

Nobel metals (Cu, Ag, Au)

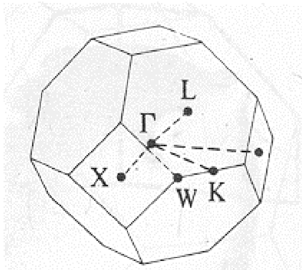
DOS of Cu

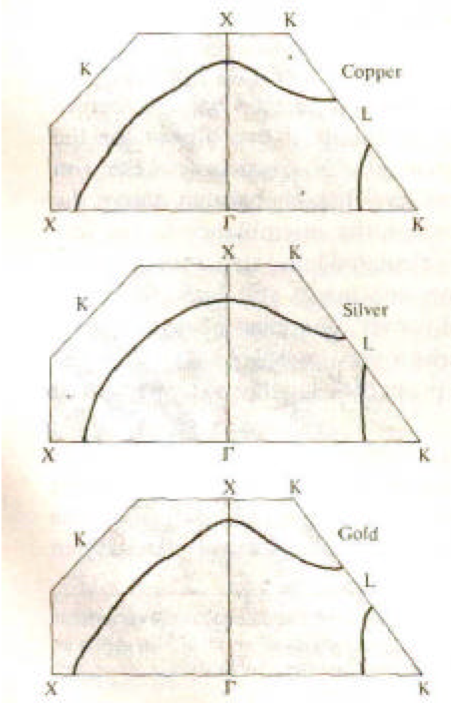






(a)





(b)

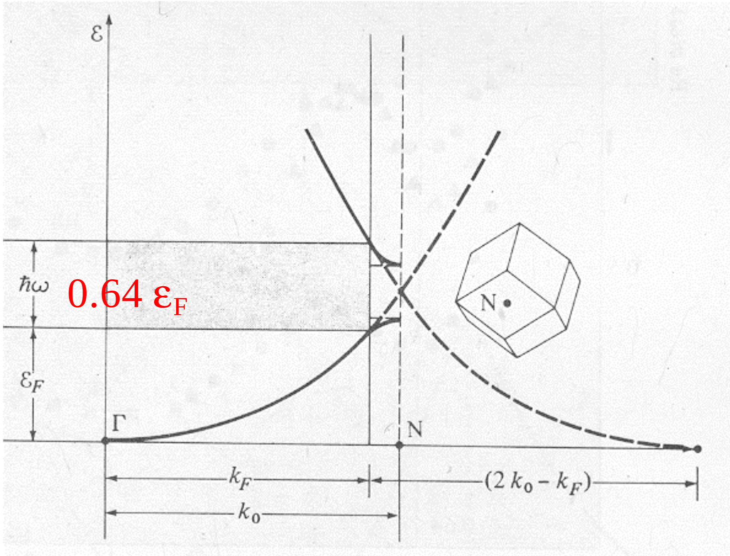
A_{111}(belly)/A_{111}(neck)=27

A_{111}(belly)/A_{111}(neck)=51

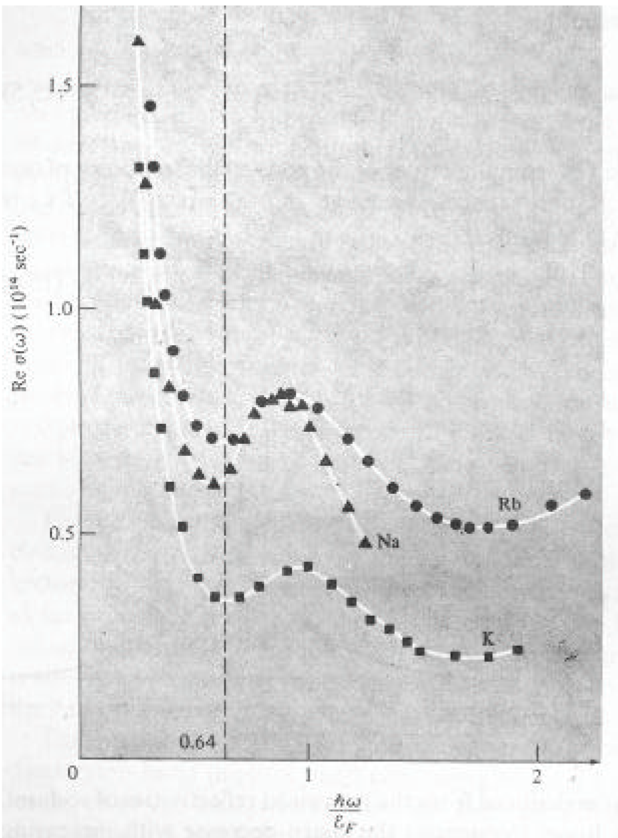
A_{111}(belly)/A_{111}(neck)=29

Optical properties of Alkali metals

5000A ≈ 10^5 /cm << 10^8 /cm → vertical transition



Re σ(ω) for Na, K, and Rb



Fermi energy

Na: 3.24 eV

K: 2.12 eV

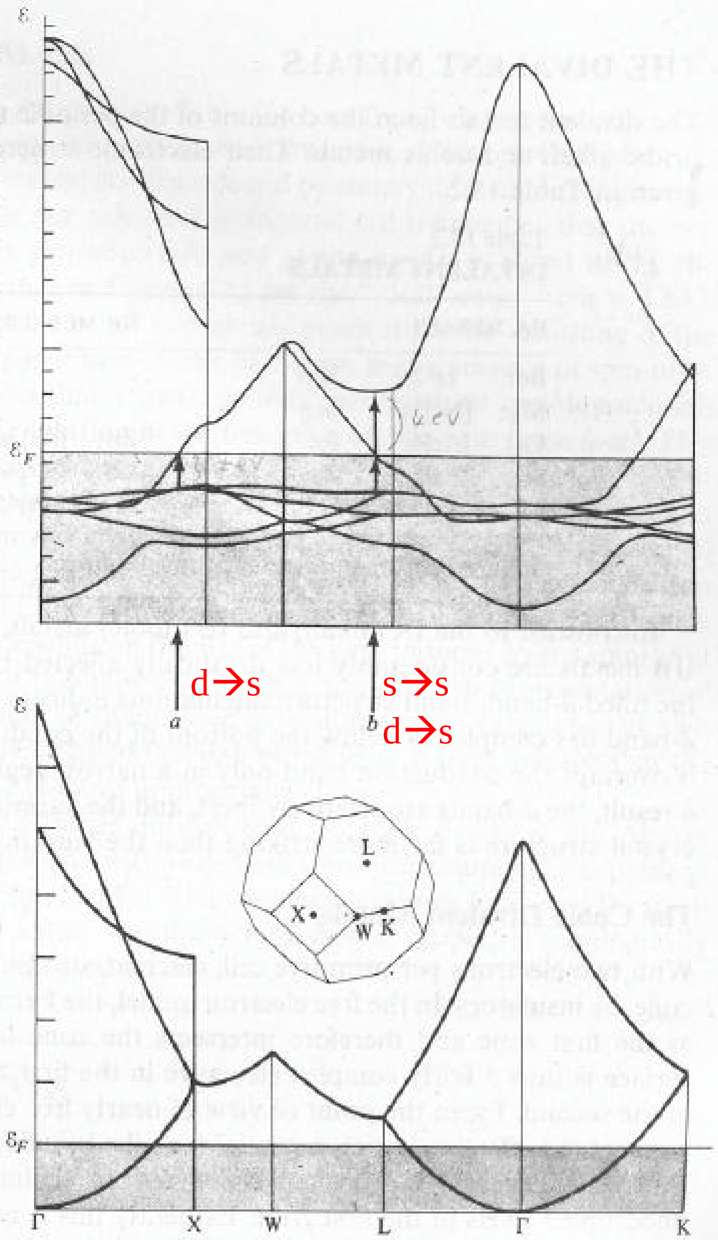
Rb:1.85 eV

EM wave in a metal: exp[i(cω/n)x], $n=(\varepsilon_0+4\pi\sigma i/\omega)^{1/2}$

Absorption ∝ Im(n) ∝ Re(σ)

Optical properties of noble metals

Figure 15.11
Burdick's calculated bands for copper, illustrating that the absorption threshold for transitions up from the conduction band is about 4 eV, while the threshold for transitions from the *d*-band to the conduction band is only about 2 eV. (The energy scale is in tenths of a rydberg (0.1 Ry = 1.36 eV).) Note the resemblance of the bands other than the *d*-bands to the free electron bands plotted below.



Cu: low threshold (2eV) Ag: high threshold (4eV)

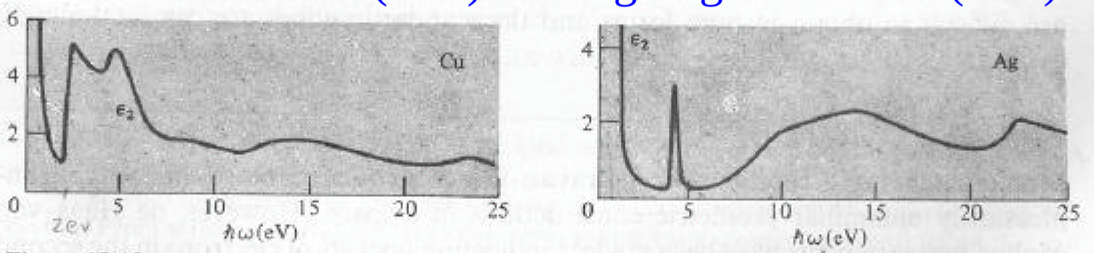


Figure 15.12
The imaginary part of the dielectric constant, $\epsilon_2(\omega) = \text{Im}\,\epsilon(\omega)$ vs. $\hbar\omega$, as deduced from reflectivity measurements. (H. Ehrenreich and H. R. Phillip, *Phys. Rev.* 128, 1622 (1962).) Note the characteristic free electron behavior ($1/\omega^3$) below about 2 eV in copper and below about 4 eV in silver. The onset of interband absorption is quite apparent.

(2) Divalent metals

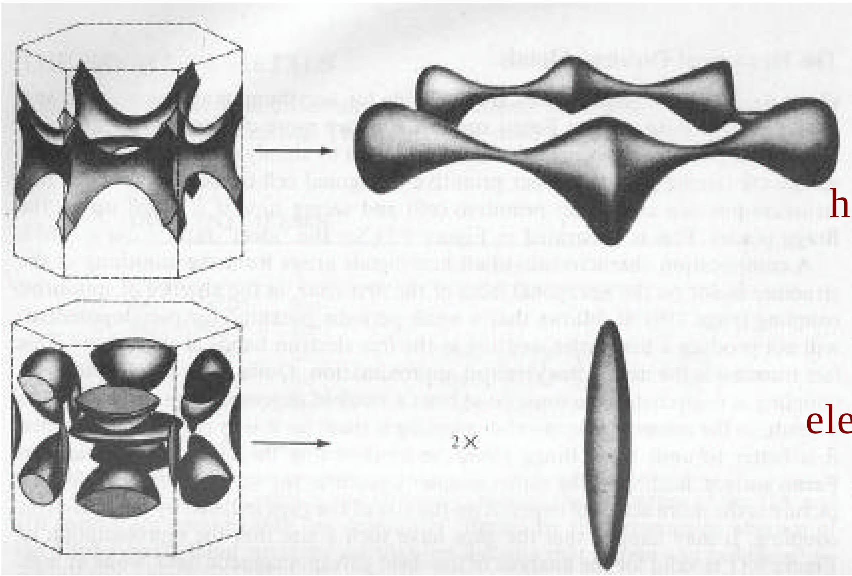
DIVALENT METALS

IIA METALS			IIB METALS		
Be:	$1s^2 2s^2$	hcp			
Mg:	$[Ne]3s^2$	hcp			
Ca:	$[Ar]4s^2$	fcc	Zn:	$[Ar]3d^{10}4s^2$	hcp
Sr:	$[Kr]5s^2$	fcc	Cd:	$[Kr]4d^{10}5s^2$	hcp
Ba:	$[Xe]6s^2$	bcc	Hg:	$[Xe]4f^{14}5d^{10}6s^2$	*

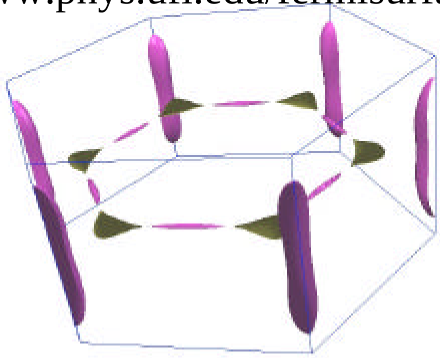
* Rhombohedral monatomic Bravais lattice.

Eg.,Fermi surfaces of Beryllium

Empty lattice actual FS

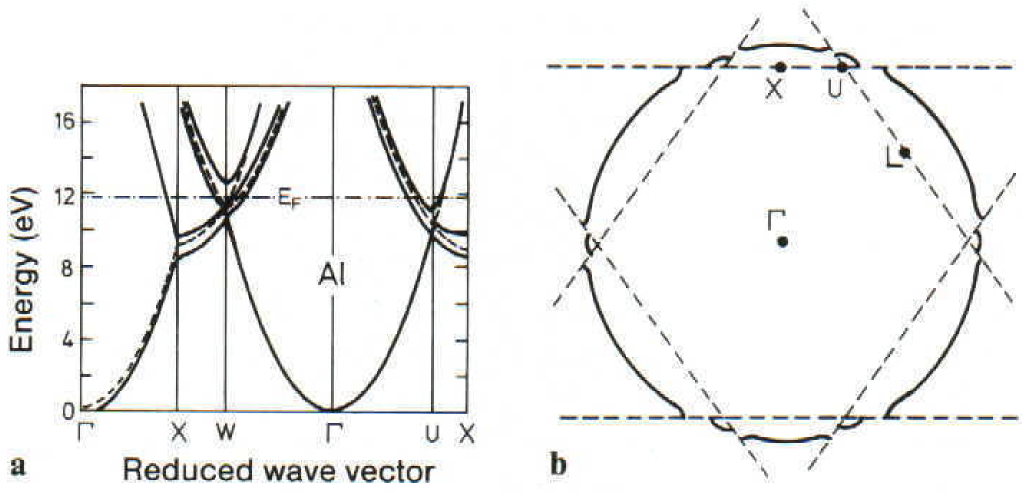


http://www.phys.ufl.edu/fermisurface/

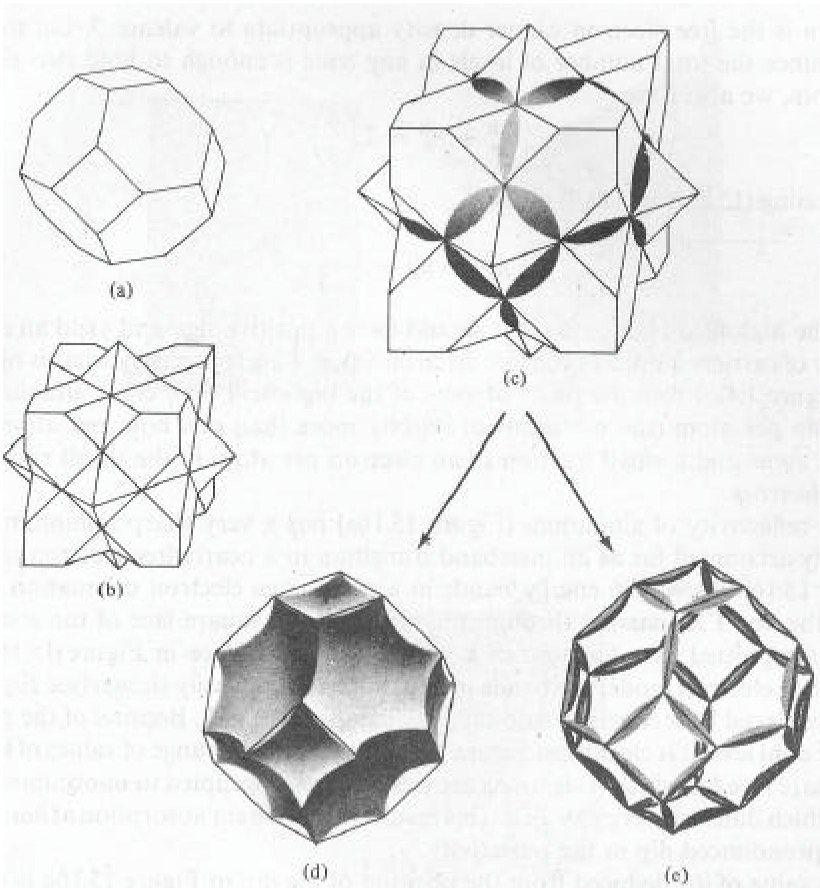


(3) Trivalent metals

Eg., Aluminum

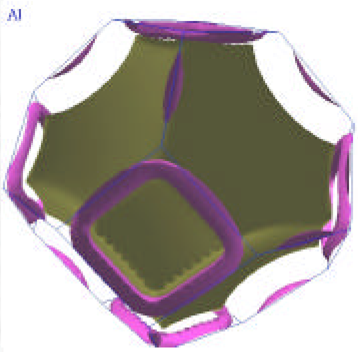


The FS from the empty lattice model:

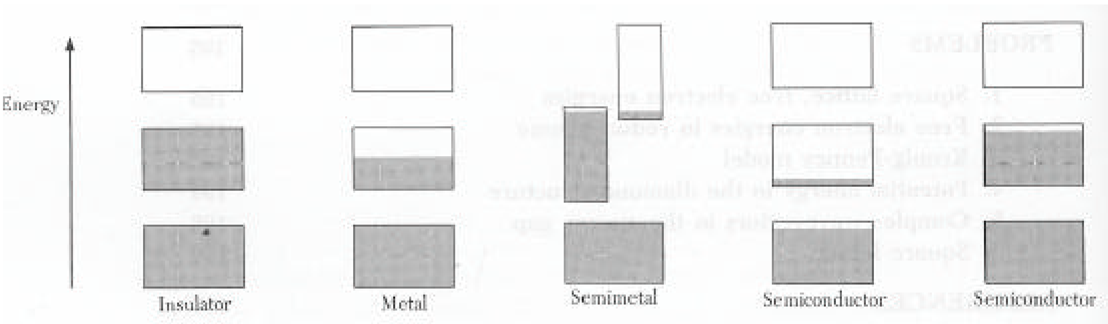


2nd BZ   3rd BZ

Actual FS



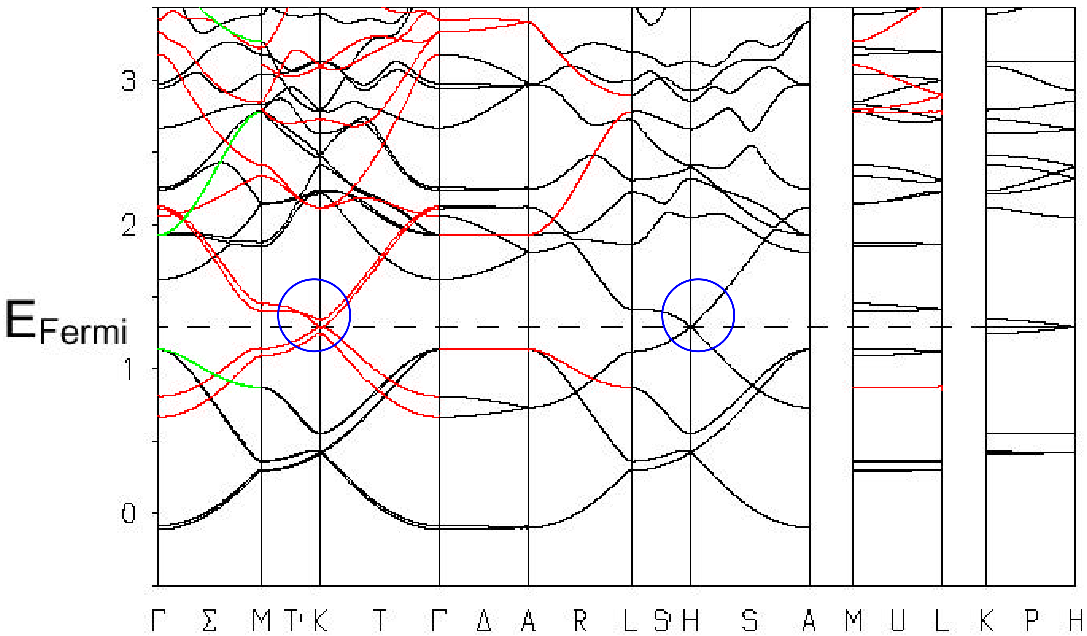
(4) Semimetal



Number of carrier << $10^{22}/cm^3$

Examples: As($4s^2 4p^3$), Sb($5s^2 5p^3$), Bi($6s^2 6p^3$); graphite

Band structure of graphite (by Bross and Alsheimer)



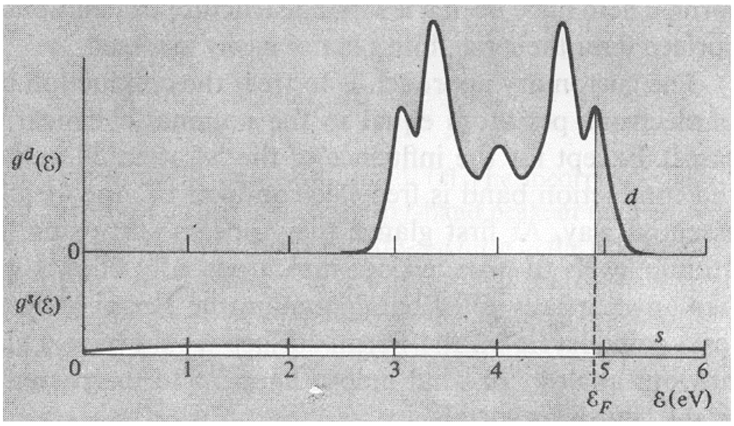
(nonzero DOS at K and H)

Pentavalent metals As, Sb, Bi have rhombohedral crystal structure (stretch a cube along its body diagonal) with 2 atoms in a unit cell (10 valence electron fill 5 energy bands)

(5) The transition metals (d metals, 3d, 4d, 5d)

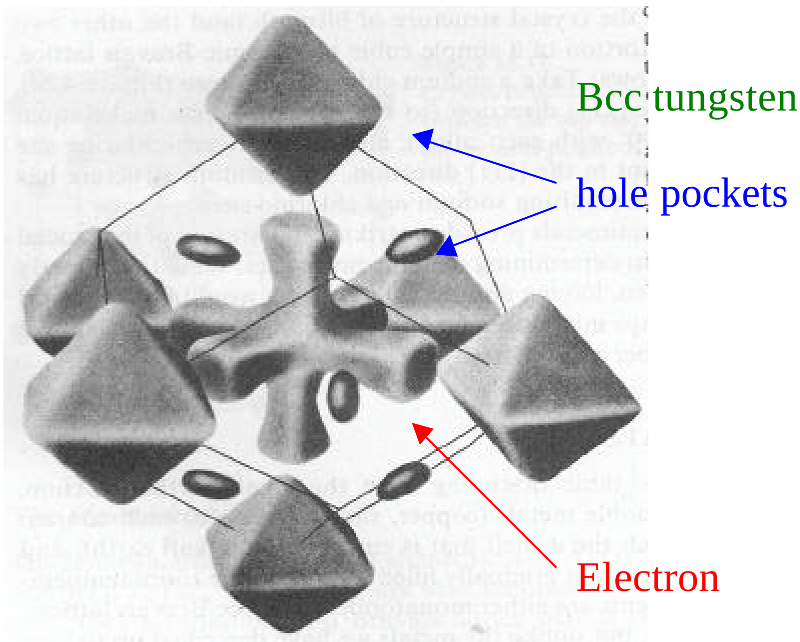
✧ Fermi energy at d-bands

→ higher DOS, larger specific heat $C \propto k_B^2 T g(E_F)$



✧ Tight-binding approx. more appropriate.

✧ Correction from e-e int maybe as large as 100%.



✧ Partially filled d-bands may give rise to magnetism.

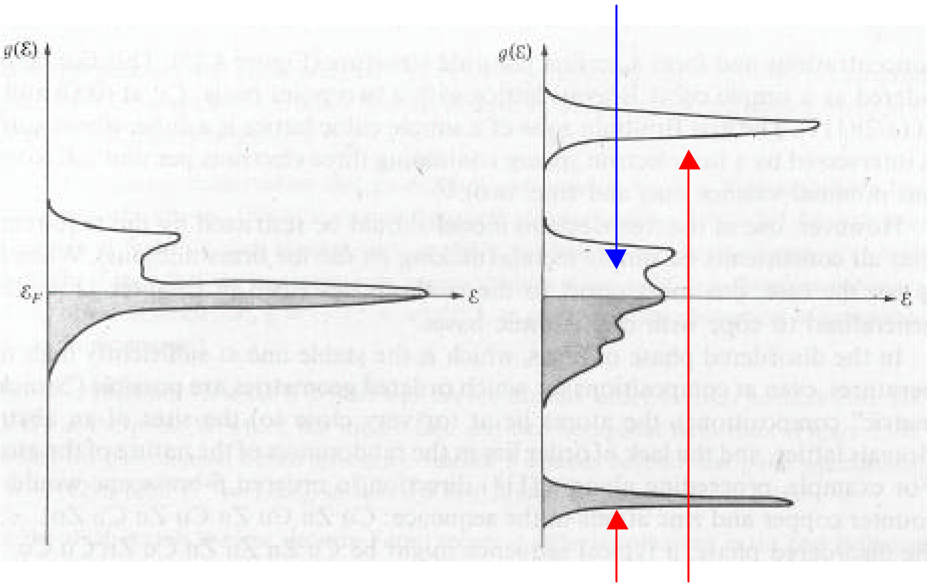
Electron spin no longer simply “a factor of 2”

(chap 32)

(6) The rare earth metals (f metals, 4f, 5f)

- Mostly hcp, similar chemical properties, difficult to get large and pure samples. Therefore, few Fermi surface data.
- Theoretical band calculation may not be reliable anyway. Expect to see f-band characters near FE, but not so!

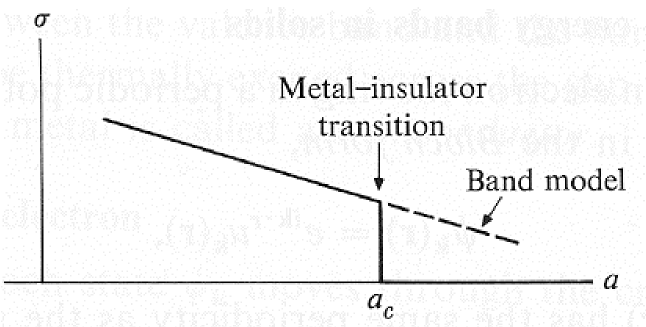
s-p-d hybridized bands in the middle



split f-bands above and below

- Simple one-electron band picture may fail altogether!

E.g. Mott transition (metal-insulator transition)



2-1

3
Li
6.939

LITHIUM, from *lithos*, meaning stone; discovered 1817: the lightest of the solid elements. Pictured here immersed in an inert oil, lithium forms a black oxide *(above)* when exposed to air. It is used in ceramics, alloys, in the H-bomb—and in treating both gout victims and manic-depressives.

2-8-1

11
Na
22.990

SODIUM, from soda; symbol Na, from its Latin name *natrium*; discovered 1807; sixth most abundant element. Metallic sodium is too violent for most everyday uses and is generally stored in kerosene as above. But its useful compounds include table salt, baking soda, borax and lye.

2-8-8-1

19
K
39.102

POTASSIUM, from potash, an impure form of potassium carbonate known to the ancients; symbol K from its Latin name *kalium*; discovered 1807. Seventh most abundant element in the earth's crust. Its radioactivity, though mild, may be one natural cause of genetic mutation in man.

2-8-18-8-1

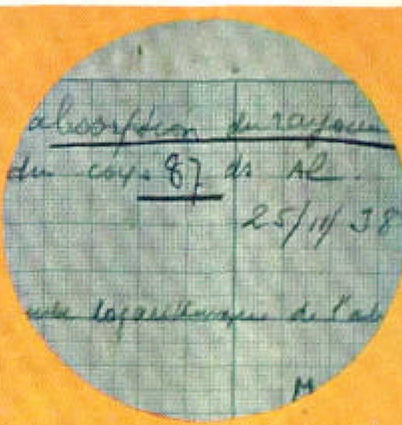
37
Rb
85.47

RUBIDIUM, from *rubidus*, or red (the color its salts impart to flames); discovered 1861. Rubidium, used in electric-eye cells, is also a potential space fuel. Like potassium, it is slightly radioactive, and has been used to locate brain tumors, as it collects in tumors but not in normal tissue.

2-8-18-18-8-1

55
Cs
132.91

CESIUM, from *caesius*, or sky-blue (its salts turn flames blue); discovered 1860: the softest metal, liquid at warm room temperature, 83° F. Extremely reactive, it finds limited use in vacuum tubes and in atomic clocks so accurate that they vary no more than five seconds in 10 generations.



2-8-18-32-18-8-1

87
Fr
(223)

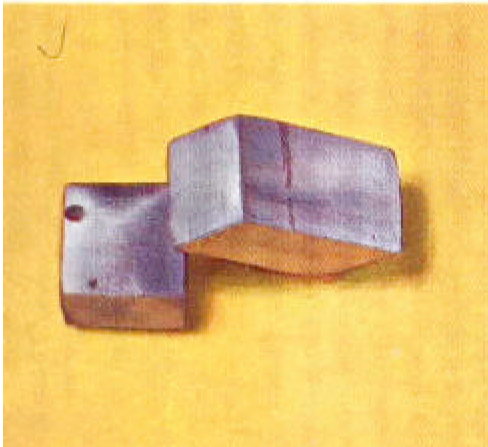
FRANCIUM, for France; discovered 1939. A short-lived product of the decay of actinium, francium has never actually been seen. The graph above which identifies francium by its radiation is from the notebook of the discoverer, Marguerite Perey, a onetime assistant to Marie Curie.

2 2 | 4 **Be** 9.0122

BERYLLIUM, from the mineral beryl, in which it was found in 1798. This element produces alloys that are extremely elastic, hence its role in making gears, springs and other machine parts. Because of its high melting point—2,345° F.—beryllium goes into making rocket nose cones.

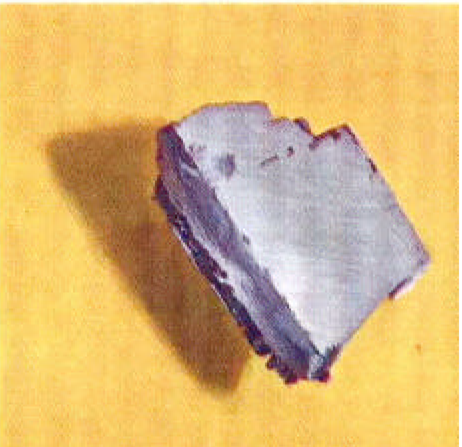
2 8 2 | 12 **Mg** 24.312

MAGNESIUM, from Magnesia, an ancient city in Asia Minor; discovered 1775; eighth most abundant element; burns as a powder or foil in firecrackers, bombs and flash bulbs. It has one odd biological effect: a deficiency in man can have the same effect as alcoholism—delirium tremens.



2 8 8 2 | 20 **Ca** 40.08

CALCIUM, from *calx*, or lime—an oxide of calcium; discovered 1808; fifth most abundant in the earth's crust. Its presence in our bodies is essential. Normal quota in an adult is about two pounds, mostly in the teeth and bones. Calcium also plays a role in regulating the heartbeat.

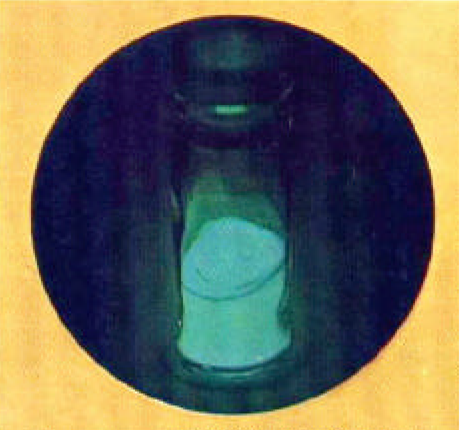


2 8 18 8 2 | 38 **Sr** 87.62

STRONTIUM, from Strontian, Scotland; discovered 1790; a rare metal which is a sort of evil alter ego of life-supporting calcium. Radioactive strontium 90 is present in atomic fallout. It is absorbed by bone tissue in place of calcium, and enough of it destroys marrow and can cause cancer.

2 8 18 18 8 2 | 56 **Ba** 137.34

BARIUM, from *barys*, heavy or dense; discovered 1808; to minimize oxidation, the sample above was photographed in argon. The white sulphate is drunk as a medical cocktail to outline the stomach and intestines for X-ray examination. Barium nitrate gives fireworks a green color.



2 8 18 32 18 8 2 | 88 **Ra** (226)

RADIUM, from *radius*, or ray; discovered 1898 by Pierre and Marie Curie; sixth rarest of the elements. Shown above is radium bromide mixed with zinc sulphide—a mixture used in luminous watch dials. The radium gives off dangerous radiation which causes the zinc sulphide to glow.

2 8 18 1

29
Cu
63.54

COPPER, from *cuprum*, derived from the ancient name for Cyprus, famed for its copper mines; known by early man. It and gold are the only two colored metals. Alloyed in most gold jewelry and silverware, copper is mixed with zinc in brass, with tin in bronze. A "copper" penny is bronze.

2 8 18 2

30
Zn
65.37

ZINC, probably from *zin*, German for tin; discovered by the alchemist Paracelsus in the 16th Century, though the zinc-copper alloy brass was known to the ancients. While not technically a colored metal, zinc has a bluish cast. An excellent coating metal, it is used to line iron water buckets.

2 8 18 18 1

47
Ag
107.87

SILVER, from Old English *seolfor*, for silver; symbol Ag from its Latin name *argentum*; prehistoric; the best conductor of heat and electricity. Its salts are basic in photography: when silver bromide is exposed to light, it undergoes a chemical change which the developer then makes visible.

2 8 18 18 2

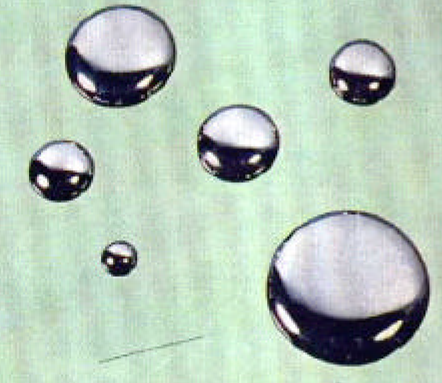
48
Cd
112.40

CADMIUM, from *kadmia*, or earth; discovered 1817. Cadmium occurs in nature with zinc. It makes excellent neutron-eating rods to slow up atomic chain reactions and finds use in nickel-cadmium batteries. Its bright sulphide makes the artist's popular pigment cadmium yellow.

2 8 18 32 18 1

79
Au
196.97

GOLD, from the old English word *geolo*, or yellow; symbol Au from its Latin name *aurum*; prehistoric; the most malleable metal. Man's lust for gold has been a delusion, for he has pursued little more than a yellow gleam. It cannot be used for much besides money, jewelry and dental work.



2 8 18 32 18 2

80
Hg
200.59

MERCURY, from the planet Mercury; symbol Hg from *hydrargyrum*, or liquid silver; prehistoric. It appears in the glass tubing of thermometers and barometers; it also finds use in "silver" dental inlays and in silent electric switches. Vaporized mercury fills modern blue-hued street lights.