Bands, Fermi surfaces, ...

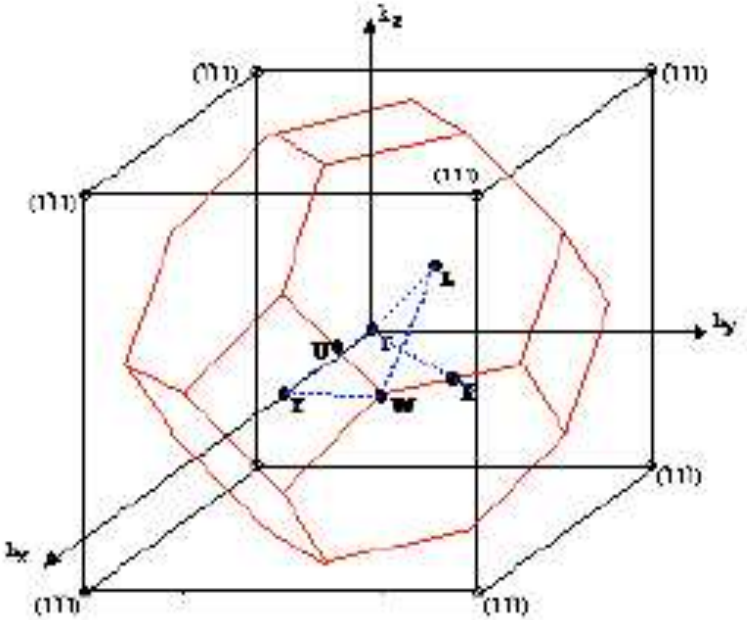
(slides for comments on representative pictures)

10 November 2023

M. Peressi

Free electron bands for FCC structures

or "empty lattice"



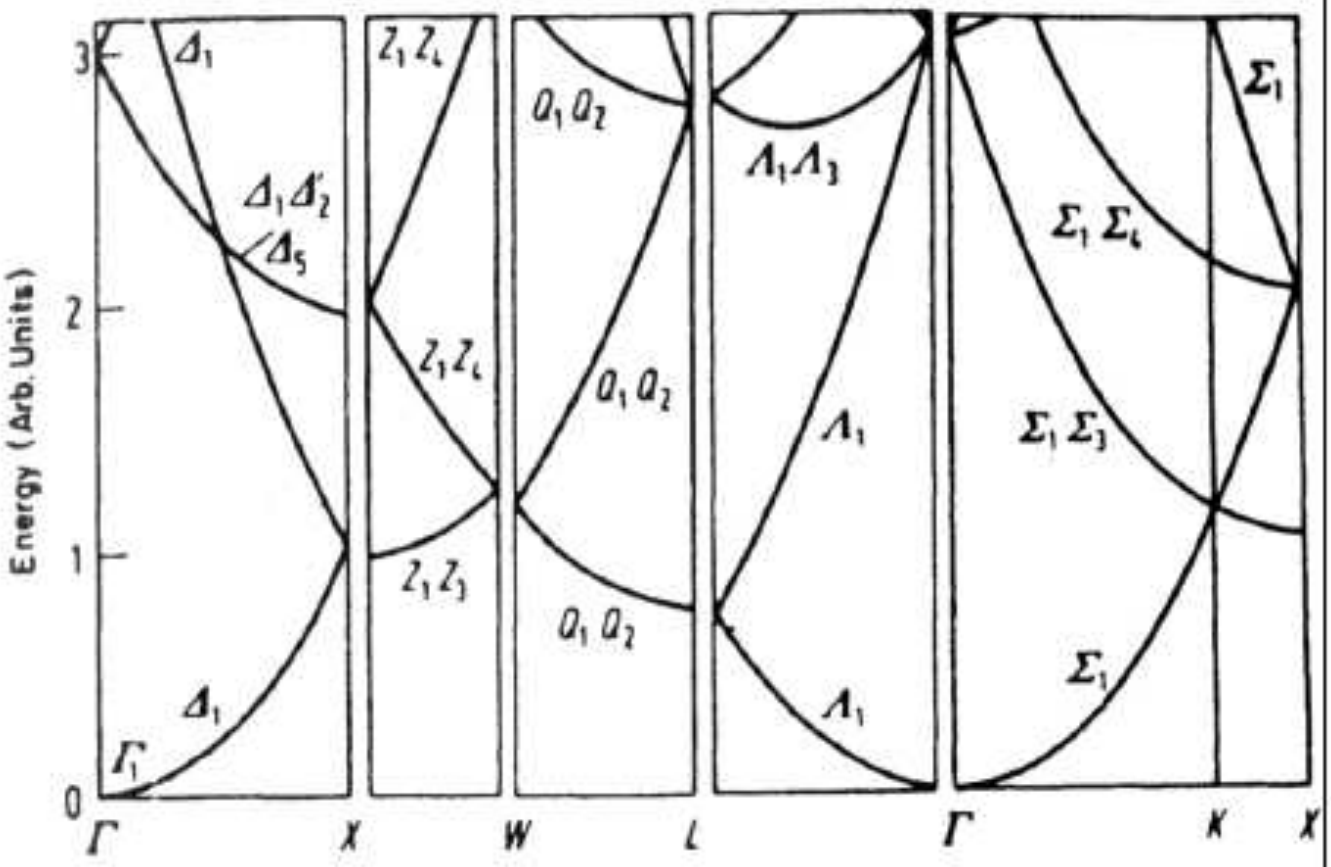
(this is interesting for full labelling)

Γ – center of the BZ

X – [100] intercept; Γ – X path Δ

K – [110] intercept; Γ – K path Σ

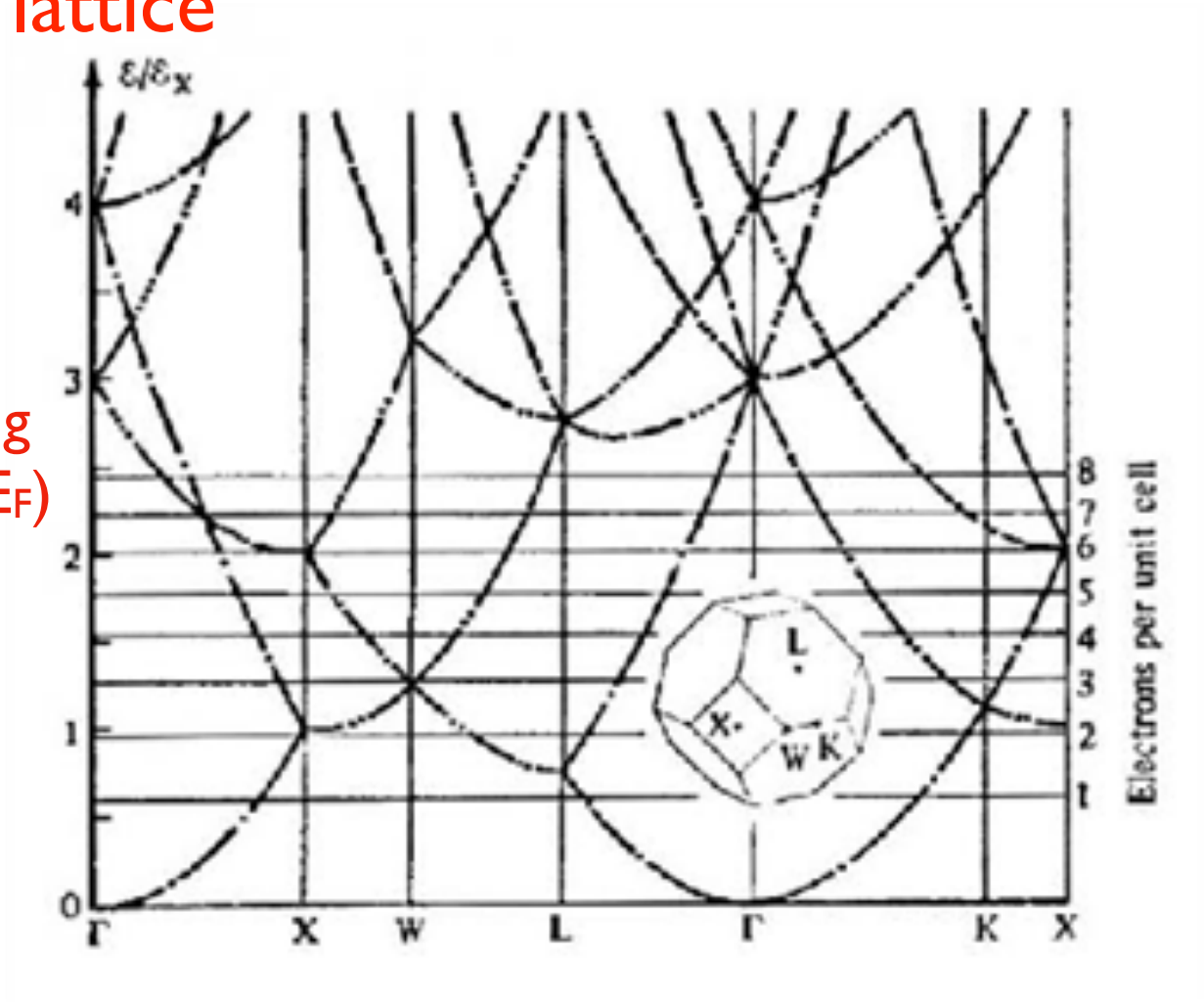
L – [111] intercept; Γ – L path Λ



Free electron bands for FCC structures

or "empty lattice"

(this is interesting for indication of E_F)

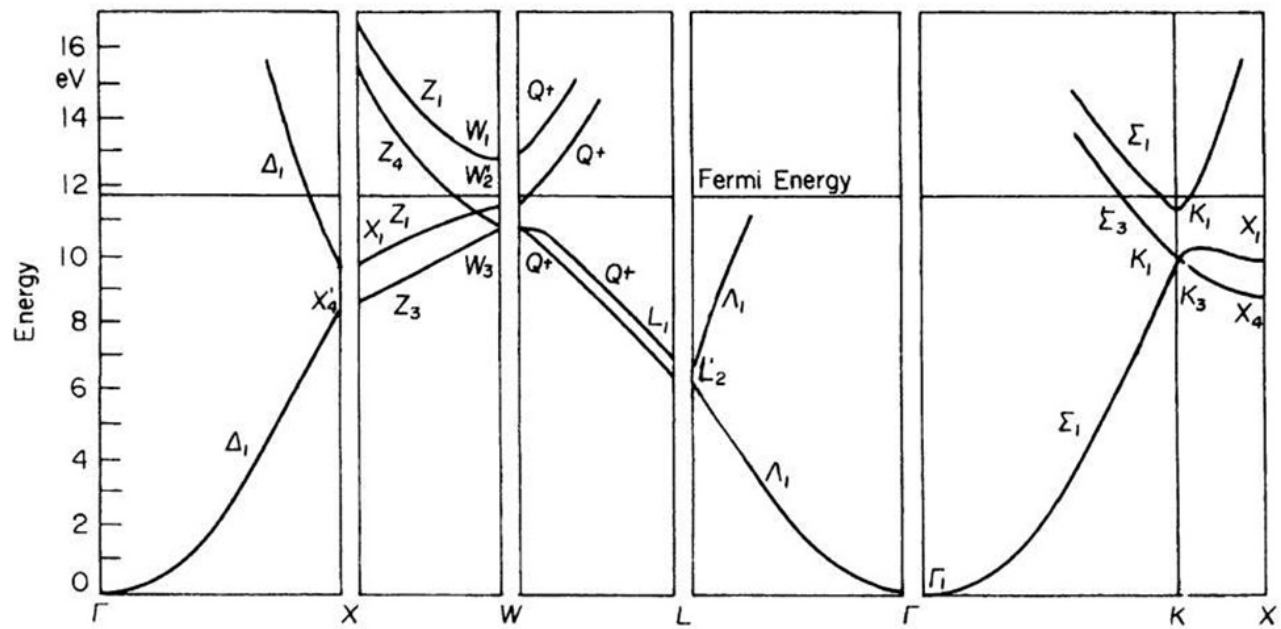


from Ashcroft & Mermin Fig. 9.5

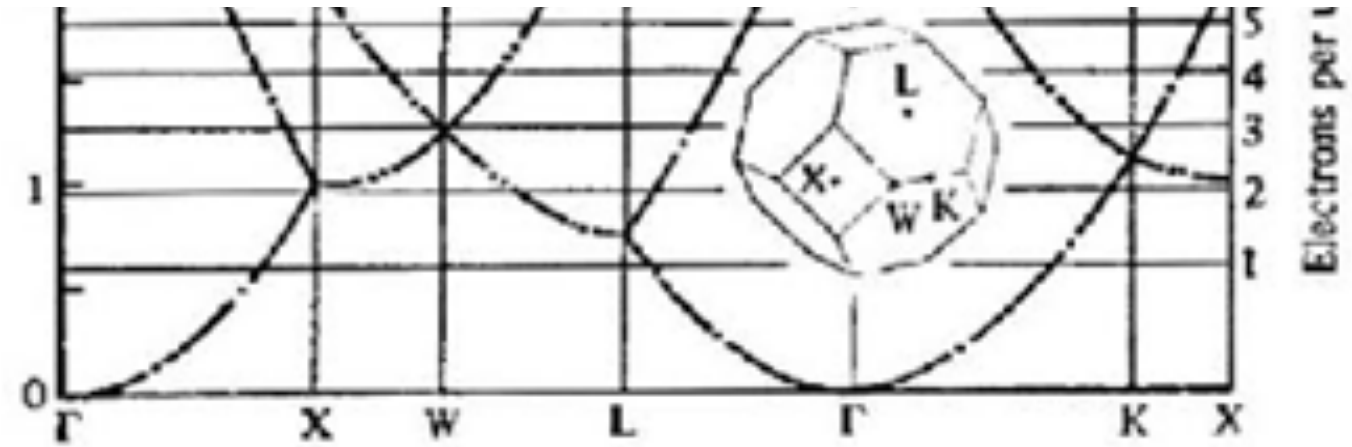
Dispersion relation in 3D for an FCC Bravais lattice. The horizontal lines give Fermi-energies for the indicated number of electrons per primitive cell. The number of dots on a curve specifies the number of degenerate free electron levels represented by the curve.

Band structure of selected metals

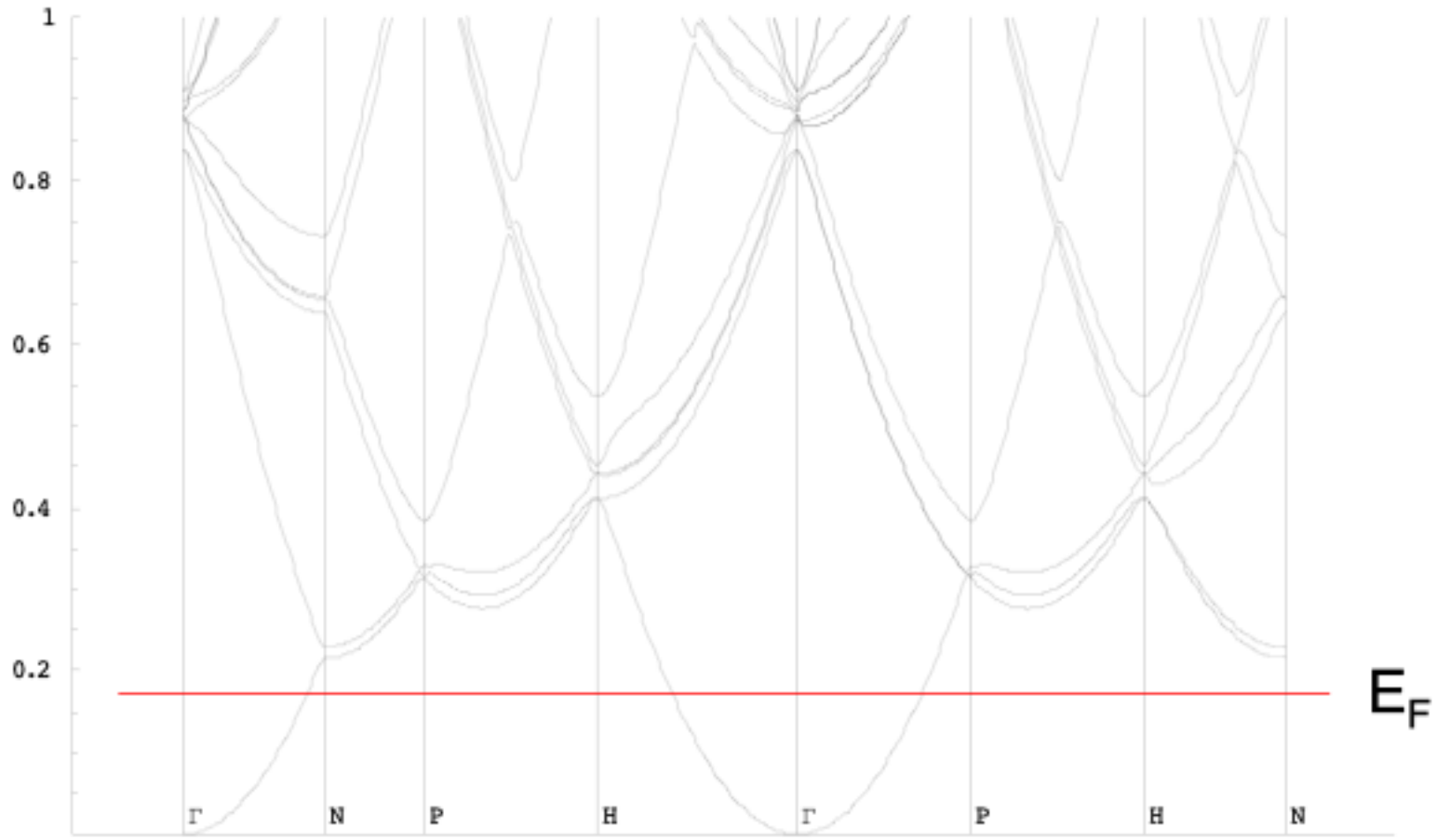
Al: FCC,
3 e/atom



FCC
free electrons
or "empty lattice"
(A&M fig 9.5)



Li: FCC,
1 e/atom



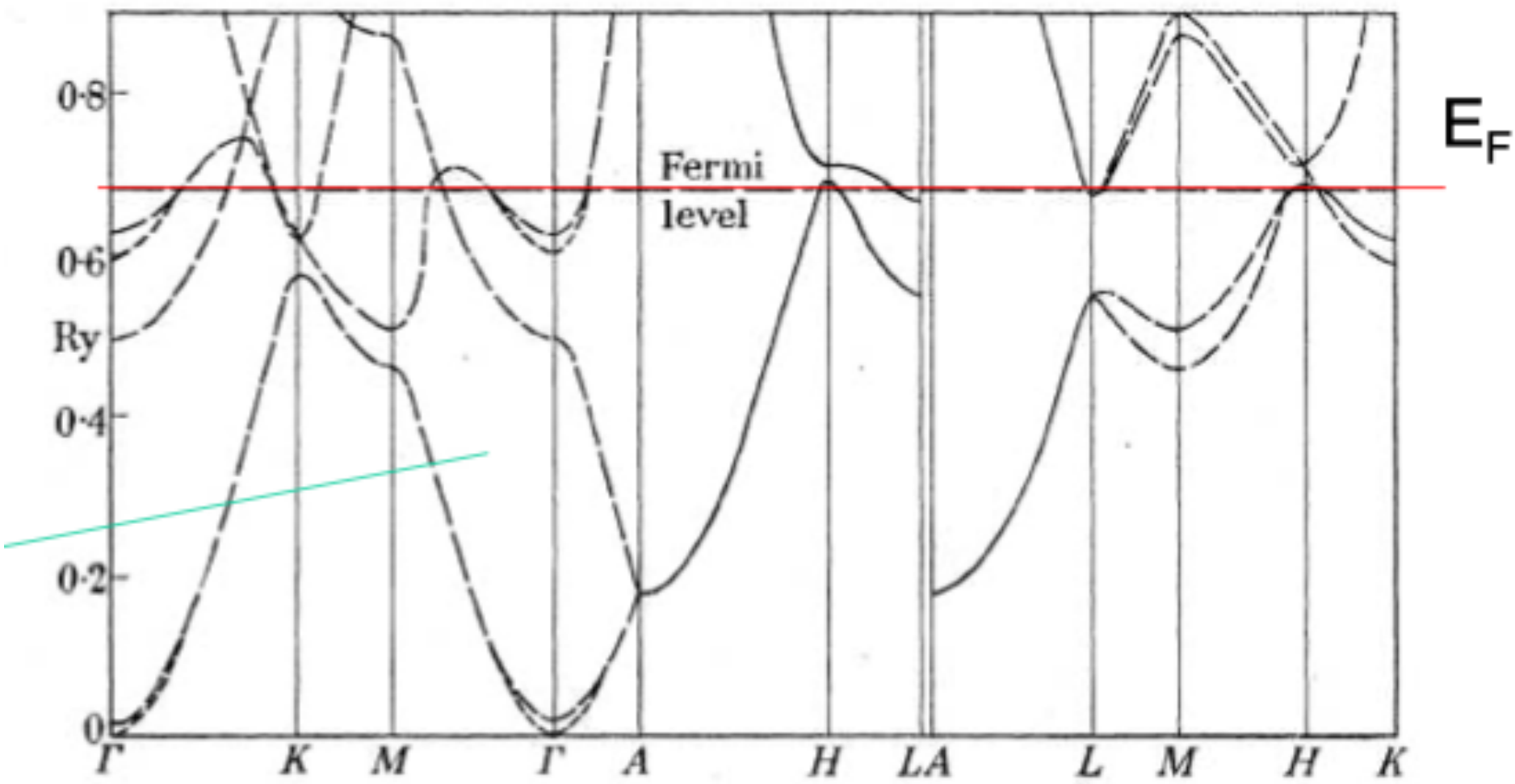
almost perfectly parabolic dispersion curve (in the occupied region)

the Fermi energy cuts the first band => the Fermi surface is fully contained in the I B.z.

Mg: HCP,

2 e/atom,

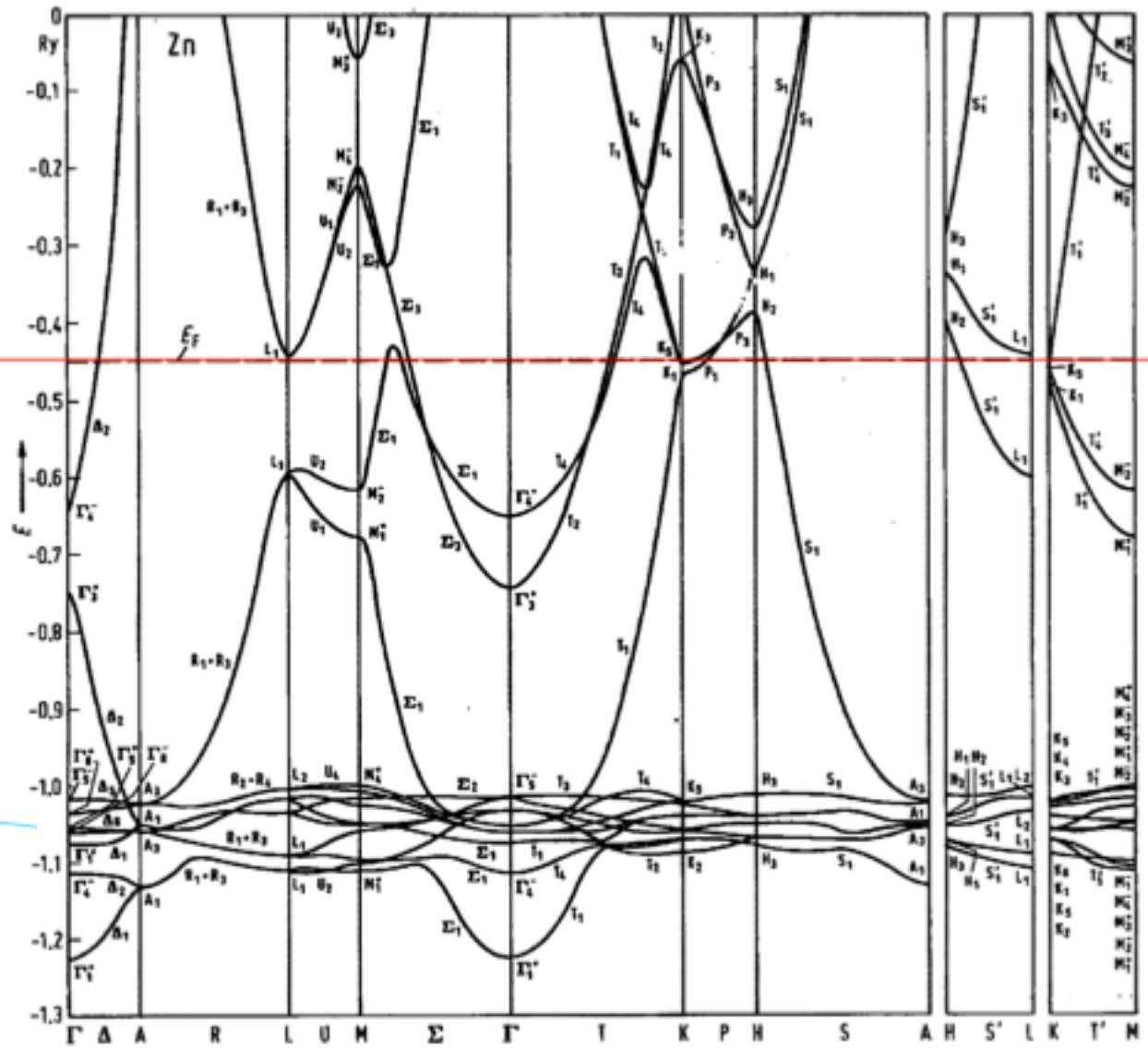
4 e/unit cell



hcp-crystal

2 s/p el./atom
4 s/p el./unit cell

Zn: HCP,
2 e/atomo,
4 e/cella unitaria

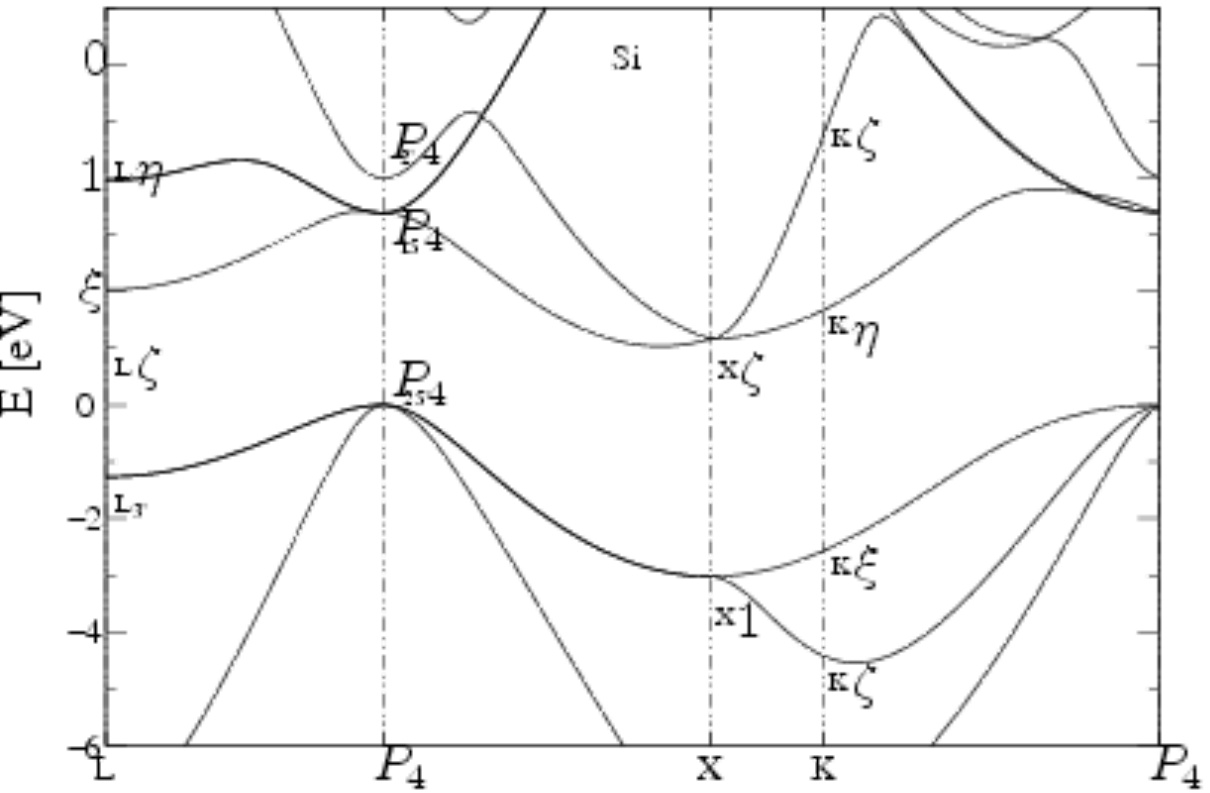


E_F

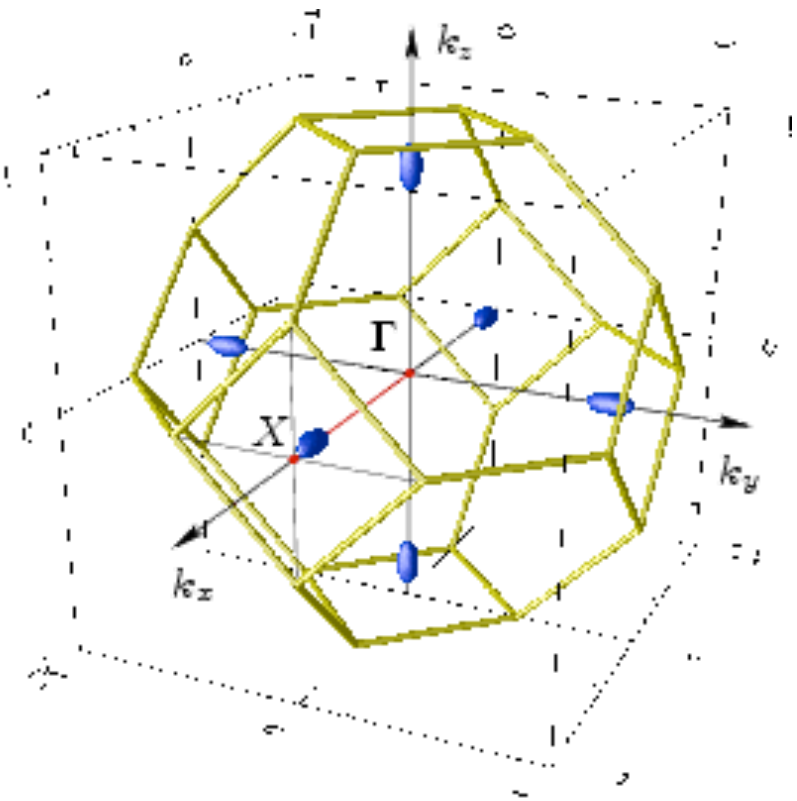
d-band
(10 bands for
20 el./unit cell)

Band structure of selected semiconductors

Si



(a) Band diagram of silicon.



(b) First conduction band valleys.

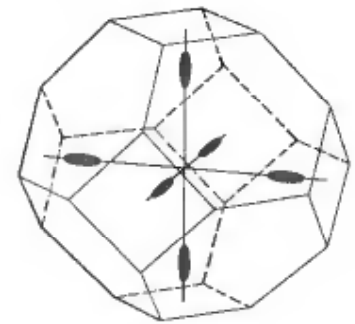
indirect gap!

Band structure of selected semiconductors

16/01/2012, II test
Ex. 2

Silicon The crystal has the diamond structure, so the first Brillouin zone is the truncated octahedron appropriate to a face-centered cubic Bravais lattice. The conduction band has six symmetry-related minima at points in the ⟨100⟩ directions, about 80 percent of the way to the zone boundary (Figure 28.5). • • •

Figure 28.5
Constant-energy surfaces near the conduction band minima in silicon. There are six symmetry-related ellipsoidal pockets. The long axes are directed along ⟨100⟩ directions.

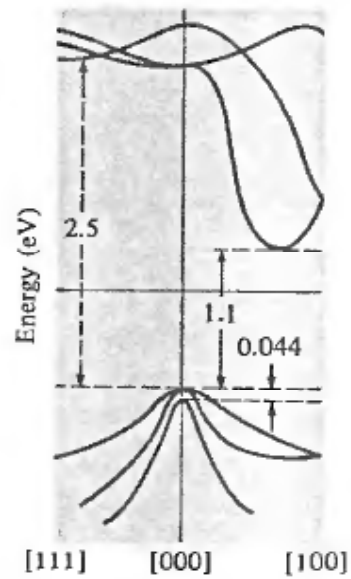


from Ashcroft-Mermin,
Ch 28, Typical semiconductor band structure, p 569

going in depth

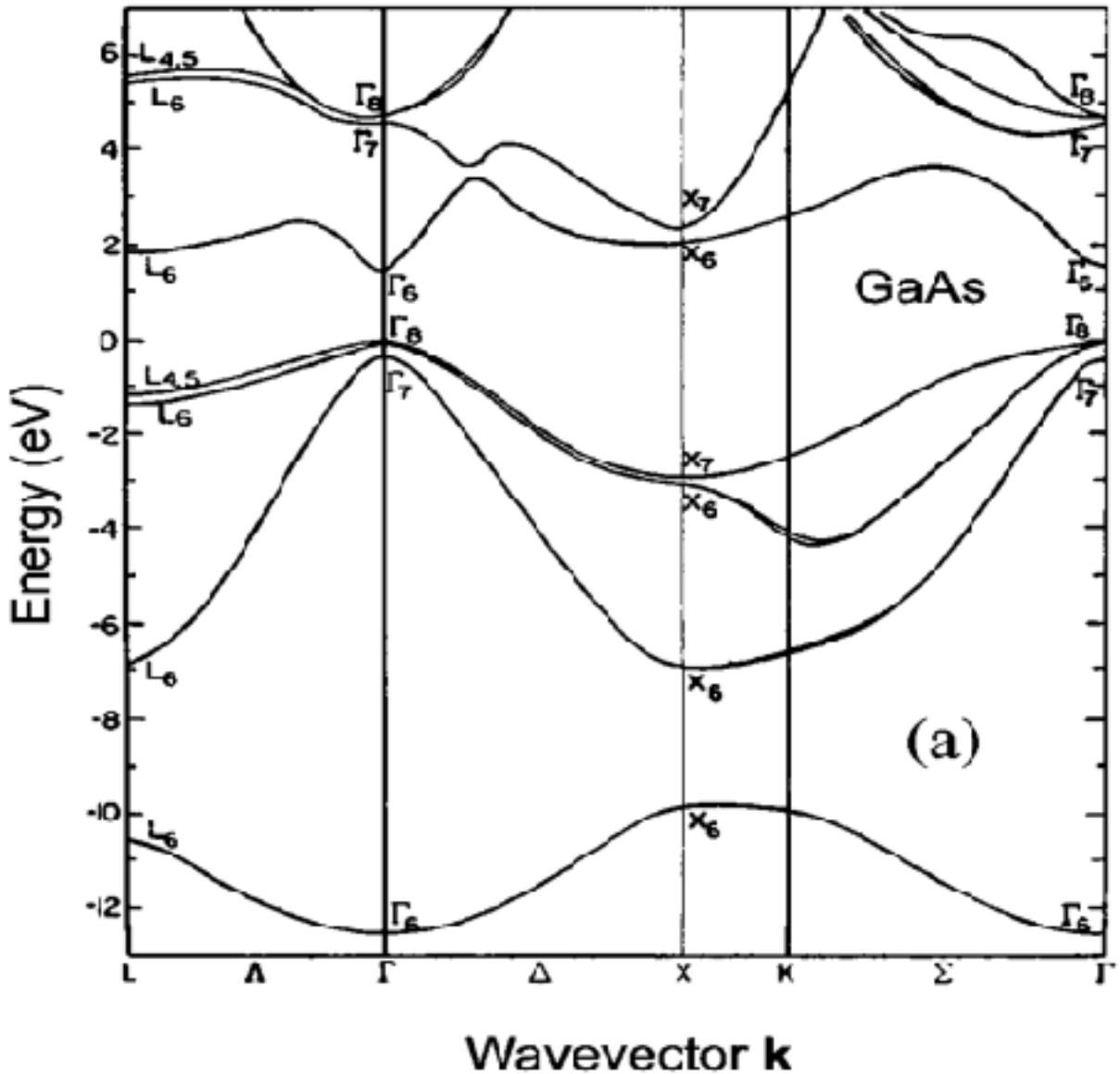
of the six ellipsoids must be an ellipsoid of revolution about a cube axis. They are quite cigar-shaped, being elongated along the cube axis. In terms of the free electron mass m, the effective mass along the axis (the longitudinal effective mass) is $m_L \approx 1.0m$ while the effective masses perpendicular to the axis (the transverse effective mass) are $m_T \approx 0.2m$. There are two degenerate valence band maxima, both located at $\mathbf{k} = \mathbf{0}$, which are spherically symmetric to the extent that the ellipsoidal expansion is valid, with masses of $0.49m$ and $0.16m$ (Figure 28.6).

Figure 28.6
Energy bands in silicon. Note the conduction band minimum along [100] that gives rise to the ellipsoids of Figure 28.5. The valence band maximum occurs at $\mathbf{k} = 0$, where two degenerate bands with different curvatures meet, giving rise to "light holes" and "heavy holes." Note also, the third band, only 0.044 eV below the valence band maximum. This band is separated from the other two only by spin-orbit coupling. At temperatures on the order of room temperature ($k_BT = 0.025$ eV) it too may be a significant source of carriers. (From C. A. Hogarth, ed., *Materials Used in Semiconductor Devices*, Interscience, New York, 1965.)



Band structure of selected semiconductors

GaAs

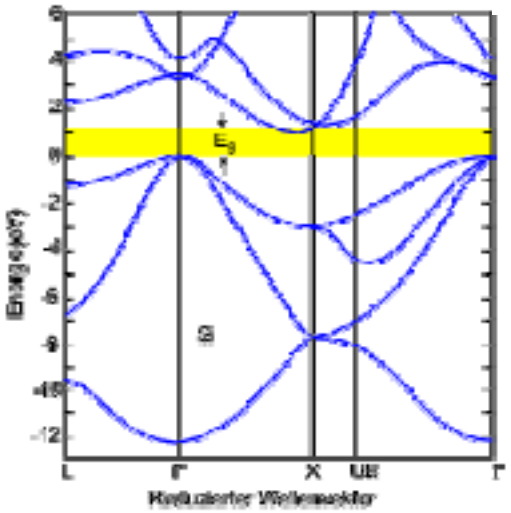


direct gap!

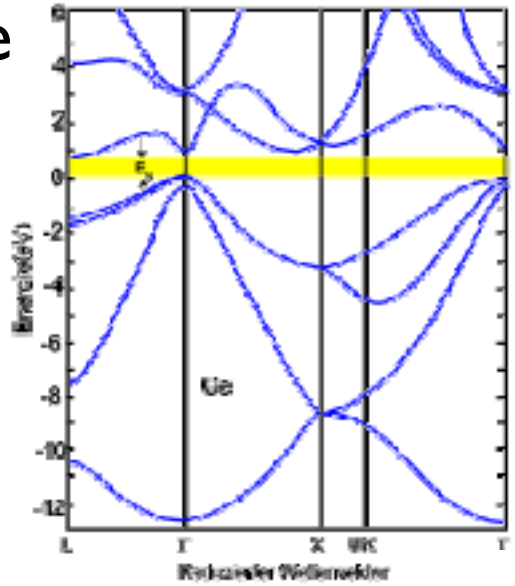
Band structure of selected semiconductors

fcc-crystal

Si



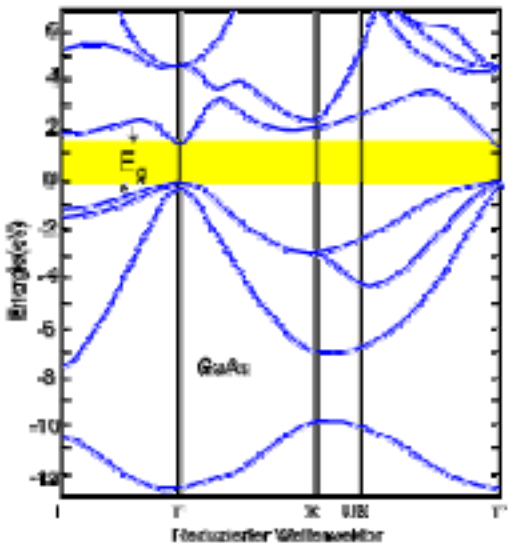
Ge

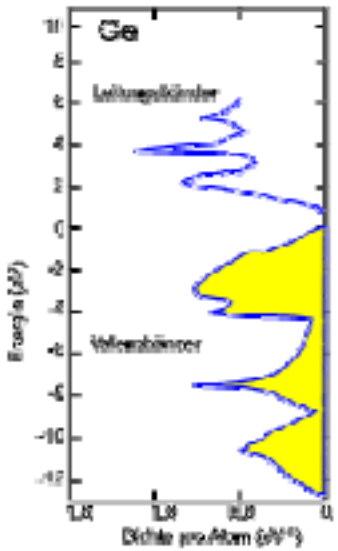


8 e
per unit cell

4 bands occ.

GaAs





density of states

Band structure of other elemental solids

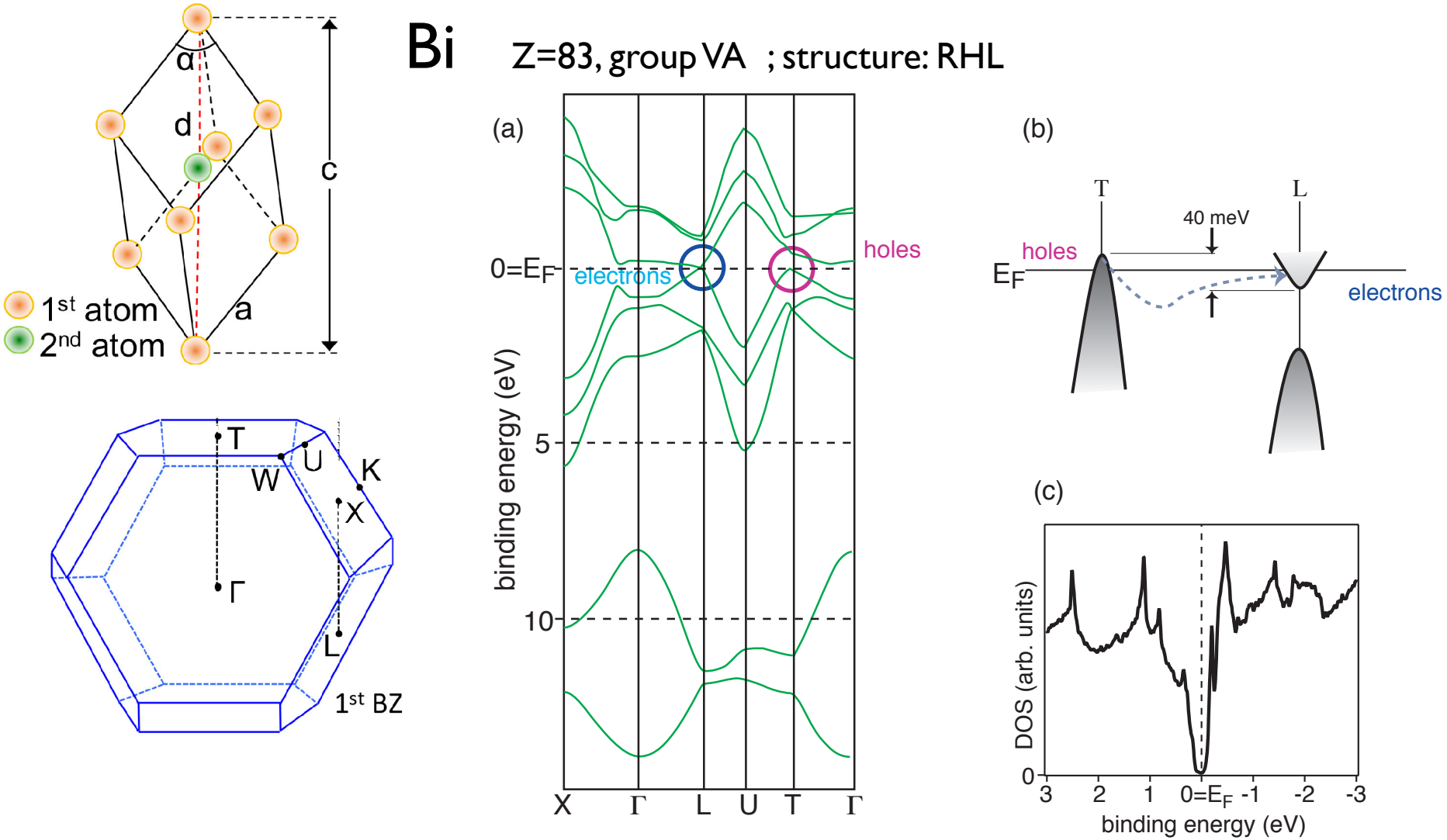


Figure 1: Electronic structure of Bismuth. (a) Bulk band dispersion in different directions of the Brillouin zone (b) Schematic band structure of the bands crossing the Fermi energy. (c) Density of states.

Bi Z=83, group VA ; structure: RHL

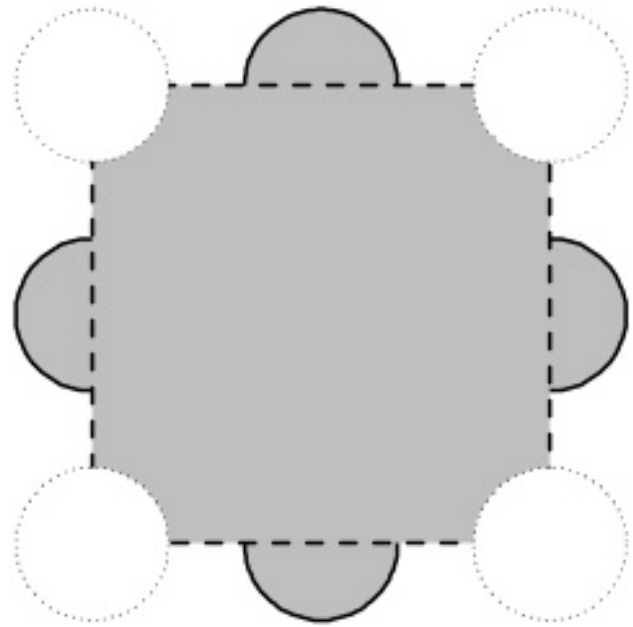
The effect of the presence of both holes and electrons on the Hall constant can be understood qualitatively from the expression for R_H:

$$R_H = \frac{p\mu_h^2 - n\mu_e^2}{e(p\mu_h + n\mu_e)^2}$$

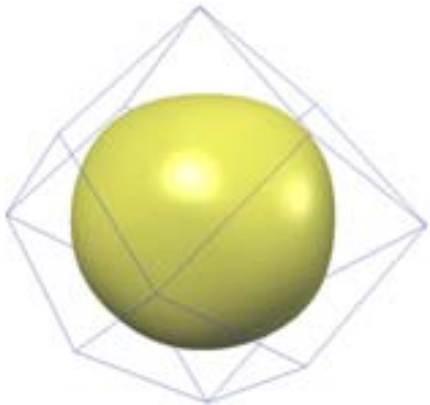
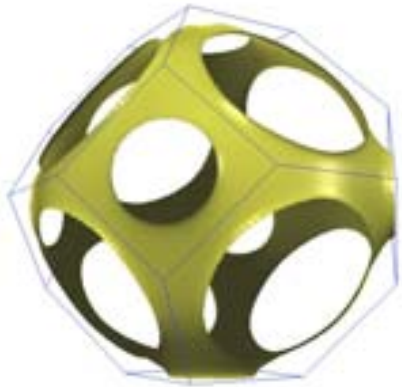
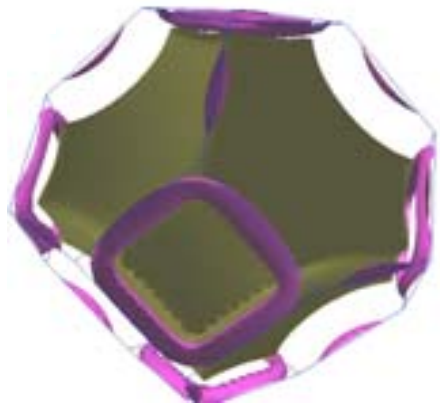
(see: Ashcroft-Mermin: problem 12.4;

written test of January 16, 2012 - problem n. 3)

(qualitative picture!)



3D Fermi Surface

1 valence e^-	2 valence e^-	3 valence e^-
		
Na	**Ca**	**Al**
BCC	FCC	FCC

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

Brillouin zones and their filling with free electrons Fermi spheres

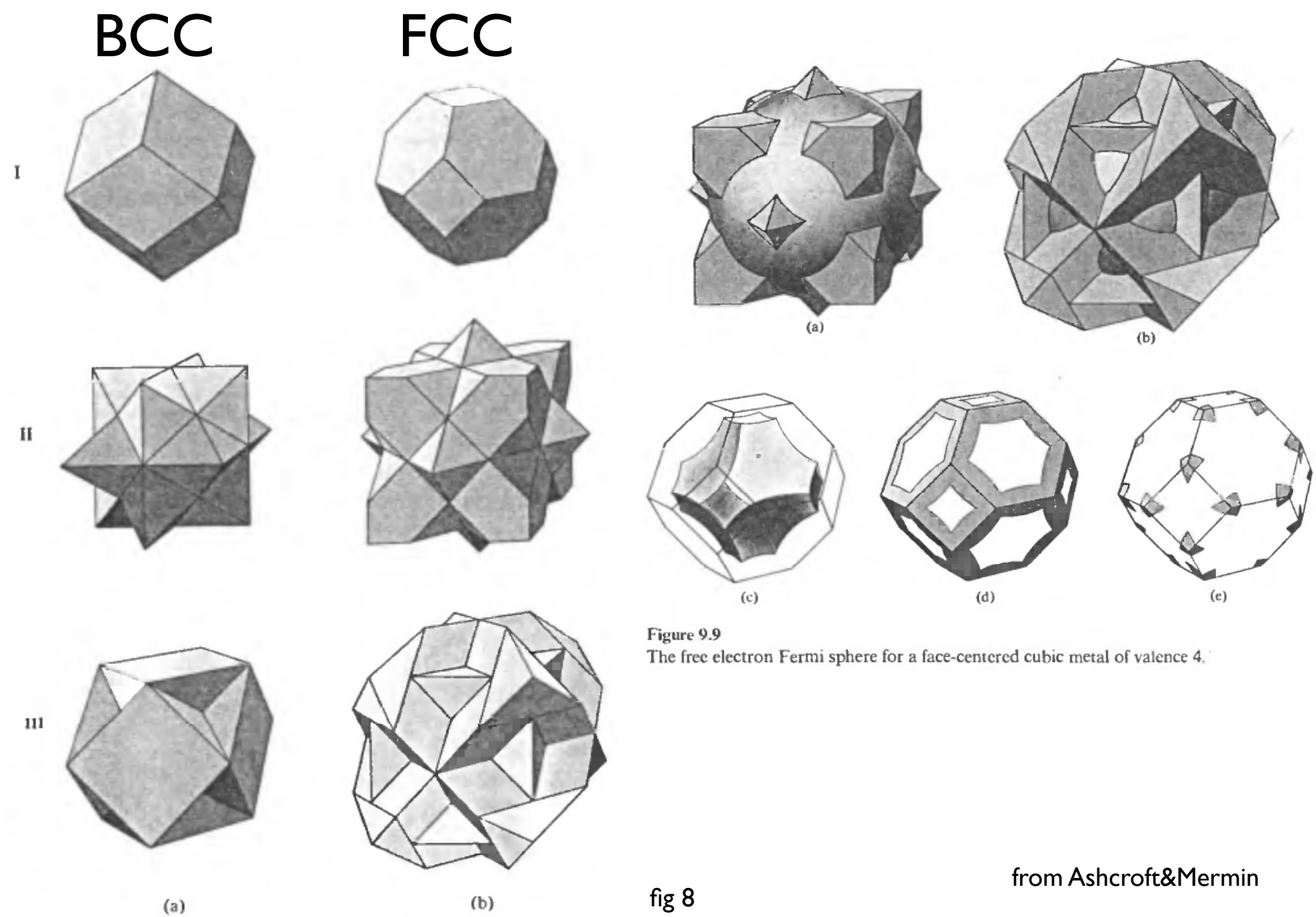


Figure 9.9
The free electron Fermi sphere for a face-centered cubic metal of valence 4.

fig 8

from Ashcroft&Mermin