Reading

Omar: 1.1-1.8, Already finished 1.9, 1.10

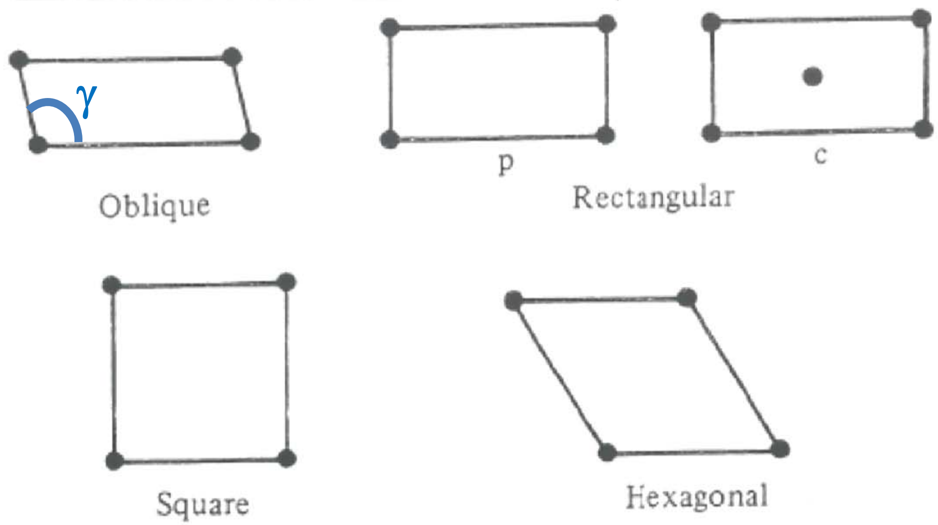
Omar: 5.1-5.3, 5.8

Ibach and Luth: Already finished all of Chapter 1, 2.1-2.5 only, lighter on 2.2

Translational order in two dimensions

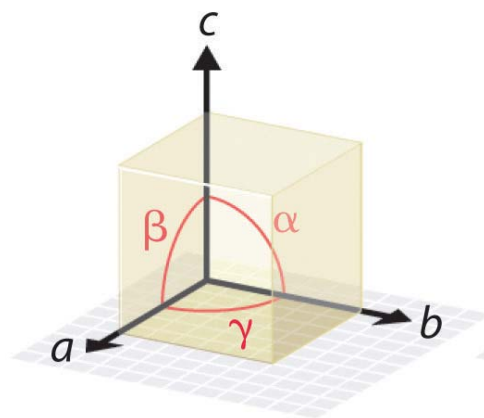
Table 2.1. *The five two-dimensional Bravais nets*

	Shape of unit mesh	Mesh symbol	Conventional rule for choice of axes	Nature of axes and angles	Name
Oblique	General parallelogram	p	None	$a \neq b$ $\gamma \neq 90°$	Oblique
Rectangular	Rectangle	p c	Two shortest, mutually perpendicular vectors	$a \neq b$ $\gamma = 90°$	Rectangular
Square	Square	p	Two shortest, mutually perpendicular vectors	$a = b$ $\gamma = 90°$	Square
Hexagonal	60° angle rhombus	p	Two shortest vectors at 120° to each other	$a = b$ $\gamma = 120°$	Hexagonal



p = primitive
c = centered

Translational order in three dimensions

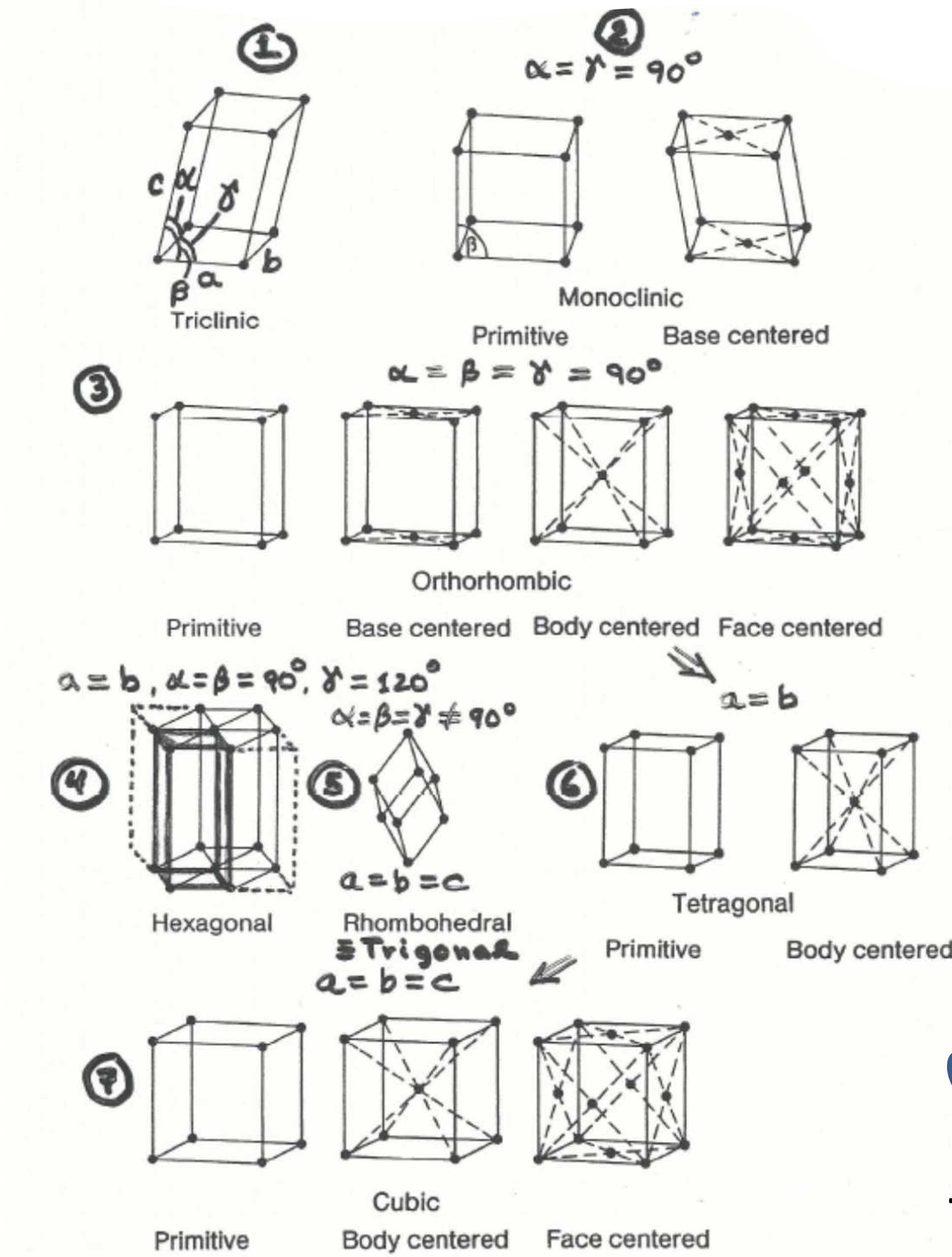


Edges and angles

Table 2.1. The seven different basis-vector systems or crystal systems. Most elements crystallize in a cubic or hexagonal structure. For this reason, and also because of their high symmetry, the cubic and hexagonal coordinate systems are particularly important

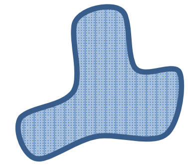
	Basis vectors/crystal axes	Angles	Crystal system
1	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90°$	triclinic
2	$a \neq b \neq c$	$\alpha = \gamma = 90°$ $\beta \neq 90°$	monoclinic
3	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90°$	orthorhombic
6	$a = b \neq c$	$\alpha = \beta = \gamma = 90°$	tetragonal
4	$a = b \neq c$	$\alpha = \beta = 90°$ $\gamma = 120°$	hexagonal
5	$a = b = c$	$\alpha = \beta = \gamma \neq 90°$	rhombohedral ≡ trigonal
7	$\alpha = b = c$	$\alpha = \beta = \gamma = 90°$	cubic

The seven 3D crystal systems and 14 Bravais Lattices

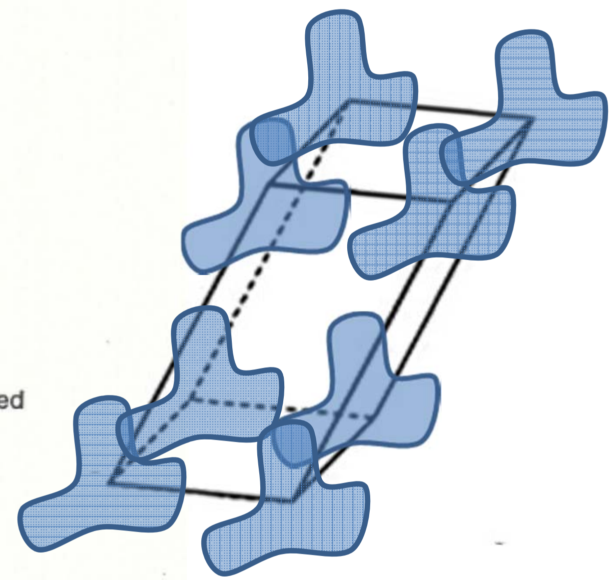


http://demonstrations.wolfram.com/TheSevenCrystalClasses/

Plus a possible Basis



= Final crystal structure

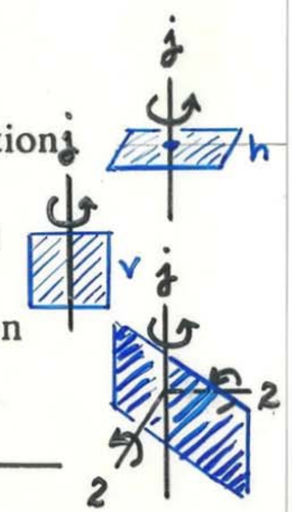


Final overall symmetry =
Translational Operations +
Basis Point Symmetry Operations

Table 2.2. The Schönflies point group symbols — one we'll use

	Symbol	Meaning
Classification according to rotation axes and principal mirror planes	C_j	(j = 2, 3, 4, 6) j-fold rotation axis
	S_j	j-fold rotation-inversion axis
	D_j	j two-fold rotation axes ⊥ to a (j-fold) principal rotation axis
	T	4 three- and 3 two-fold rotation axes as in a tetrahedron
	O	4 three- and 3 four-fold rotation axes as in an octahedron
	C_i	a center of inversion
	C_s	a mirror plane
Additional symbols for mirror planes	h	horizontal = perpendicular to the (main) rotation axis
	v	vertical = parallel to the main rotation axis
	d	diagonal = parallel to the main rotation axis in the plane bisecting the 2-fold rotation axes

5, 7, ... FOR MOLECULES, CLUSTERS
∞ FOR LINEAR MOLECULES



CRYSTAL STRUCTURE

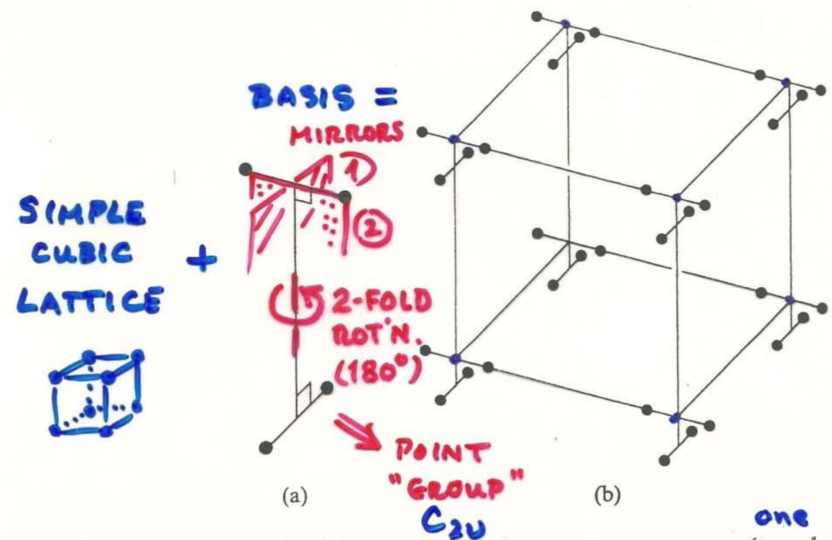


Fig. 1.9 (a) A basis which has a ~~D_{2d}~~ C_{2v} point group symmetry (~~two horizontal~~ one 2-fold axes plus two vertical reflection planes). (b) A simple tetragonal lattice with a basis having the ~~D_{2d}~~ C_{2v} point group.

GROUP = SET OF "SYMMETRY OPERATIONS" BRINGING OBJECT BACK INTO ITSELF

SYMMETRY OPERATIONS INCLUDE:

TRANSLATIONS BY $\bar{r} = n_1 a + n_2 b + n_3 c$

n_1, n_2, n_3 = INTEGERS

⇒ TRANSLATION GROUP

+ OPERATIONS ON BASIS ALONE THRU CTR. OF MASS

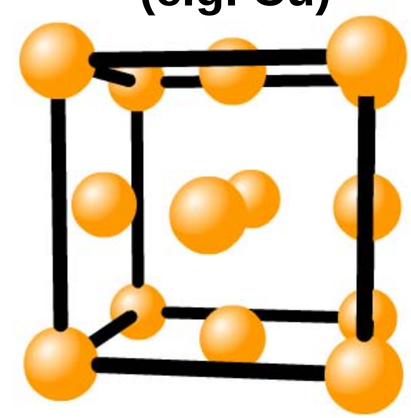
- ROTATION BY $2\pi/n$
- REFLECTION IN A PLANE
- INVERSION ($\bar{r} \to -\bar{r}$)

⇒ POINT GROUP

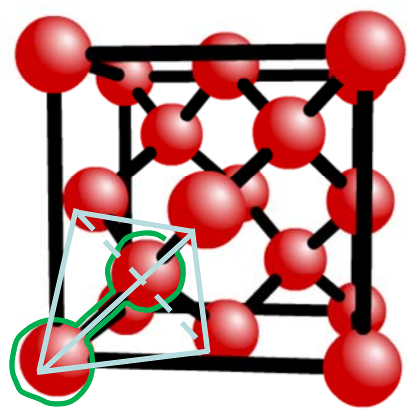
SPACE GROUP = TRANS. GRP. × POINT GRP

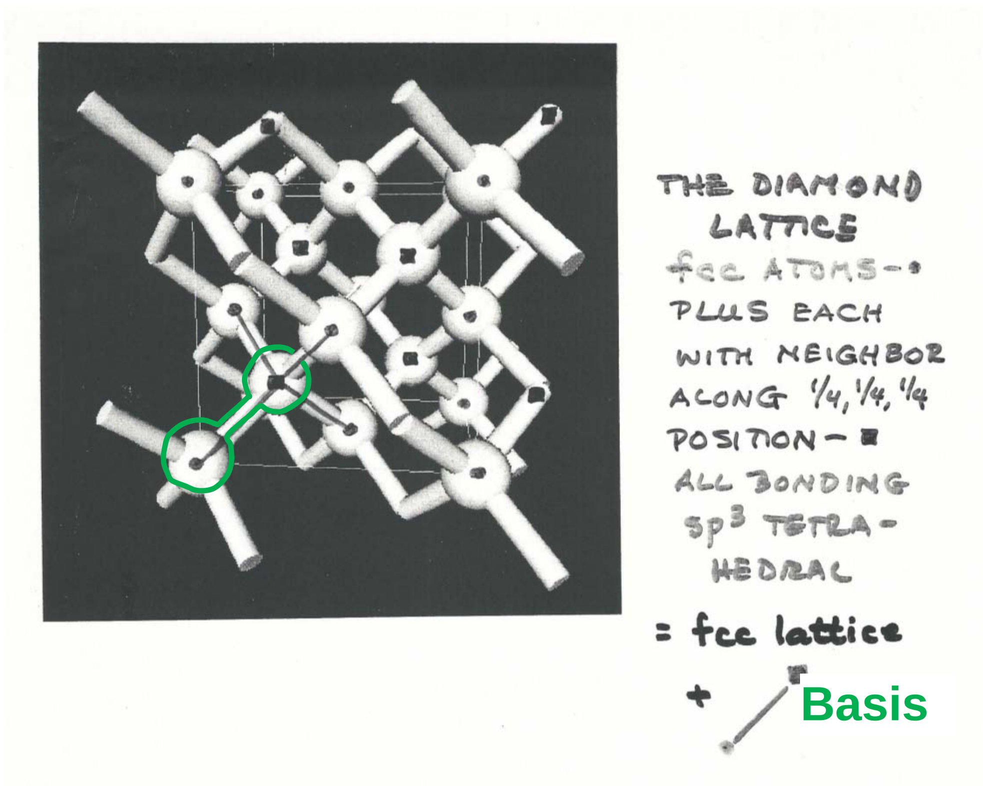
Ordered packing of atoms in solids

Face-centered cubic (e.g. Cu)



Diamond (e.g., C, Si, Ge)

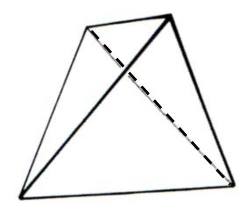




Good websites/downloads for simple structures: http://www.dawgsdk.org/crystal/en/library/fcc#0002

http://demonstrations.wolfram.com/CrystalViewer/

Tetrahedron



And another website for various structures, orbitals, etc: http://www.chemtube3d.com/solidstate/_simplecubic(final).htm

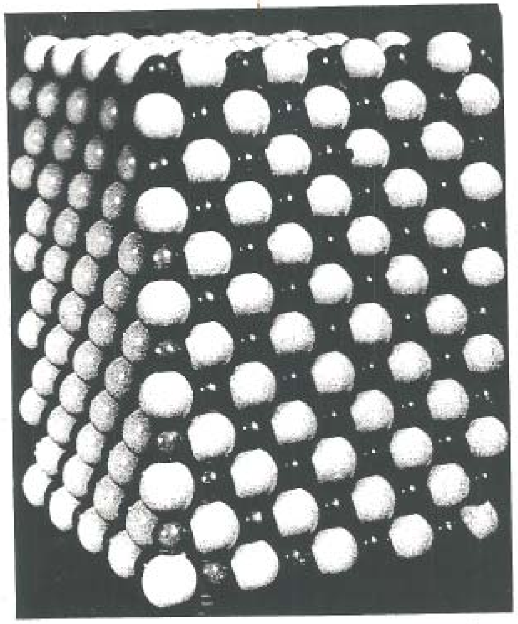


Figure 23 Model of sodium chloride. The sodium ions are smaller than the chlorine ions. (Courtesy of A. N. Holden and P. Singer, from *Crystals and crystal growing*.)

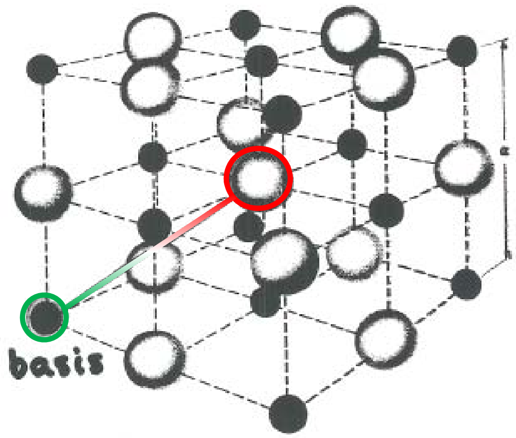


Figure 24 The sodium chloride crystal structure. The Bravais lattice is fcc, and the basis has one Na^+ ion at 0 0 0 and one Cl^- ion at $\frac{1}{2}\frac{1}{2}\frac{1}{2}$.

NaCl

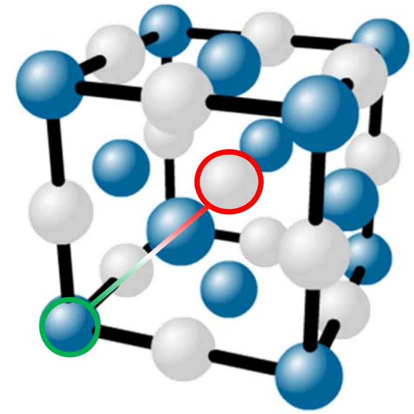


Figure 25 Natural crystals of lead sulfide, PbS, which has the NaCl crystal structure. (Photograph by Betsy Burleson.)

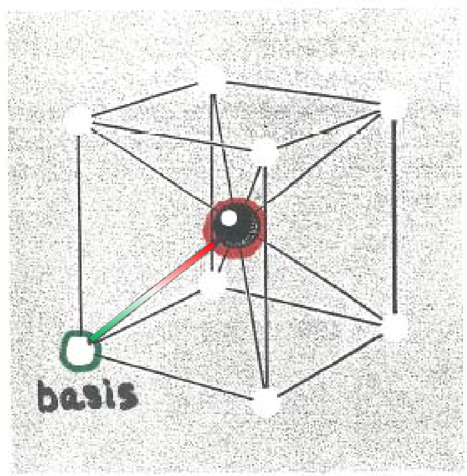
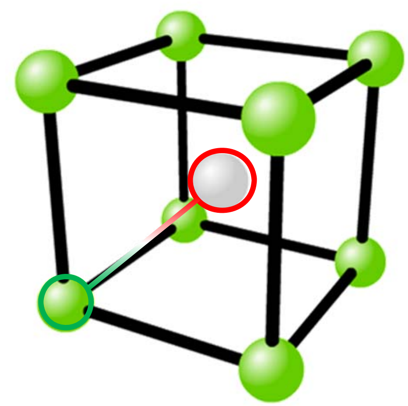
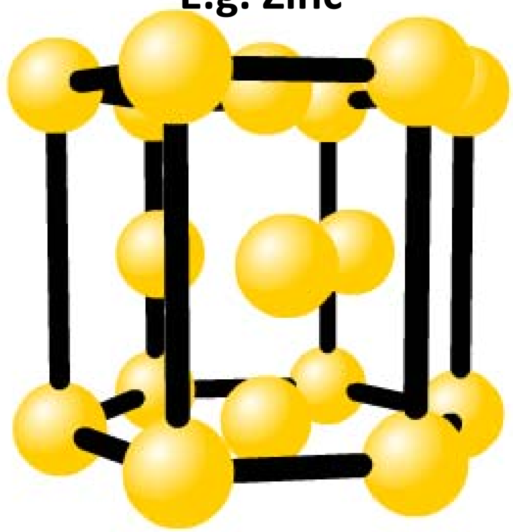


Figure 26 The cesium chloride crystal structure. The Bravais lattice is simple cubic, and the basis has one Cs^+ ion at 0 0 0 and one Cl^- ion at $\frac{1}{2}\frac{1}{2}\frac{1}{2}$.

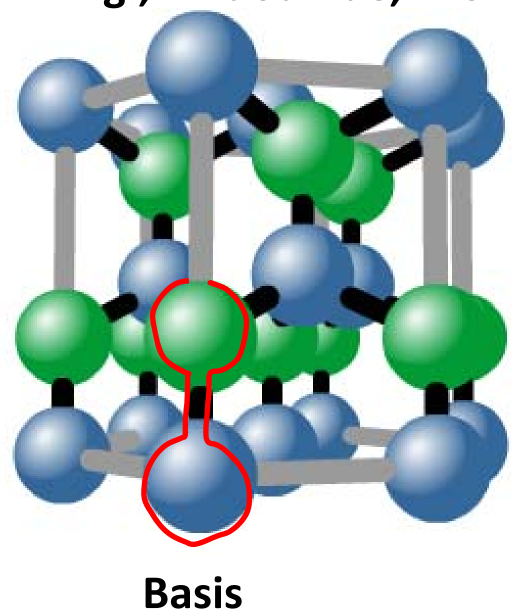
CsCl



Hexagonal close-packed
E.g. Zinc

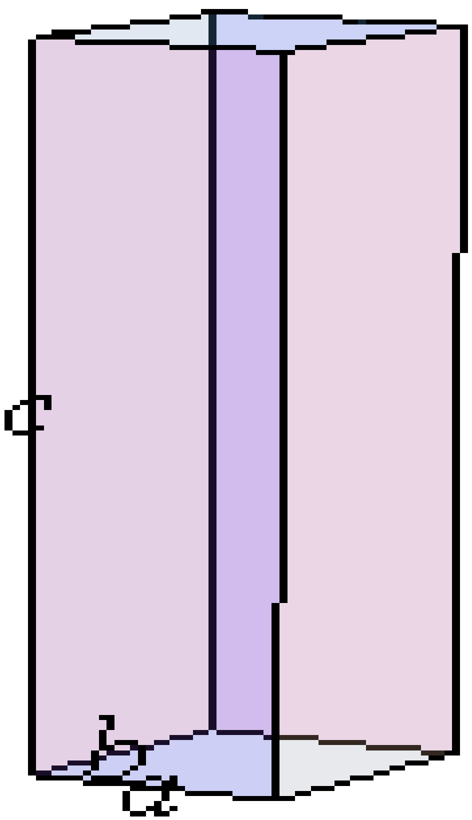


Wurzite
E.g., Zinc Sulfide, ZnS

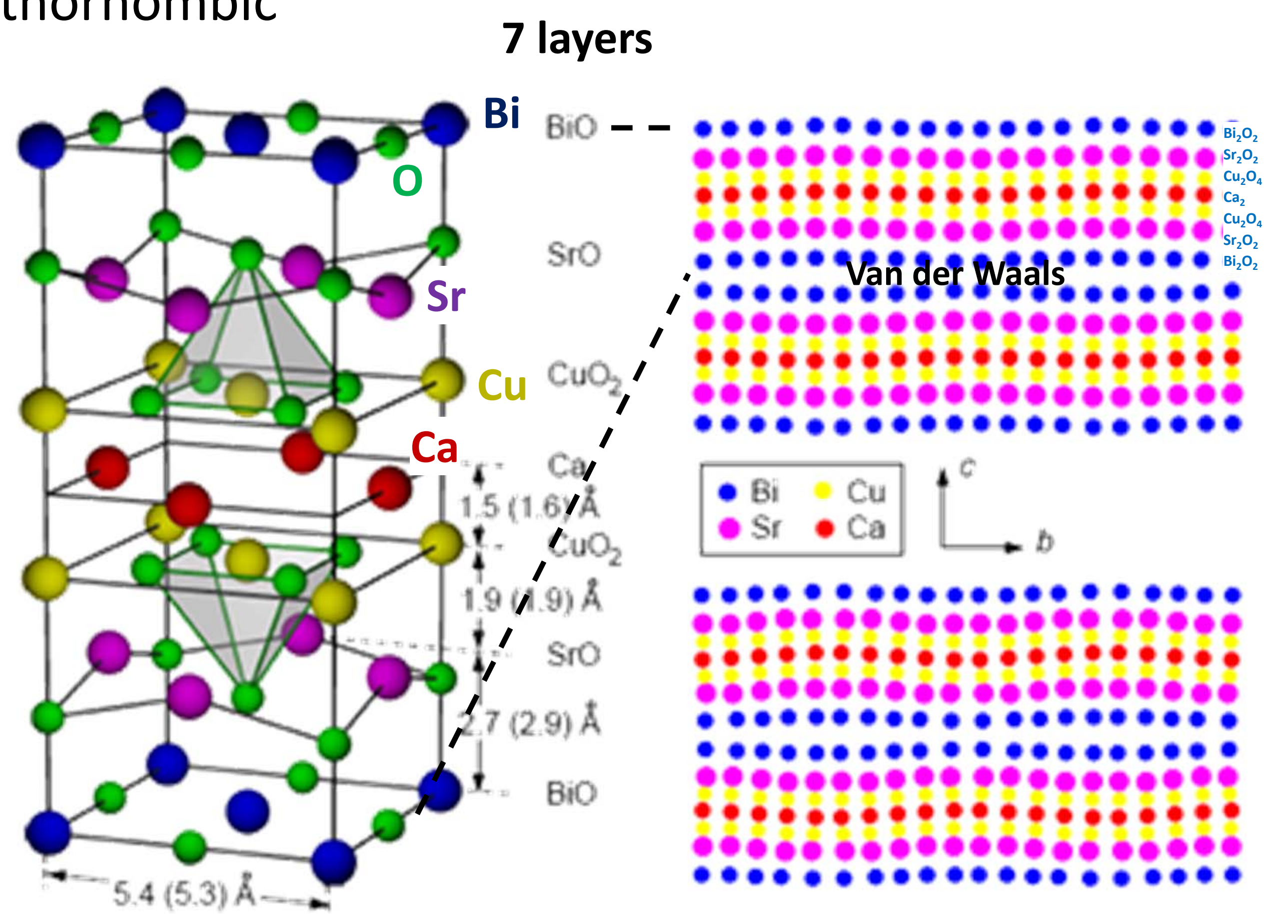


A high-temperature superconductor: $Bi_2Sr_2CaCu_2O_{8+x}$ ("BSSCO")

Simple Orthorhombic

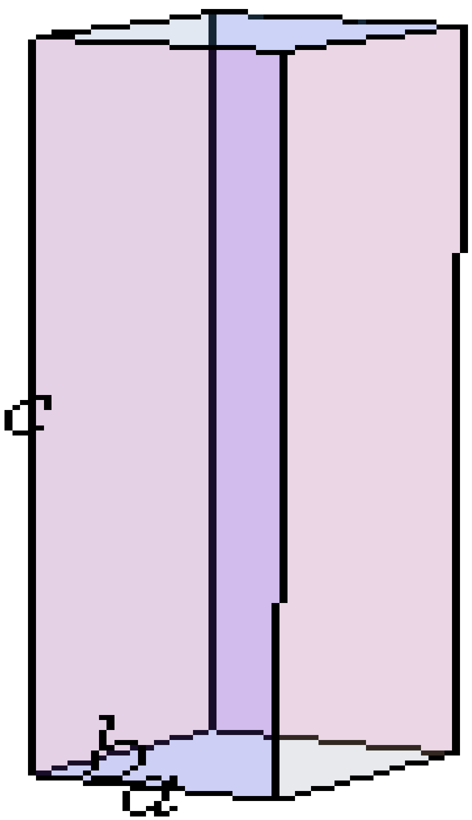


$a = b$

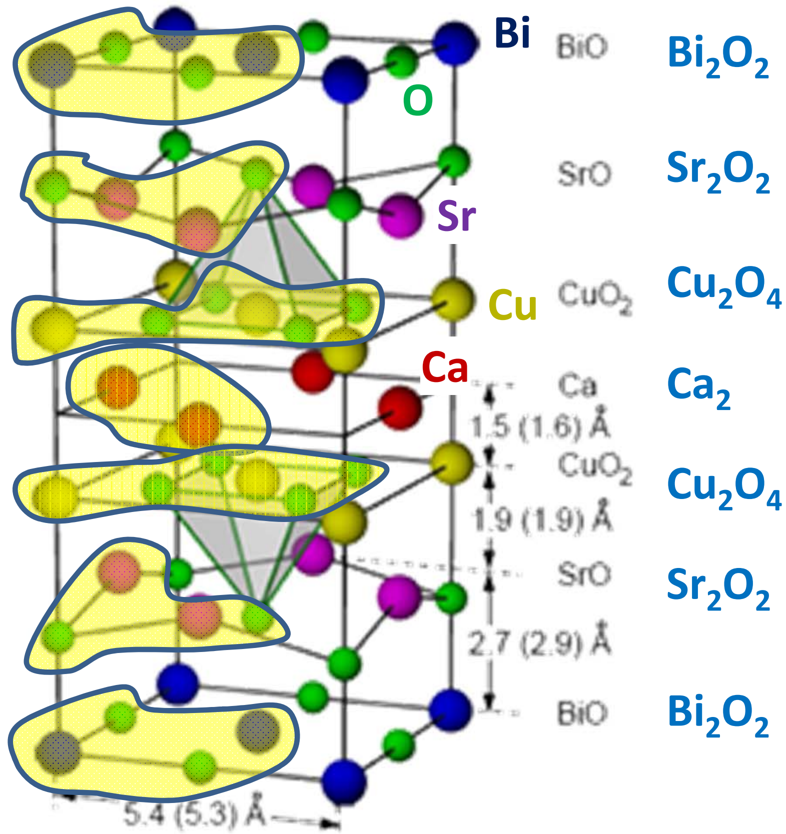


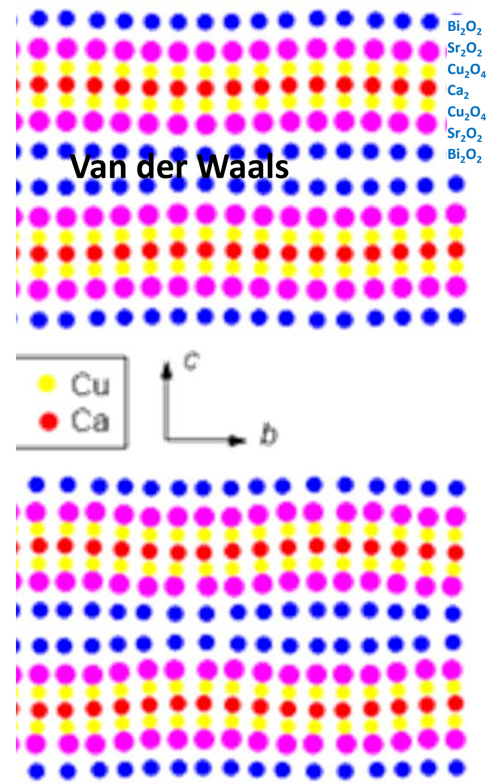
A high-temperature superconductor: $Bi_2Sr_2CaCu_2O_{8+x}$ (“BSSCO”)

Simple Orthorhombic



$a = b$





The Basis: $Bi_4Sr_4Ca2Cu_4O_{16+x}$

Electrons in crystalline solids—are everywhere

For all states in crystalline (ordered) solids:

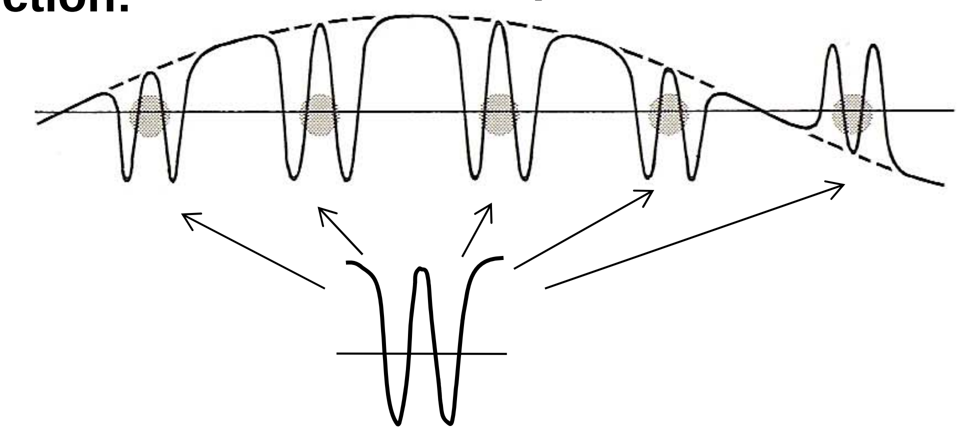
$$\Psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})e^{i\vec{k}\bullet\vec{r}}, \textit{ where } u_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r}+\vec{A}), \textit{ this is a "Bloch function"}$$

with probability density of

$$\Psi_{\vec{k}}^*(\vec{r})\Psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}^*(\vec{r})e^{-i\vec{k}\bullet\vec{r}}u_{\vec{k}}(\vec{r})e^{i\vec{k}\bullet\vec{r}} = u_{\vec{k}}(\vec{r})^2, \textit{ the same on every atom!}$$

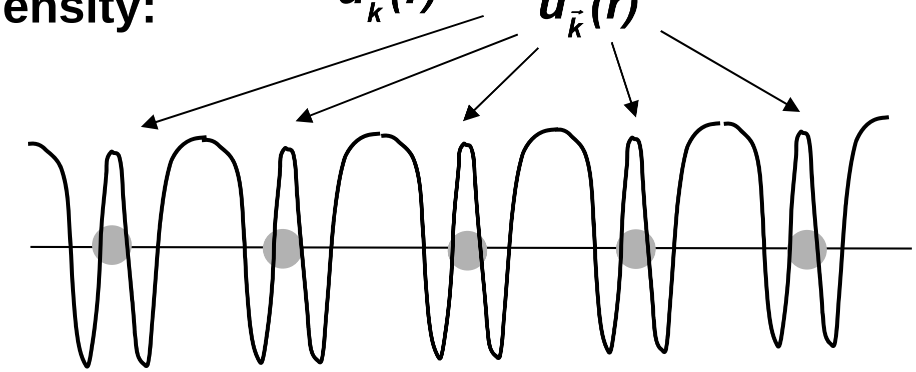
A typical Bloch function:

Re or Im part of $e^{i\vec{k}\bullet\vec{r}}$ ***: coskr or sinkr***



And its probability density:

$u_{\vec{k}}(\vec{r})$ $u_{\vec{k}}(\vec{r})^2$



Omar, Sections 5.1-5.3

For many cases, we can again use atomic orbitals as the basis functions: theTight Binding Model

Recall for a molecule:

$$\varphi_j^{MO}(\vec{r}) = \sum_{\substack{\text{Atoms } A \\ \text{Orbitals } i}}^{N} C_{Ai,j}\,\varphi_{Ai}^{AO}(\vec{r} - \vec{R}_A)$$

For a solid with N atoms: (Omar, Section 5.8)

$$\varphi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})e^{i\vec{k}\bullet\vec{r}} = \sum_{\substack{\text{Atoms } A \\ \text{Orbitals } i}}^{N} e^{i\vec{k}\bullet\vec{R}_A} C_{Ai,\vec{k}}\,\varphi_{Ai}^{AO}(\vec{r} - \vec{R}_A)$$

Is it Bloch?

$$= e^{i\vec{k}\bullet\vec{r}} \sum_{\substack{\text{Atoms } A \\ \text{Orbitals } i}}^{N} e^{-i\vec{k}\bullet(\vec{r}-\vec{R}_A)} C_{Ai,\vec{k}}\,\varphi_{Ai}^{AO}(\vec{r} - \vec{R}_A)$$

Yes!

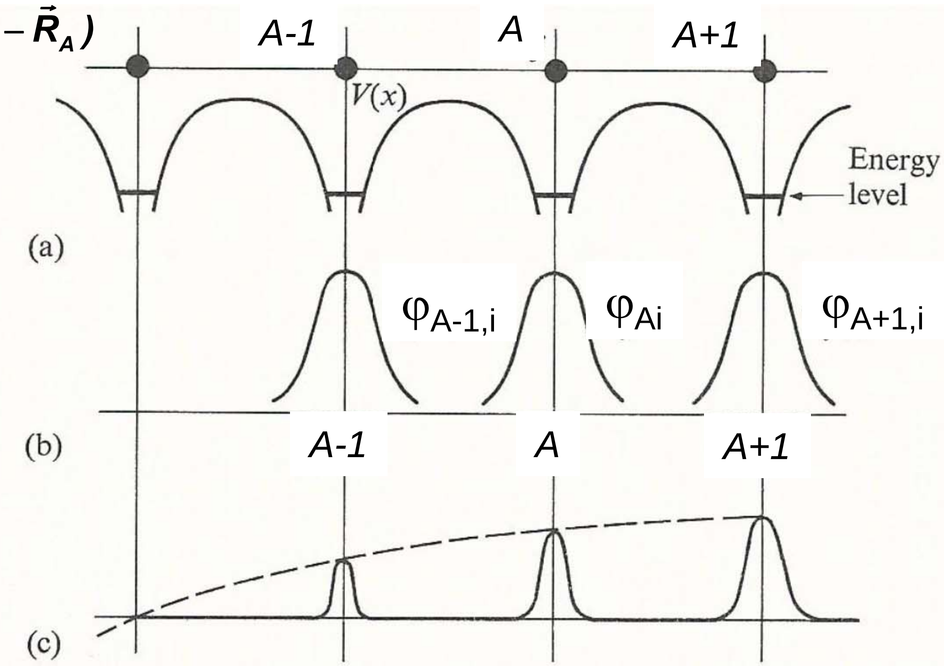
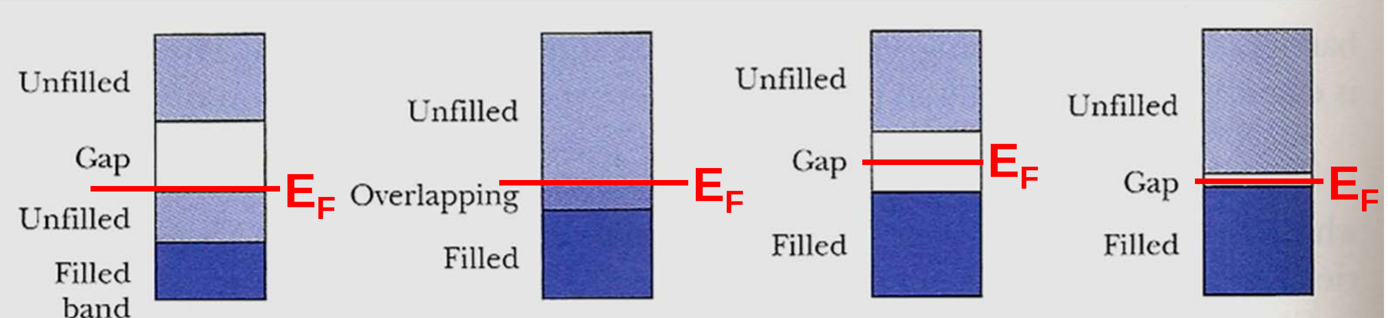


Fig. 5.14 The tight-binding model. (a) The crystal potential. (b) The atomic wave functions. (c) The corresponding Bloch function.

The types of band structures-by conductive behavior

Figure 11.6 Possible band structures: (a) a conductor with an unfilled valence band, (b) a conductor with overlapping valence and conduction bands (a semimetal), (c) an insulator due to its large band gap, and (d) a semiconductor (due to its small band gap).

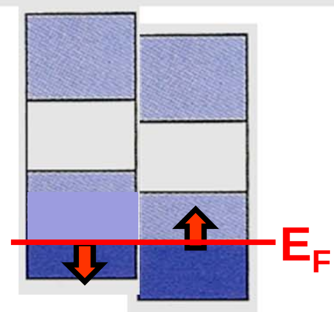


(a) Conductor (unfilled valence band)

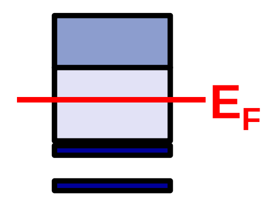
(b) Semimetal (overlapping bands)

(c) Insulator (large band gap)

(d) Semiconductor (small band gap)



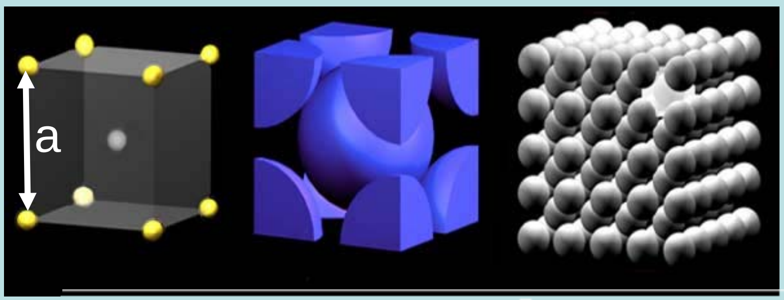
(e)
Spin-down Spin-up
Ferromagnetic Conductor
(The exchange interaction)

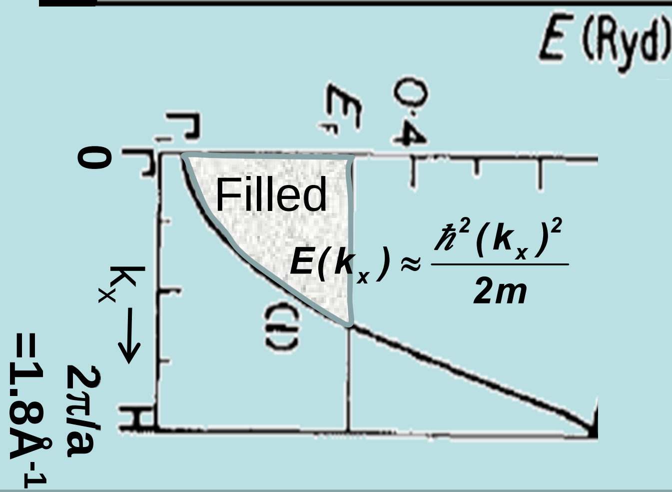


(f)
Ionic solid:
Very narrow atomic/ionic filled bands

Electronic bands and density of states for “free-electron” metals-
Rydberg = 13.605 eV

Lithium—bcc, a = 3.49 Å
$1s^2 2s^1$



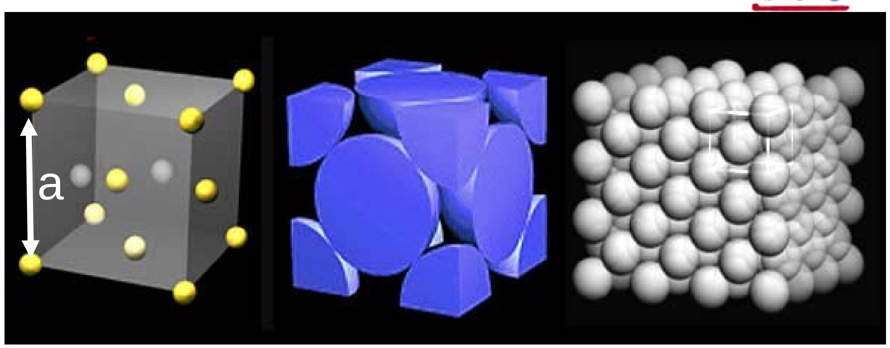


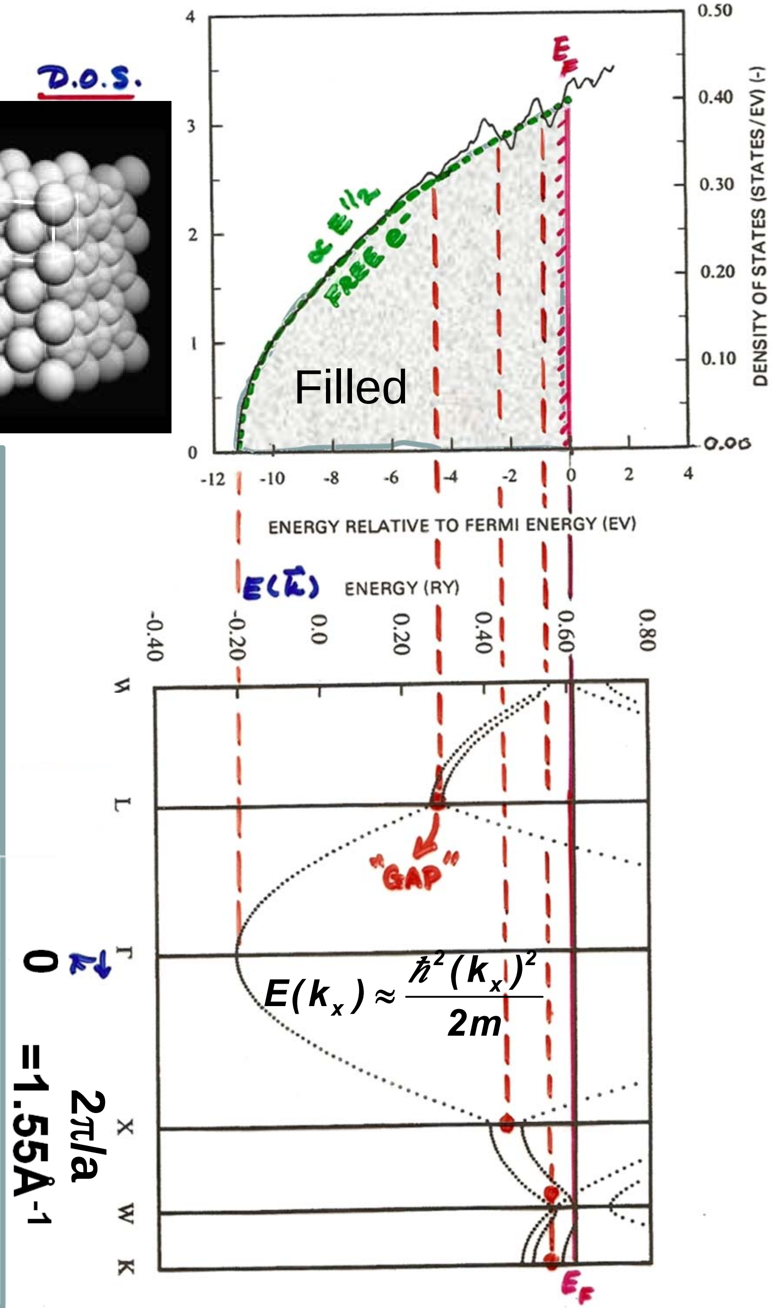
Ryd = 13.6 eV

Electronic bands and density of states for “free-electron” metals-

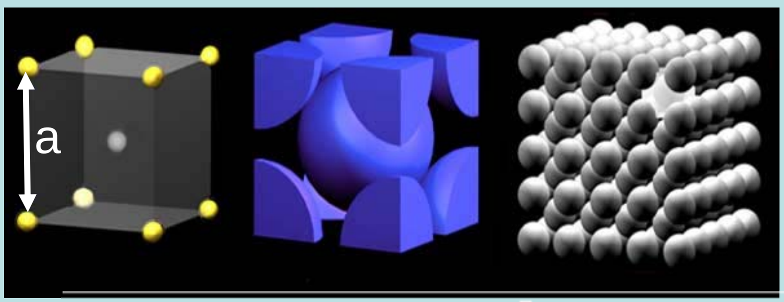
Rydberg = 13.605 eV

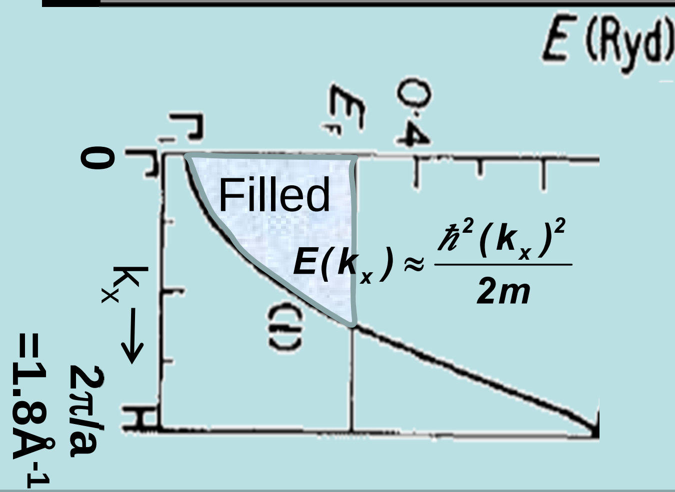
Aluminum—fcc,
a = 4.05 Å
$1s^2 2s^2 2p^6 3s^2 3p^1$





Lithium—bcc, a = 3.49 Å
$1s^2 2s^1$





Ryd = 13.6 eV

Electronic bands and density of states for a transition metal-Copper

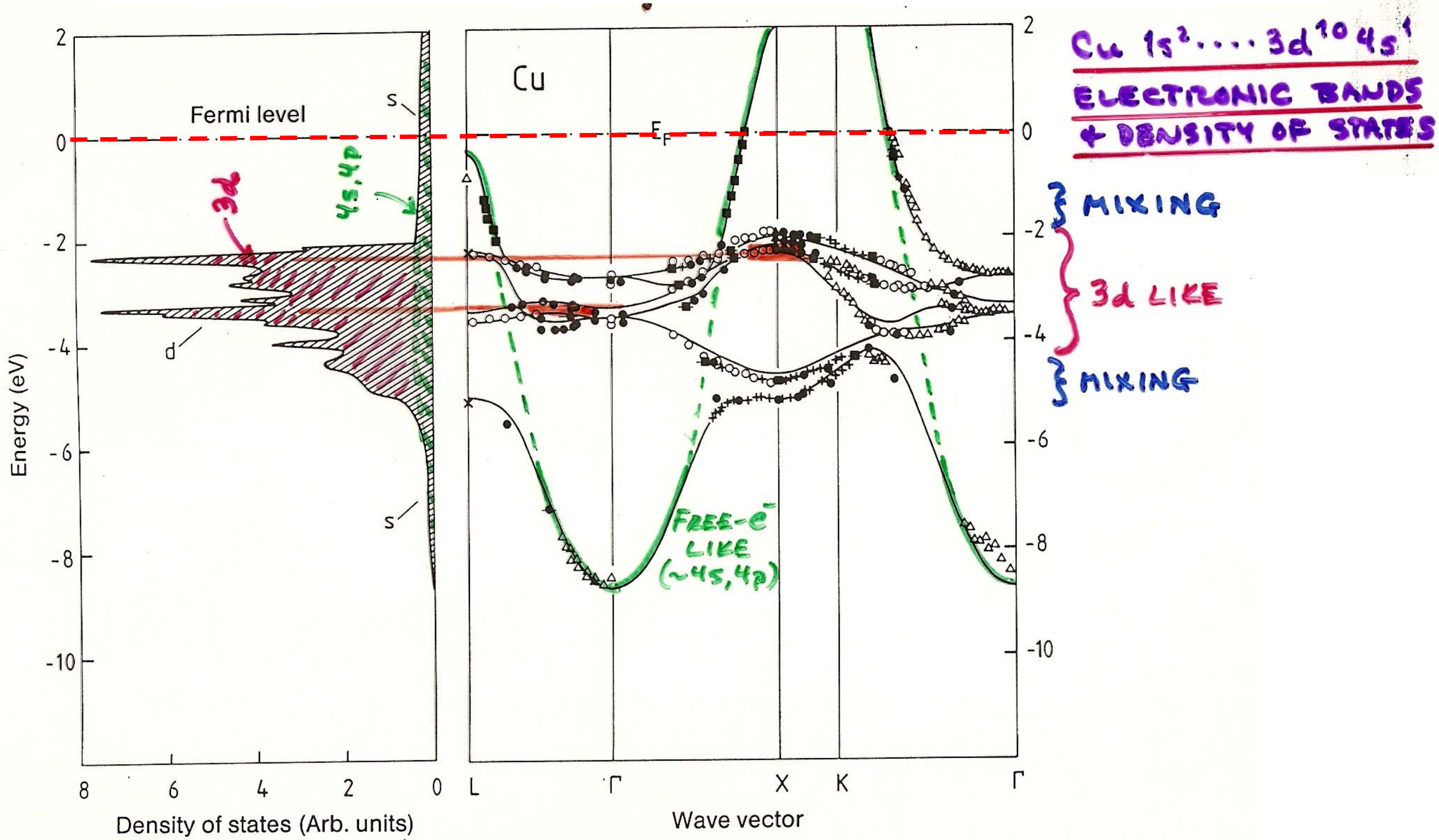
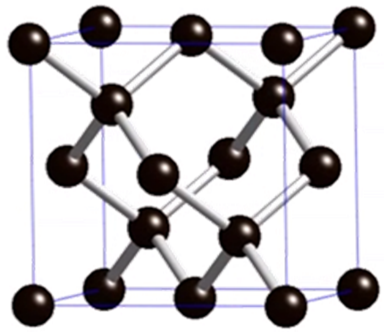
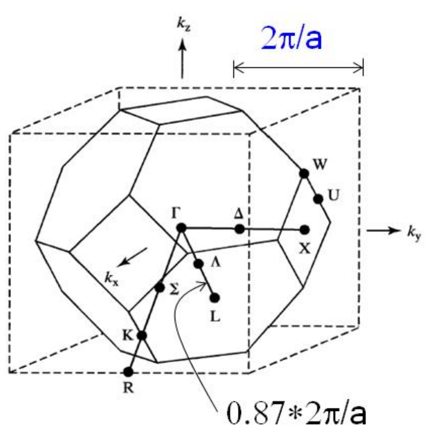


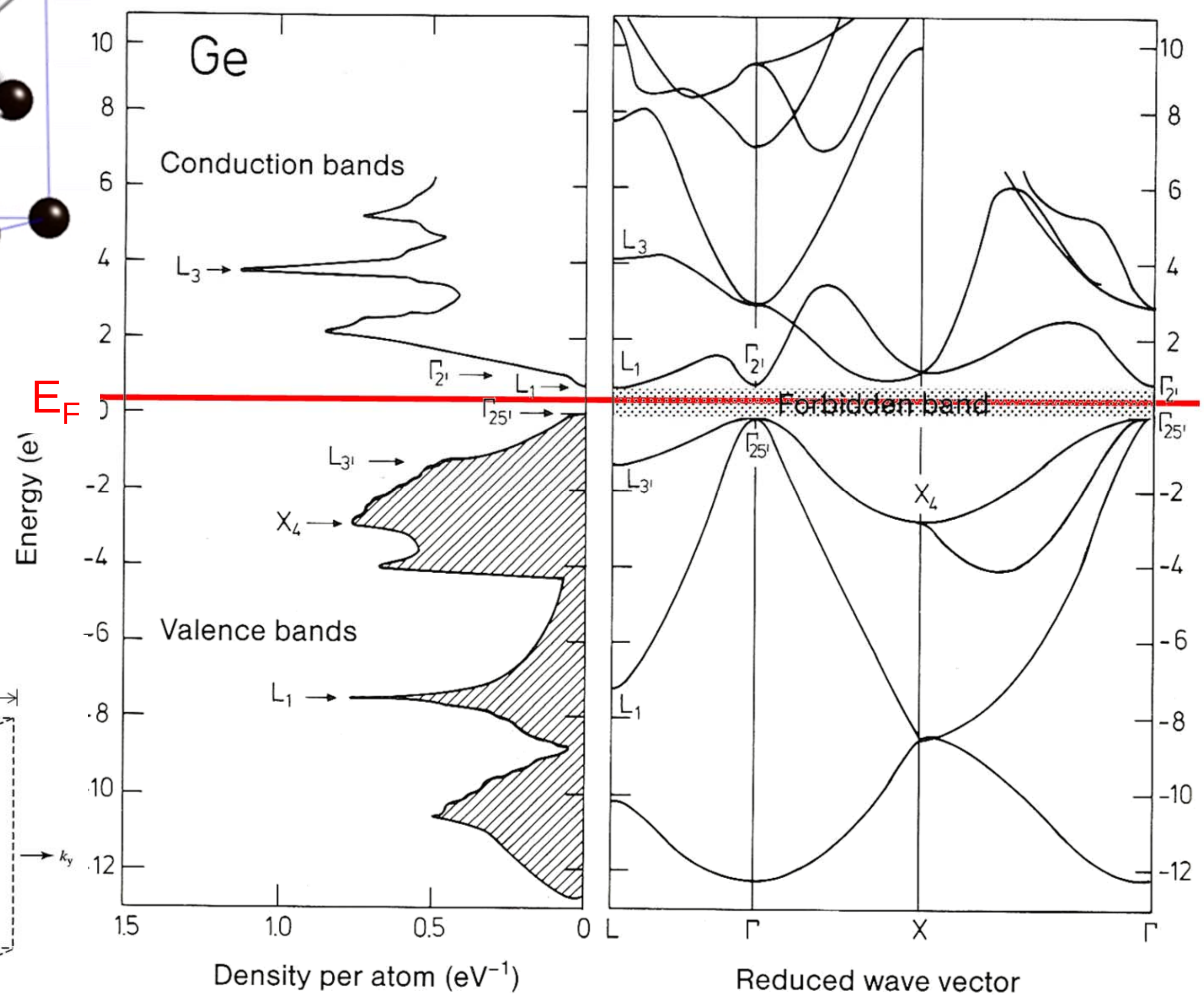
Fig. 7.12. Bandstructure $E(k)$ for copper along directions of high crystal symmetry (*right*). The experimental data were measured by various authors and were presented collectively by Courths and Hüfner [7.4]. The full lines showing the calculated energy bands and the density of states (*left*) are from [7.5]. The experimental data agree very well, not only among themselves, but also with the calculation

Electronic bands and density of states for a semiconductor-Germanium—
$1s^2 2s^2\ 2p^6 3s^2\ 3p^6 3d^{10} 4s^2 4p^2$



Diamond Structure = fcc + 2-atom basis





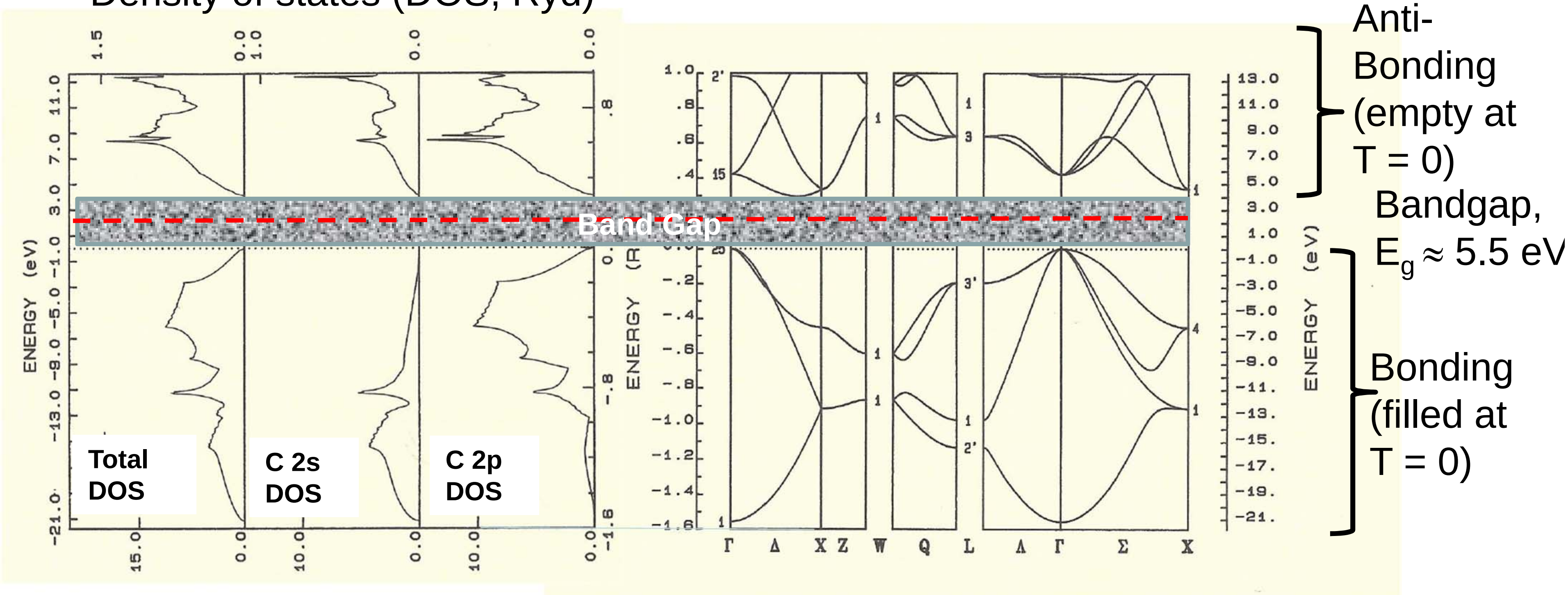
Anti-Bonding (empty at T = 0)

Bandgap, $E_g \approx 0.7$ eV

Bonding (filled at T = 0)

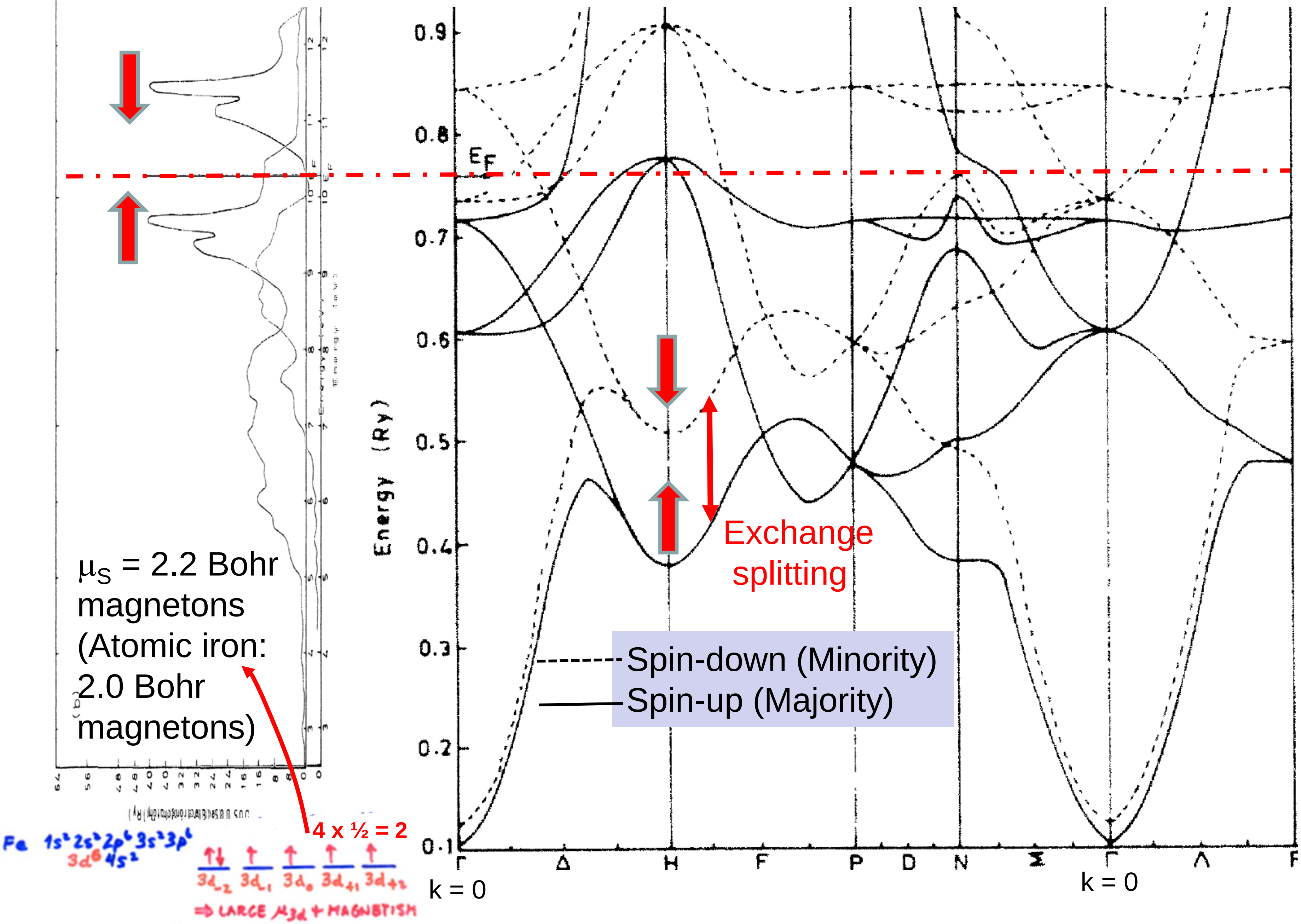
Electronic bands and density of states for an insulator-Carbon: Diamond—$1s^2 2s^2 2p^2$

Density of states (DOS, Ryd)

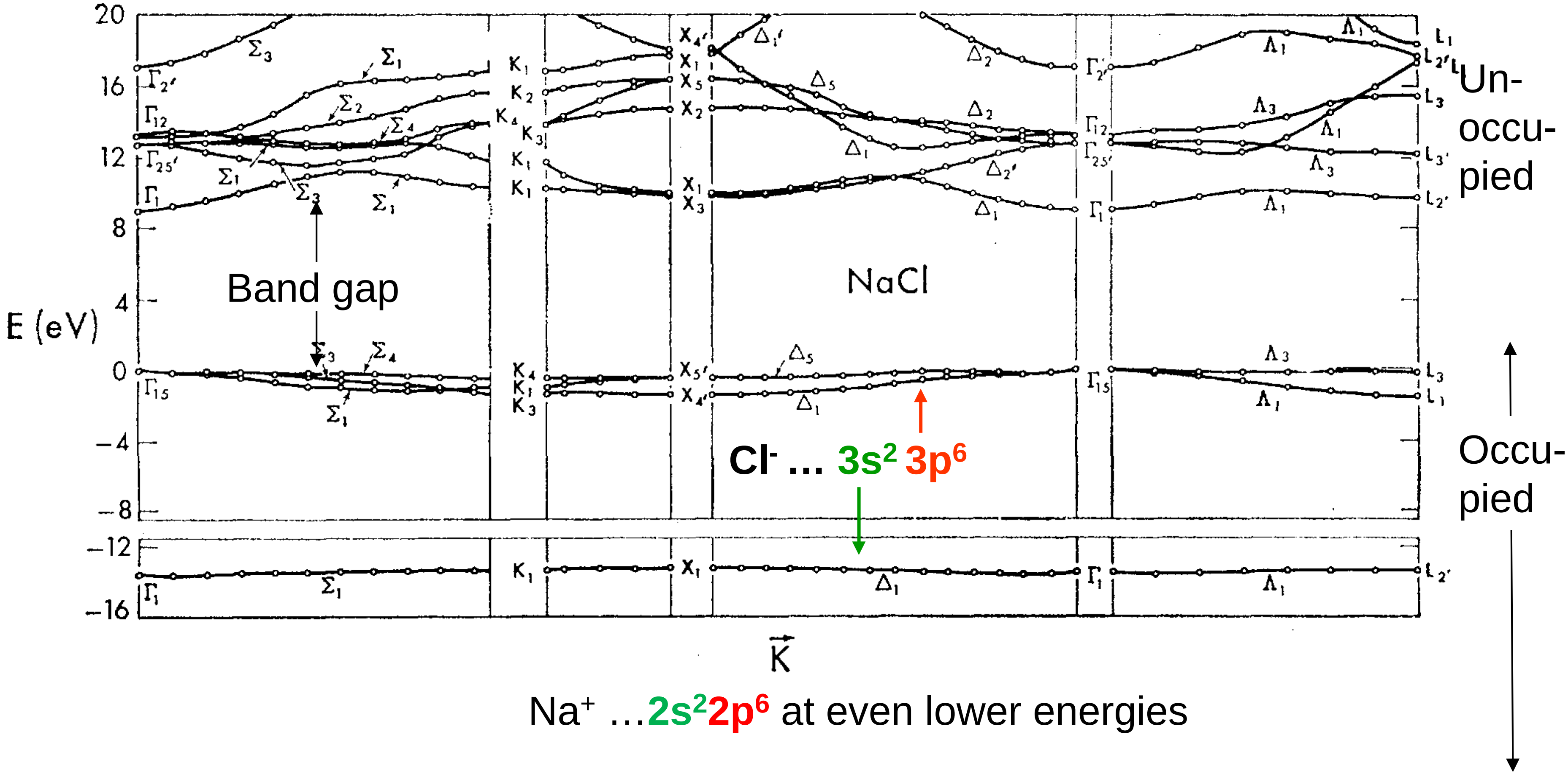


Density of states (DOS, eV)

The electronic bands and densities of states of metallic ferromagnetic iron (face-centered cubic)



Ionic solids—another limit: e.g NaCl
The band structure



Na^{+} …$2s^2 2p^6$ at even lower energies

Flat bands→ Highly localized, immobile electrons

ELASTIC SCATTERING OF LIGHT BY AN ATOM:

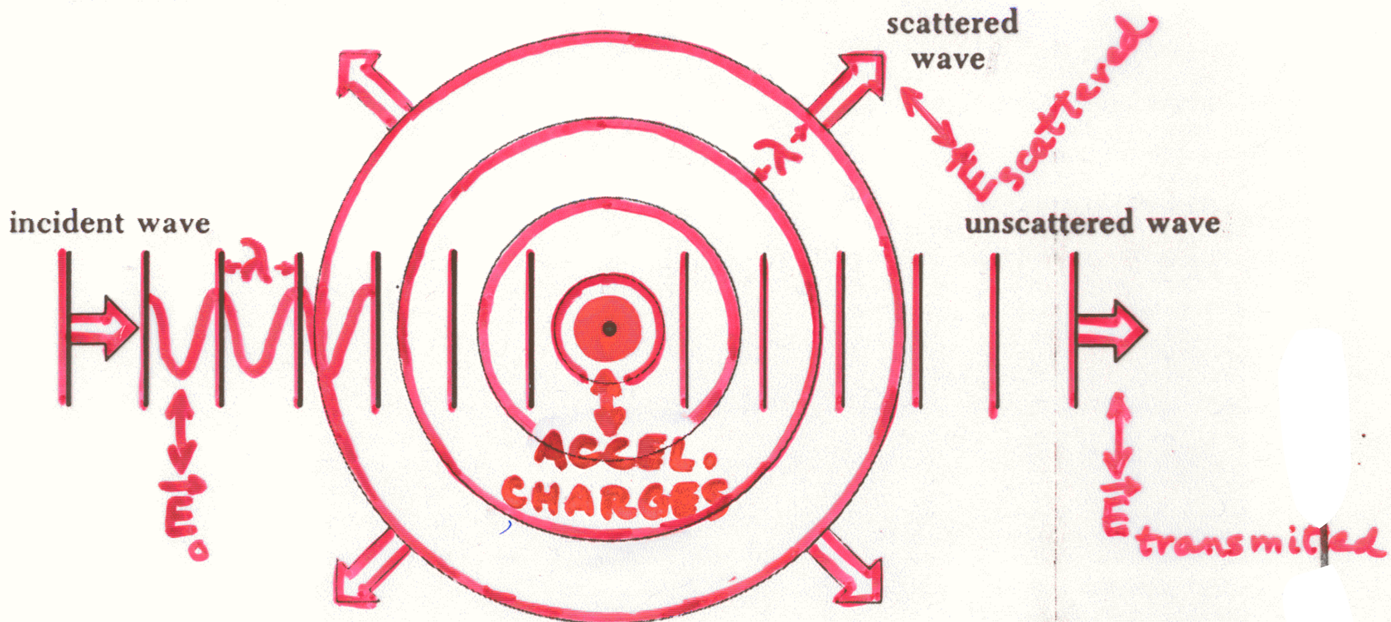
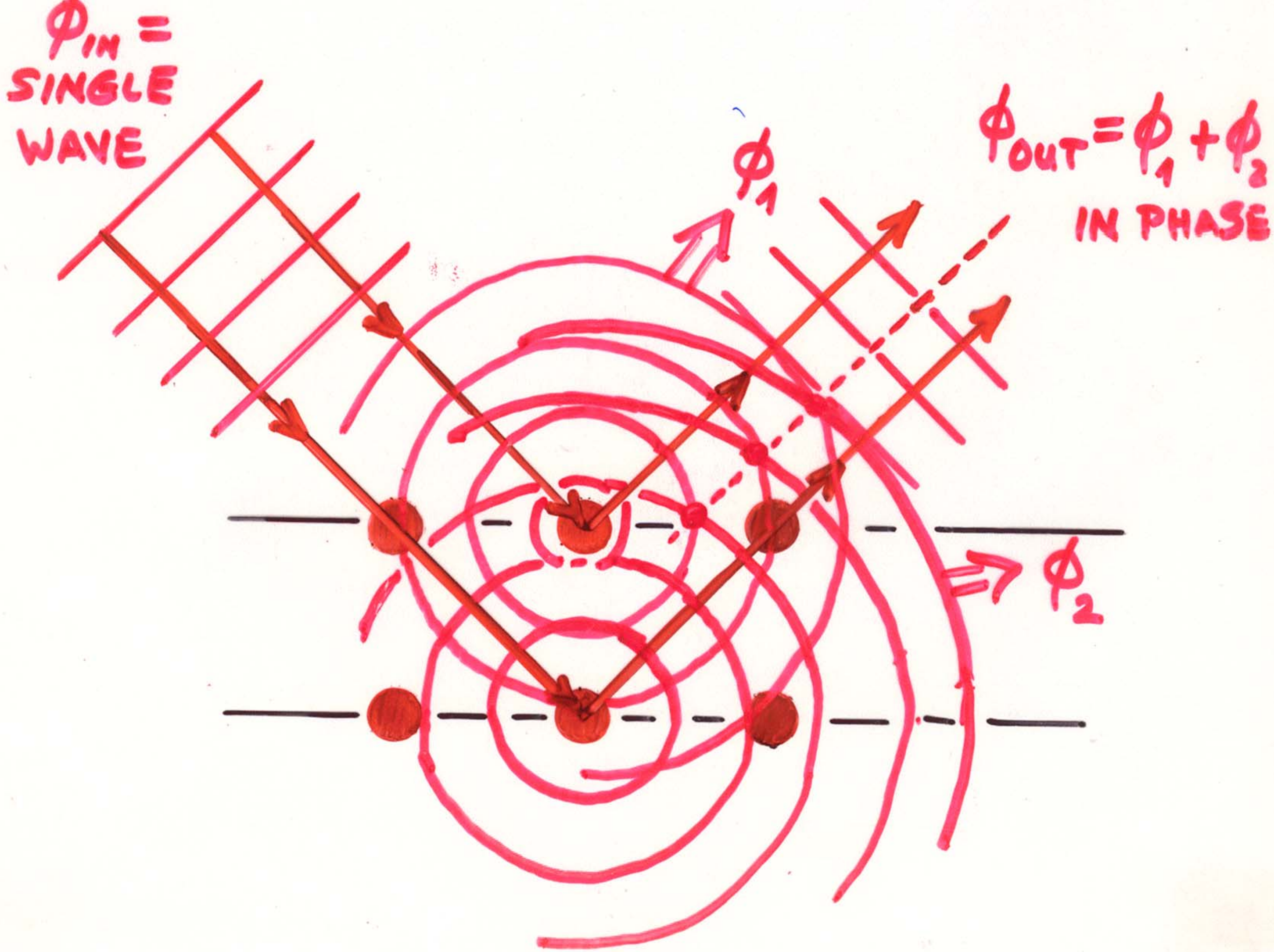
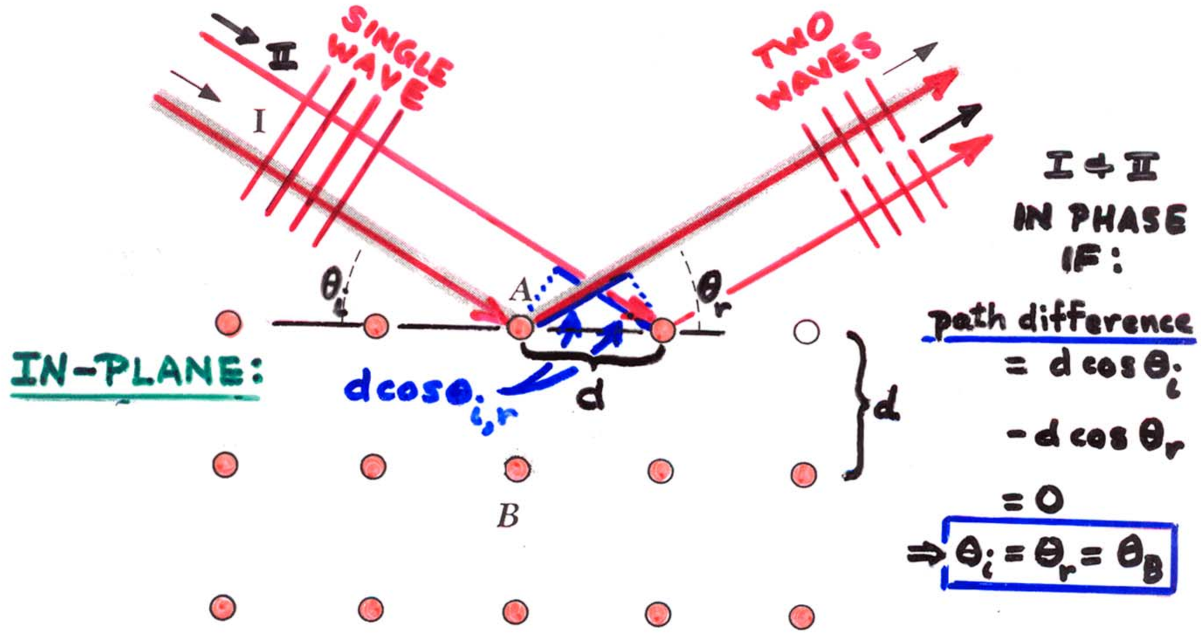
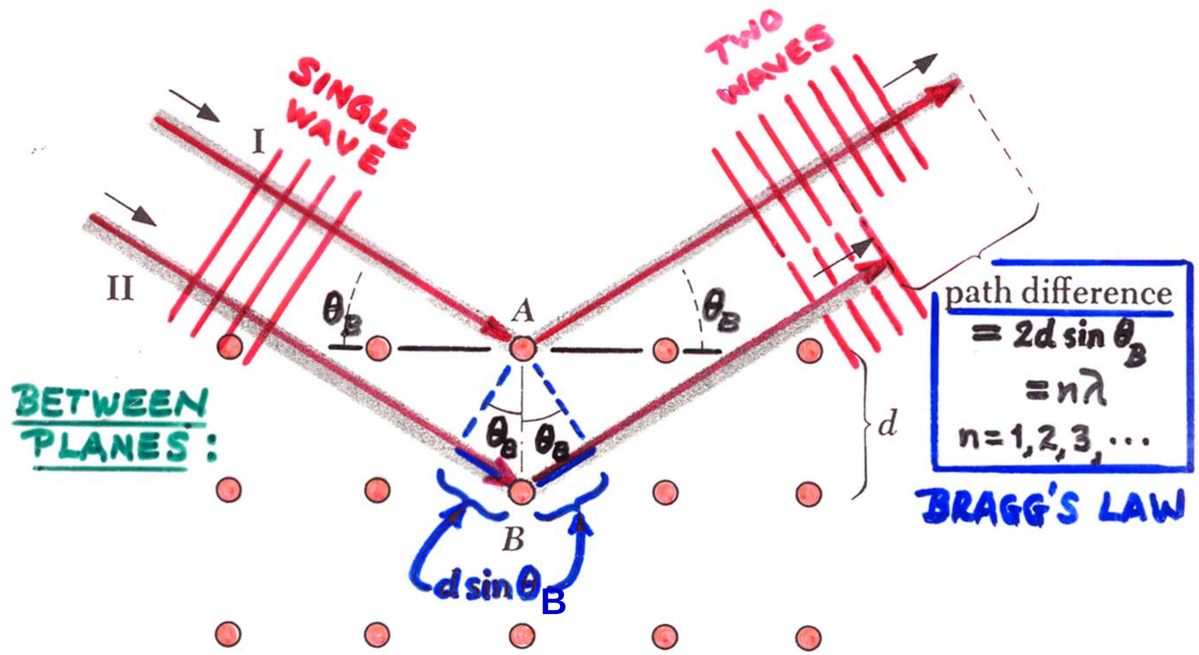


FIGURE 2.15 The scattering of electromagnetic radiation by a group of atoms. Incident plane waves are reemitted as spherical waves.

BRAGG SCATTERING FROM A CRYSTAL:

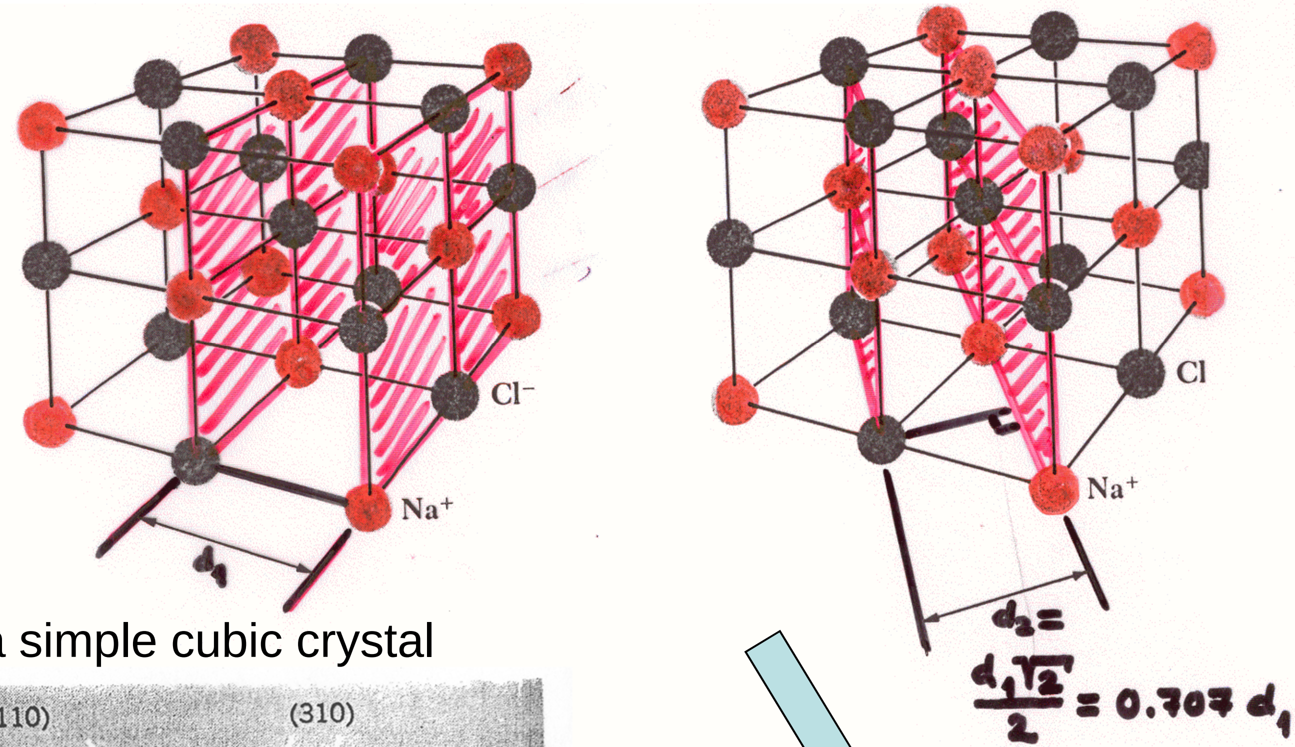




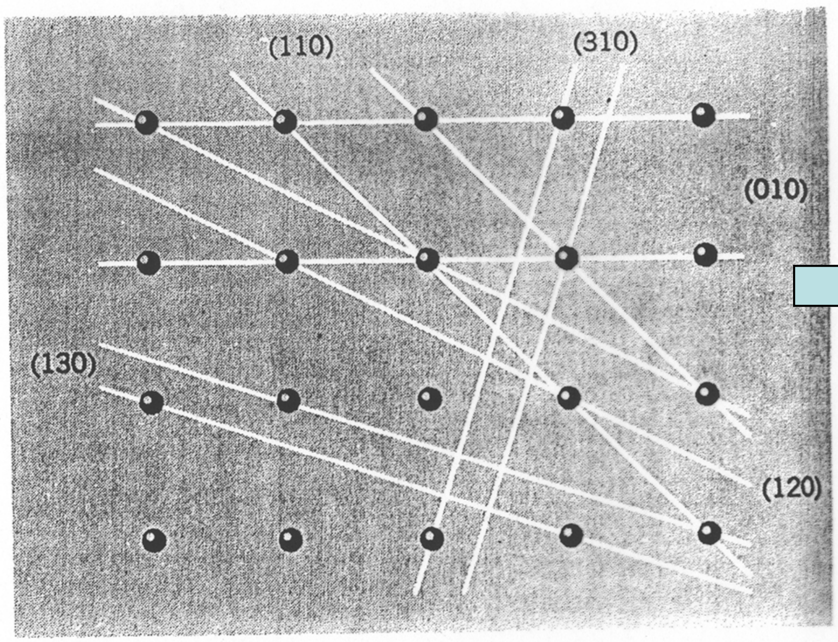


X-ray scattering from a cubic crystal.

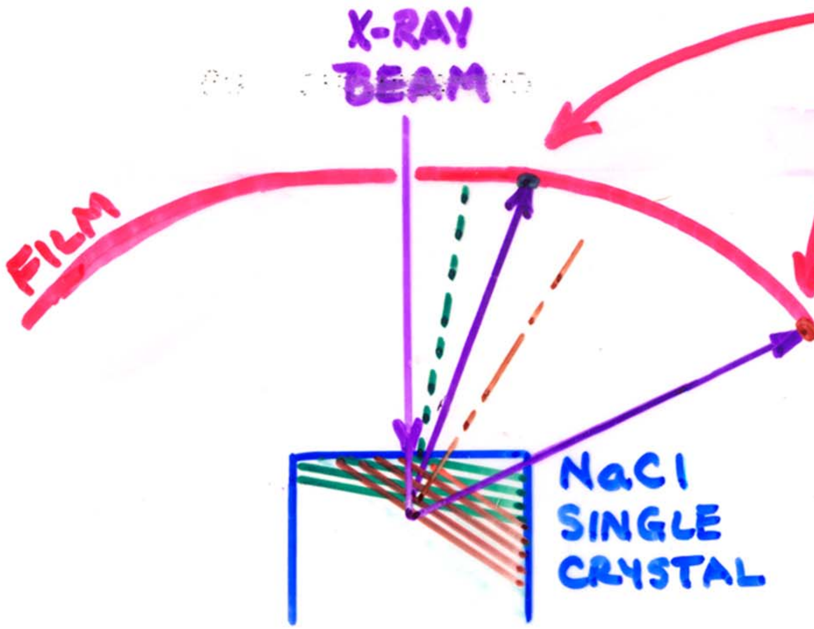
Two sets of atomic planes in a sodium chloride crystal

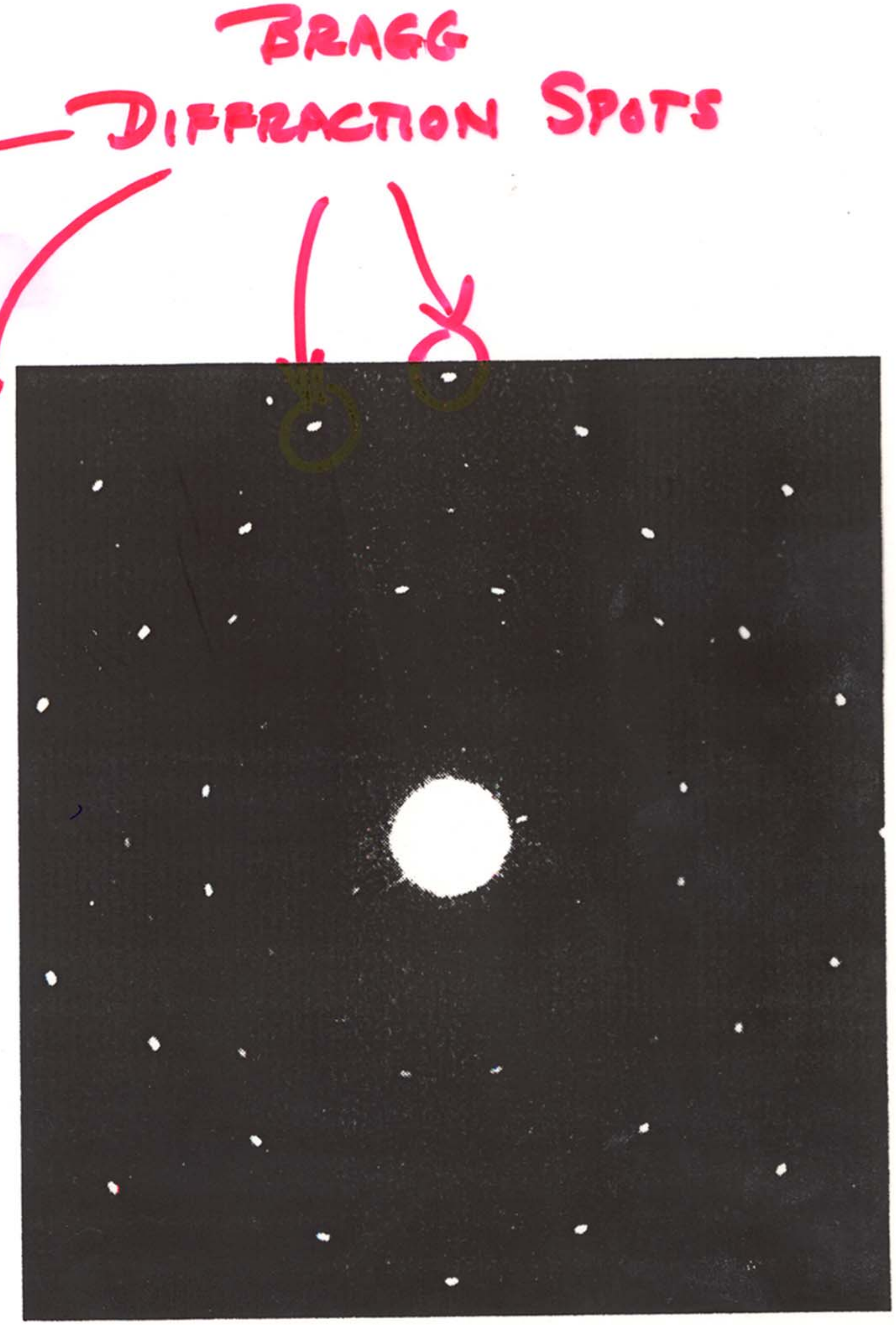


Planes in a simple cubic crystal



Many sets of planes to diffract from
In any crystal, some stronger than others





The interference pattern produced by the scattering of x-rays from ions in a crystal of sodium chloride. The bright spots are the places where x-rays scattered from various layers in the crystal come in step. The cubic pattern of the sodium chloride lattice is suggested by the fourfold symmetry of the x-ray photograph.

Atomic planes and Miller Indices:

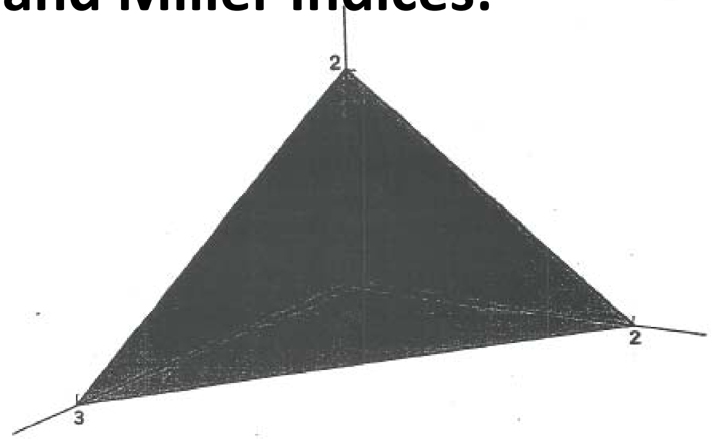


Figure 20 This plane intercepts the a, b, c axes at 3a, 2b, 2c. The reciprocals of these numbers are $\frac{1}{3}, \frac{1}{2}, \frac{1}{2}$. The smallest three integers having the same ratio are 2, 3, 3, and thus the Miller indices of the plane are (233).

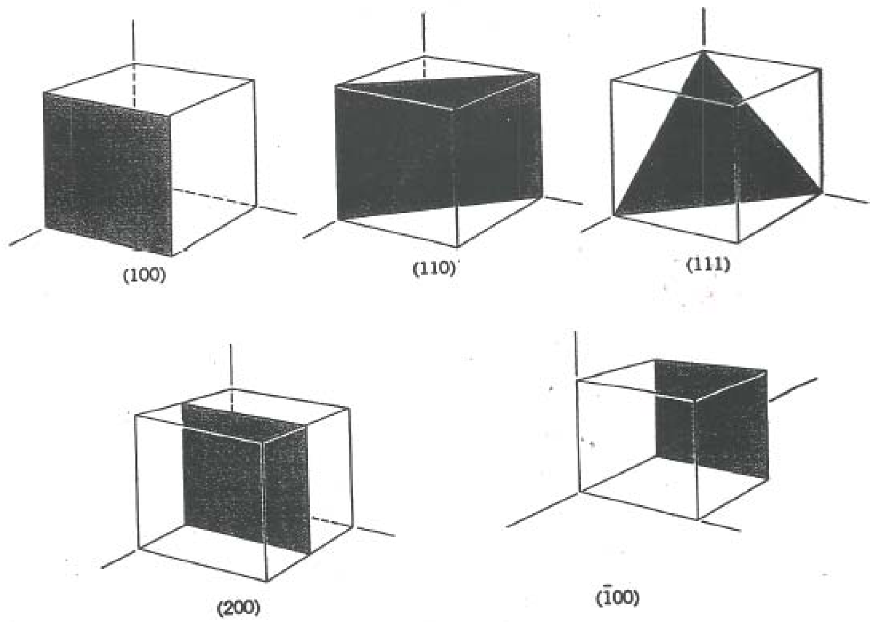


Figure 21 Miller indices of some important planes in a cubic crystal. The plane (200) is parallel to (100).

Spacing between planes with $\alpha = \beta = \gamma = 90^\circ$ given by:

$$d_{hk\ell} = \frac{n}{\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{\ell^2}{c^2}\right]^{1/2}}$$