

Crystal structures

Crystal Structure

Atoms are arranged in a periodic pattern in a crystal.

The atomic arrangement affects the macroscopic properties of a material.

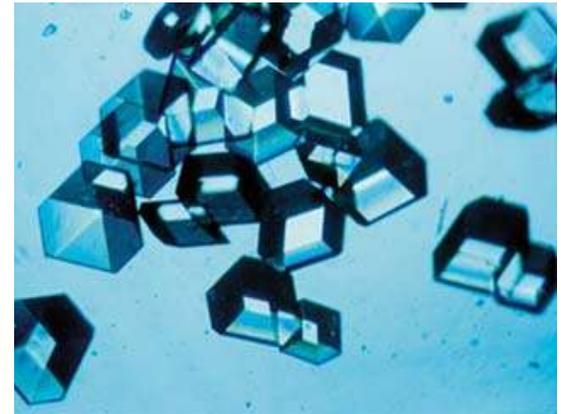
Many important materials (silicon, steel) are crystals



Gallium crystals

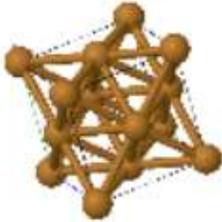


quartz



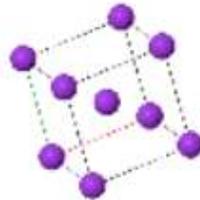
Insulin crystals

Crystal structures



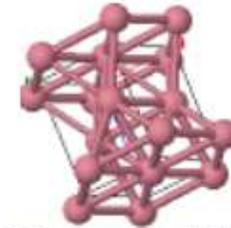
Face Centered
Cubic

Al, Cu, Ni, Ag, Pt, Au,
Pb



Body Centered
Cubic

W, Cr, Fe, Mo, Ta



Hexagonal Close
Packed

Ti, Co, Zn, Zr



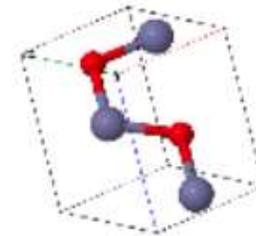
Diamond

C, Si, Ge, α -Sn



Zincblende

GaAs, InP, GaP, InAs,
AlAs



Wurtzite

ZnO, GaN, AlN, CdSe

Miller indices: Crystal planes

$$[hkl] = \text{vector in direction } h\vec{a}_1 + k\vec{a}_2 + l\vec{a}_3$$

[] specific direction

< > family of equivalent directions

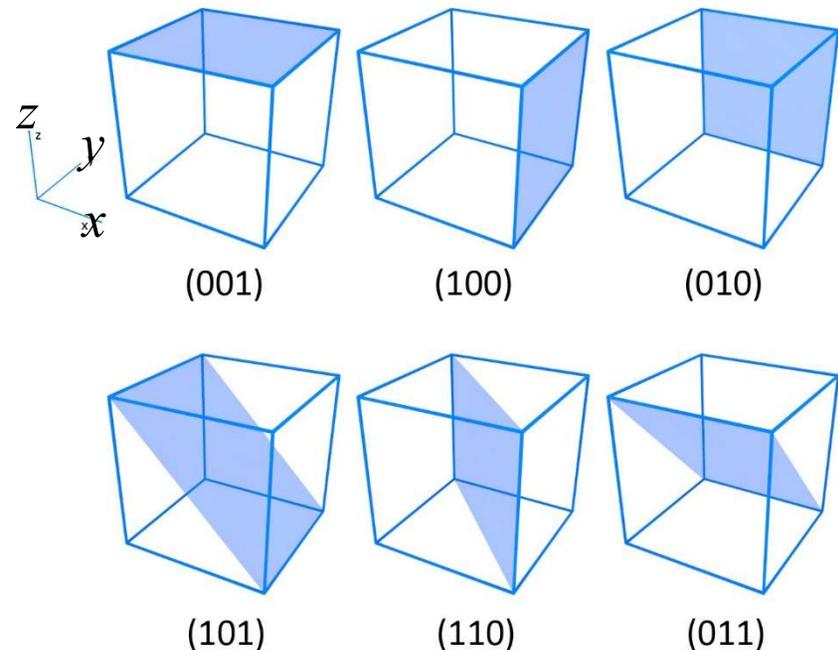
always use integers for h, k, l

() specific plane

{ } family of equivalent planes

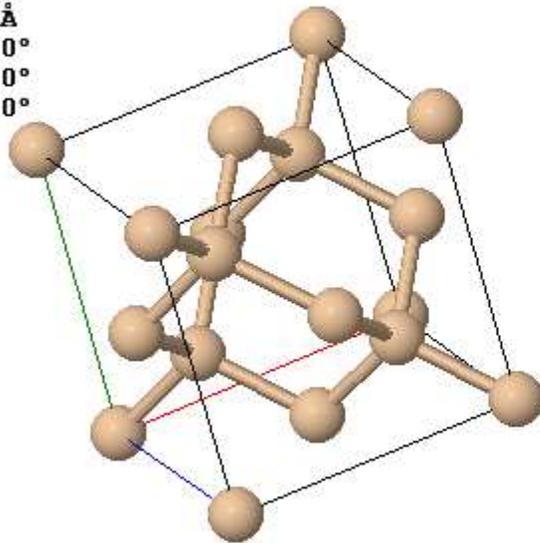


MOSFETs are made on {100} wafers



silicon

HM: $F d \bar{3} m S$
a=5.430Å
b=5.430Å
c=5.430Å
 $\alpha=90.000^\circ$
 $\beta=90.000^\circ$
 $\gamma=90.000^\circ$



Conventional unit cell Primitive unit cell Asymmetric unit

2 x 2 x 2 3 x 3 x 3 5 x 5 x 5

Ball and Stick Spacefill

H: K: L:

show HKL plane hide HKL plane

draw atoms in HKL plane

Thickness of HKL planes:

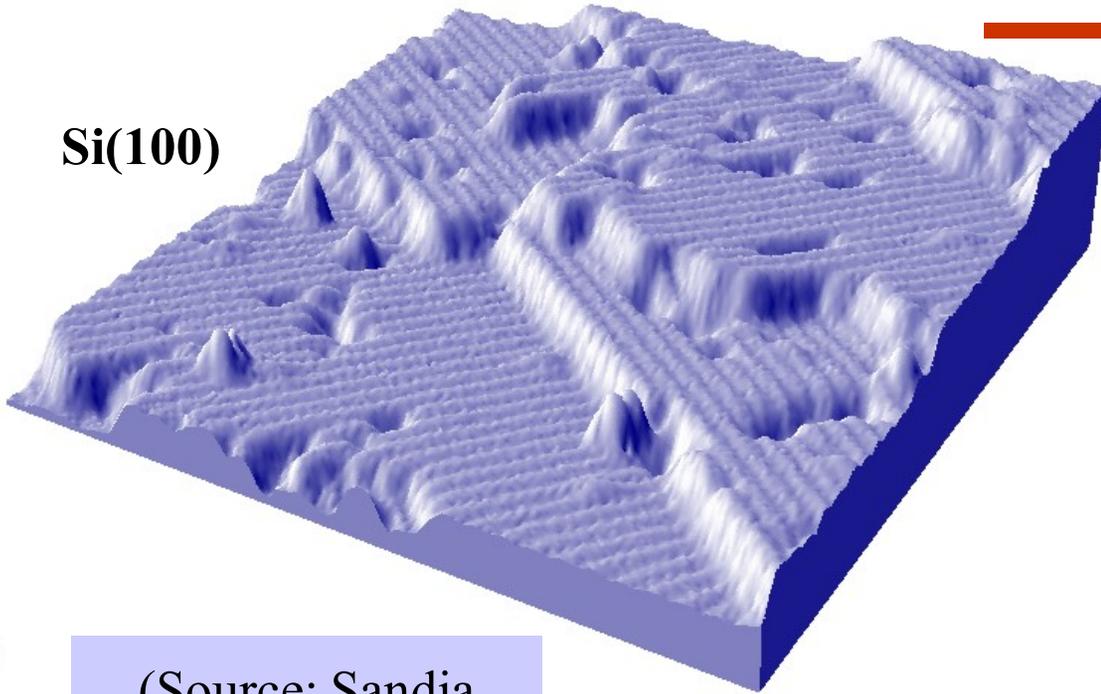
The conventional unit cell is a cube with sides of 0.543 nm. There are 8 atoms in the conventional unit cell. (The image can be rotated with a mouse.)

JSmol

<http://lampx.tugraz.at/~hadley/memmm/materials/silicon/silicon.php>

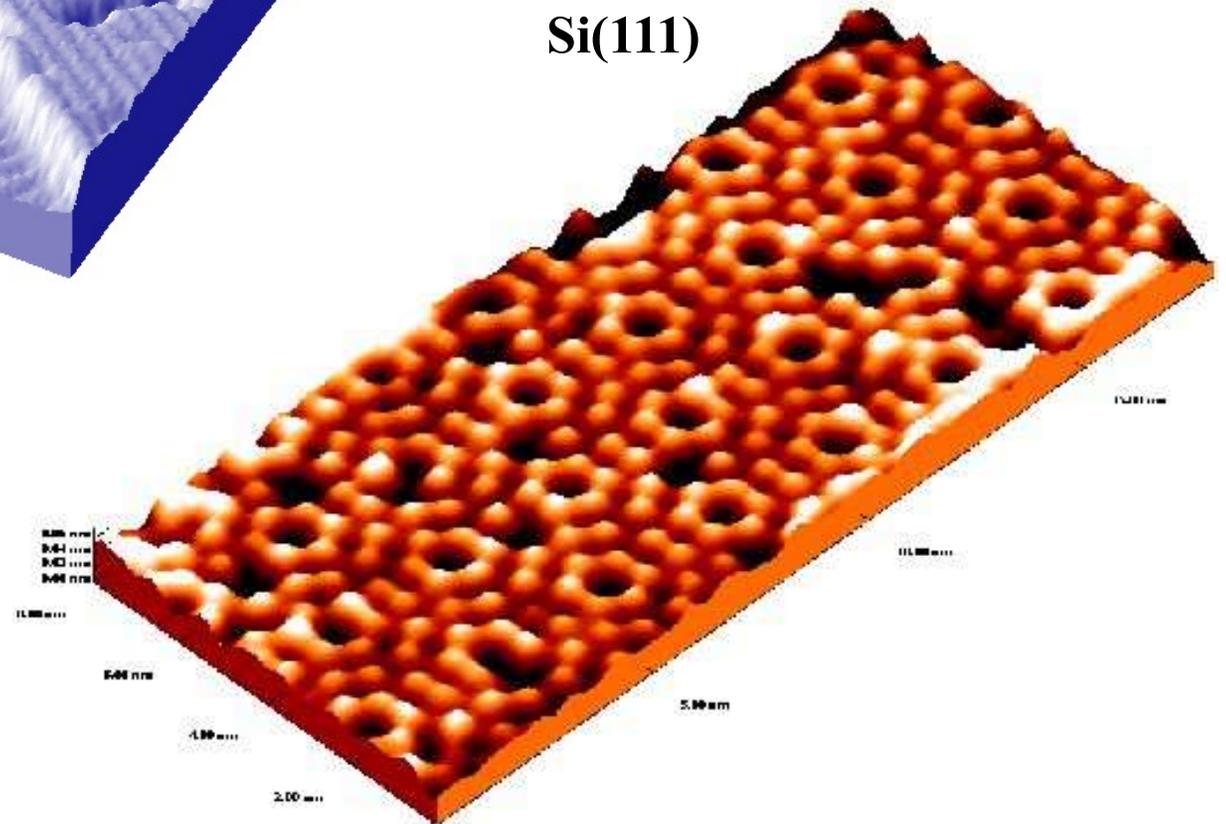
Silicon surfaces

Si(100)

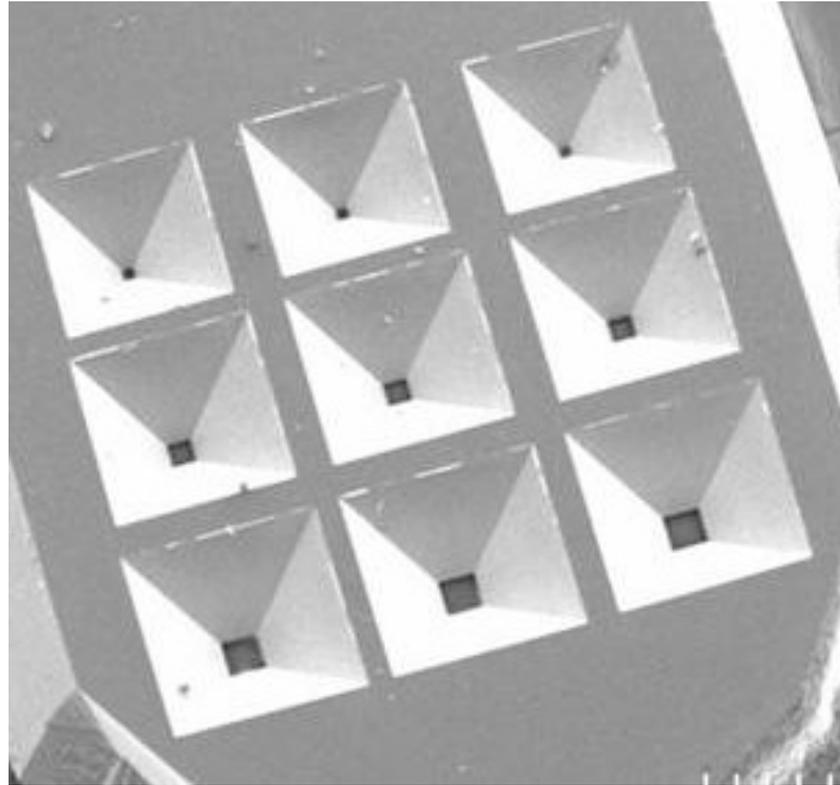


(Source: Sandia
Nat.Labs.)

Si(111)



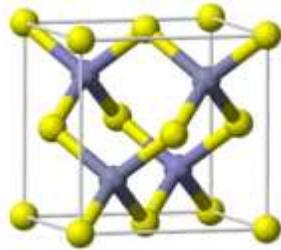
KOH etching of silicon



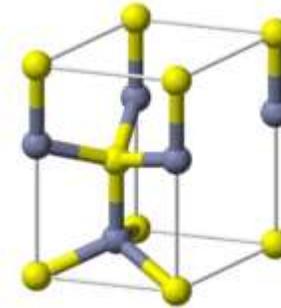
KOH etches Si $\{110\} > \{100\} > \{111\}$, producing a characteristic anisotropic V-etch, with sidewalls that form a 54.7° angle with the surface (35.3° from the normal).

http://www.ece.uncc.edu/research/clean_room/fabprocesses/KOH-EtchingAndDecon.pdf

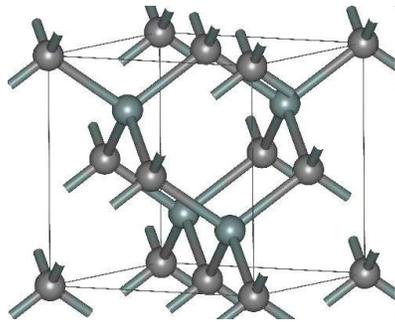
Structural phase transitions



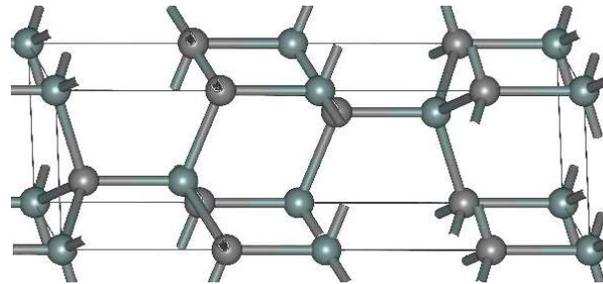
GaAs, Zinblende



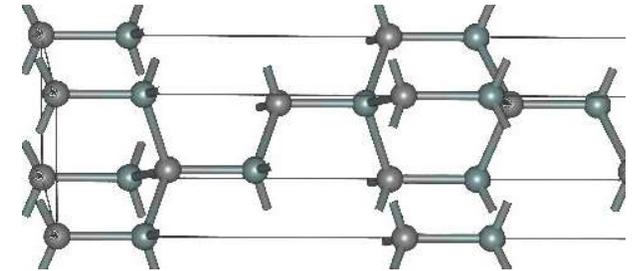
GaAs, Wurtzite



3C - SiC



4H - SiC



6H - SiC

SiC has about 100 polytypes

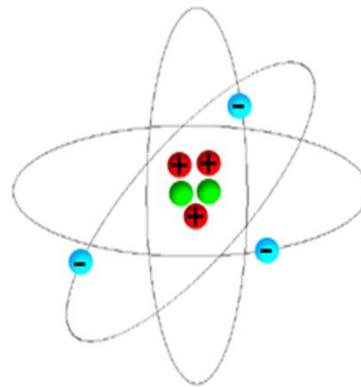
Electrons in Crystals

Electrons

Charge = -1.6022×10^{-19} C

Mass = 9.11×10^{-31} kg

Radius = ?



0.15 nm

www.alnaden.ibm.com/vis/stm/atomo.html

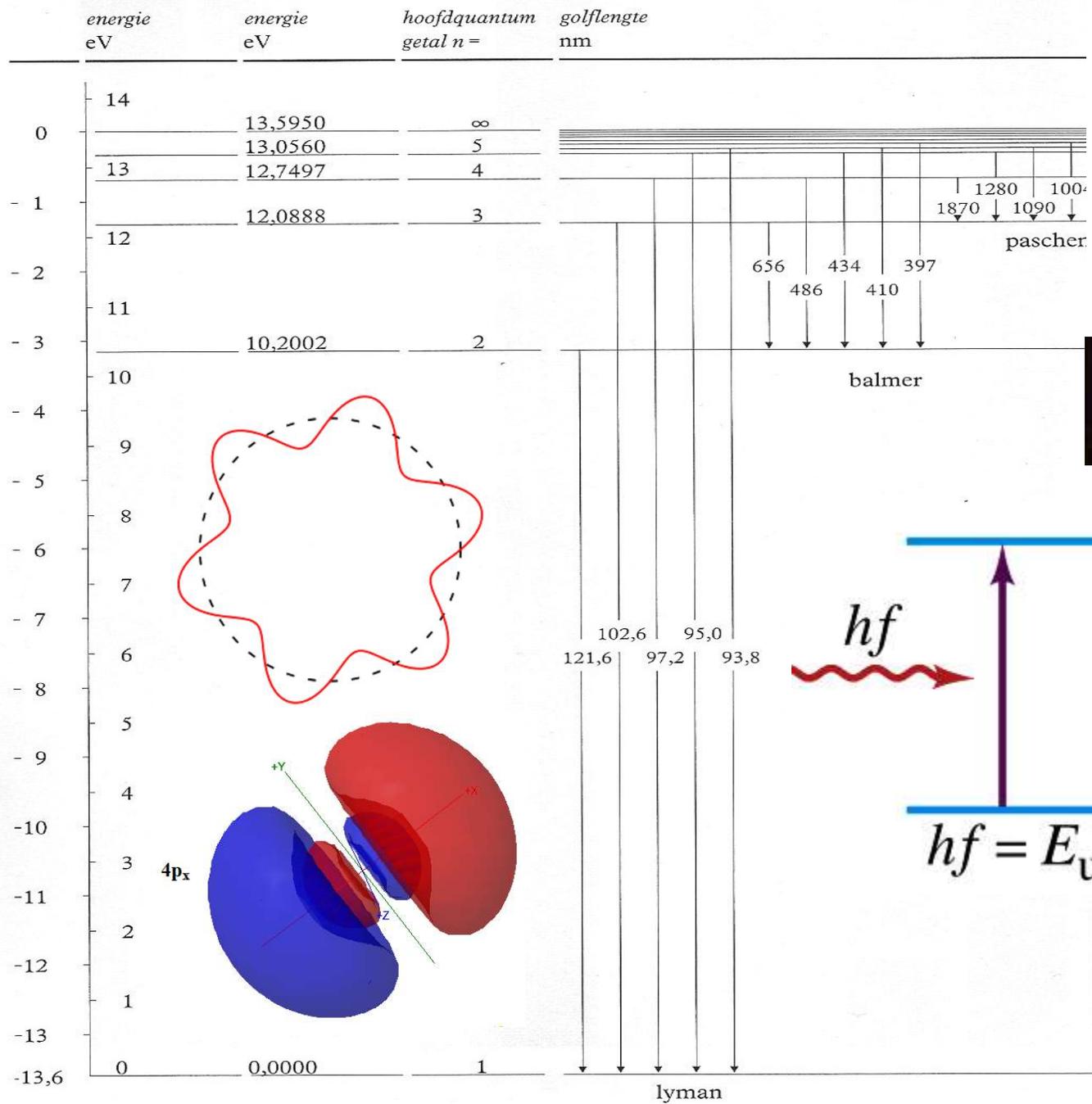
Quantum Mechanics

Everything moves like a wave but exchanges energy and momentum like a particle.

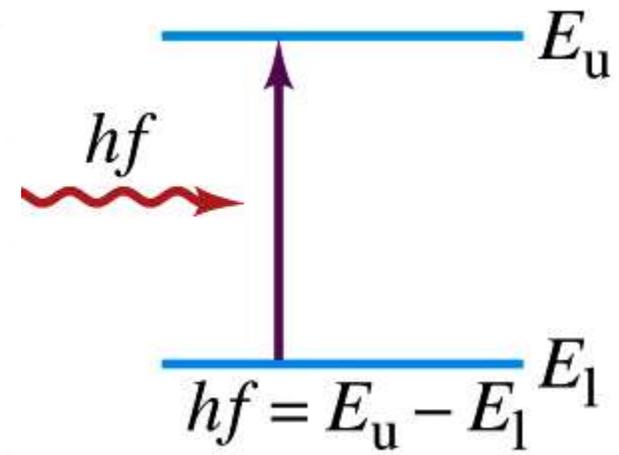
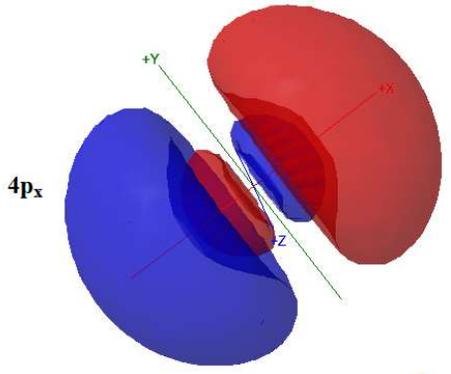
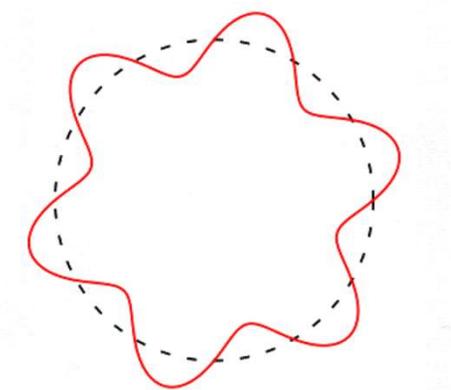
Everything moves like a wave but exchanges energy and momentum like a particle.



de aangegeven golflengten gelden in vacuüm

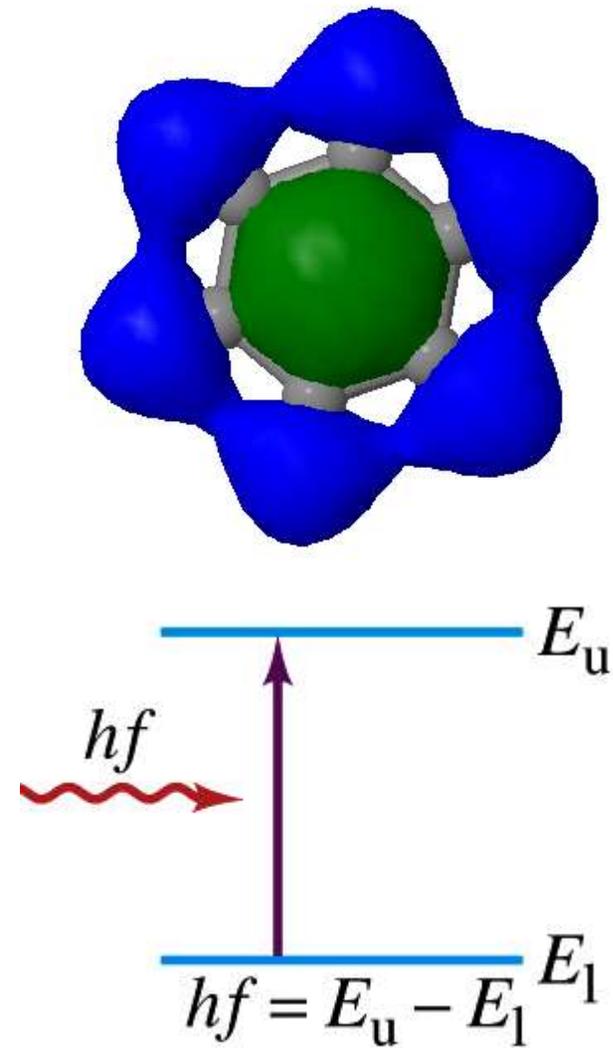
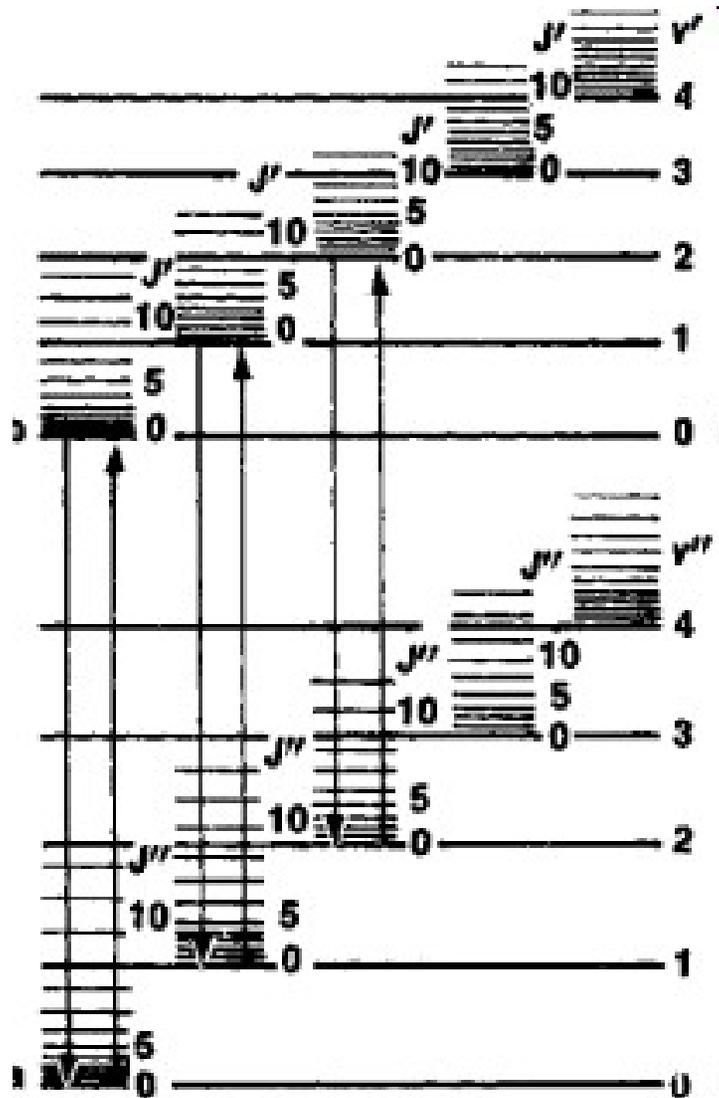


Fluorescent lamp

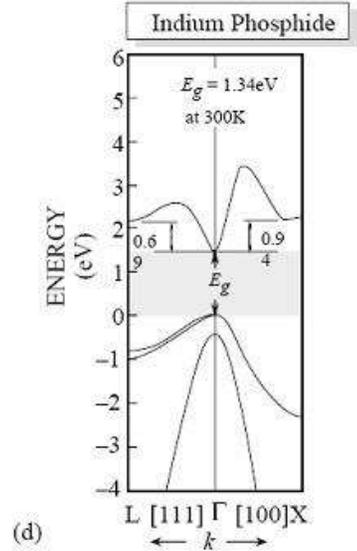
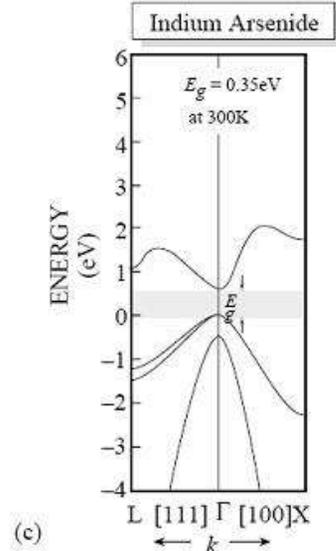
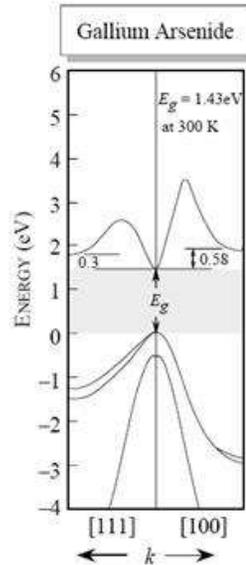
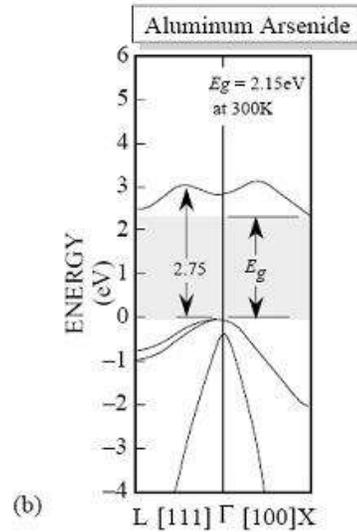
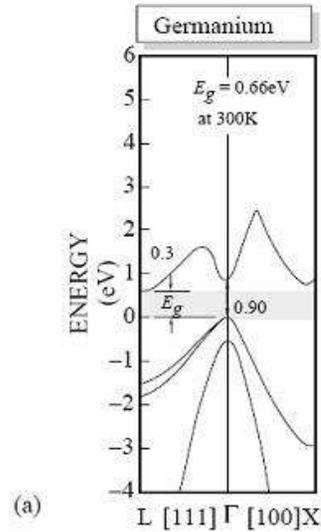
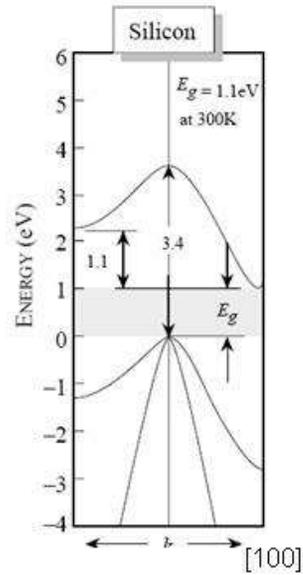


lyman

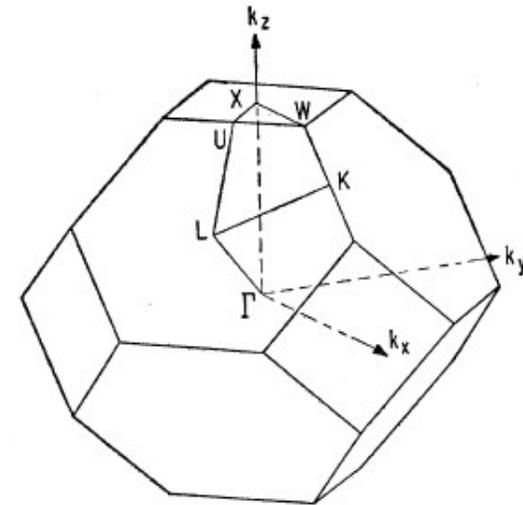
Molecular energy levels



Semiconductors



valence band
 conduction band
 band gap



molecular orbitals
 are plane waves

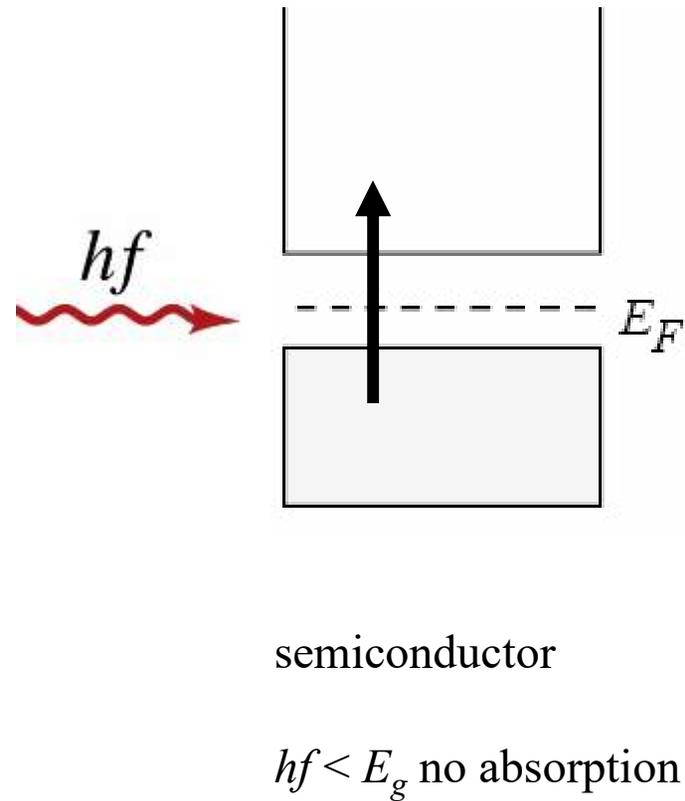
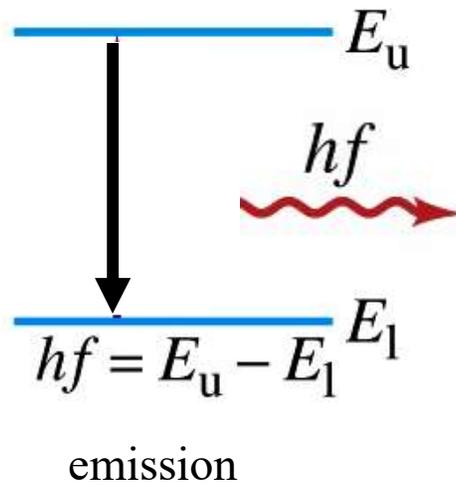
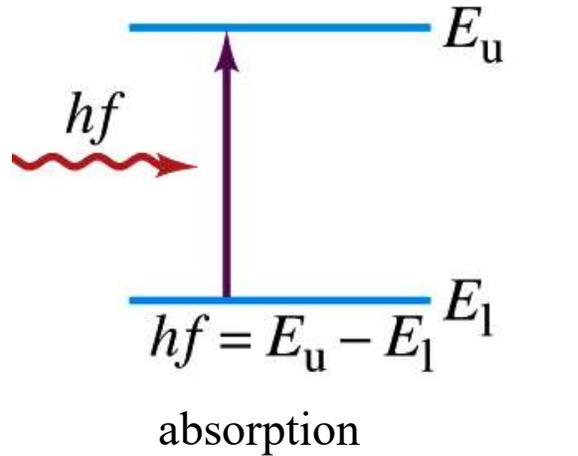
wave vector k

A k -vector points in the direction a wave is propagating.

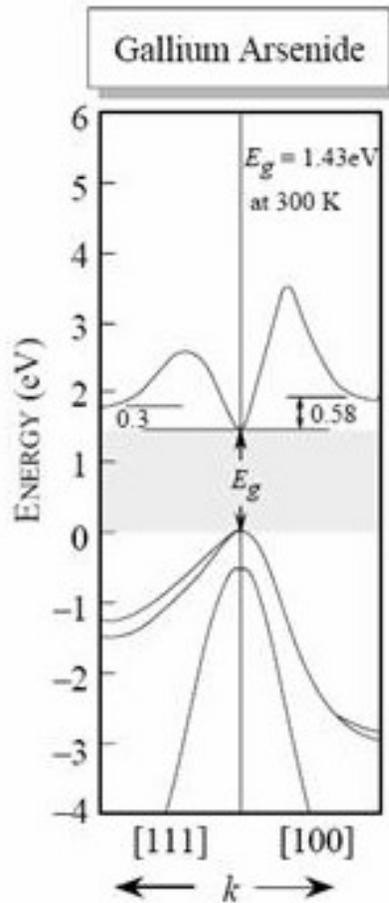
wavelength: $\lambda = \frac{2\pi}{|\vec{k}|}$

momentum: $\vec{p} = \hbar\vec{k}$

Absorption and emission of photons



What color light does a GaAs LED emit?



$$E = 1.6022 \times 10^{-19} \times 1.43 \text{ J} = hf = \frac{hc}{\lambda}$$

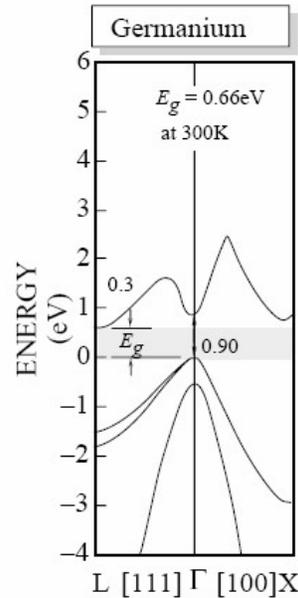
$$\lambda = 867 \text{ nm} \quad \text{infrared}$$

Direct and indirect band gaps

indirect bandgap

$$\Delta k \neq 0$$

phonons are emitted

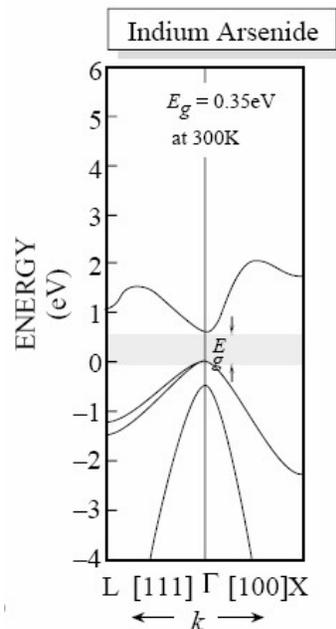


Momentum must be conserved when photons are absorbed or emitted.

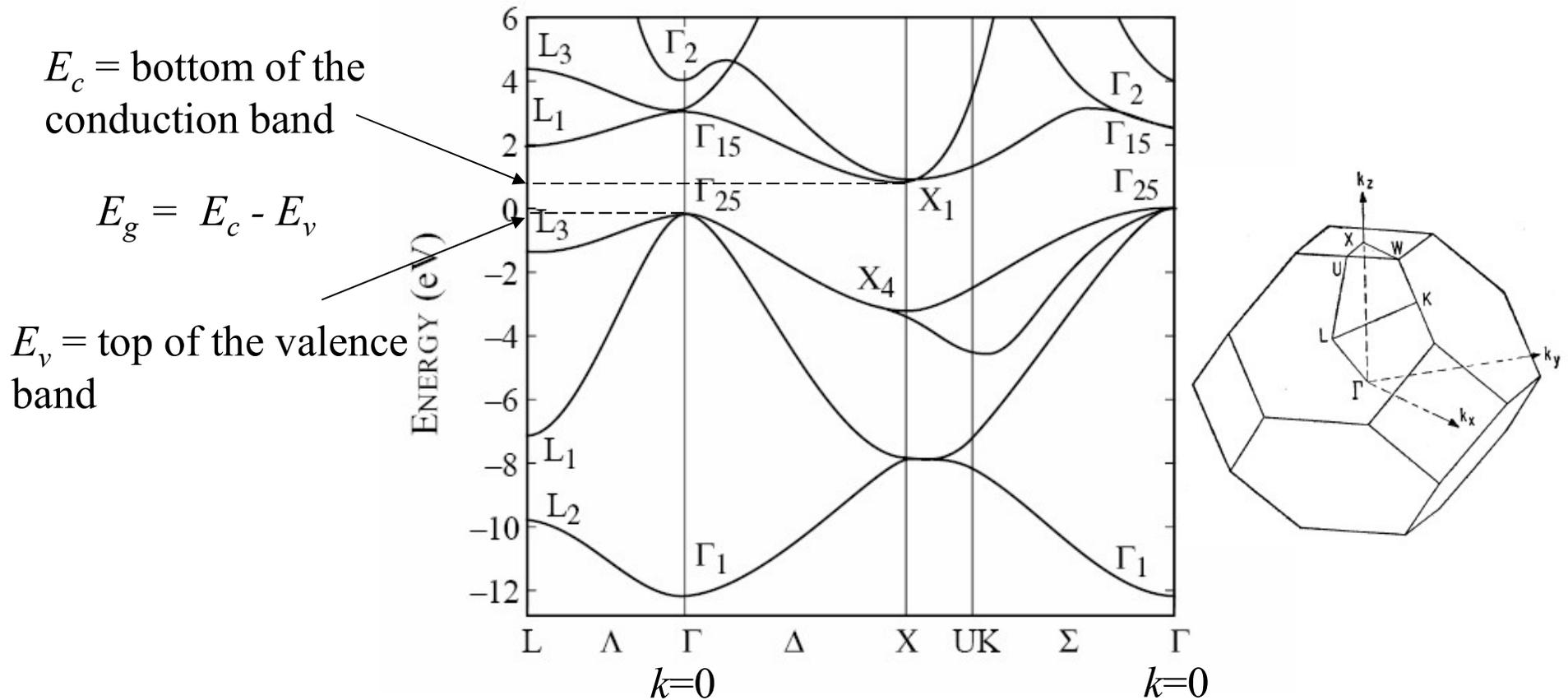
direct bandgap:

$$\Delta k = 0$$

photons can be emitted



Silicon band structure

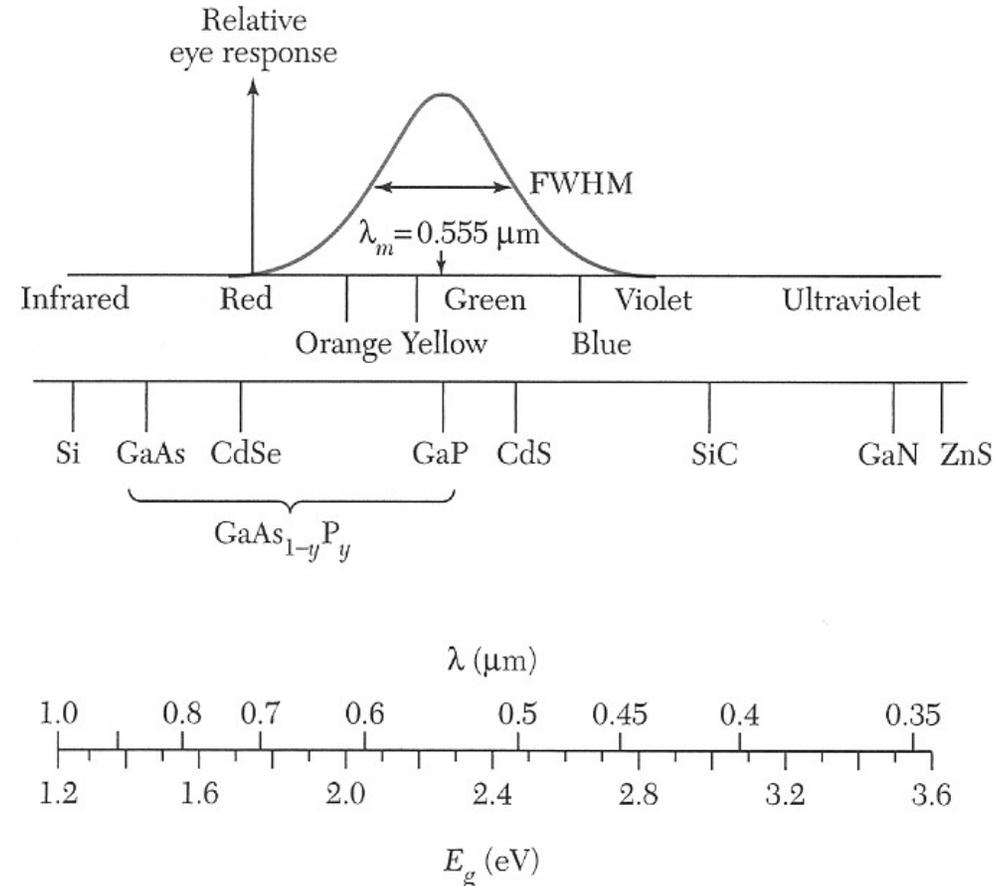


Electrons with energies in the gap are reflected out of the crystal.

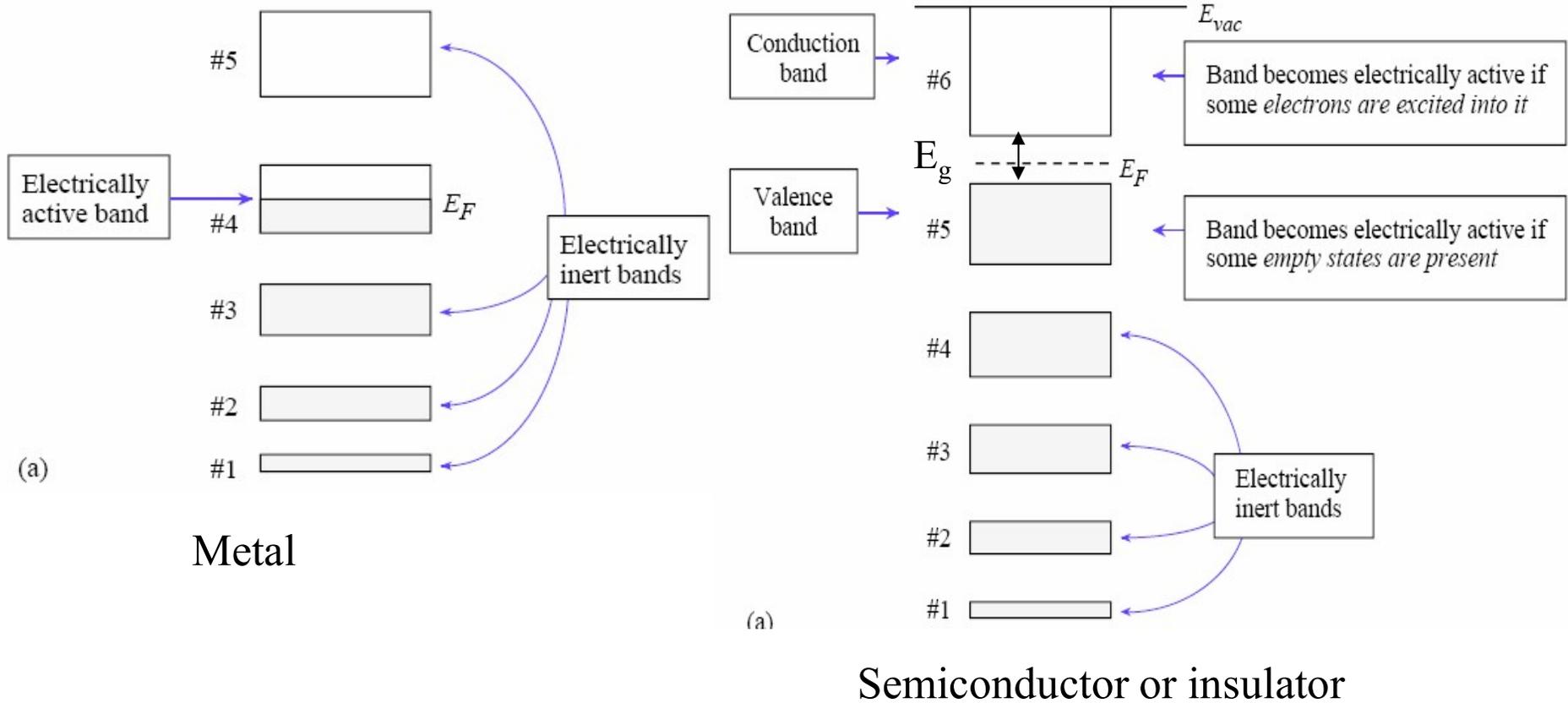
TABLE 1 Common III-V materials used to produce LEDs and their emission wavelengths.

Material	Wavelength (nm)
InAsSbP/InAs	4200
InAs	3800
GaInAsP/GaSb	2000
GaSb	1800
$Ga_xIn_{1-x}As_{1-y}P_y$	1100-1600
$Ga_{0.47}In_{0.53}As$	1550
$Ga_{0.27}In_{0.73}As_{0.63}P_{0.37}$	1300
GaAs:Er, InP:Er	1540
Si:C	1300
GaAs:Yb, InP:Yb	1000
$Al_xGa_{1-x}As:Si$	650-940
GaAs:Si	940
$Al_{0.11}Ga_{0.89}As:Si$	830
$Al_{0.4}Ga_{0.6}As:Si$	650
$GaAs_{0.6}P_{0.4}$	660
$GaAs_{0.4}P_{0.6}$	620
$GaAs_{0.15}P_{0.85}$	590
$(Al_xGa_{1-x})_{0.5}In_{0.5}P$	655
GaP	690
GaP:N	550-570
$Ga_xIn_{1-x}N$	340,430,590
SiC	400-460
BN	260,310,490

Light emitting diodes



Metals, semiconductors, insulators

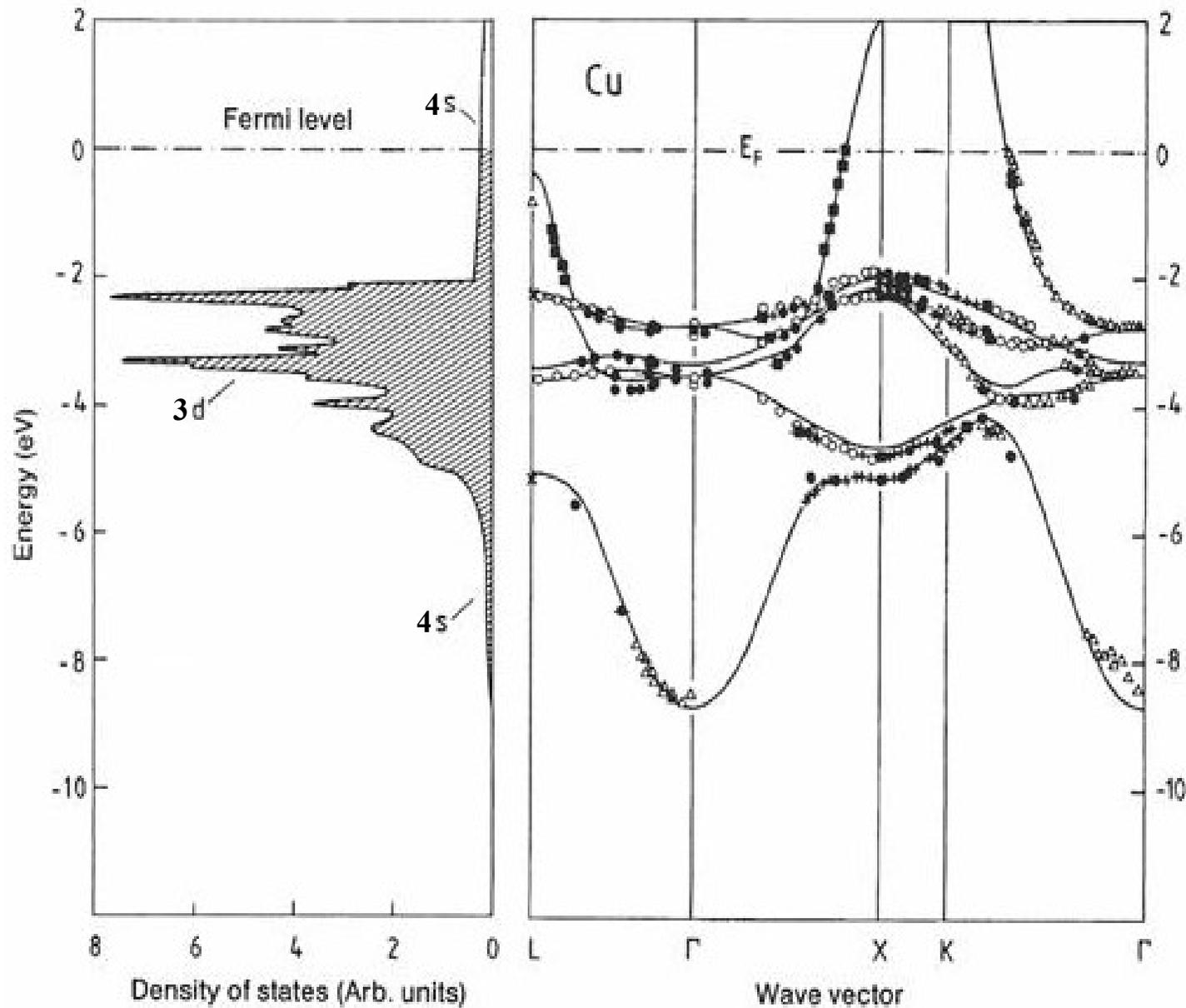


$E_g < 3\text{eV} = \text{Semiconductor}$

$E_g > 3\text{eV} = \text{Insulator}$

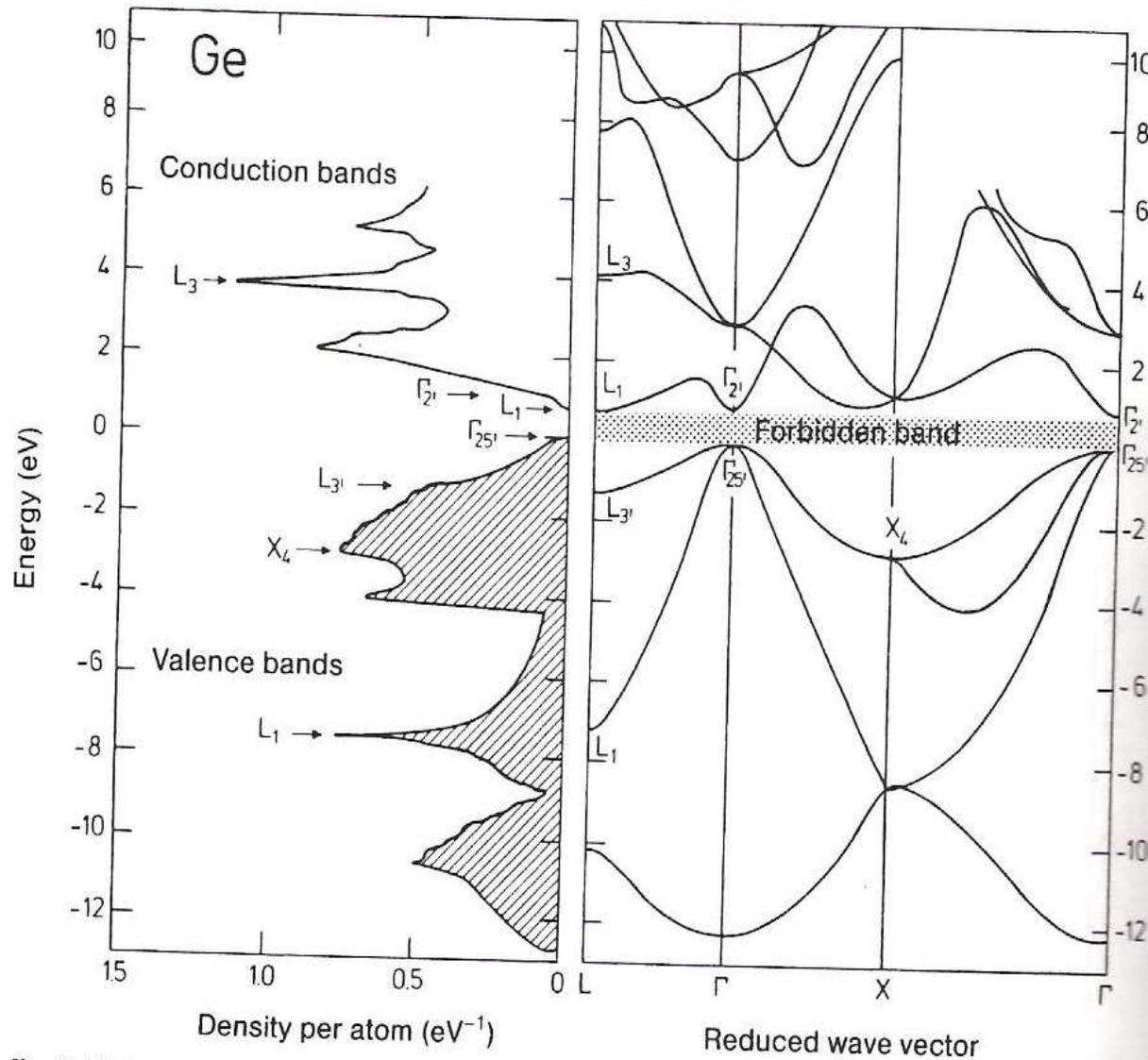
from: Singh

Copper dispersion relation and density of states



from Ibach & Lueth

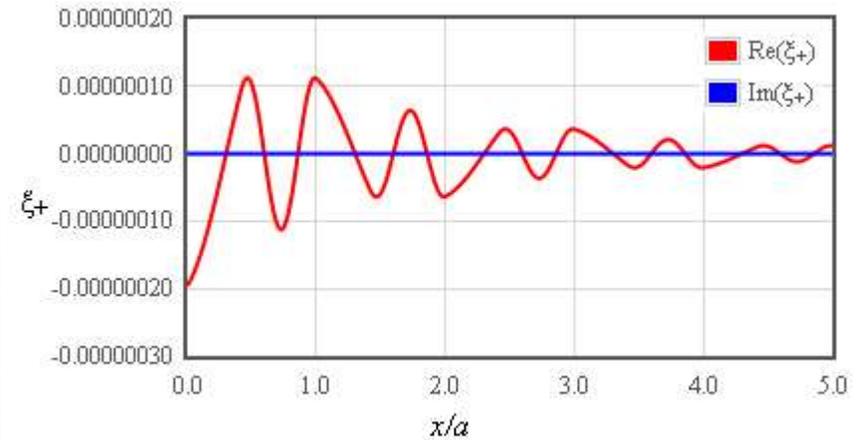
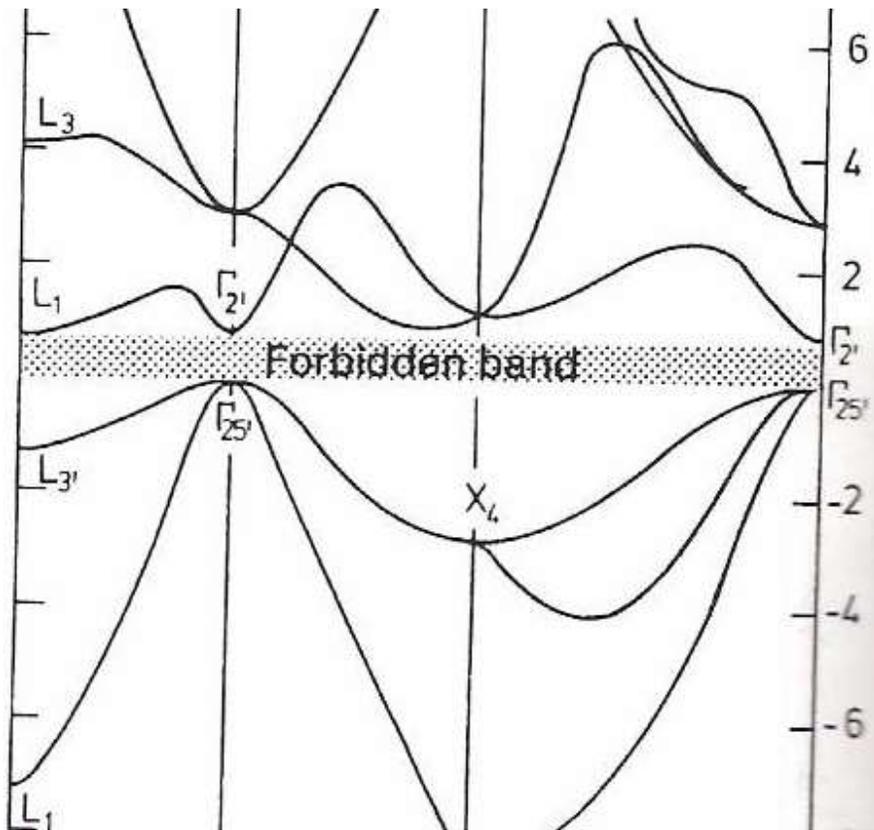
Germanium



from Ibach & Lueth

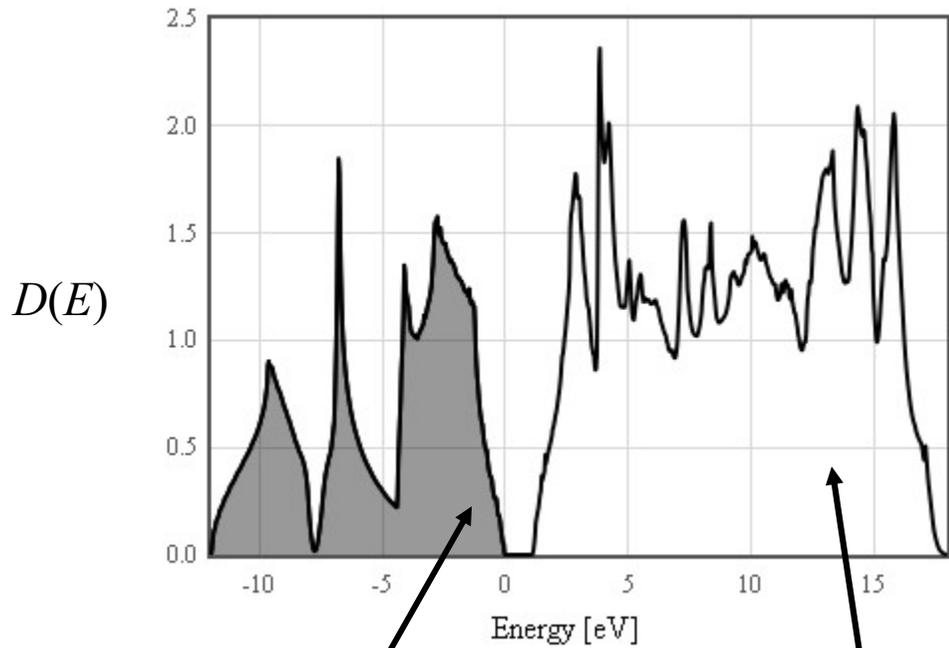
Band gap

Electrons with energies in the gap are reflected out of the crystal.



Density of states

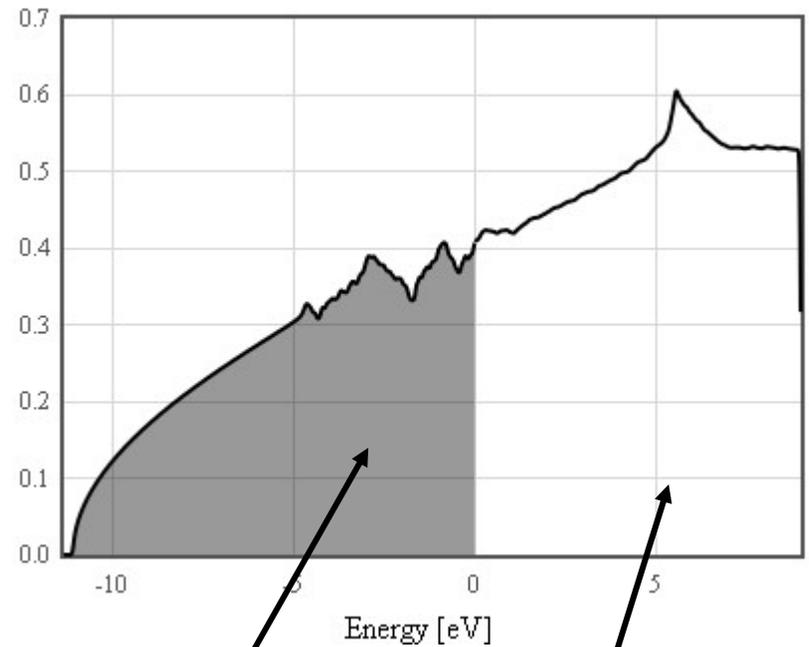
Silicon



filled states

empty states

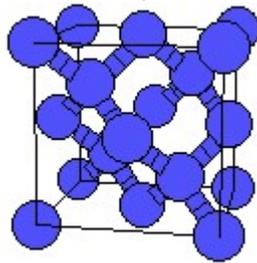
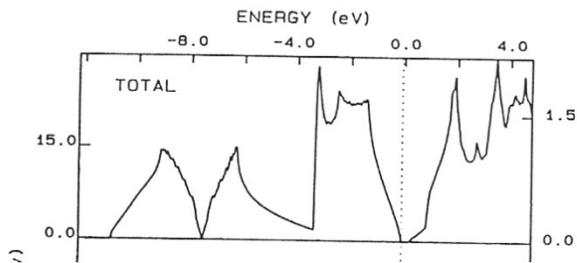
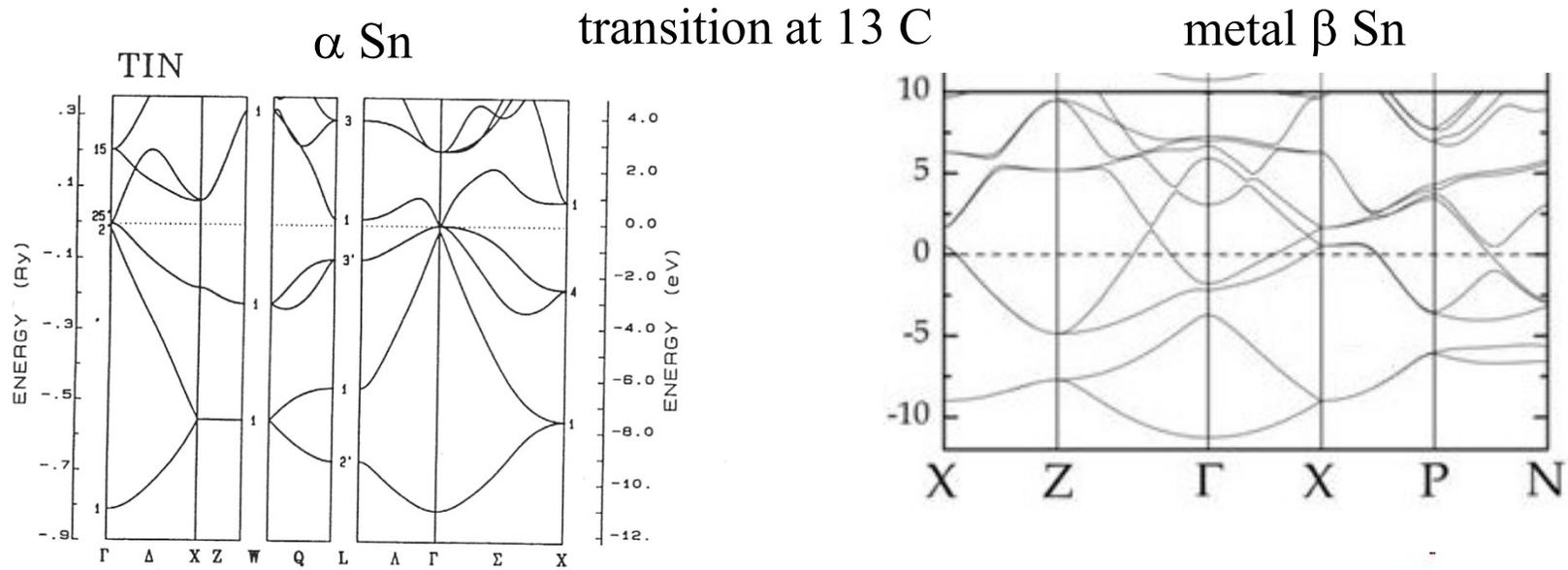
Aluminum



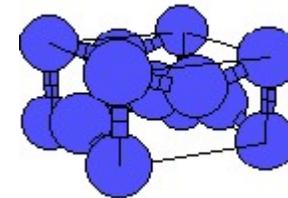
filled states

empty states

Structural phase transition in Sn

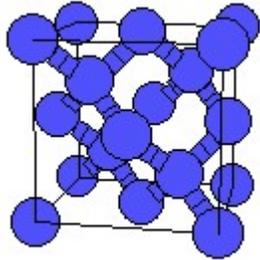


α -Sn, gray tin, diamond structure

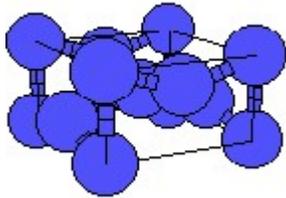


β -Sn, white tin, tetragonal

Structural phase transitions



Si, diamond structure



Si II, β -Sn, tetragonal

silicon makes a diamond to β -Sn transition under pressure

