Crystal Structure

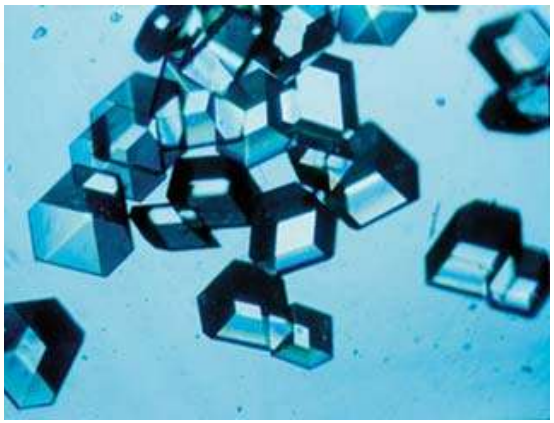
Atoms are arranged in a periodic pattern in a crystal.

The atomic arrangement affects the macroscopic properties of a material.

Many important materials (silicon, steel) are crystals

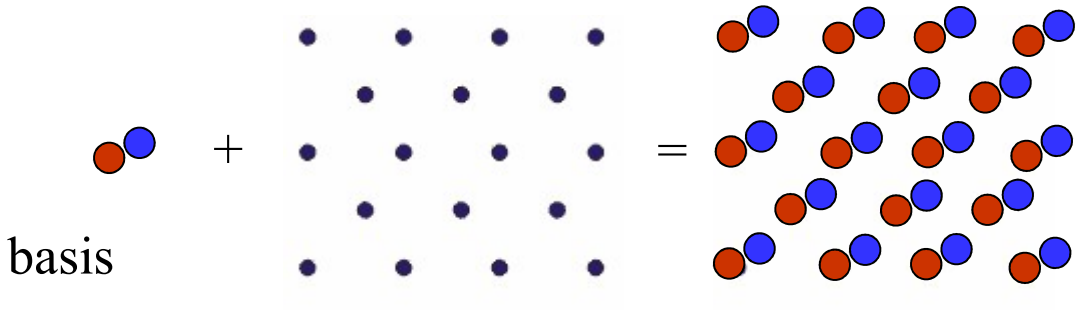
Gallium crystals

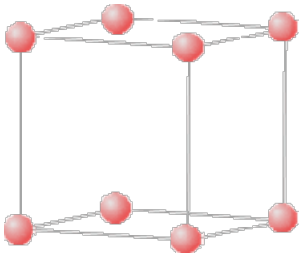
quartz



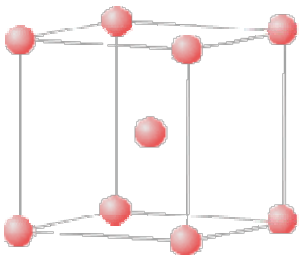
Insulin crystals

Crystal Structure

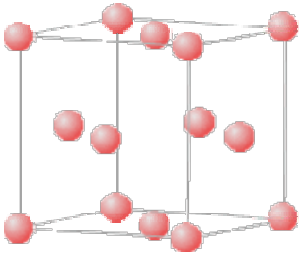




simple cubic

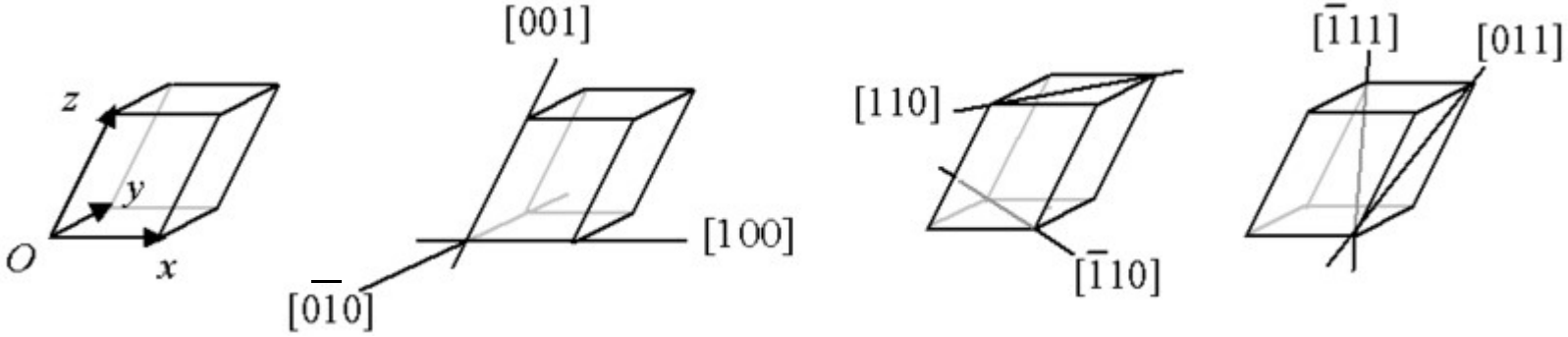


body centered cubic, bcc

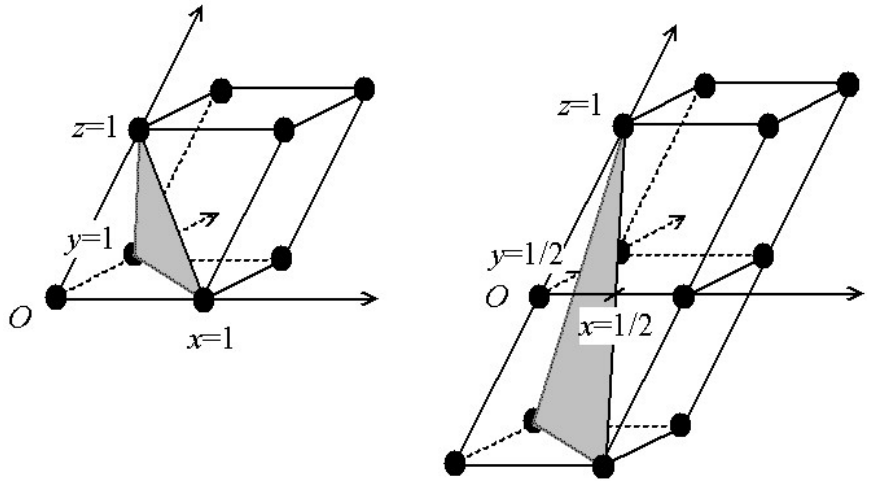


face centered cubic, fcc

Crystal planes and directions: Miller indices



plan (111) plan (221)

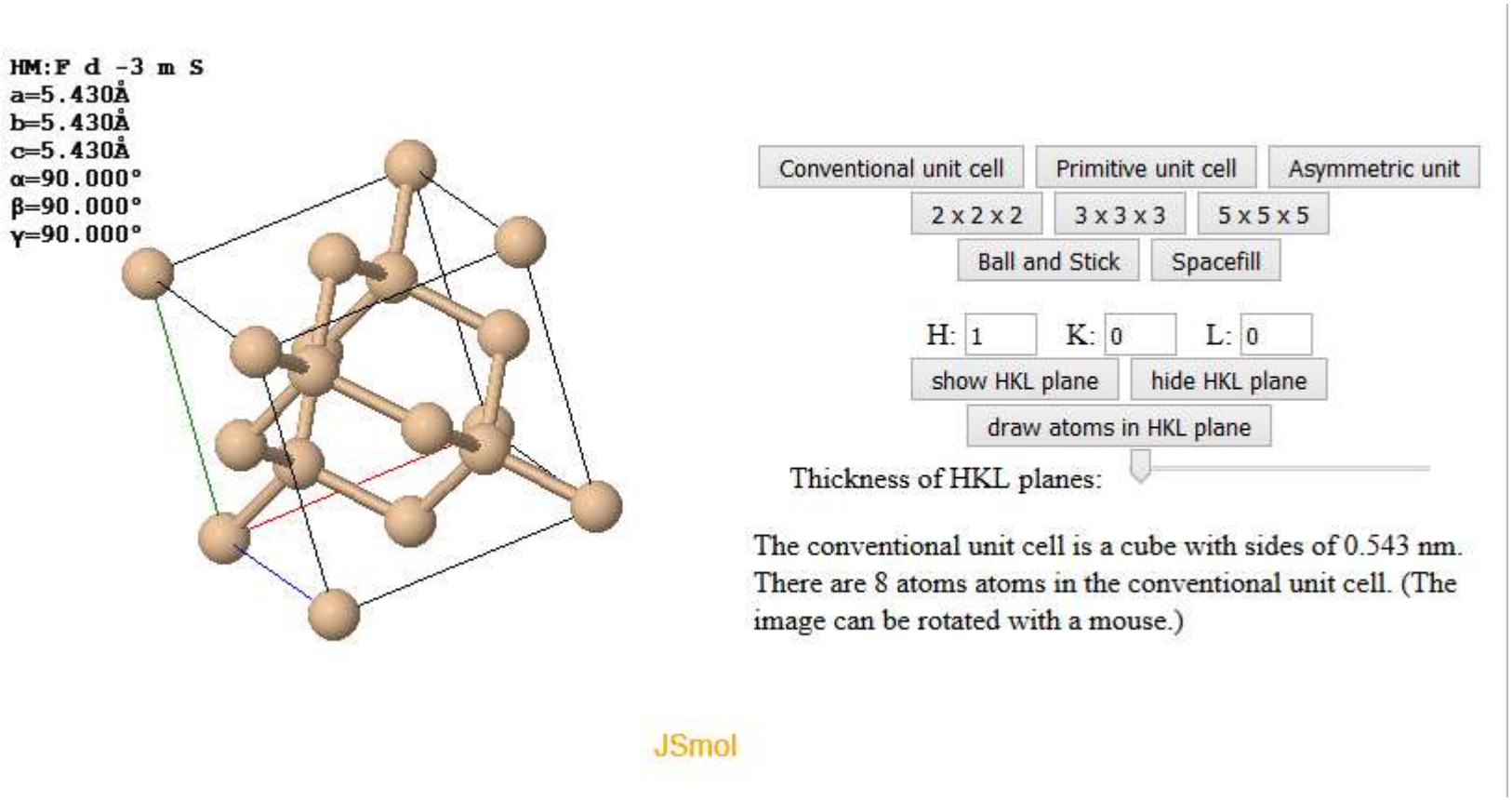


A plane with the intercepts $1/h$, $1/k$, $1/l$ is the (h,k,l) plane.

[ ] specific direction
< > family of equivalent directions
( ) specific plane
{ } family of equivalent planes

MOSFETs are made on <100> wafers

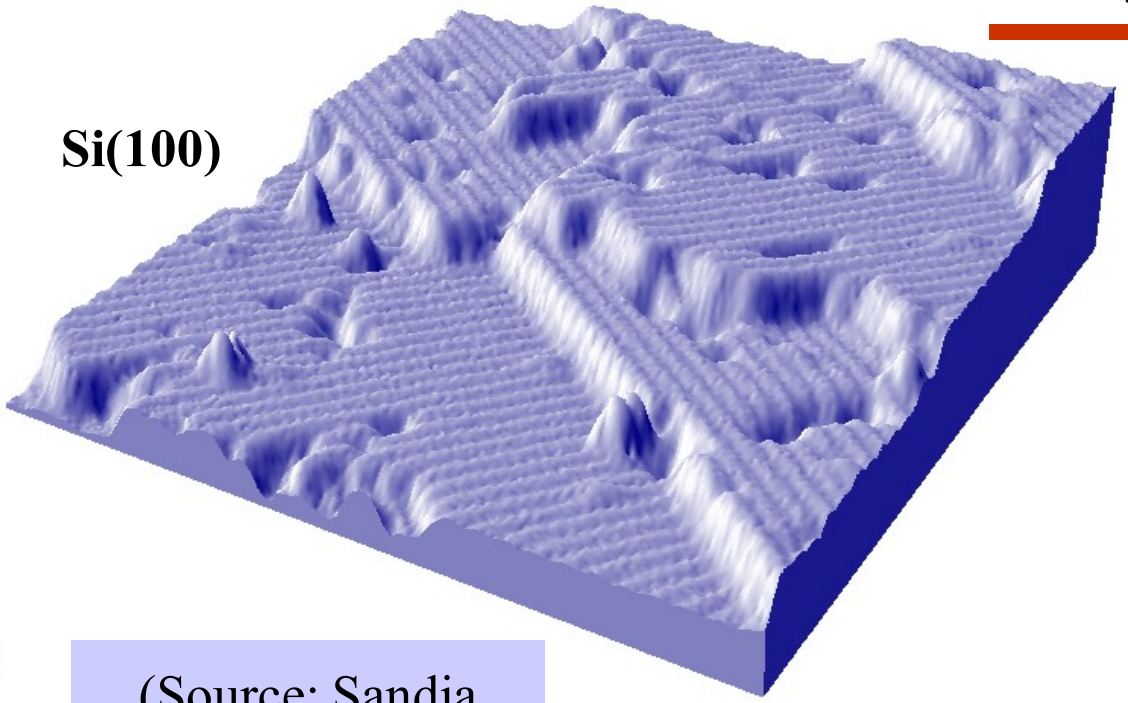
Diamond Crystal Structure



http://lampx.tugraz.at/~hadley/memm/materials/silicon/silicon.php

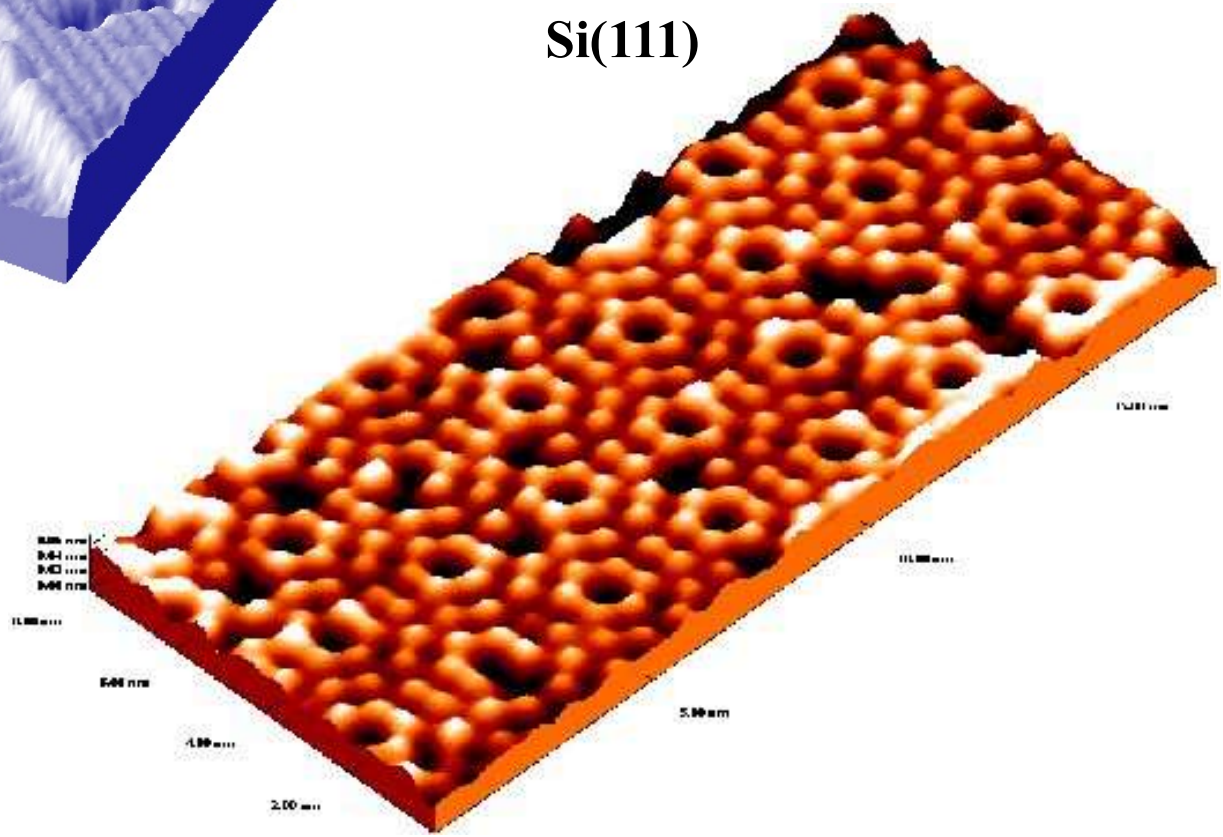
Silicon surfaces

Si(100)

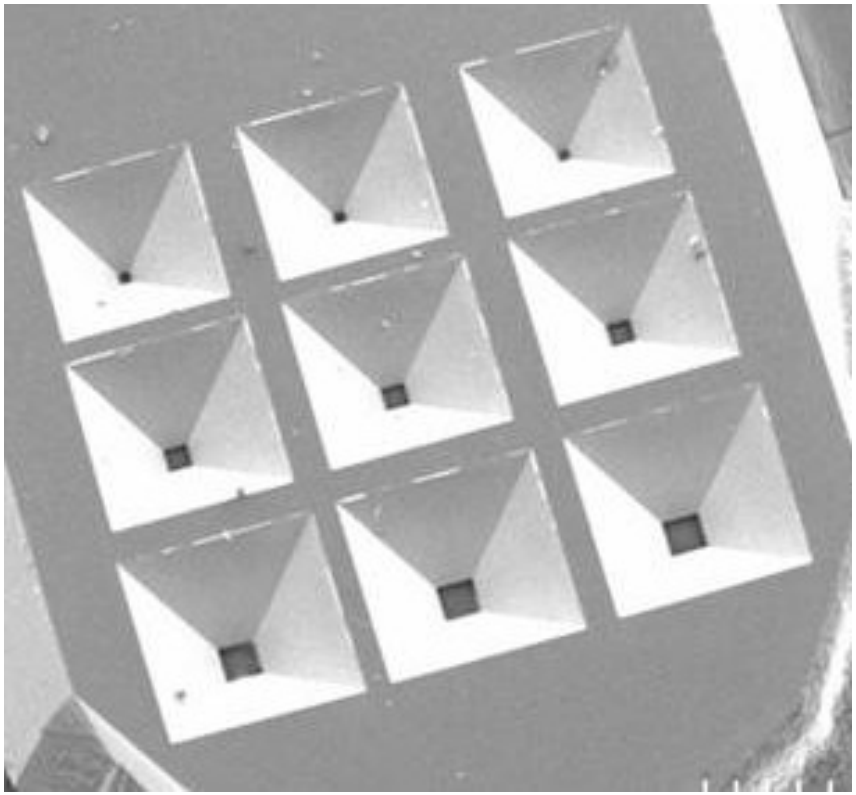


(Source: Sandia Nat.Labs.)

Si(111)



KOH etching of silicon

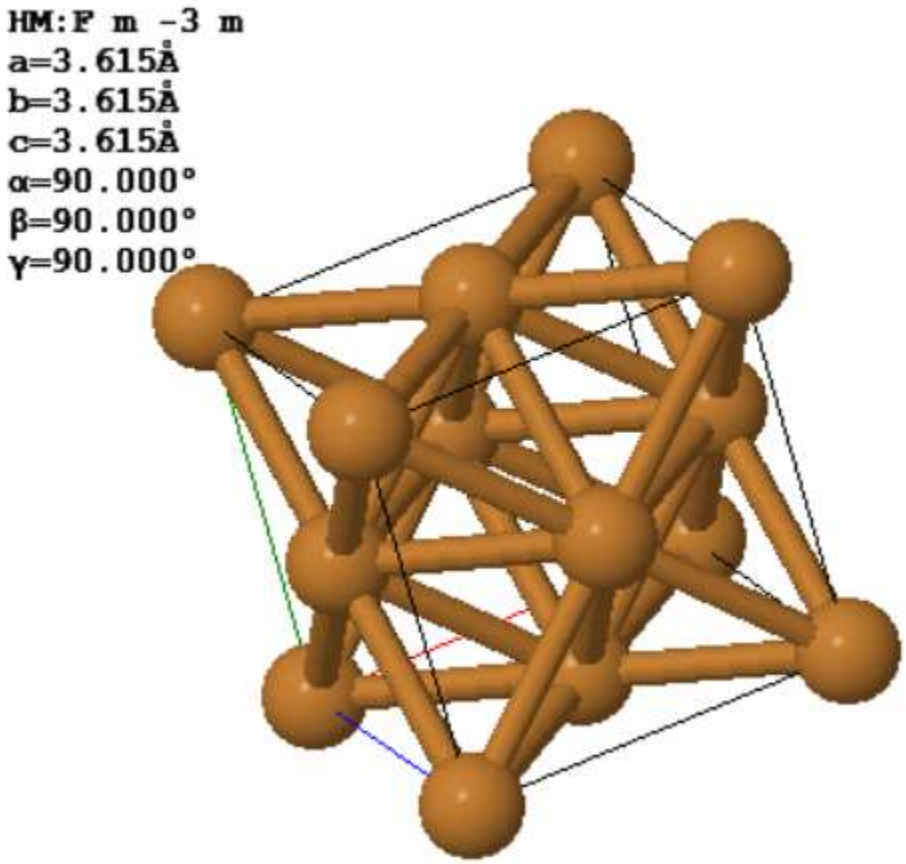


KOH etches Si {110} > {100} > {111}, producing a characteristic anisotropic V-etch, with sidewalls that form a 54.7° angle with the surface (35.3° from the normal).

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

face centered cubic (fcc)

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

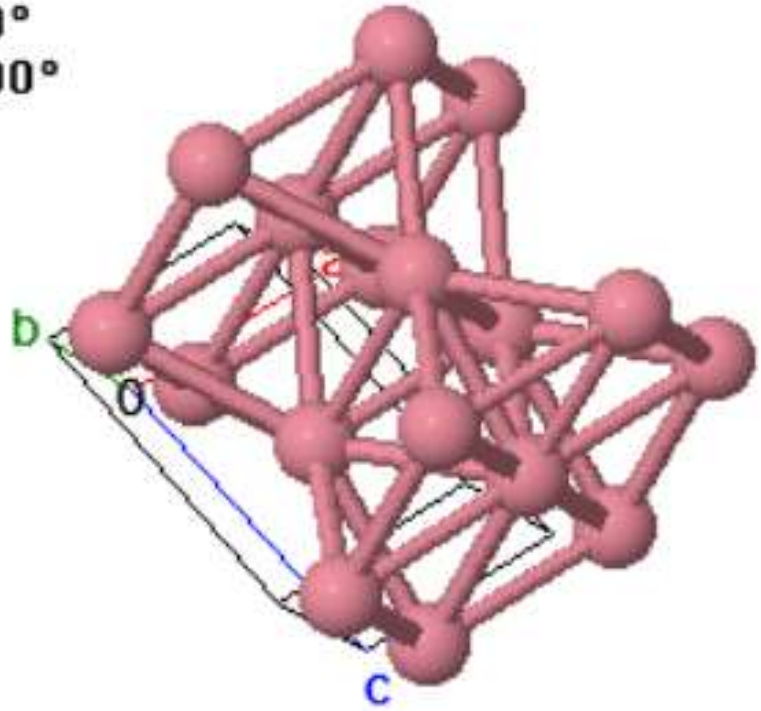


http://lampx.tugraz.at/~hadley/ss1/crystalstructure/structures/fcc/fcc_jsmol.php

hexangonal close pack (hcp)

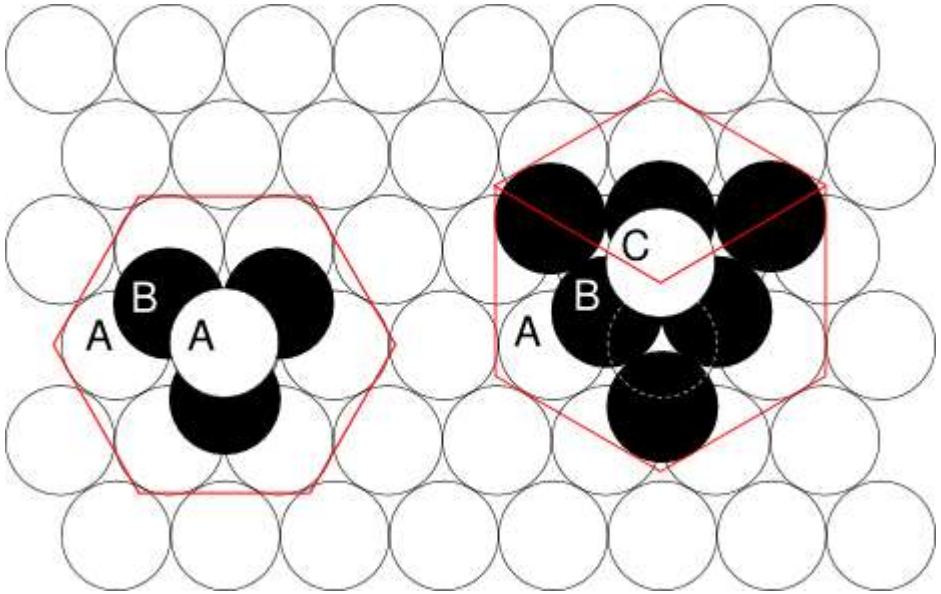
Ti, Co,
Zn, Zr,

HM:P 63/m m c
a=2.507Å
b=2.507Å
c=4.069Å
α=90.000°
β=90.000°
γ=120.000°

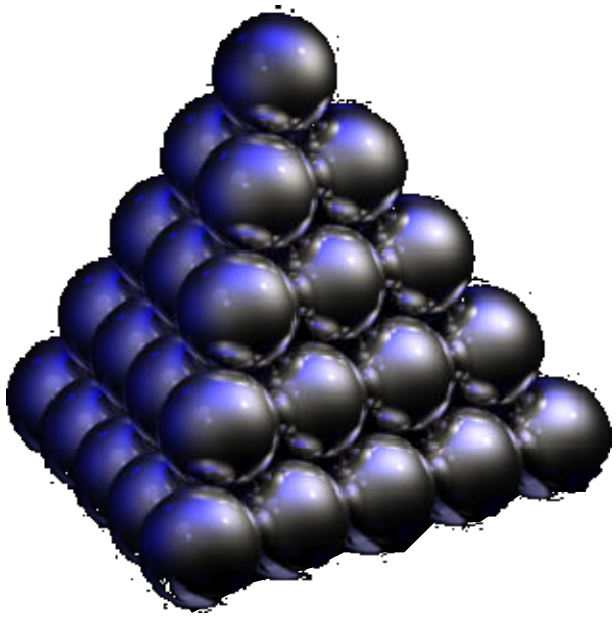


http://lampx.tugraz.at/~hadley/ss1/crystalstructure/structures/hcp/hcp_jsmol.php

Close packing



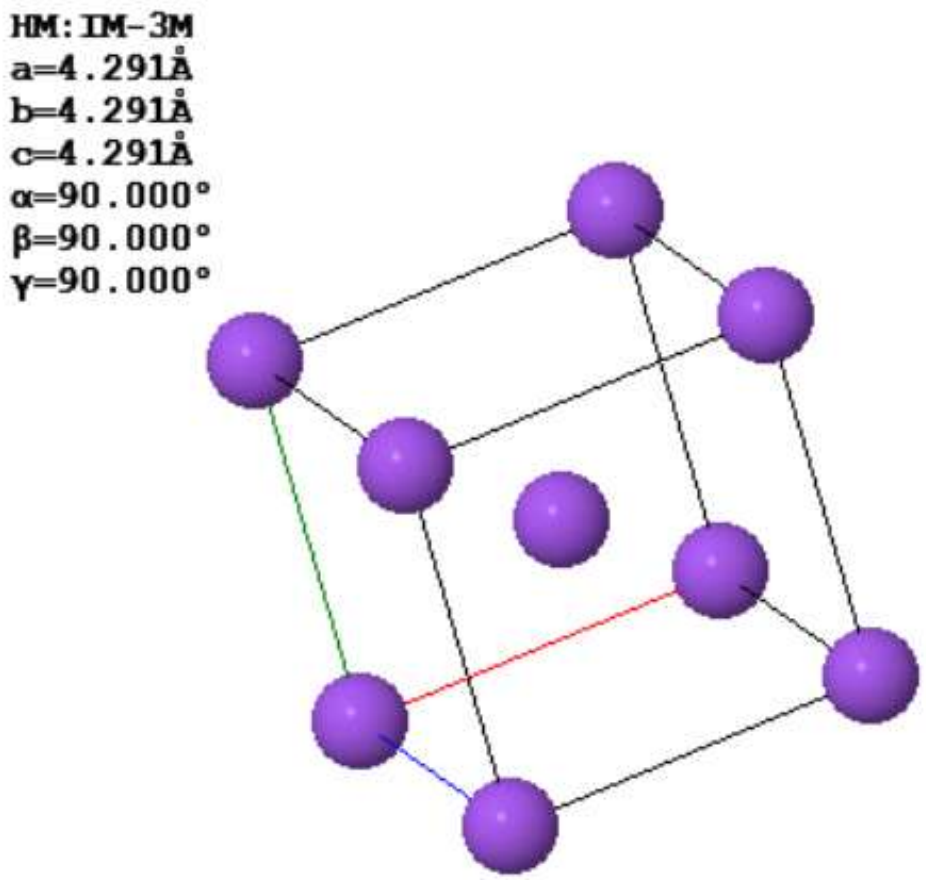
HCP FCC



HCP = Hexagonal close pack
Hexagonal Bravais lattice with two atoms in the basis.

body centered cubic bcc

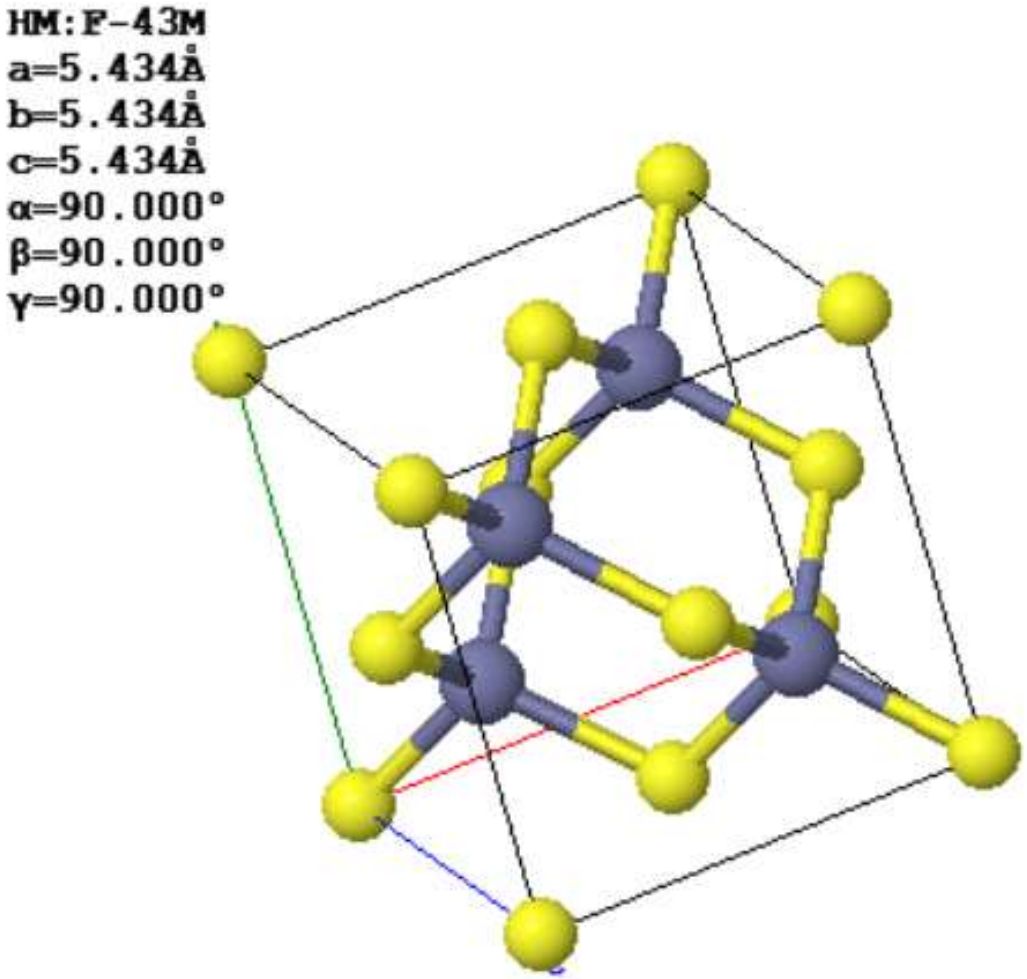
W
Cr
Fe
Mo
Ta



http://lampx.tugraz.at/~hadley/ss1/crystalstructure/structures/bcc/bcc_jsmol.php

zincblende

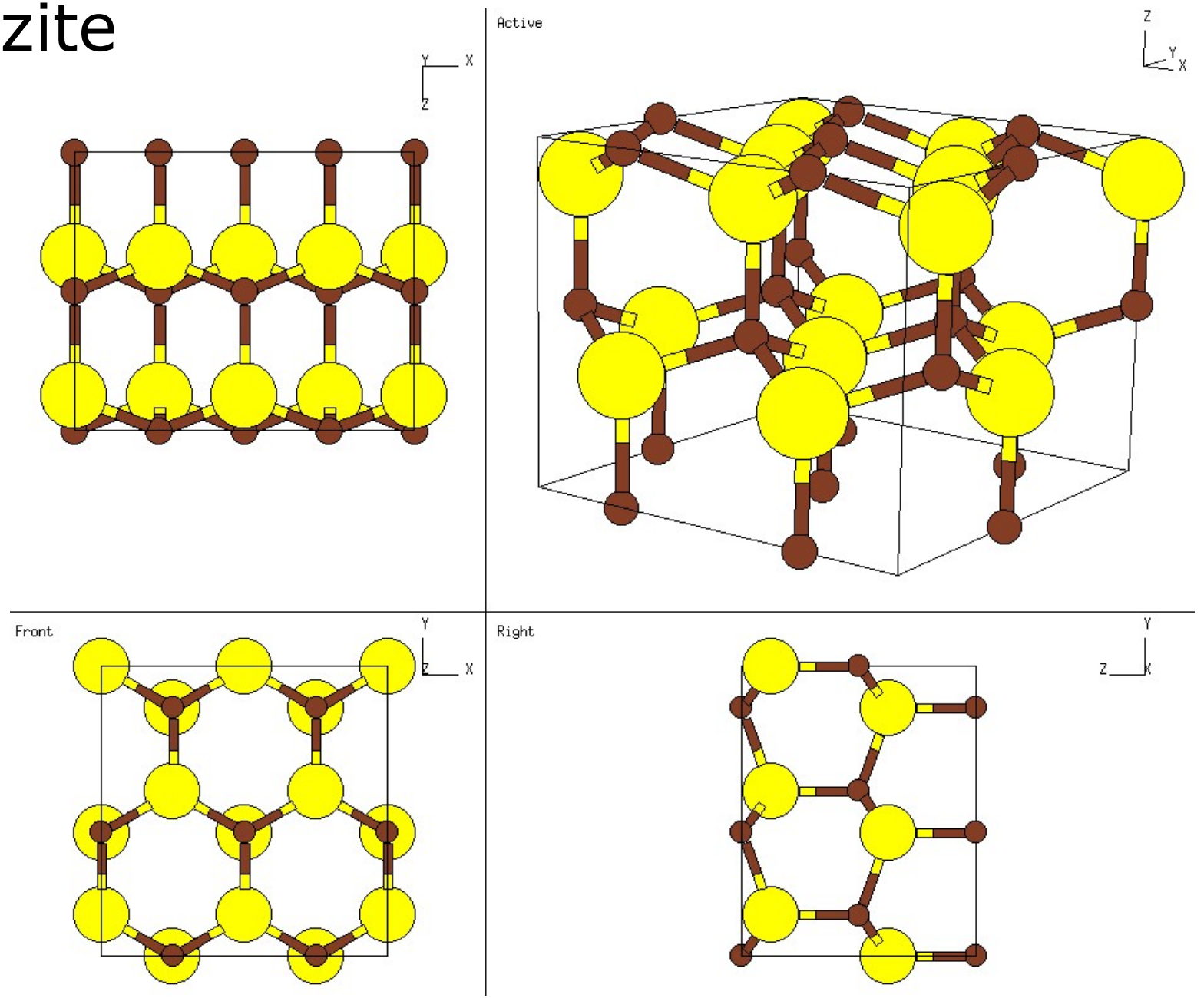
ZnS
GaAs
InP
GaP
InAs
AlAs



http://lampx.tugraz.at/~hadley/ss1/crystalstructure/structures/zincblende/zincblende_jsmol.php

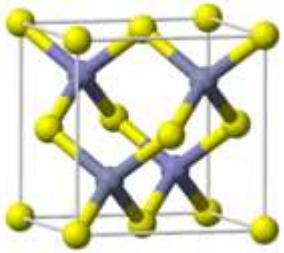
wurtzite

ZnO
CdS
CdSe
GaN
AlN



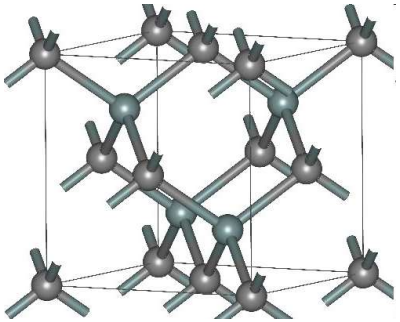
http://cst-www.nrl.navy.mil/lattice/

Structural phase transitions

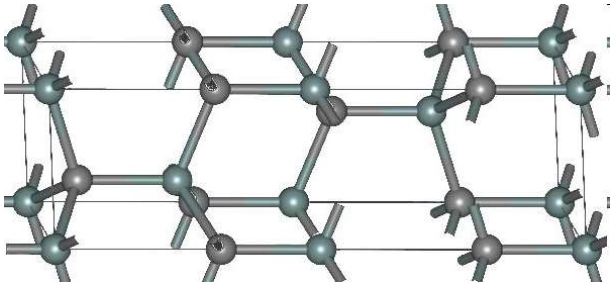


GaAs, Zincblende

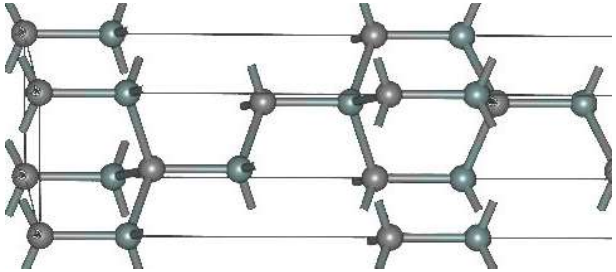
GaAs, Wurtzite



3C - SiC



4H - SiC



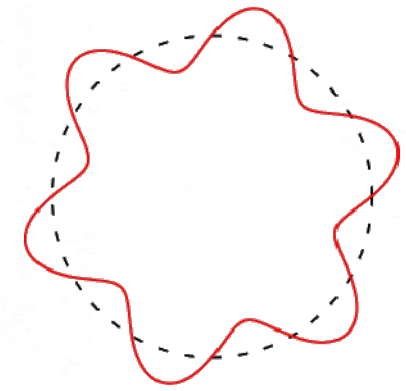
6H - SiC

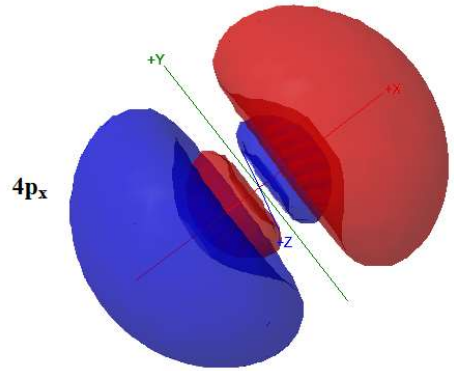
SiC has about 100 polytypes

de aangegeven golflengten gelden in vacuüm

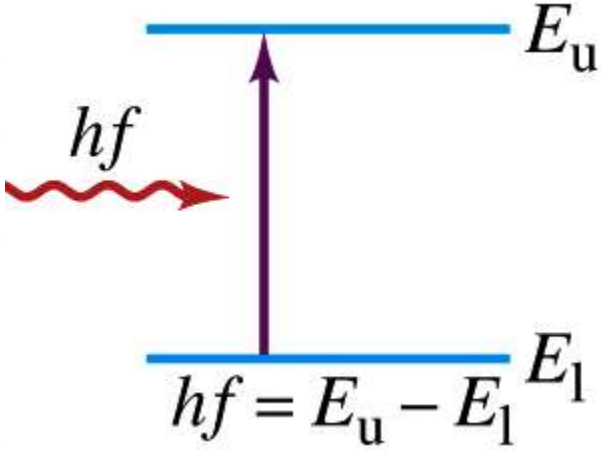
energie eV	*energie* eV	*hoofdquantum getal n =*	*golflengte* nm
14			
0	13,5950	∞	
	13,0560	5	
13	12,7497	4	
- 1	12,0888	3	
12			
- 2			
11			
- 3	10,2002	2	
10			
- 4			
9			
- 5			
8			
- 6			
7			
- 7			
6			
- 8			
5			
- 9			
4			
-10			
3			
-11			
2			
-12			
1			
-13			
-13,6	0	0,0000	1

1280 100
1870 1090
pascher
656 434 397
486 410
balmer
102,6 95,0
121,6 97,2 93,8
lyman

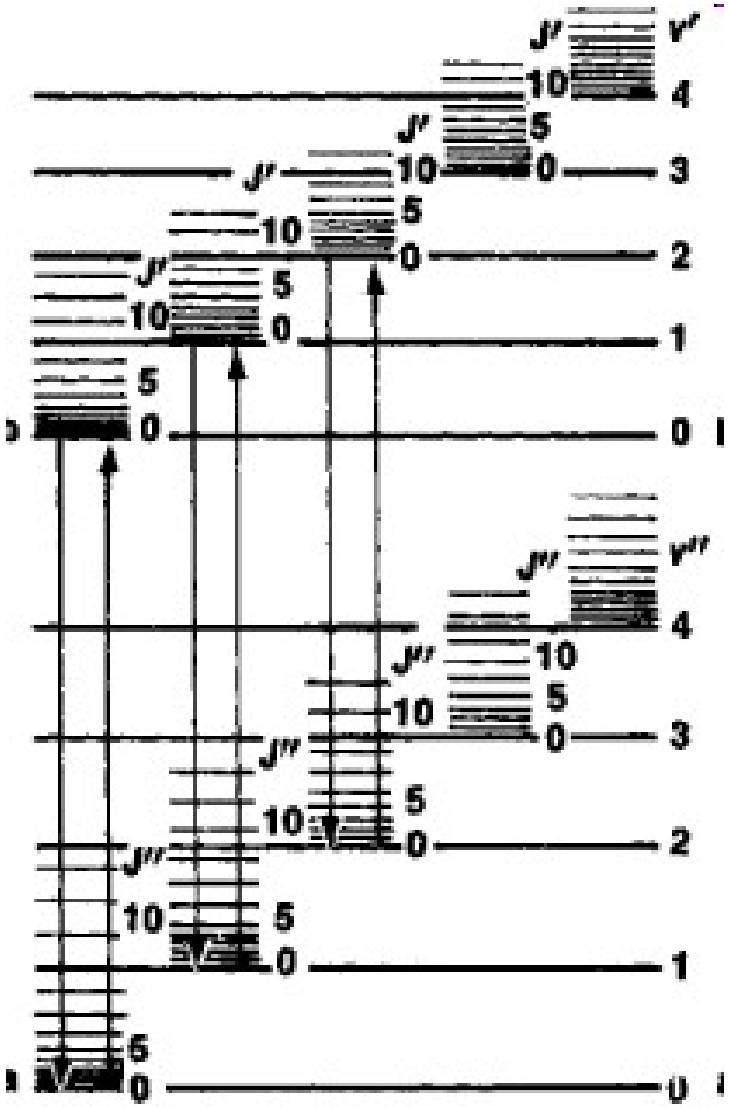


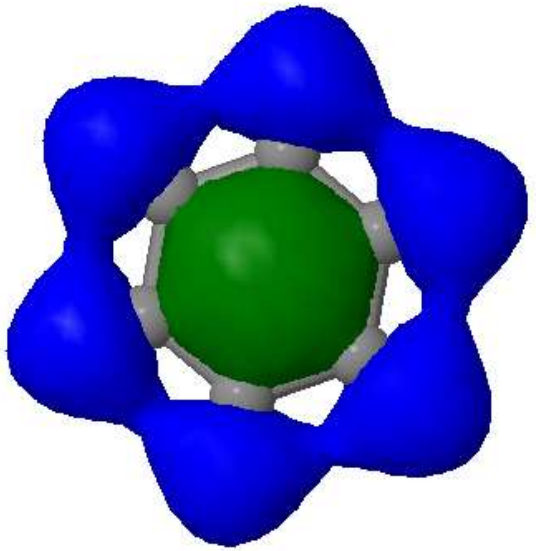


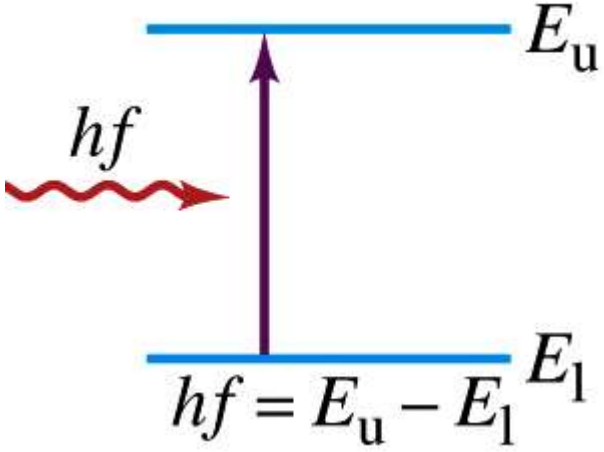
Fluorescent lamp



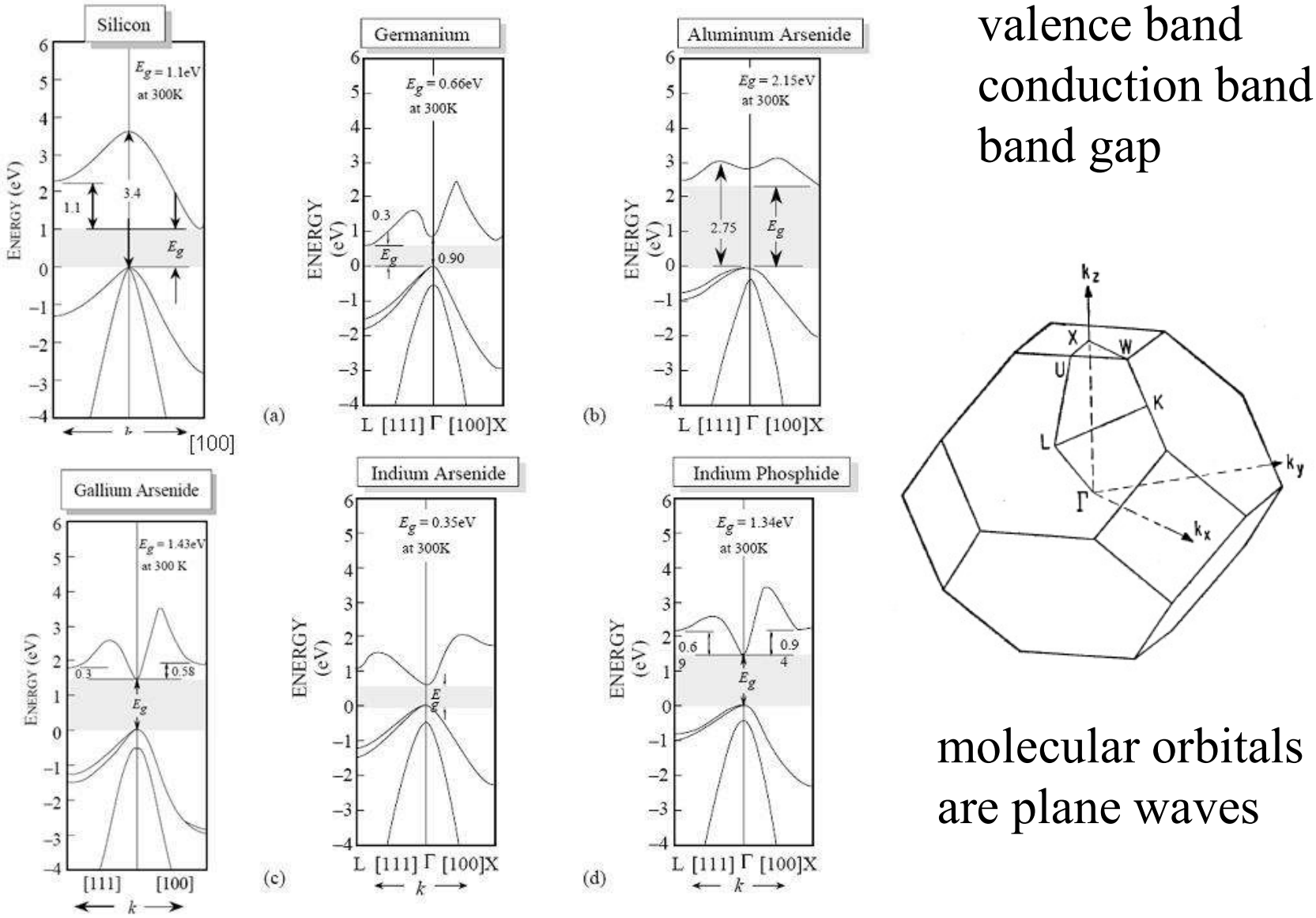
Molecular energy levels







Semiconductors



valence band
conduction band
band gap

molecular orbitals
are plane waves

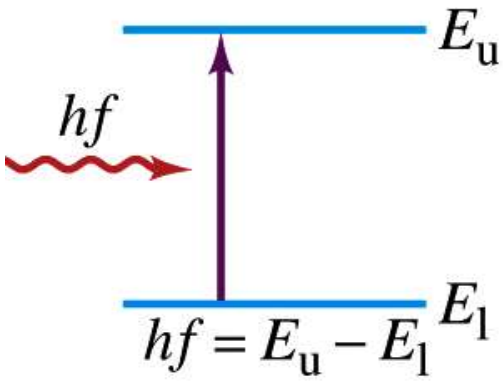
wave vector k

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

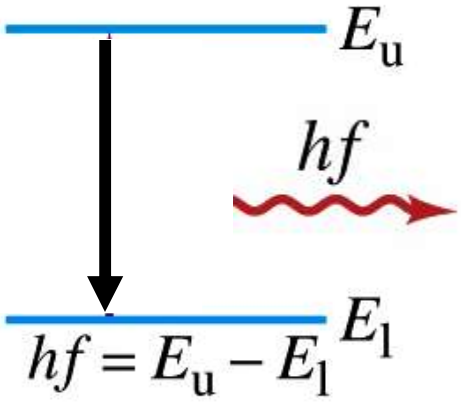
wavelength: $$\lambda = \frac{2\pi}{|\vec{k}|}$$

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

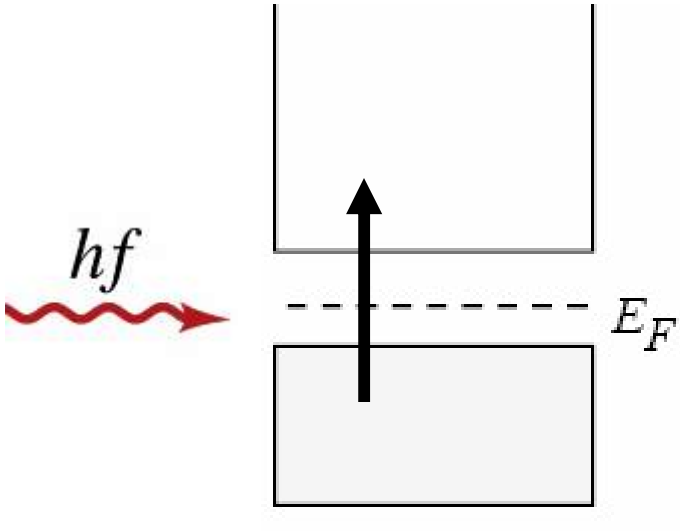
Absorption and emission of photons



absorption



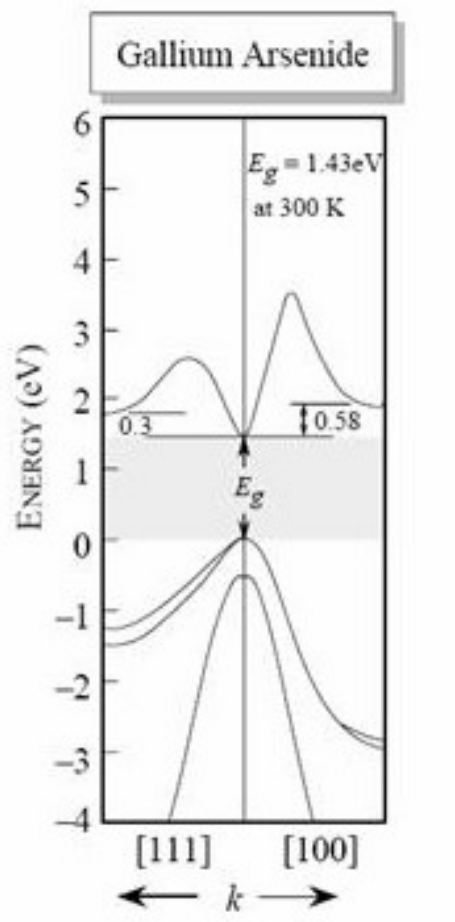
emission



semiconductor

$hf < E_g$ no absorption

What color light does a GaAs LED emit?



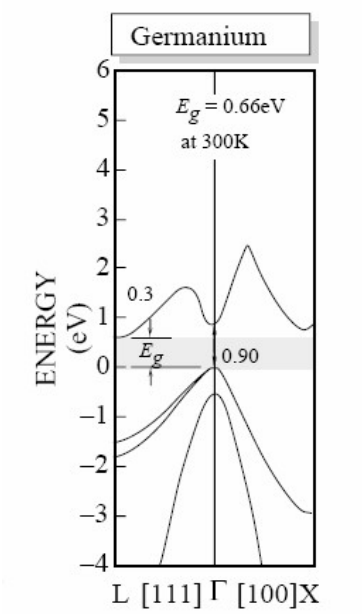
$$E = 1.6022 \times 10^{-19} \times 1.43 \text{ J} = hf = \frac{hc}{\lambda}$$

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

Direct and indirect band gaps

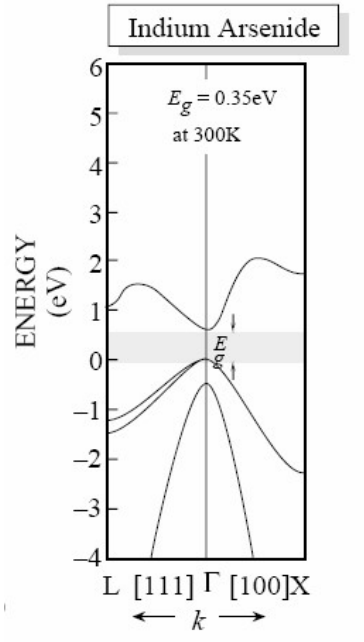
indirect bandgap
$\Delta k \neq 0$

phonons are emitted



direct bandgap:
$\Delta k = 0$

photons can be emitted



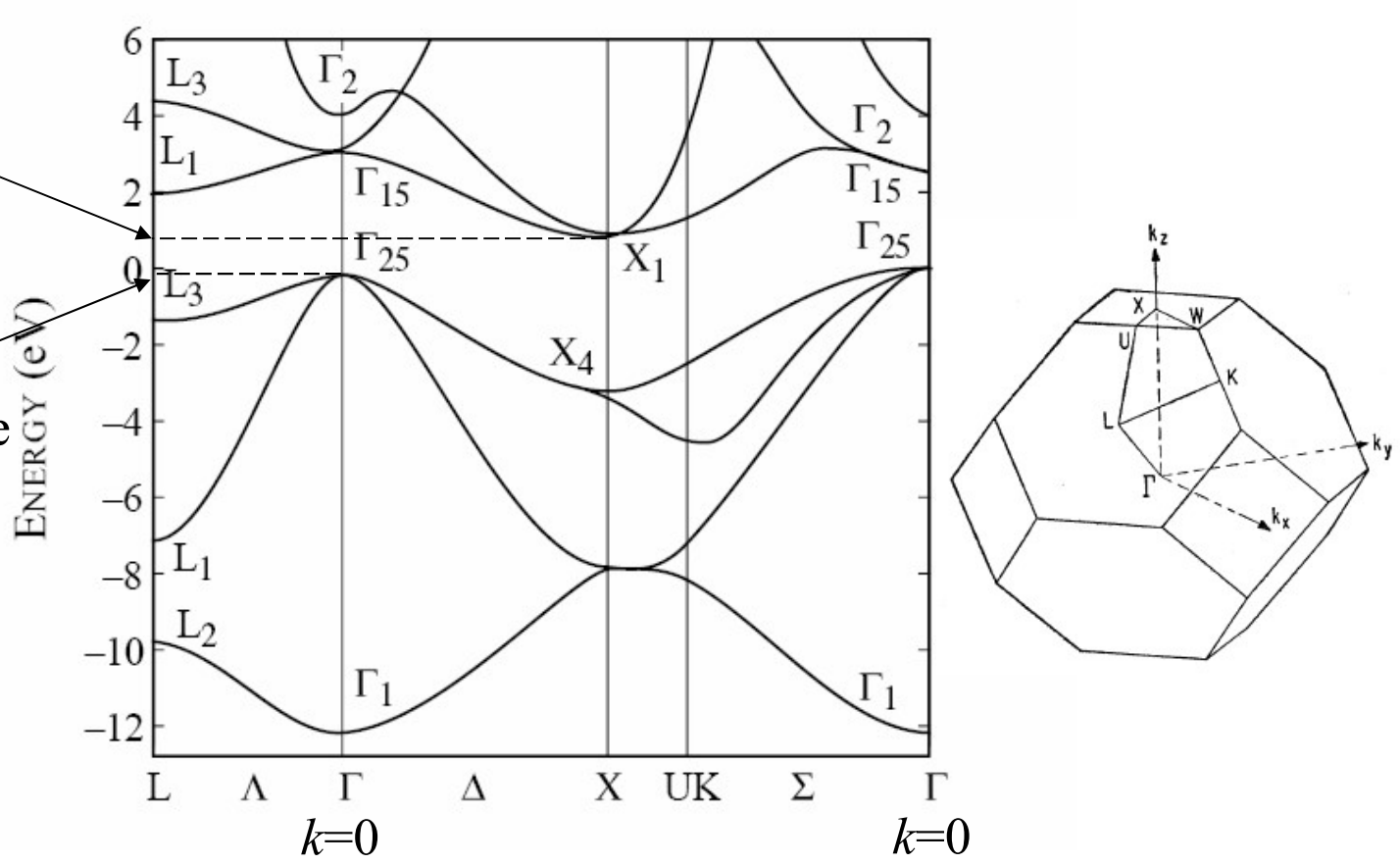
Momentum must be conserved when photons are absorbed or emitted.

Silicon band structure

E_c = bottom of the conduction band

$E_g = E_c - E_v$

E_v = top of the valence band

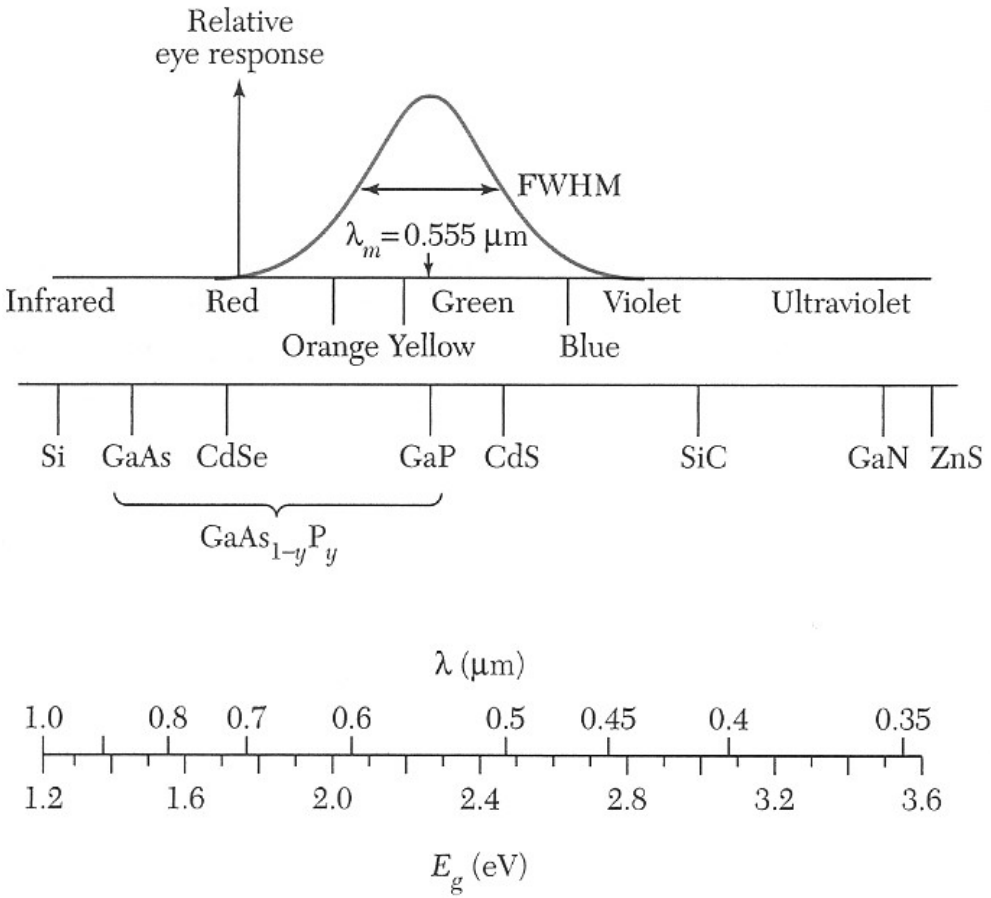


Electrons with energies in the gap are reflected out of the crystal.

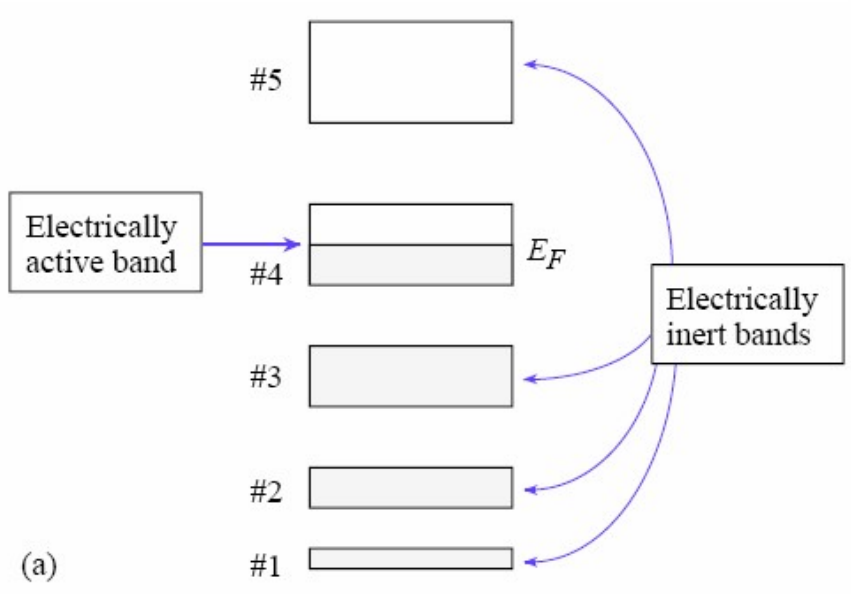
Light emitting diodes

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

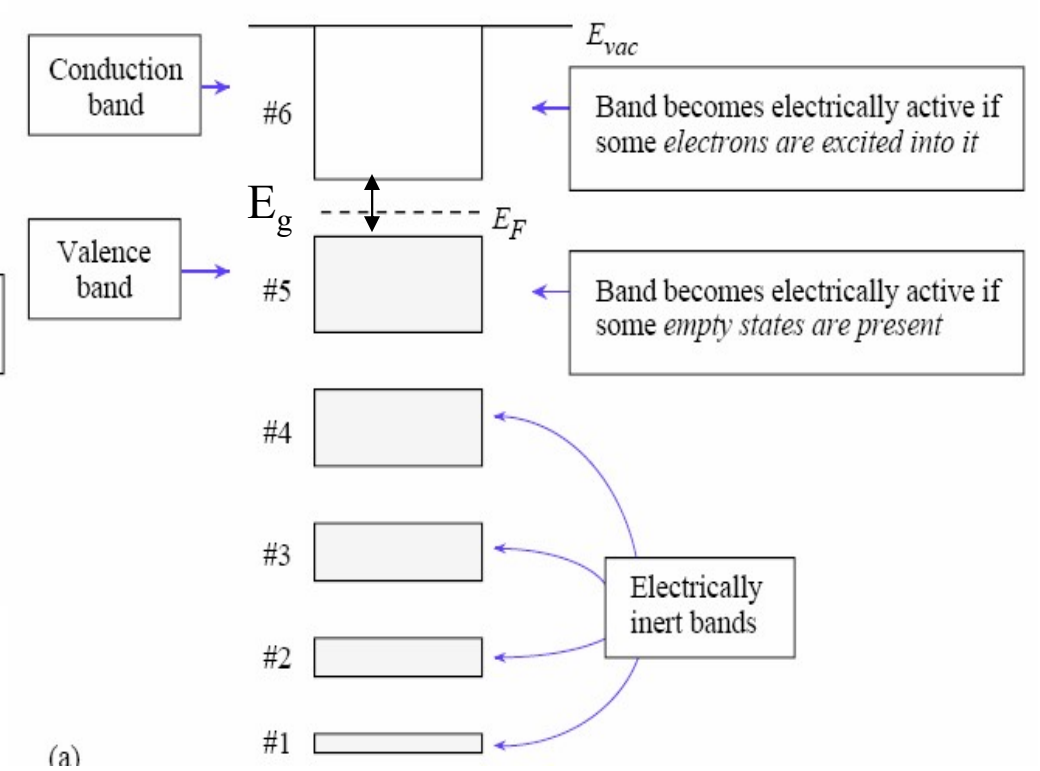
Material	Wavelength (nm)
InAsSbP/InAs	4200
InAs	3800
GaInAsP/GaSb	2000
GaSb	1800
$Ga_xIn_{1-x}As_{1-y}P_y$	1100-1600
$Ga_{0.47}In_{0.53}As$	1550
$Ga_{0.27}In_{0.73}As_{0.63}P_{0.37}$	1300
GaAs:Er,InP:Er	1540
Si:C	1300
GaAs:Yb,InP:Yb	1000
$Al_xGa_{1-x}As$:Si	650-940
GaAs:Si	940
$Al_{0.11}Ga_{0.89}As$:Si	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



Metals, semiconductors, insulators



Metal



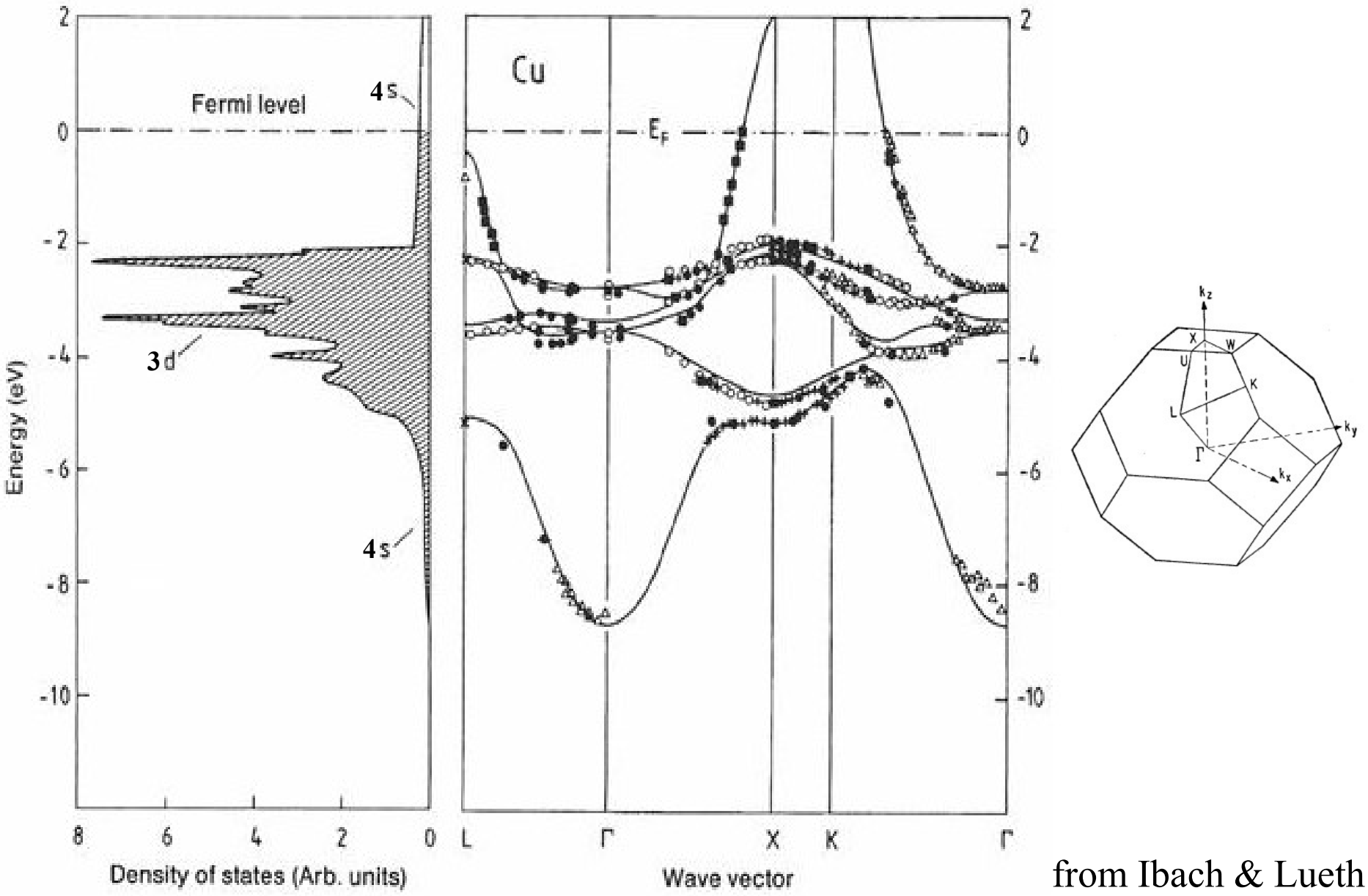
Semiconductor or insulator

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

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

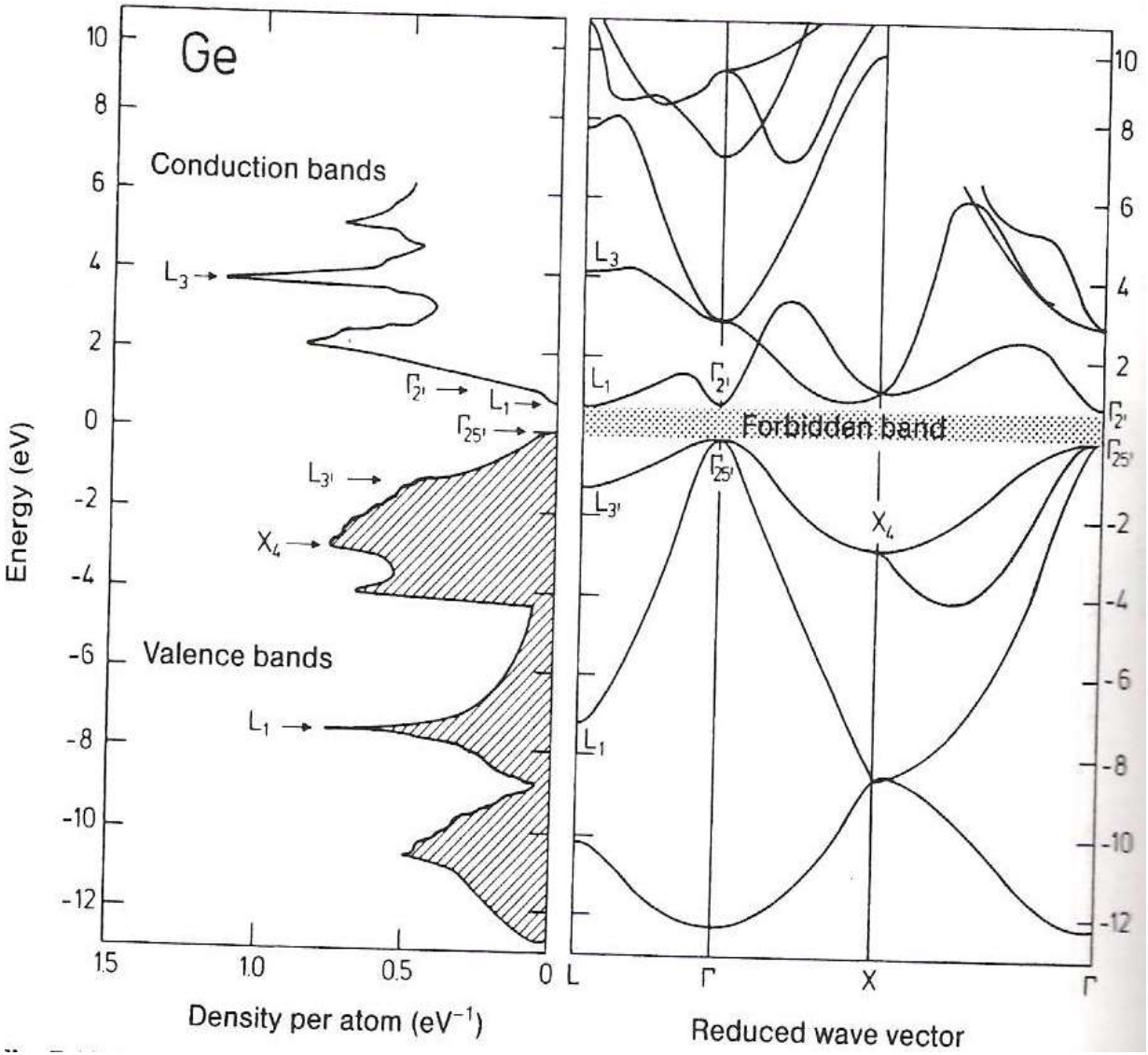
from: Singh

Copper dispersion relation and density of states



from Ibach & Lueth

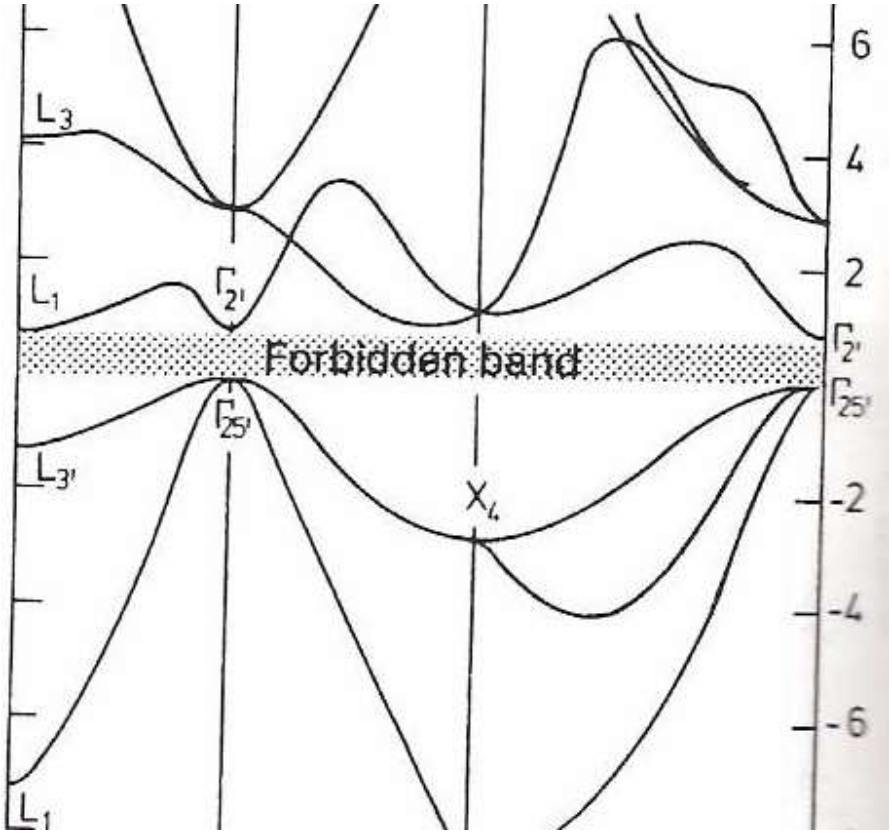
Germanium

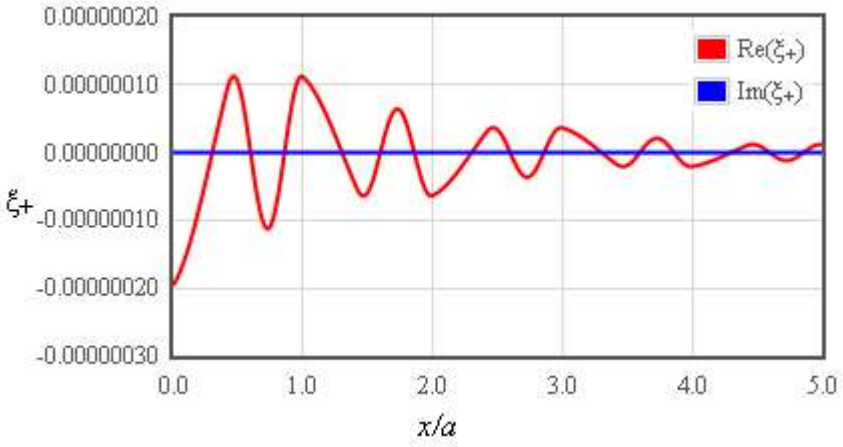


from Ibach & Lueth

Band gap

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



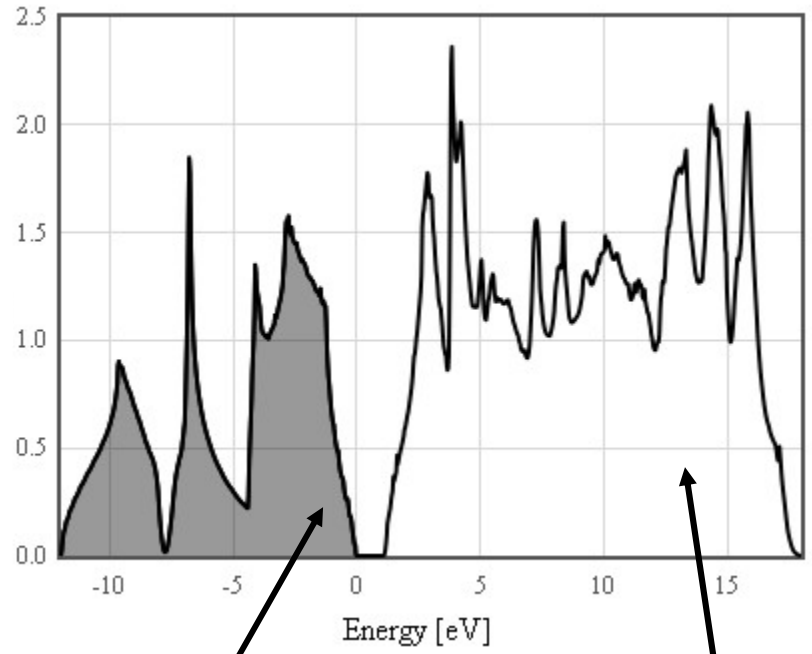


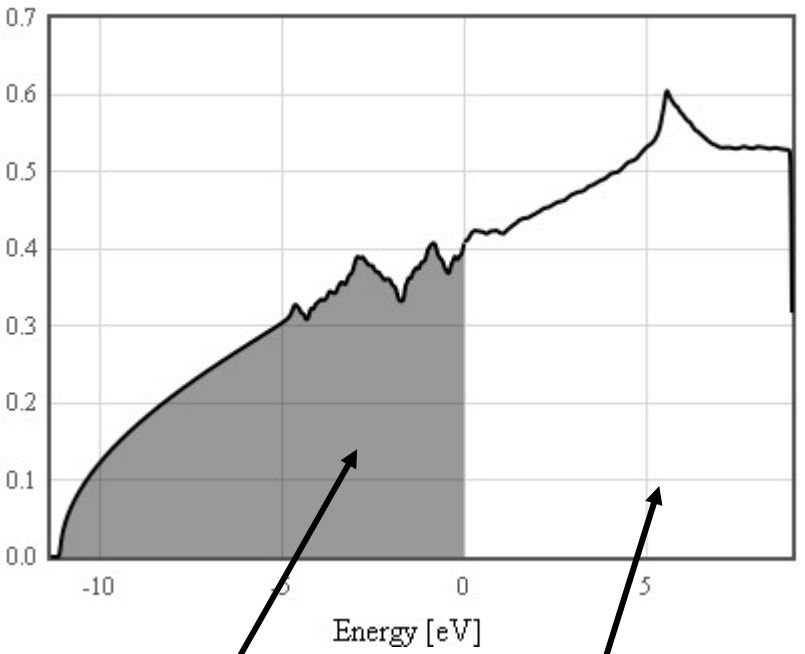
Density of states

Silicon

Aluminum

$D(E)$





filled states

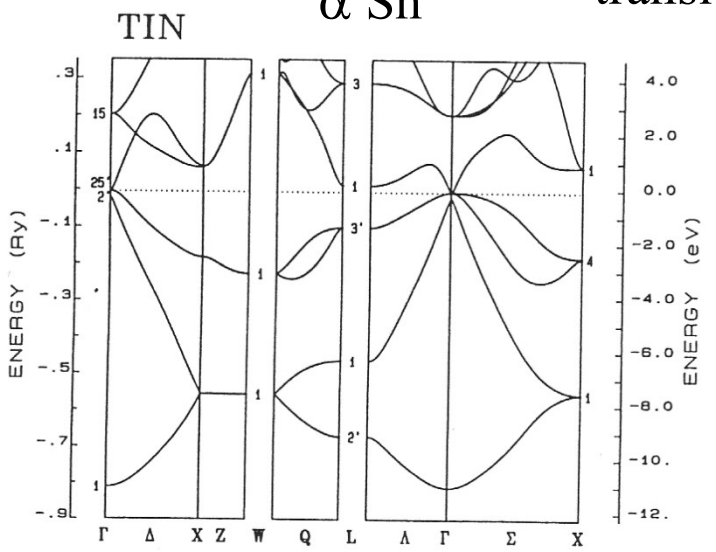
empty states

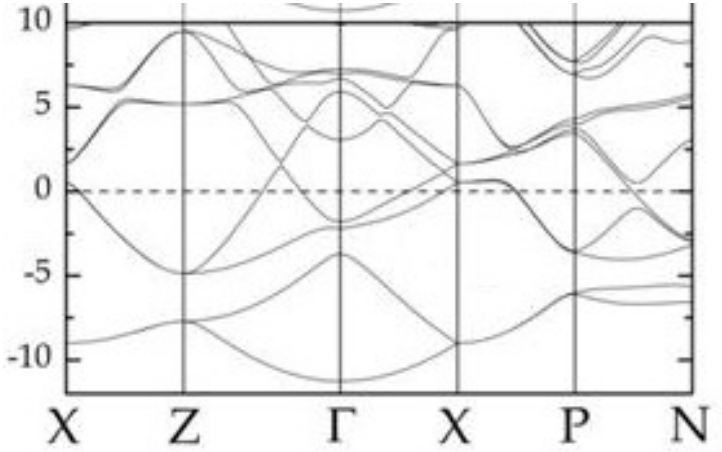
filled states

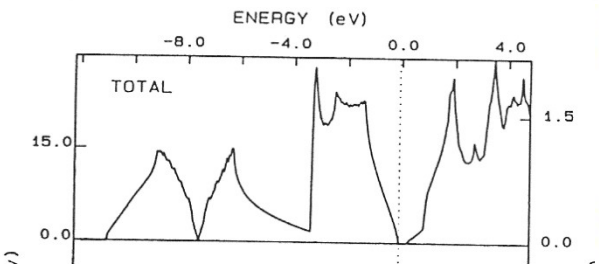
empty states

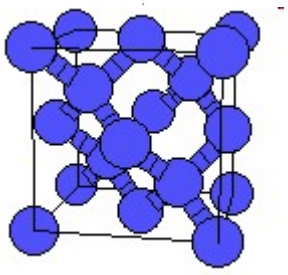
Structural phase transition in Sn

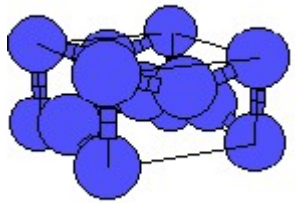
α Sn transition at 13 C metal β Sn







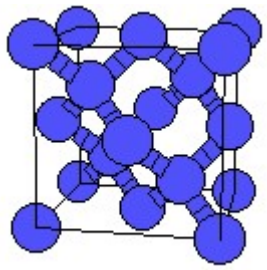




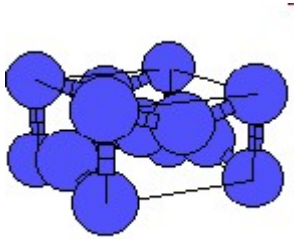
α-Sn, gray tin, diamond structure

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