Crystal Structure

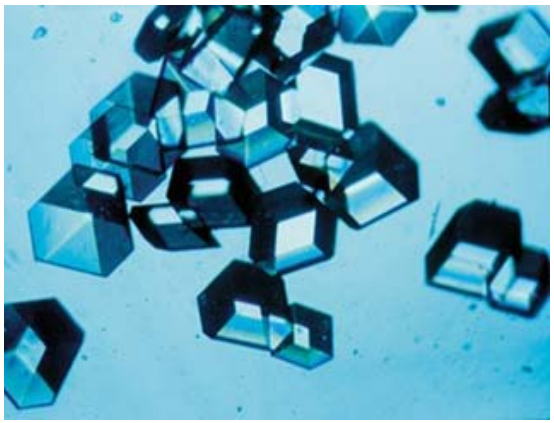
Atoms are arranged in a periodic pattern in a crystal.

The atomic arrangement affects the macroscopic properties of a material.

Many important materials (silicon, steel) are crystals

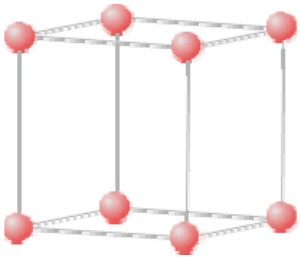
Gallium crystals

quartz

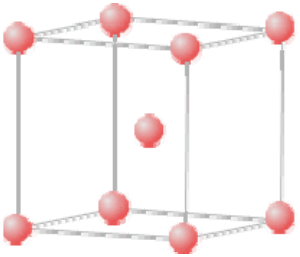


Insulin crystals

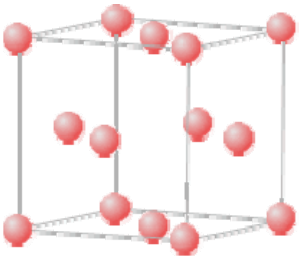
Crystal Structure



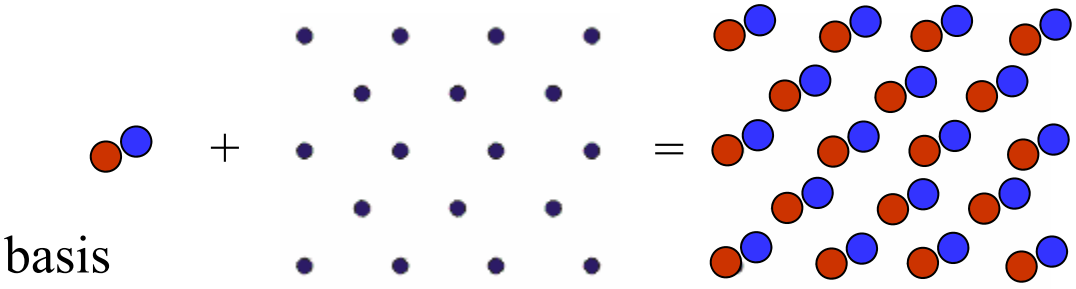
simple cubic



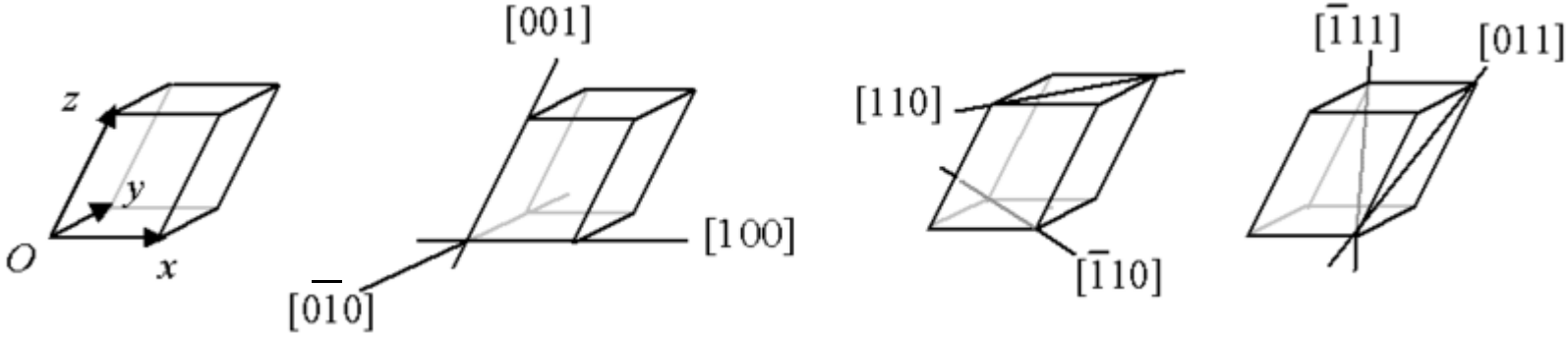
body centered cubic, bcc



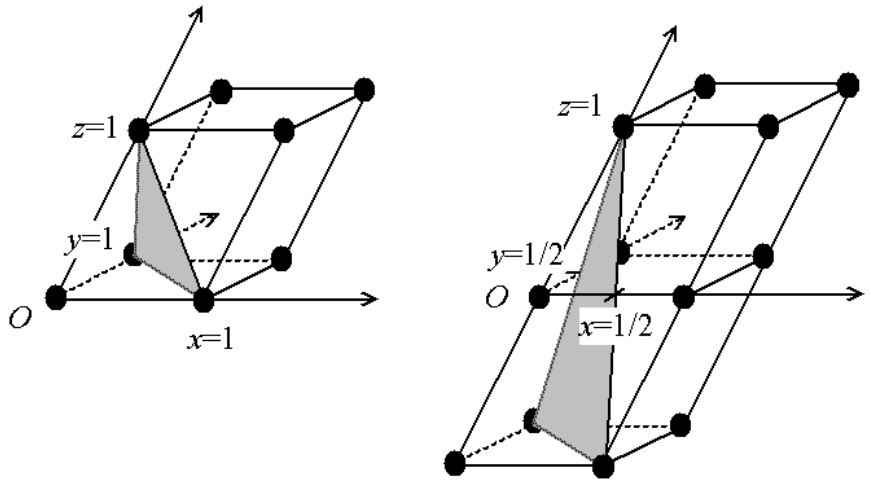
face centered cubic, fcc



Crystal planes and directions: Miller indices



plan (111) plan (221)

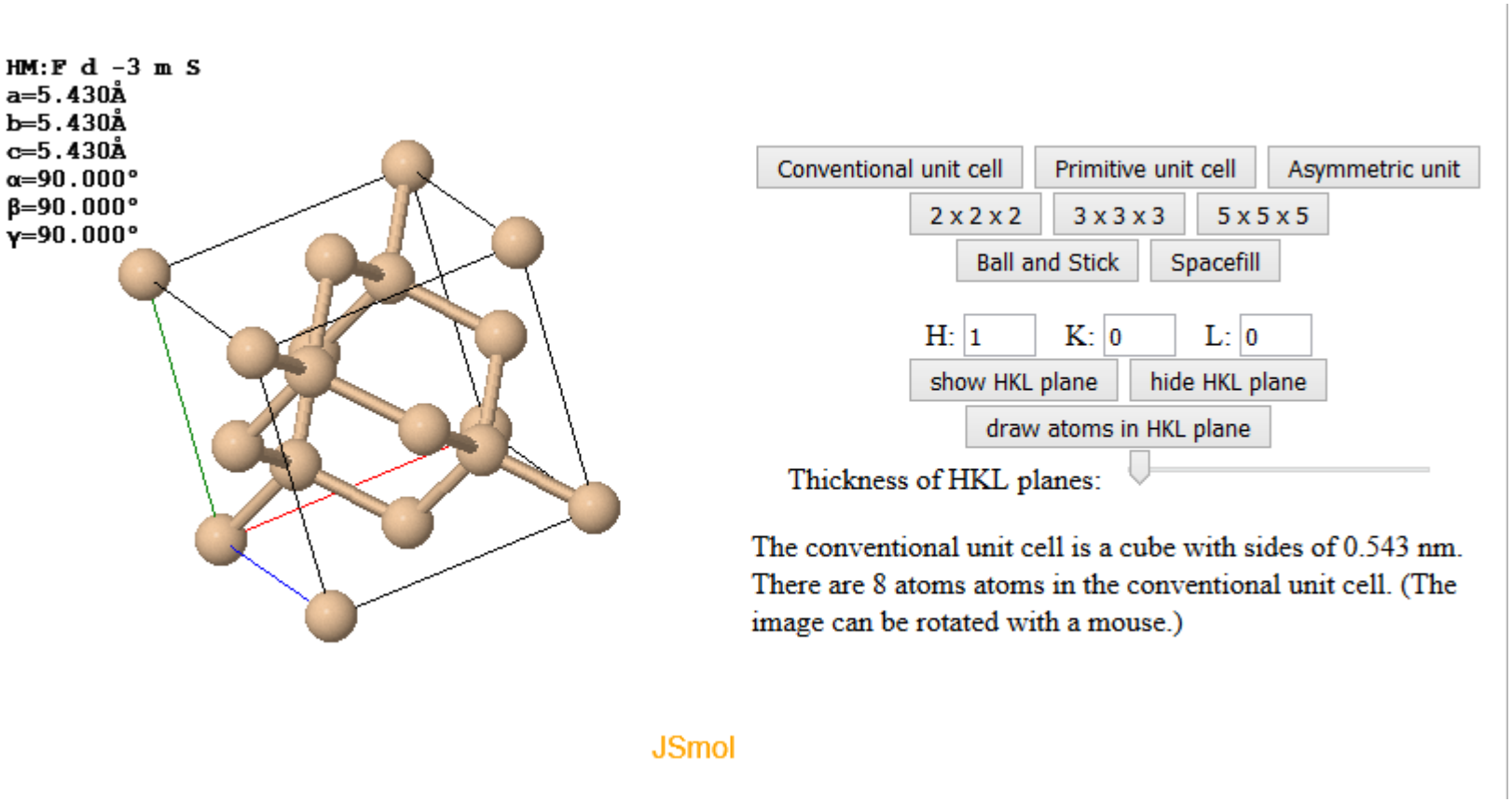


A plane with the intercepts $1/h$, $1/k$, $1/l$ is the (h,k,l) plane.

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

MOSFETs are made on <100> wafers

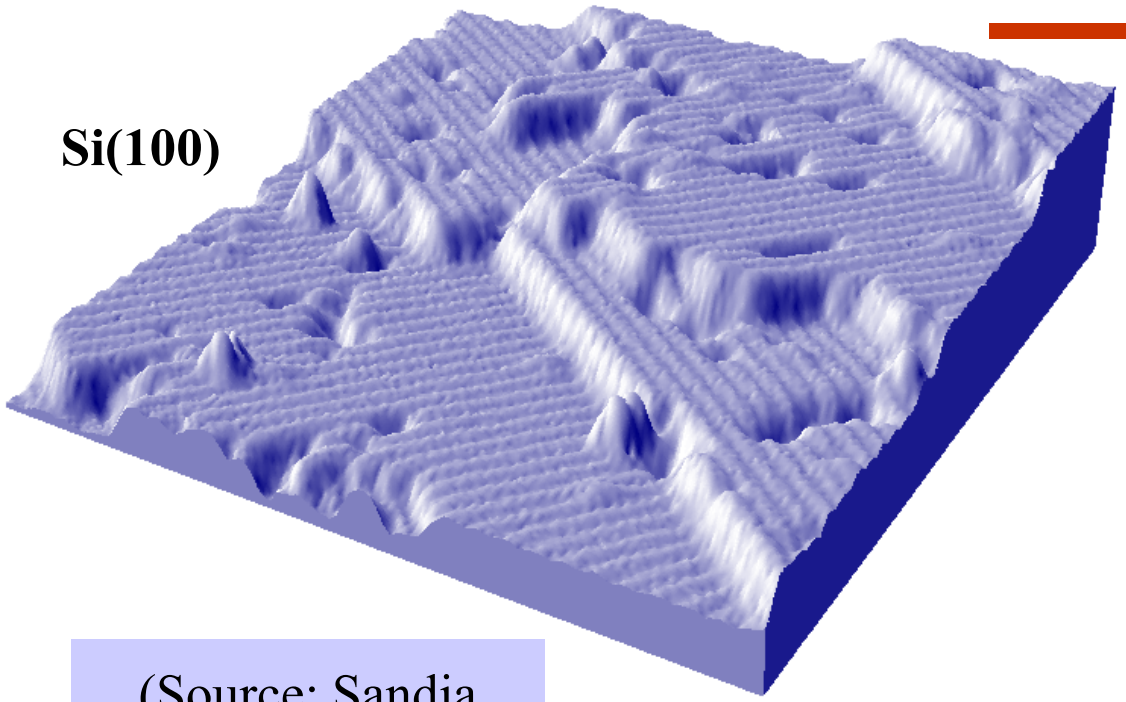
diamond



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

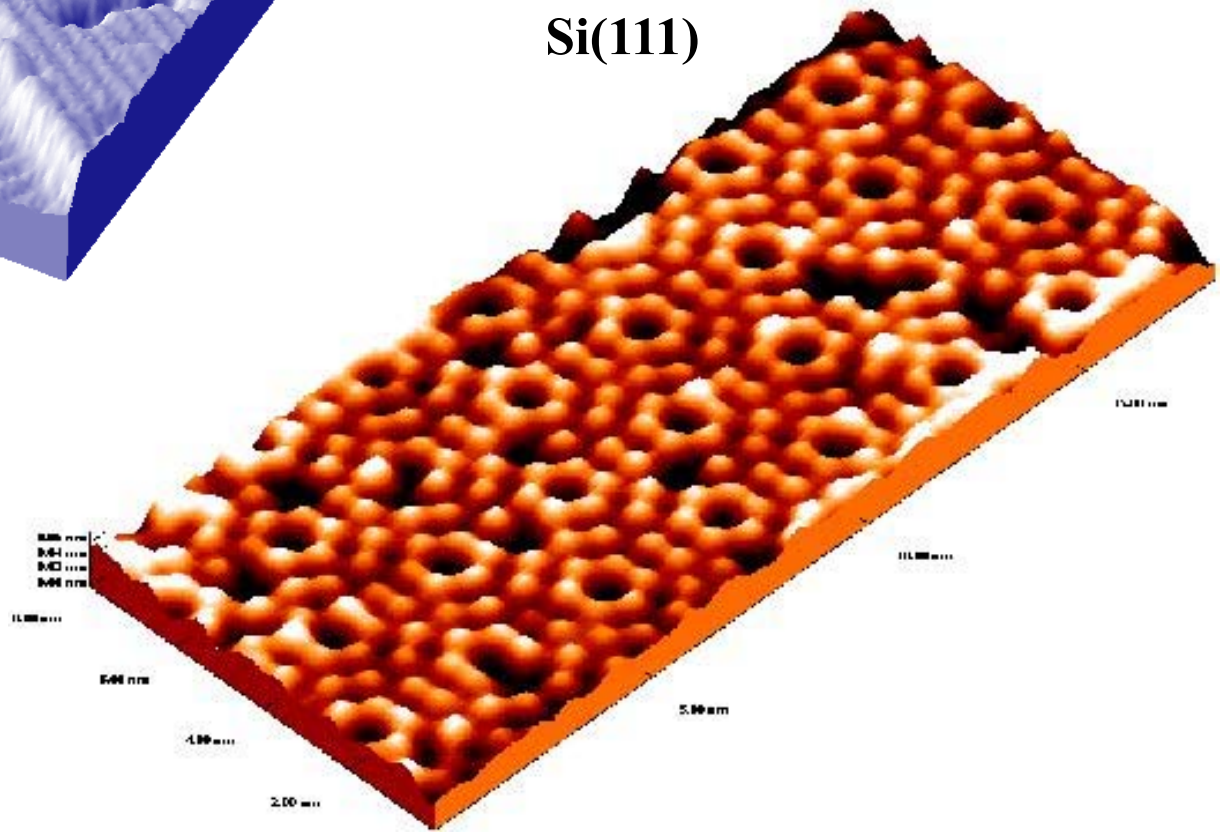
Silicon surfaces

Si(100)

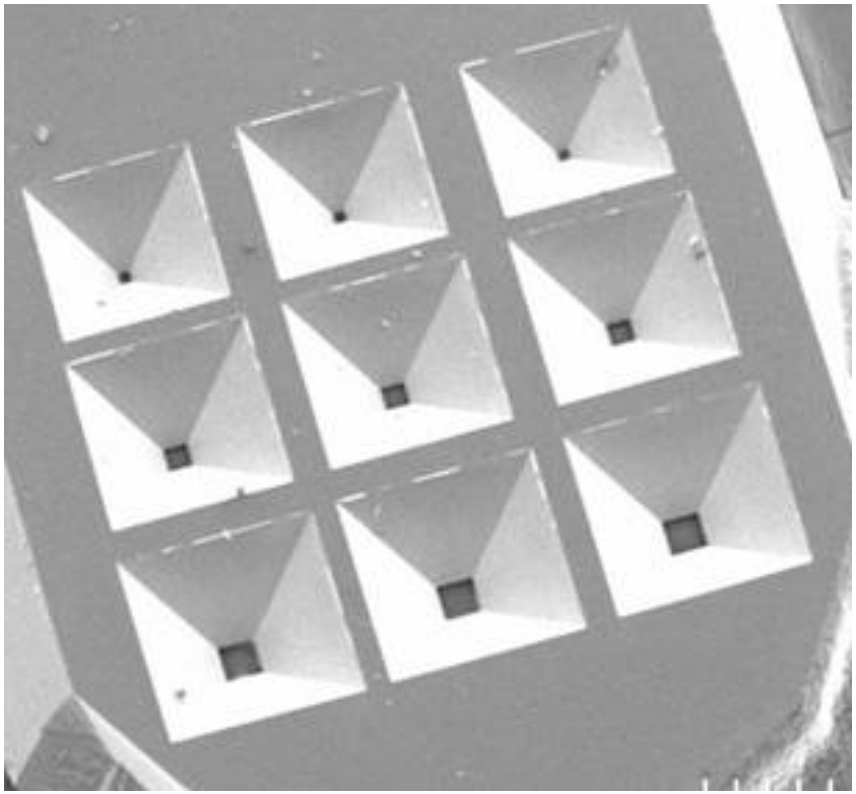


(Source: Sandia Nat.Labs.)

Si(111)



KOH etching of silicon

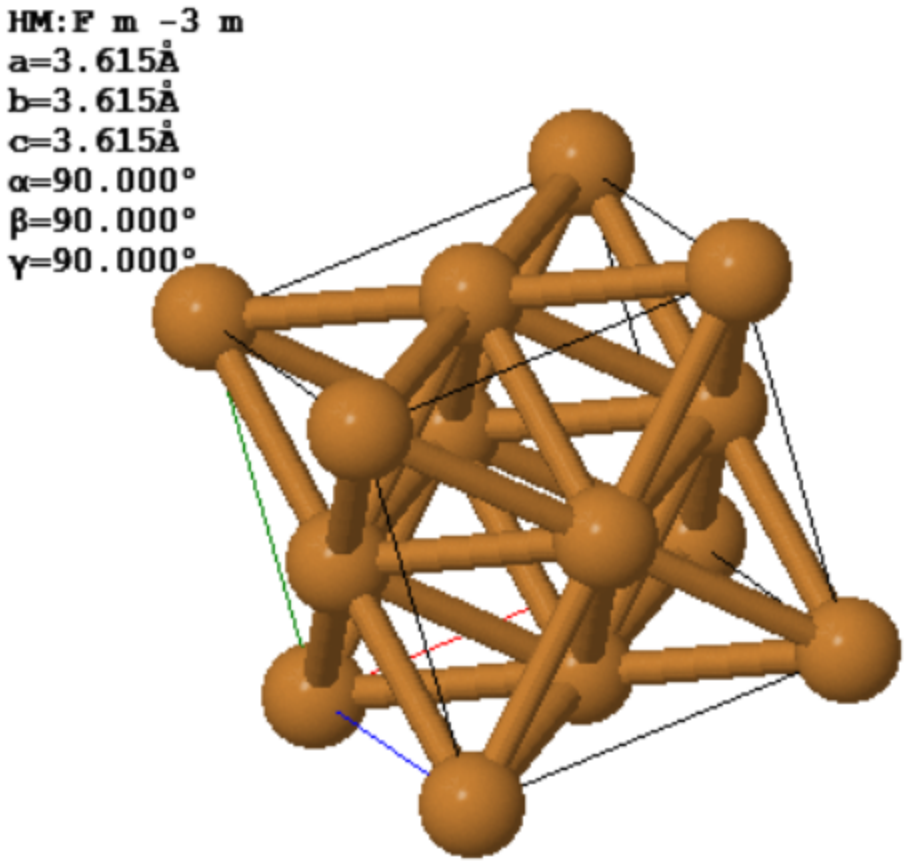


KOH etches Si {110} > {100} > {111}, producing a characteristic anisotropic V-etch, with sidewalls that form a 54.7° angle with the surface (35.3° from the normal).

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

face centered cubic (fcc)

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

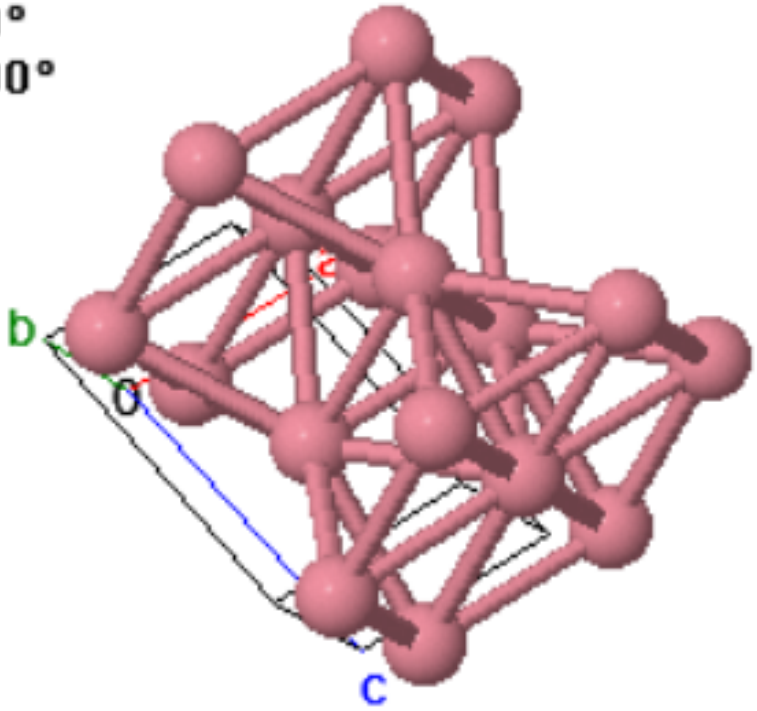


http://lampx.tugraz.at/~hadley/ss1/crystalstructure/structures/fcc/fcc_jsmol.php

hexangonal close pack (hcp)

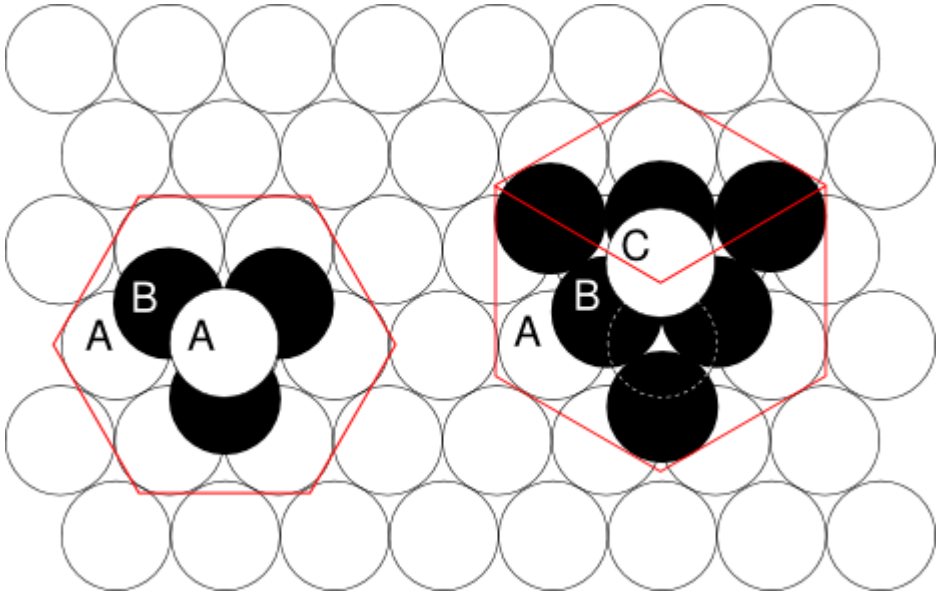
Ti, Co,
Zn, Zr,

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

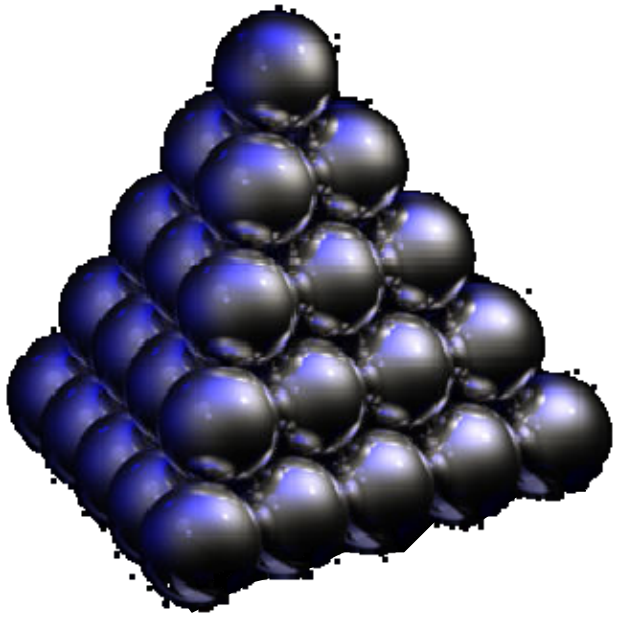


http://lampx.tugraz.at/~hadley/ss1/crystalstructure/structures/hcp/hcp_jsmol.php

Close packing



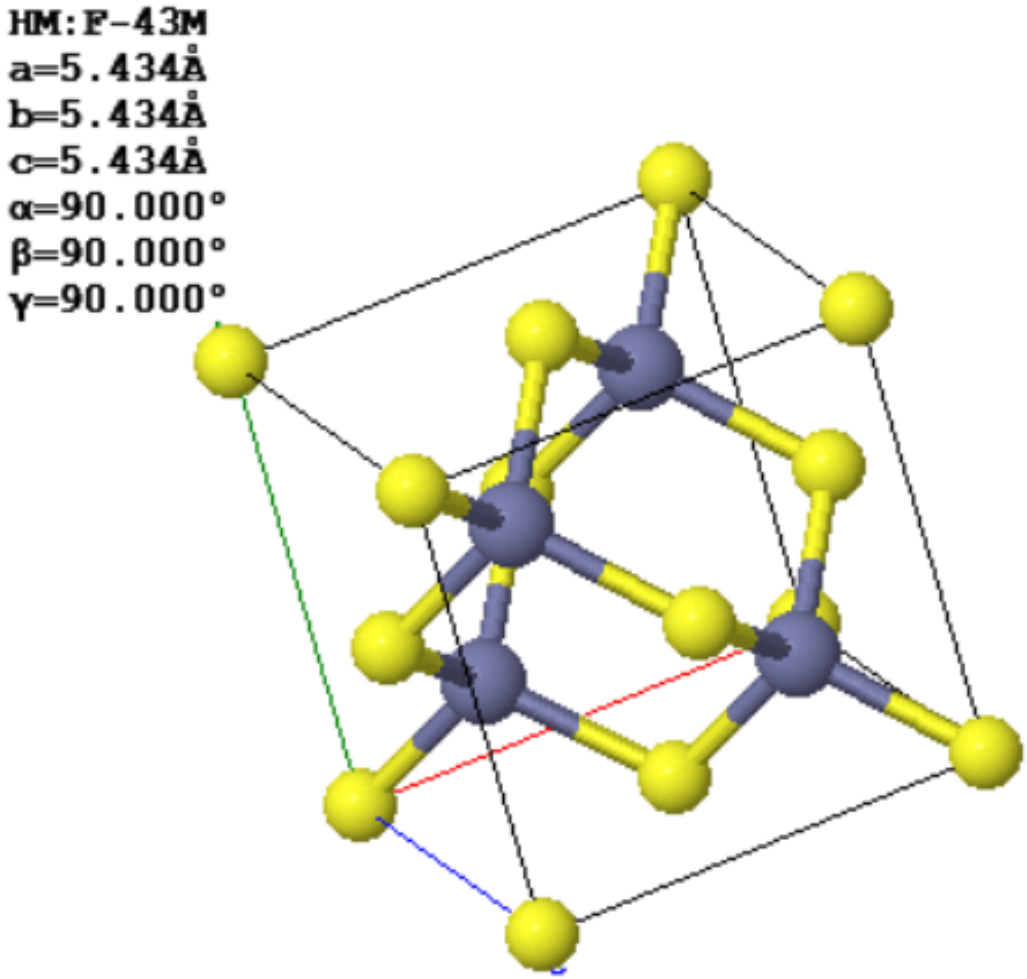
HCP FCC



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

zincblende

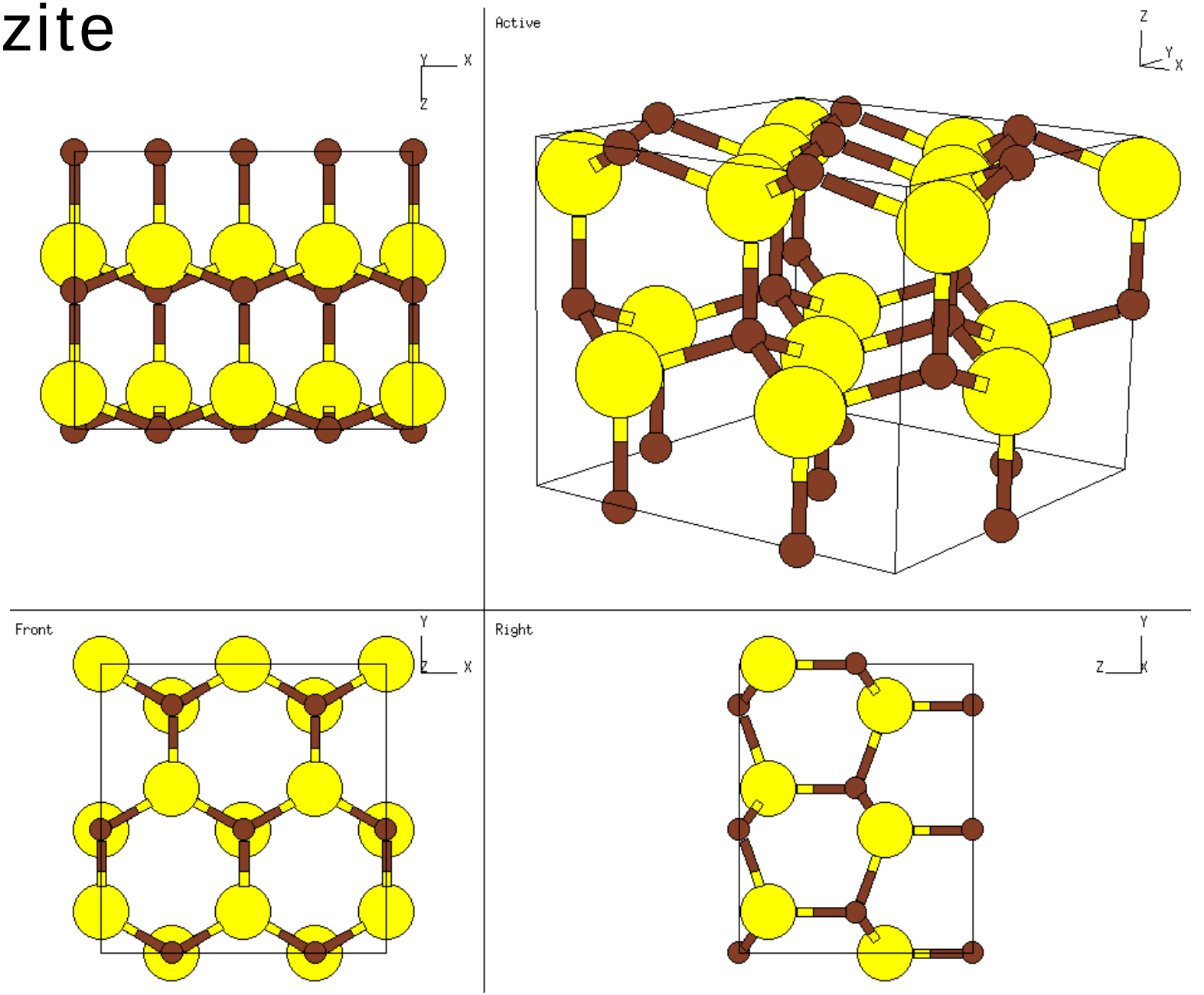
ZnS
GaAs
InP
GaP
InAs
AlAs



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

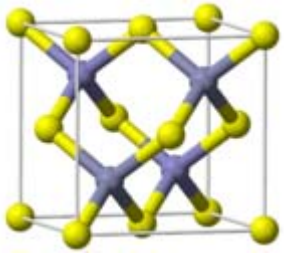
wurtzite

ZnO
CdS
CdSe
GaN
AlN



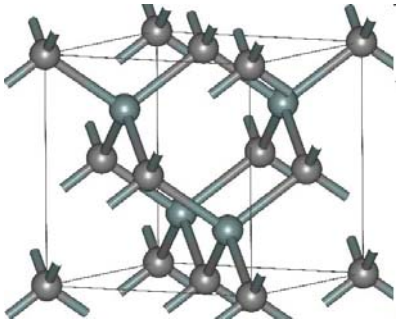
http://cst-www.nrl.navy.mil/lattice/

Structural phase transitions

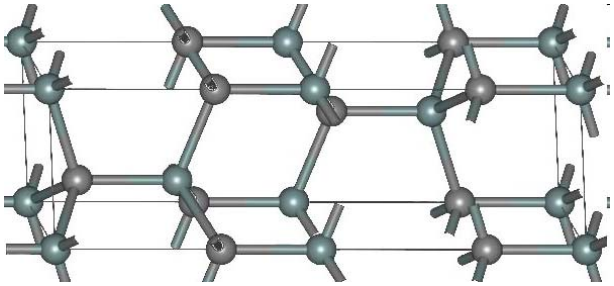


GaAs, Zincblende

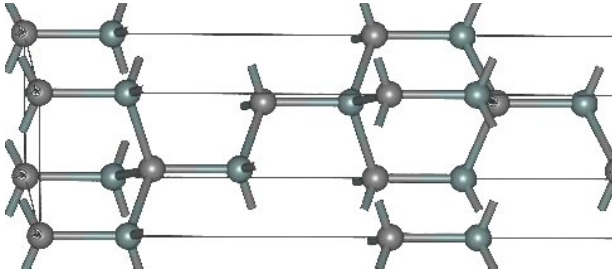
GaAs, Wurtzite



3C - SiC



4H - SiC

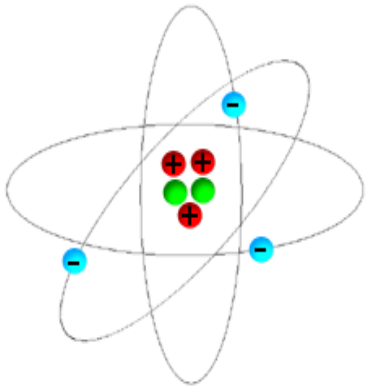


6H - SiC

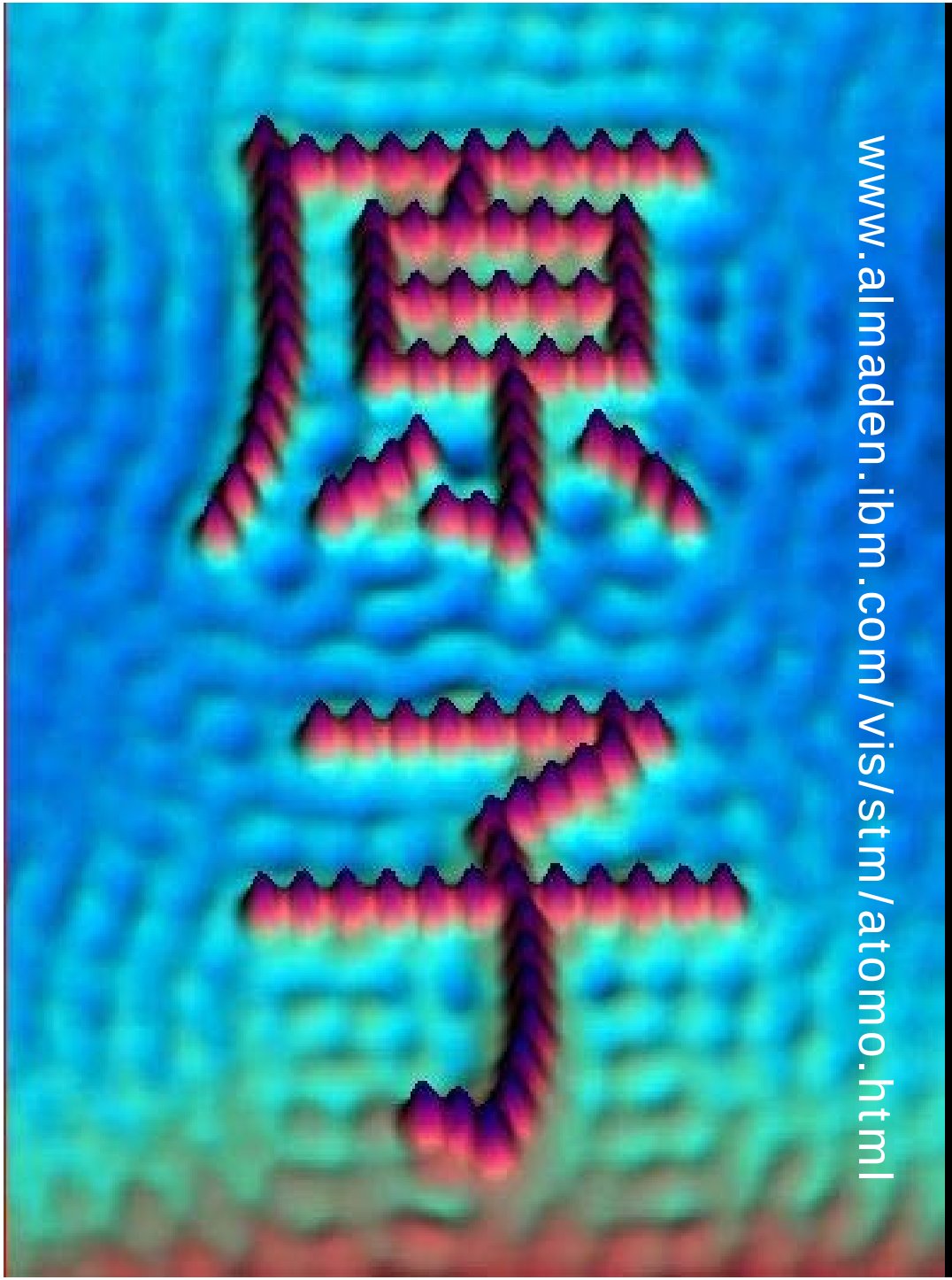
SiC has about 100 polytypes

Electrons

Charge = -1.6022×10^{-19} C
Mass = 9.11×10^{-31} kg
Radius = ?



0.15 nm



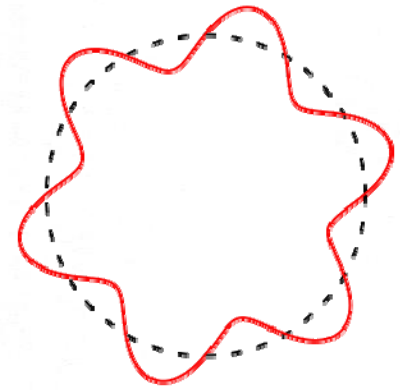
Quantum Mechanics

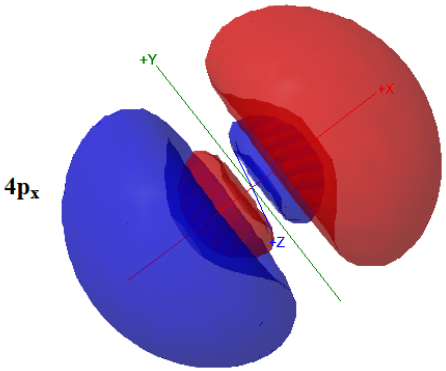
Everything moves like a wave but exchanges energy and momentum like a particle.

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

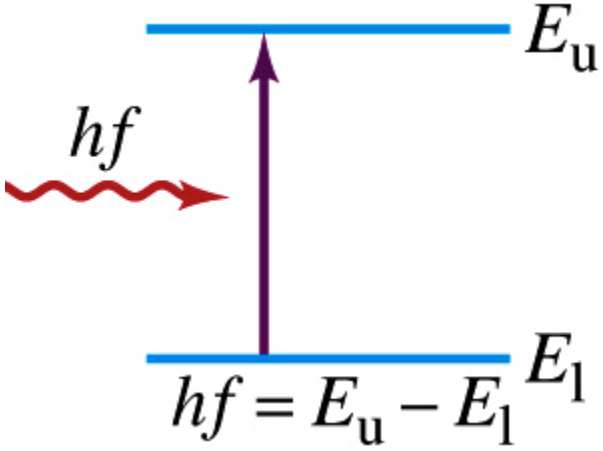
de aangegeven golflengten gelden in vacuüm

	energie eV	*energie* eV	*hoofdquantum getal n =*	*golflengte* nm
0	14			
		13,5950	∞	
		13,0560	5	
	13	12,7497	4	
- 1				1280 100
		12,0888	3	1870 1090
	12			pascher
- 2				656 434 397
				486 410
	11			
- 3		10,2002	2	
	10			balmer
- 4				
	9			
- 5				
	8			
- 6				
	7			
- 7				
	6			102,6 95,0
- 8				121,6 97,2 93,8
	5			
- 9				
	4			
-10				
	3			
-11				
	2			
-12				
	1			
-13				
-13,6	0	0,0000	1	lyman

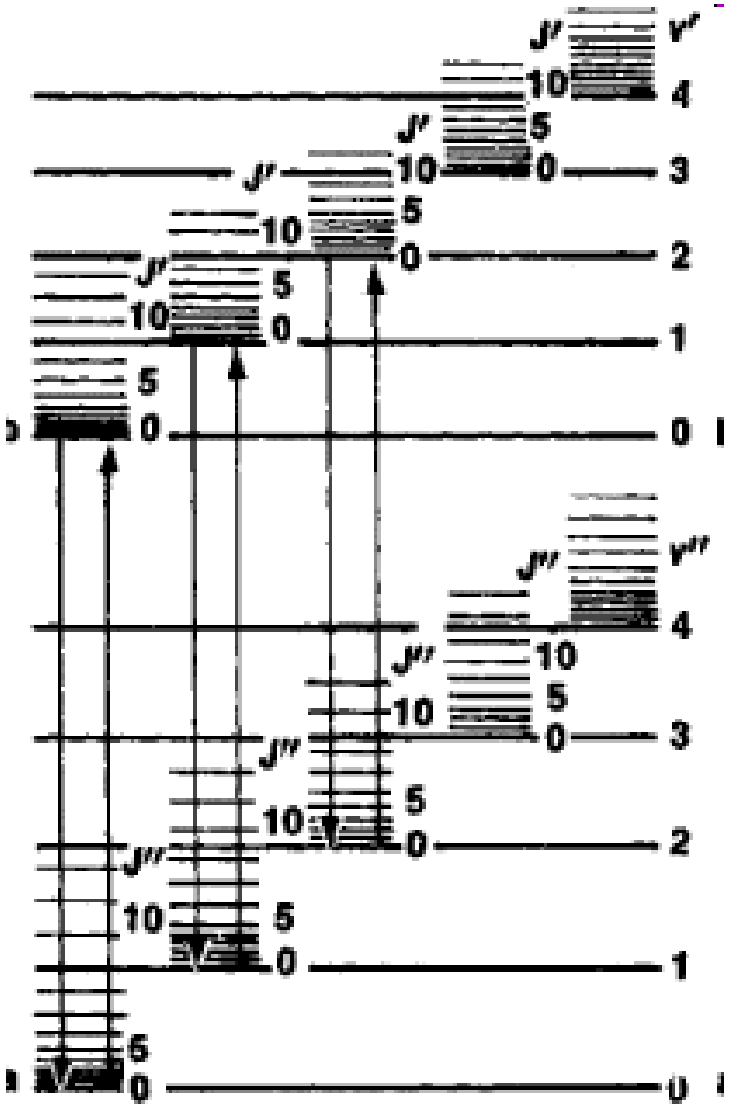


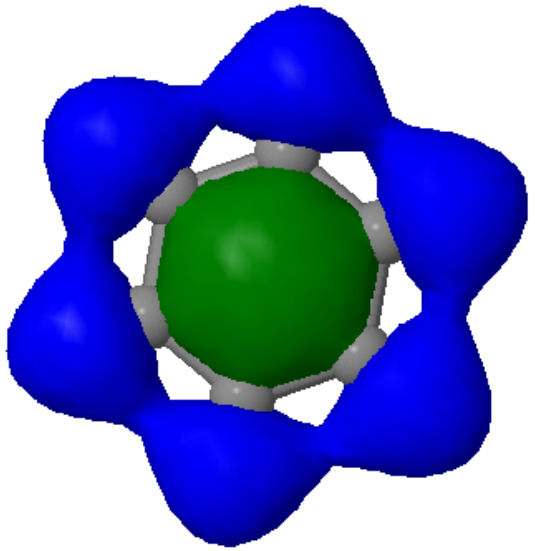


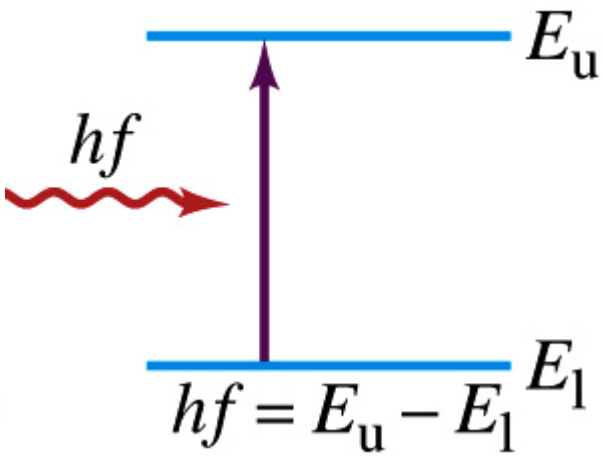
Fluorescent lamp



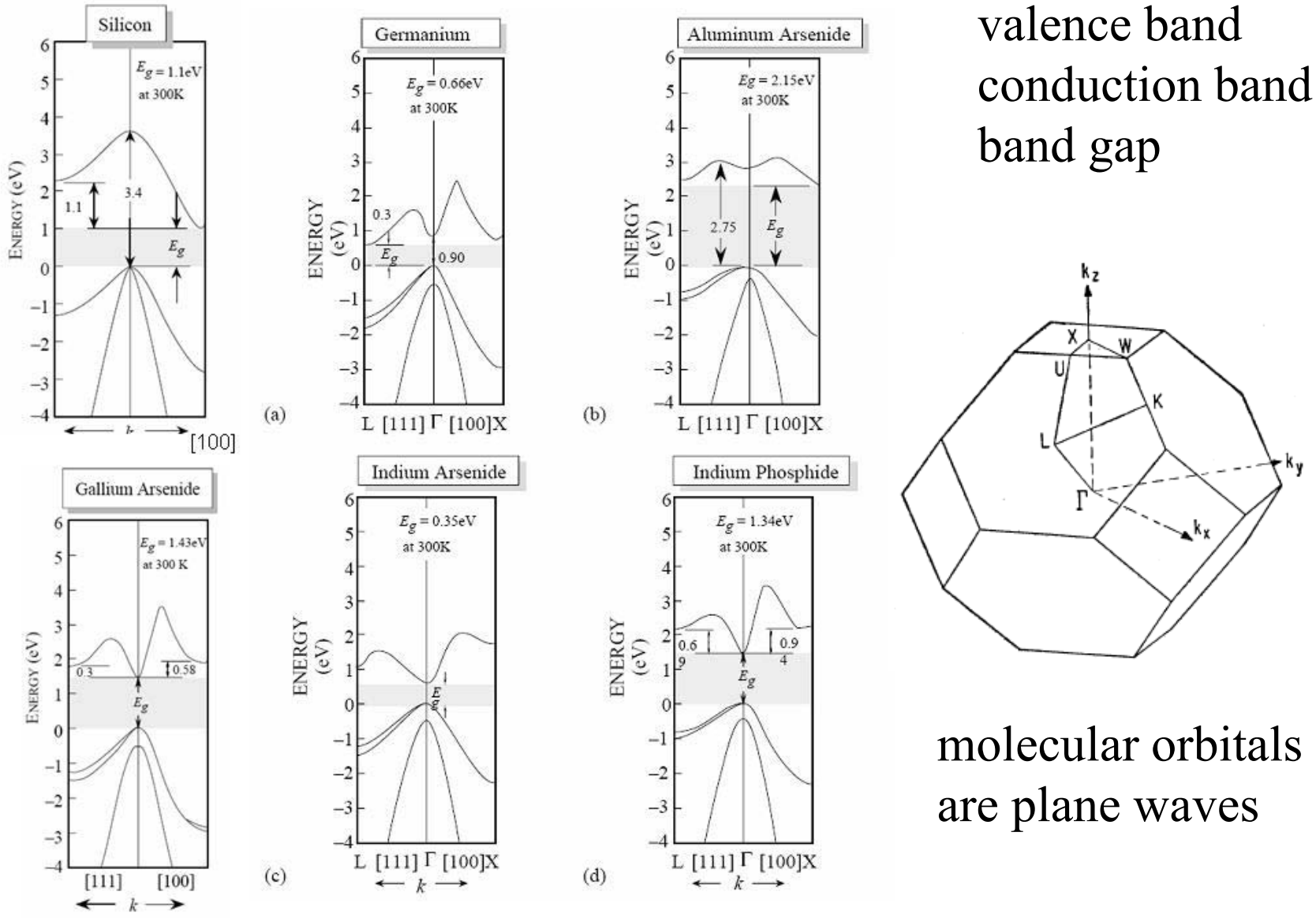
Molecular energy levels







Semiconductors



valence band
conduction band
band gap

molecular orbitals
are plane waves

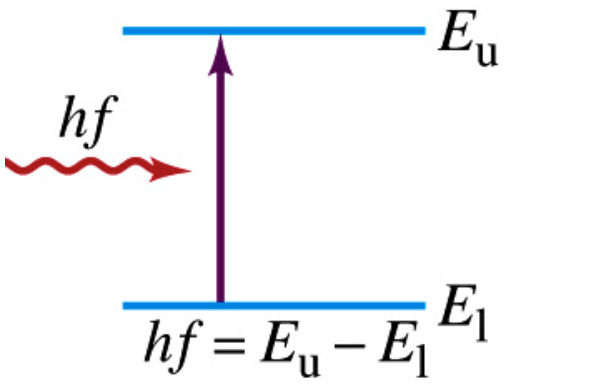
wave vector k

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

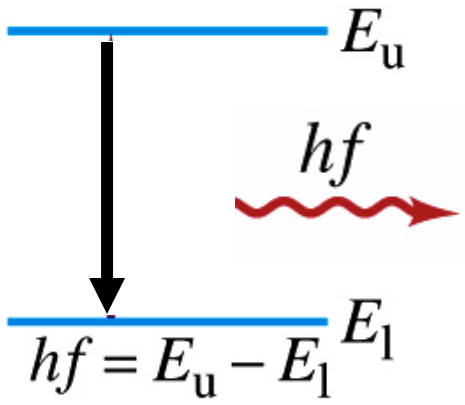
wavelength: $$\lambda = \frac{2\pi}{|\vec{k}|}$$

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

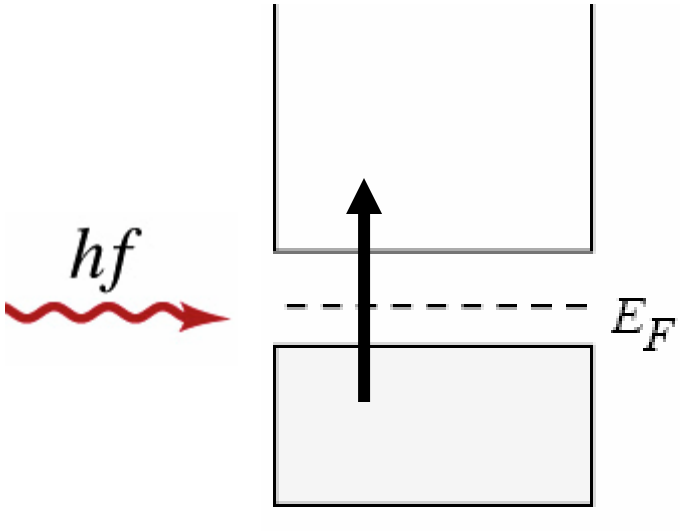
Absorption and emission of photons



absorption



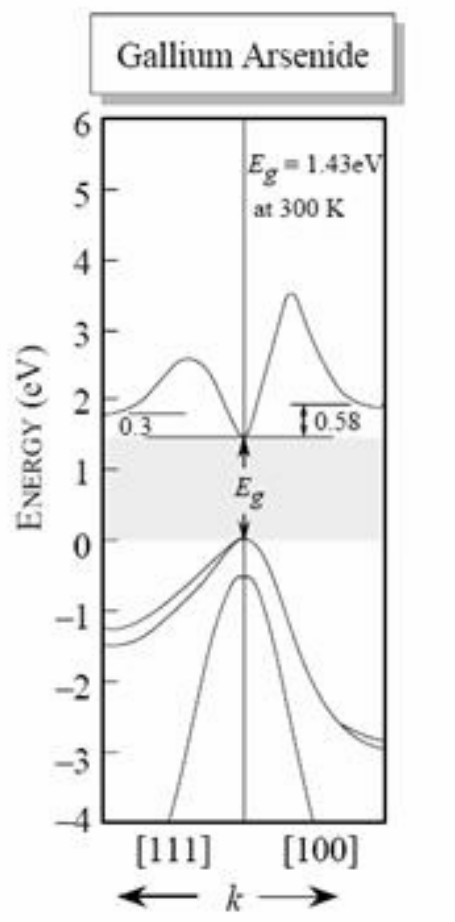
emission



semiconductor

$hf < E_g$ no absorption

What color light does a GaAs LED emit?



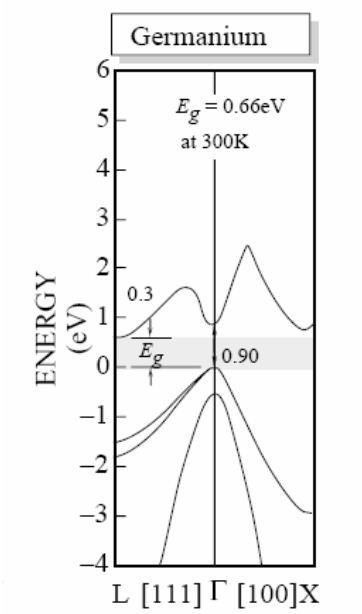
$$E = 1.6022 \times 10^{-19} \times 1.43 \text{ J} = hf = \frac{hc}{\lambda}$$

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

Direct and indirect band gaps

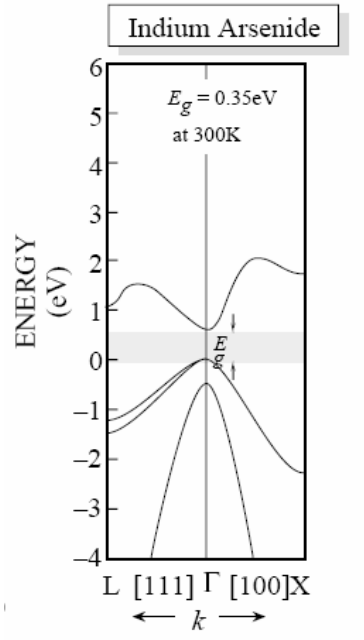
indirect bandgap
$\Delta k \neq 0$

phonons are emitted



direct bandgap:
$\Delta k = 0$

photons can be emitted



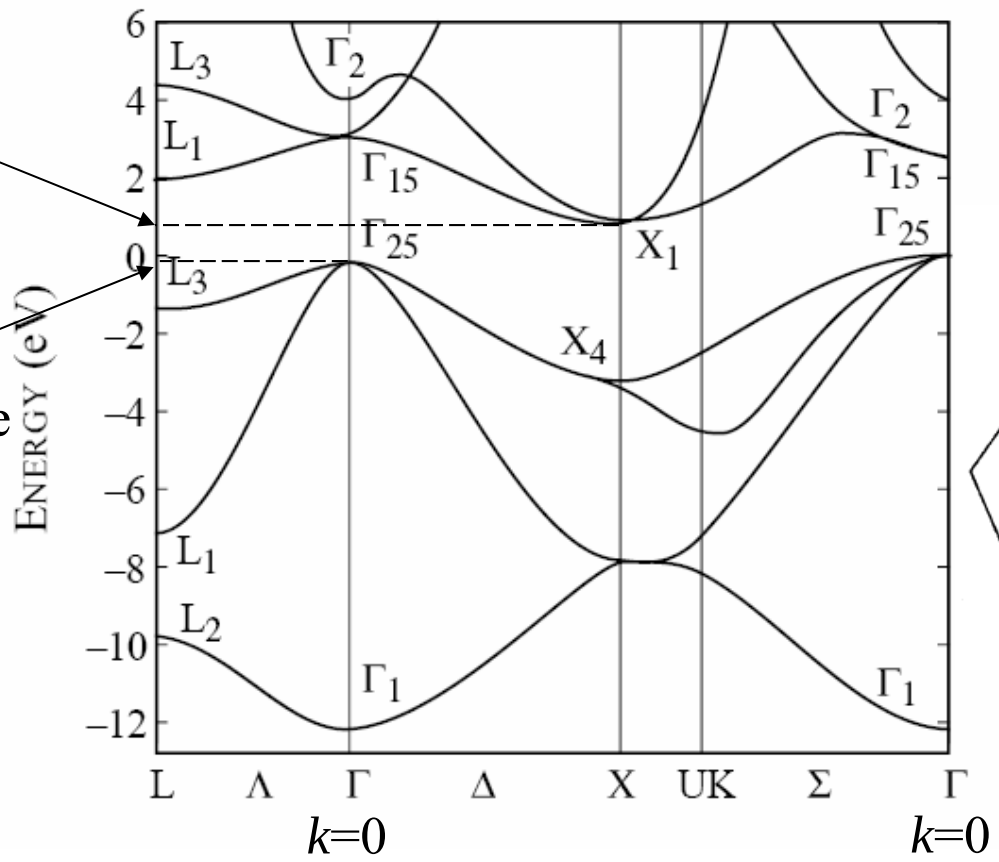
Momentum must be conserved when photons are absorbed or emitted.

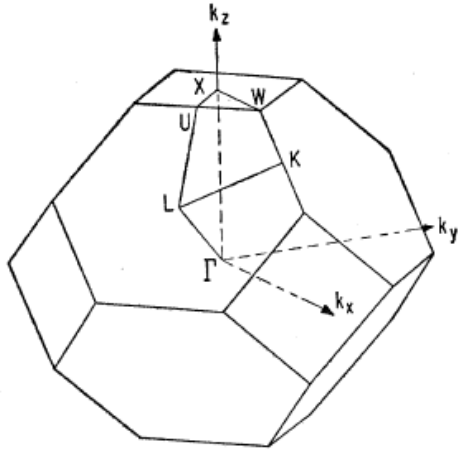
Silicon band structure

E_c = bottom of the conduction band

$E_g = E_c - E_v$

E_v = top of the valence band



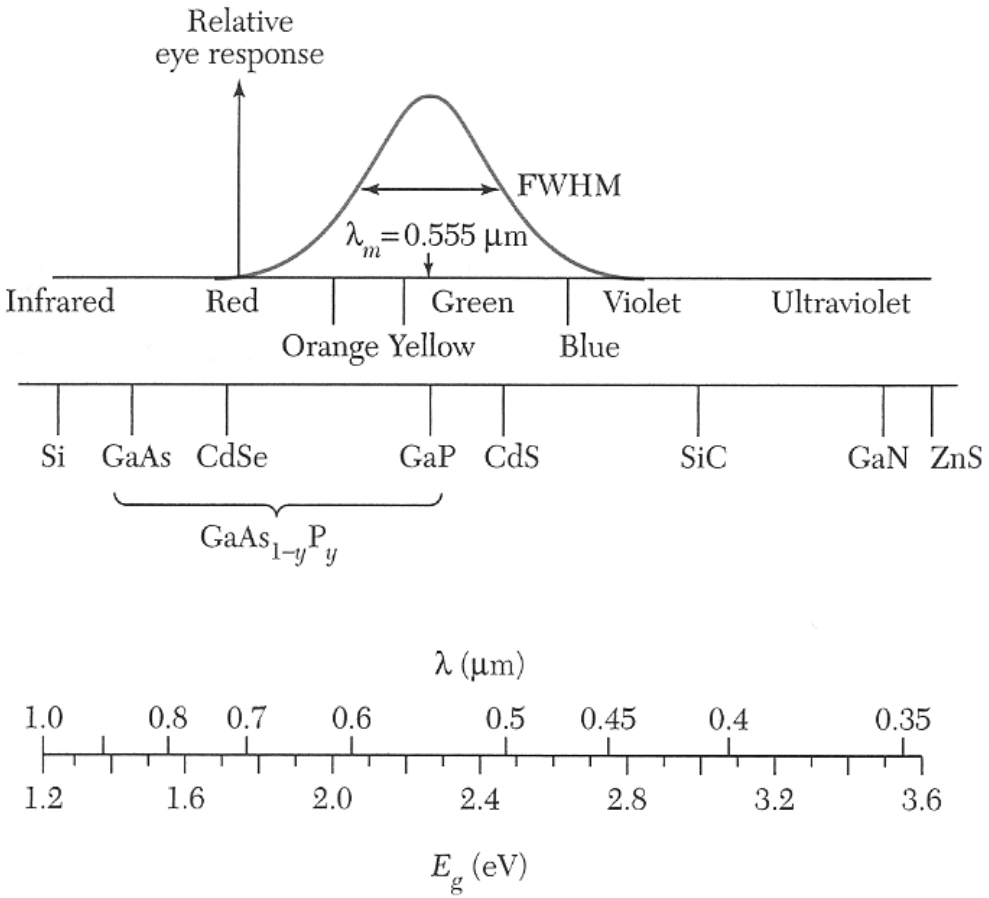


Electrons with energies in the gap are reflected out of the crystal.

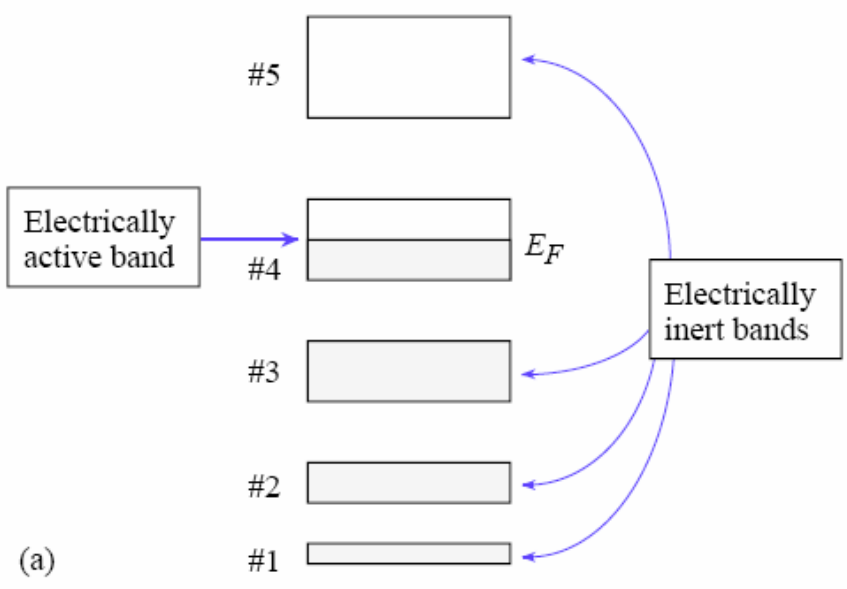
Light emitting diodes

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

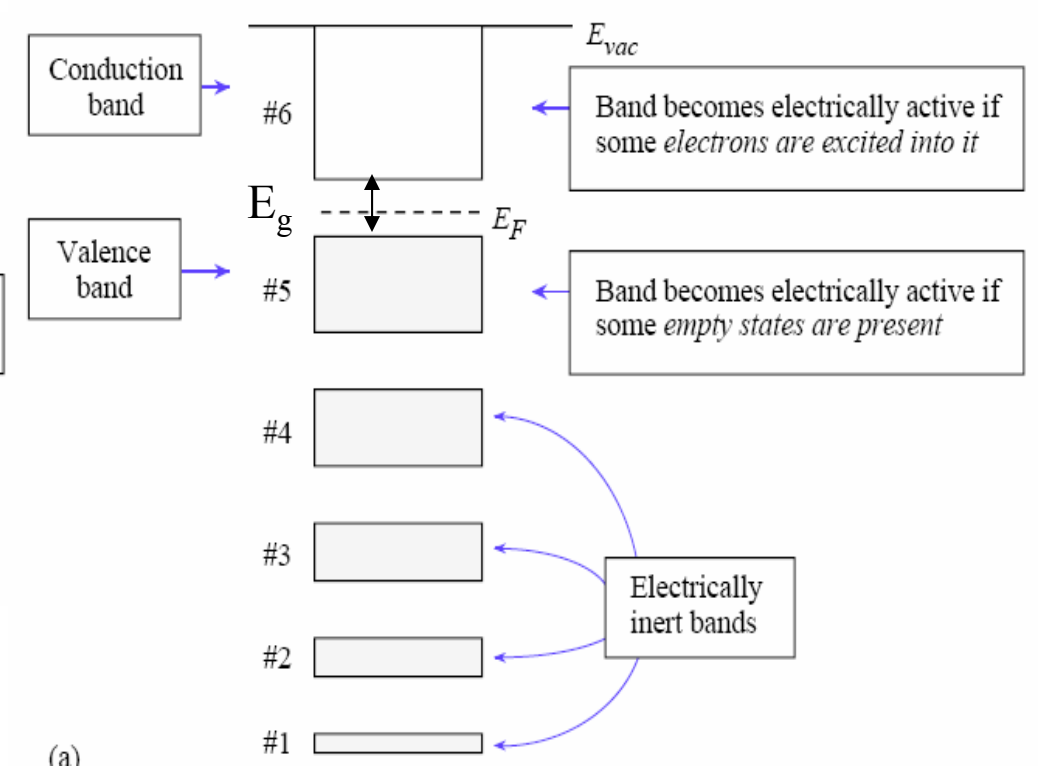
Material	Wavelength (nm)
InAsSbP/InAs	4200
InAs	3800
GaInAsP/GaSb	2000
GaSb	1800
$Ga_xIn_{1-x}As_{1-y}P_y$	1100-1600
$Ga_{0.47}In_{0.53}As$	1550
$Ga_{0.27}In_{0.73}As_{0.63}P_{0.37}$	1300
GaAs:Er,InP:Er	1540
Si:C	1300
GaAs:Yb,InP:Yb	1000
$Al_xGa_{1-x}As$:Si	650-940
GaAs:Si	940
$Al_{0.11}Ga_{0.89}As$:Si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



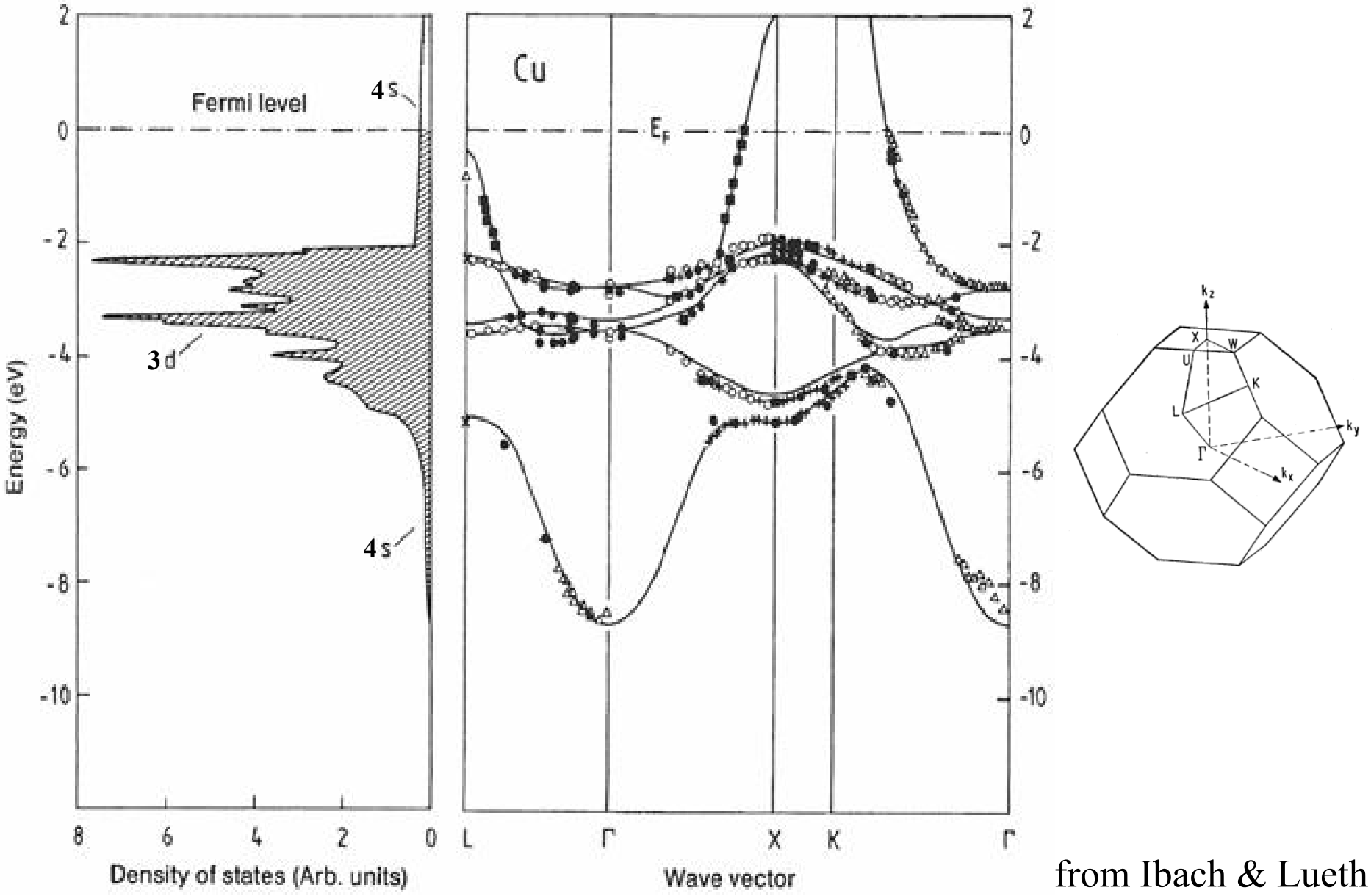
Semiconductor or insulator

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

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

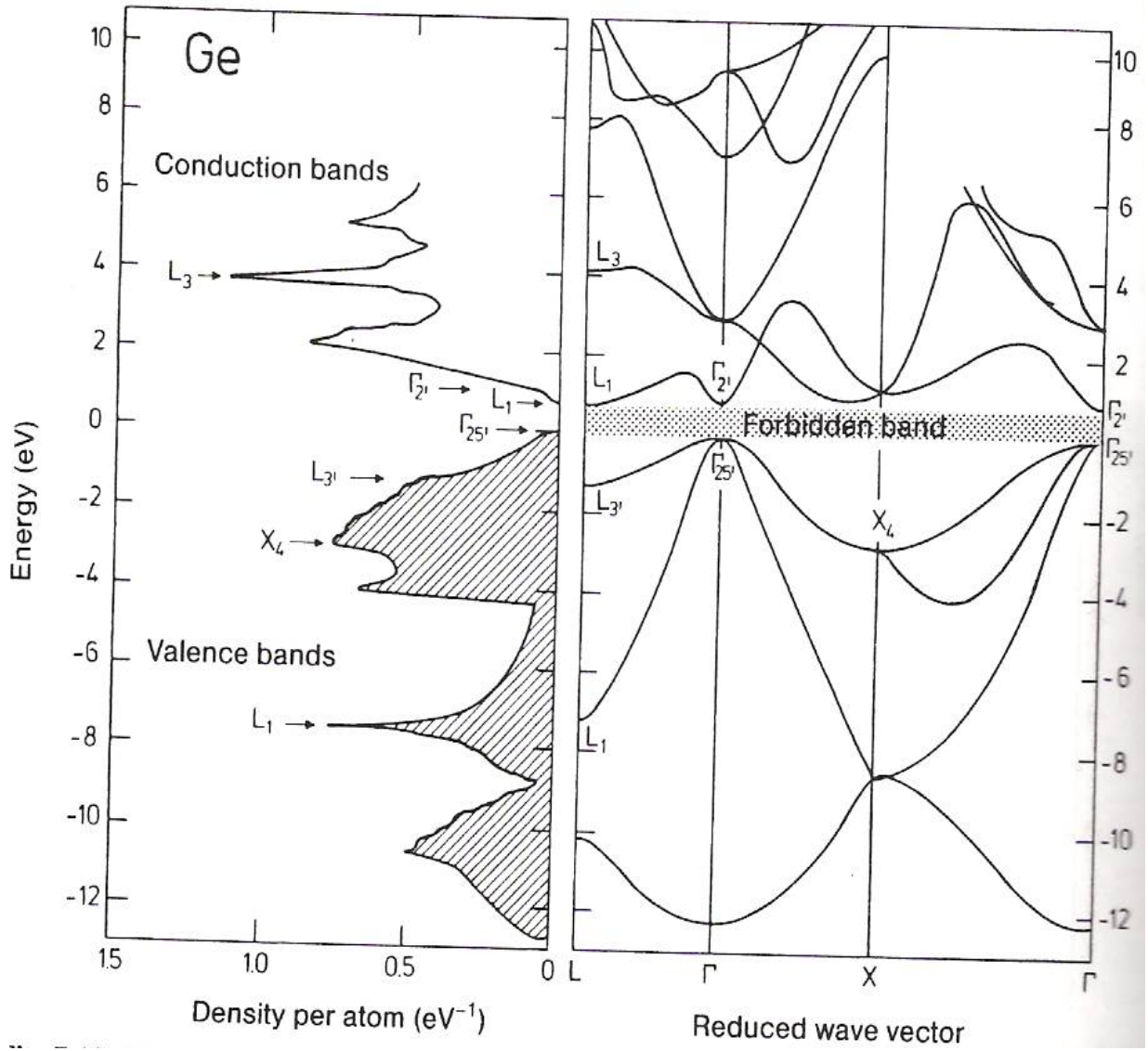
from: Singh

Copper dispersion relation and density of states



from Ibach & Lueth

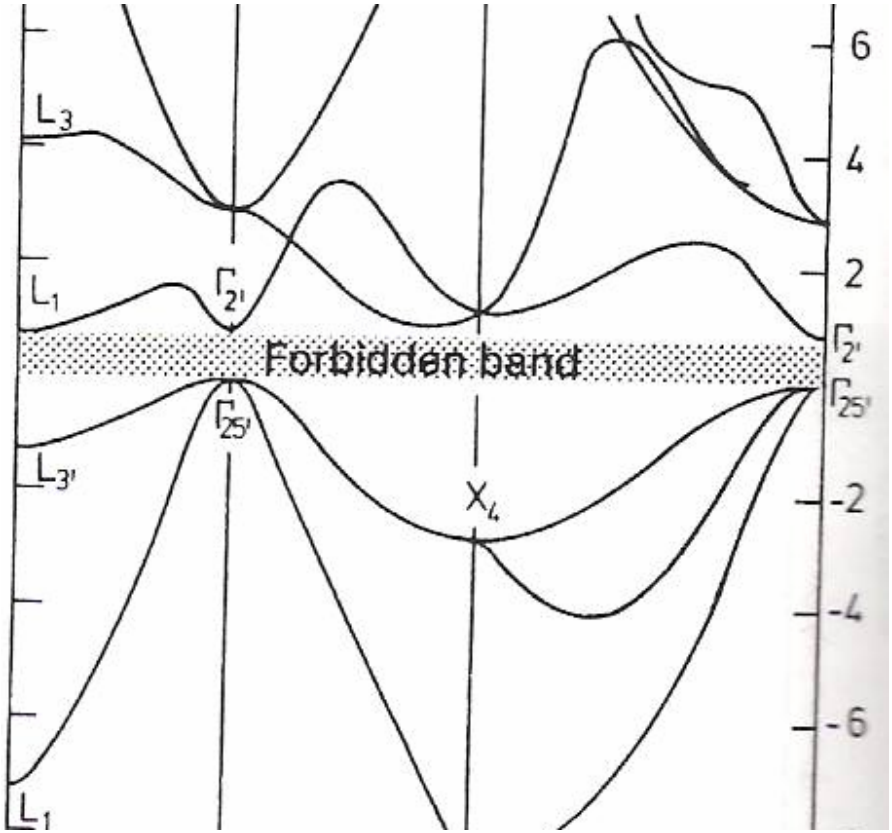
Germanium

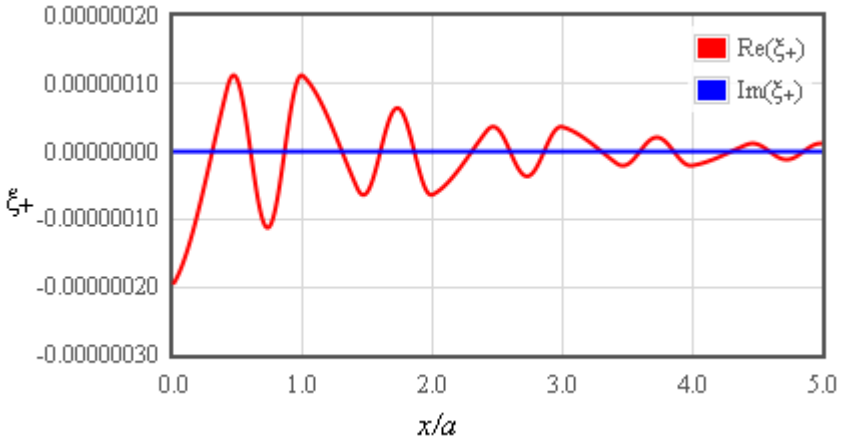


from Ibach & Lueth

Band gap

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



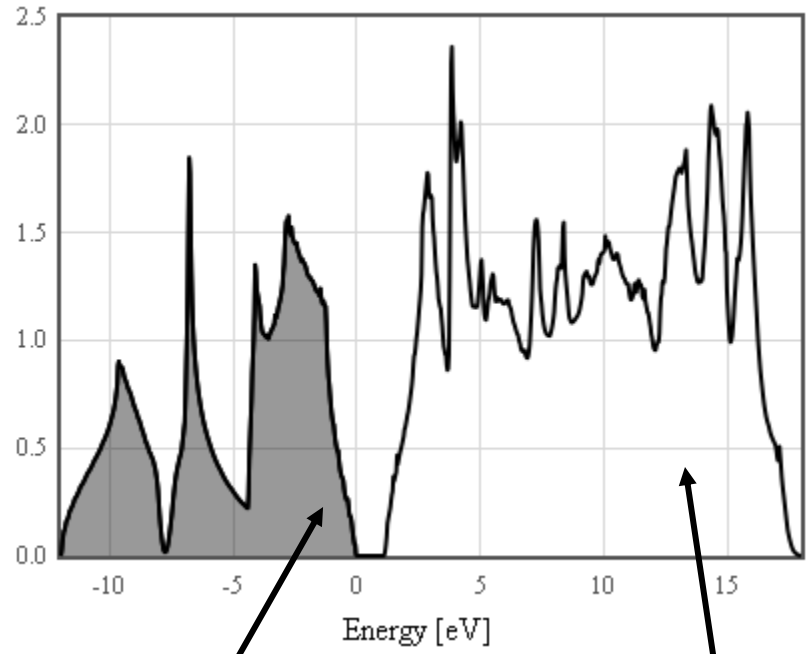


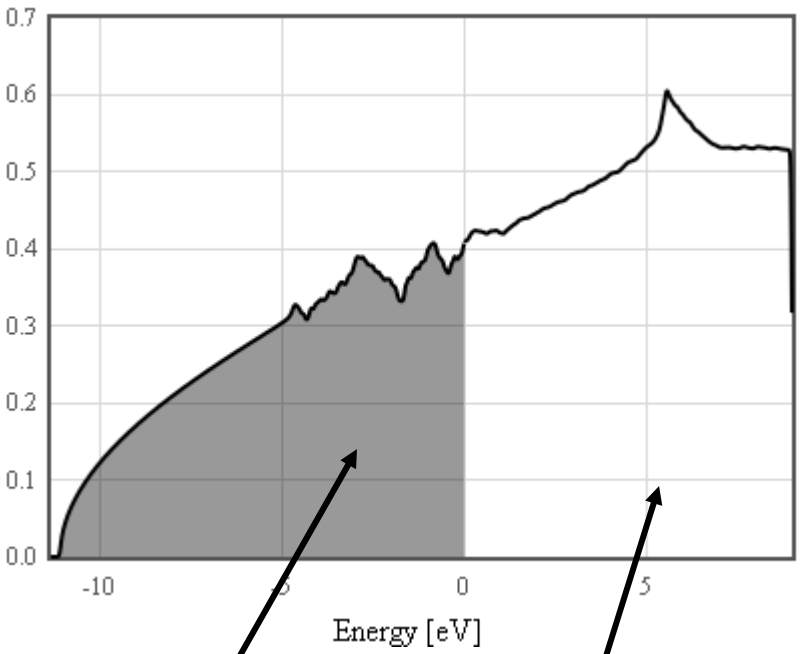
Density of states

Silicon

Aluminum

$D(E)$





filled states

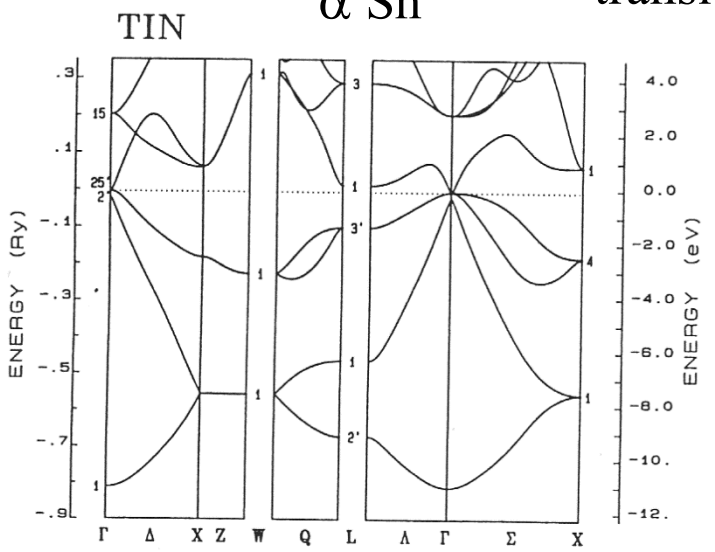
empty states

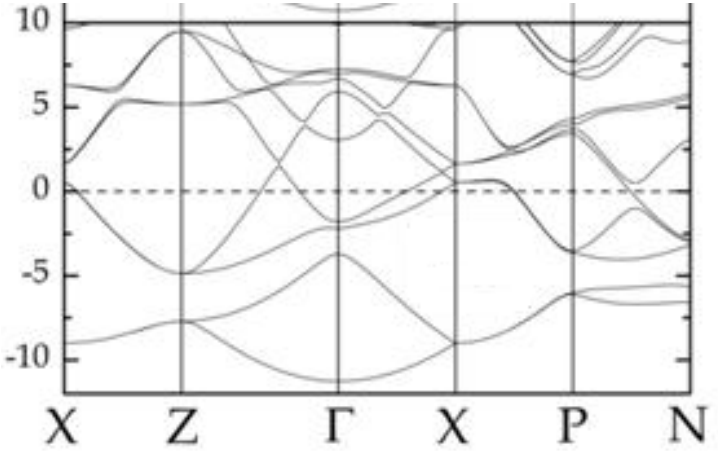
filled states

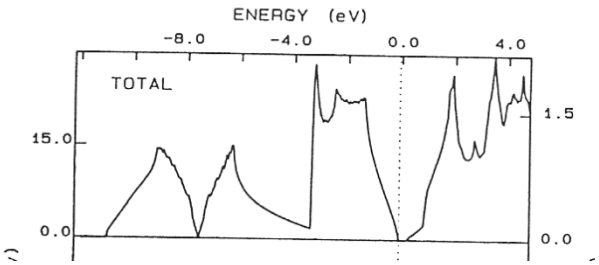
empty states

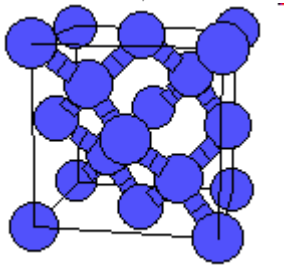
Structural phase transition in Sn

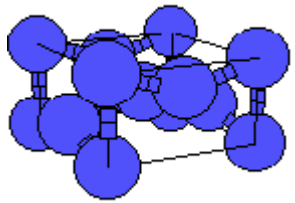
α Sn transition at 13 C metal β Sn







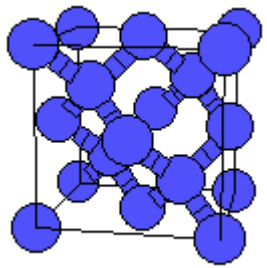




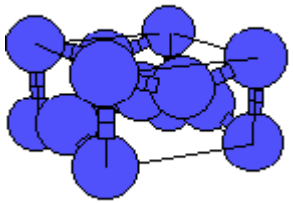
α-Sn, gray tin, diamond structure

β-Sn, white tin, tetragonal

Structural phase transitions

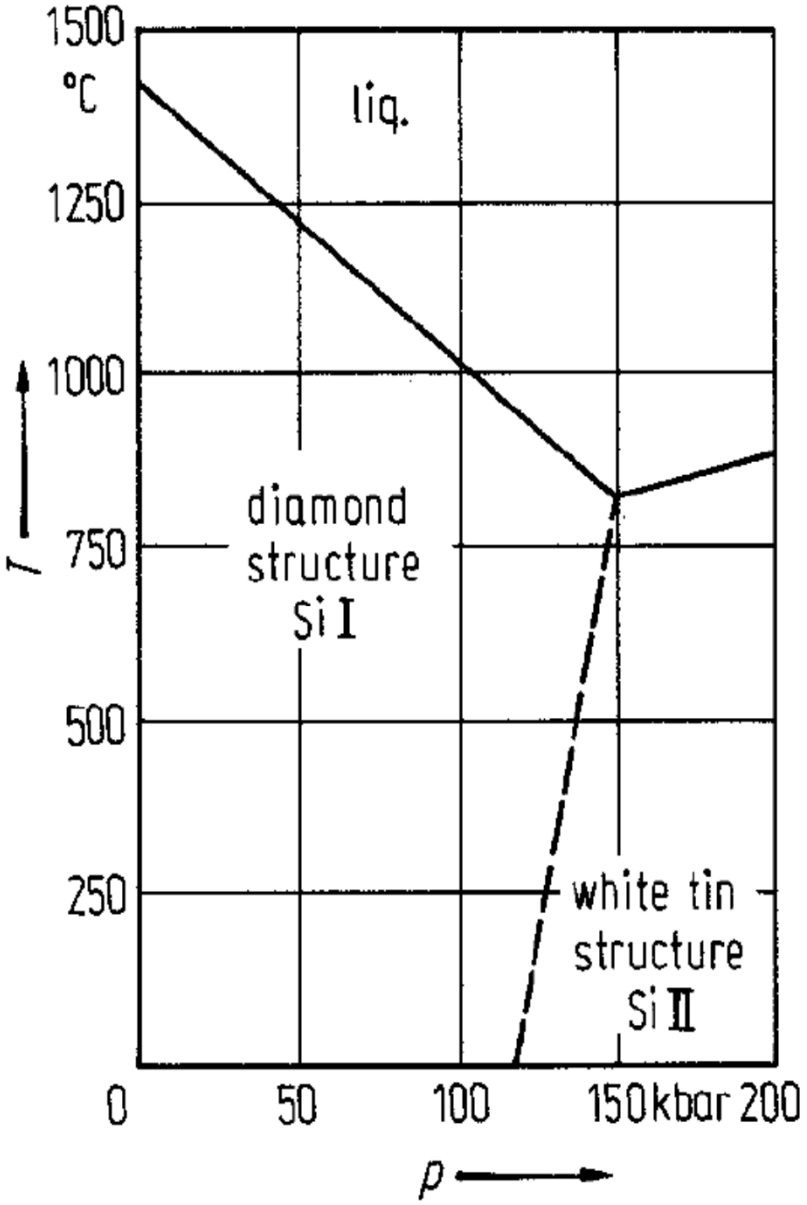


Si, diamond structure



Si II, β-Sn, tetragonal

silicon makes a diamond to β-Sn transition under pressure



Fermi function

$f(E)$ is the probability that a state at energy E is occupied.

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)}$$