Crystal structures

Crystal Structure

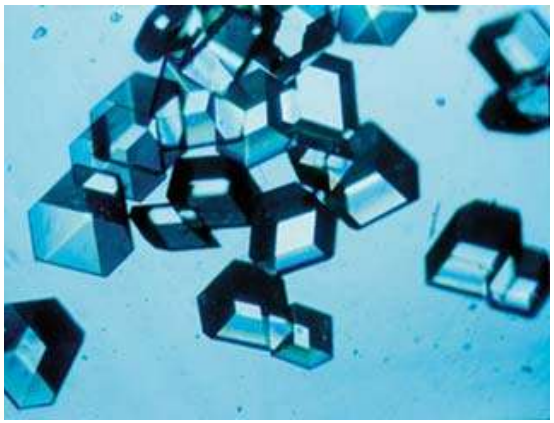
Atoms are arranged in a periodic pattern in a crystal.

The atomic arrangement affects the macroscopic properties of a material.

Many important materials (silicon, steel) are crystals

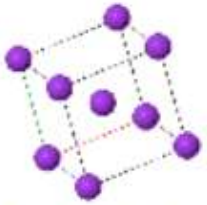
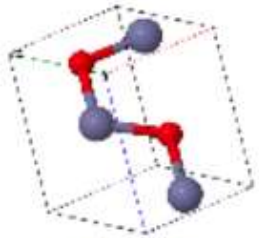
Gallium crystals

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	 Wurzite ZnO, GaN, AlN, CdSe

Miller indices: Crystal planes

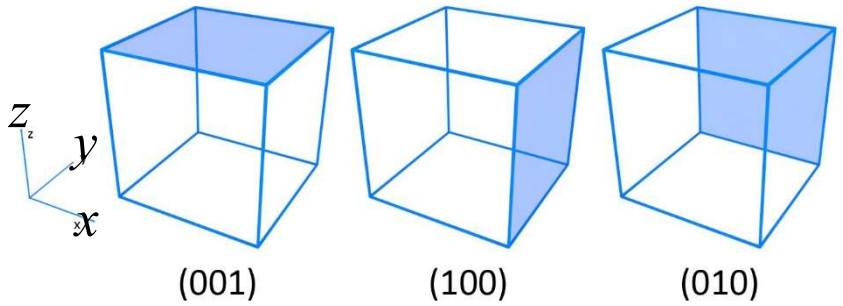
$[hkl]$ = vector in direction $h\vec{a}_1 + k\vec{a}_2 + l\vec{a}_3$

[ ] specific direction
< > family of equivalent directions

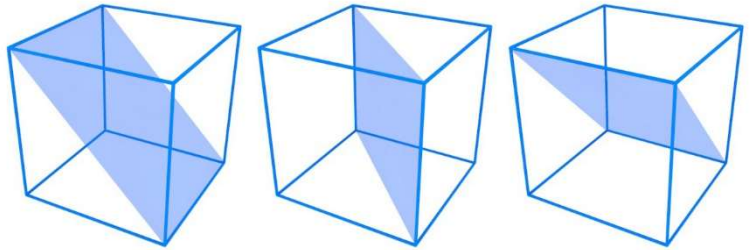
always use integers for *h,k,l*

( ) specific plane
{ } family of equivalent planes

MOSFETs are made on {100} wafers

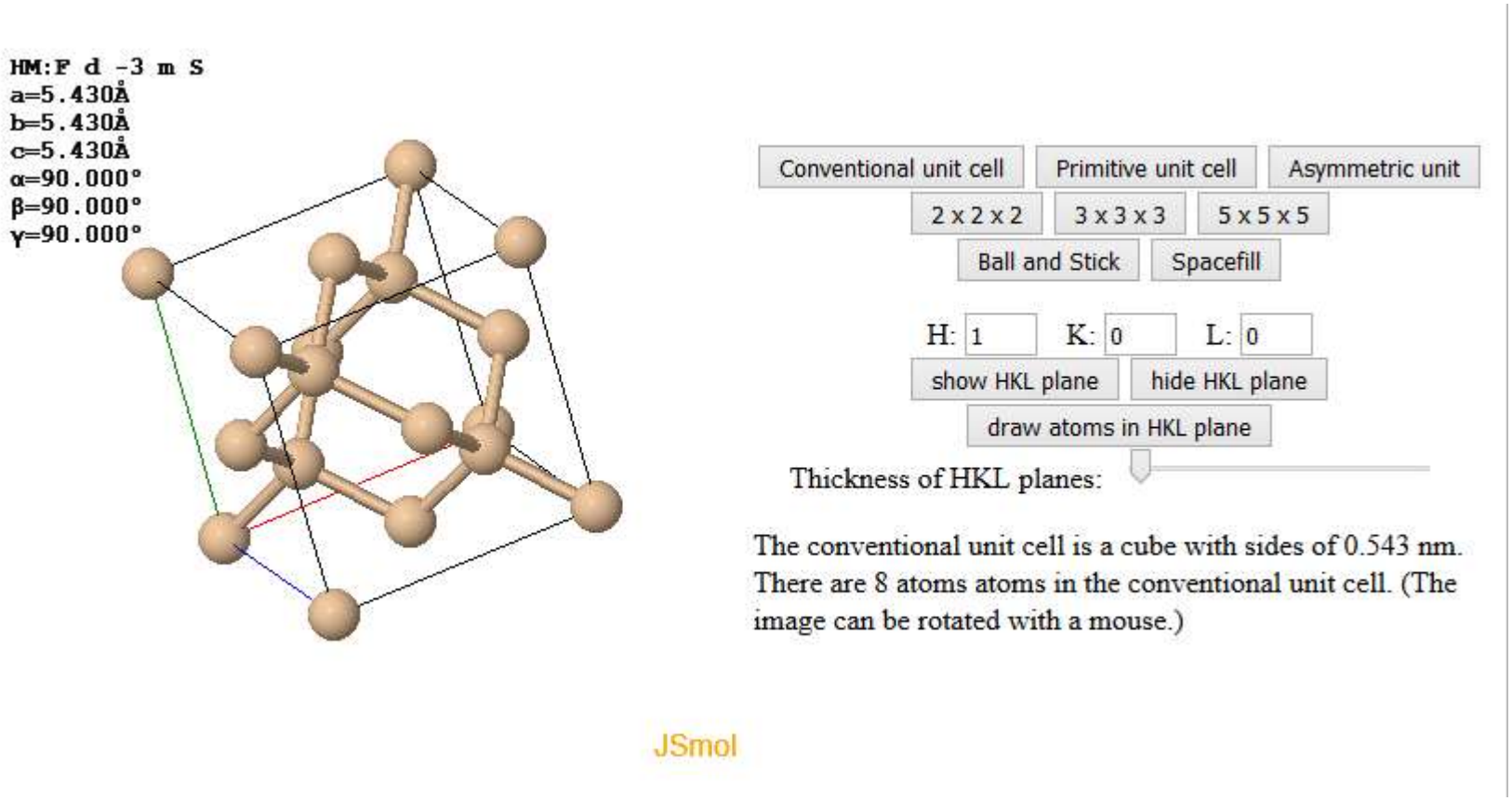


(001) (100) (010)



(101) (110) (011)

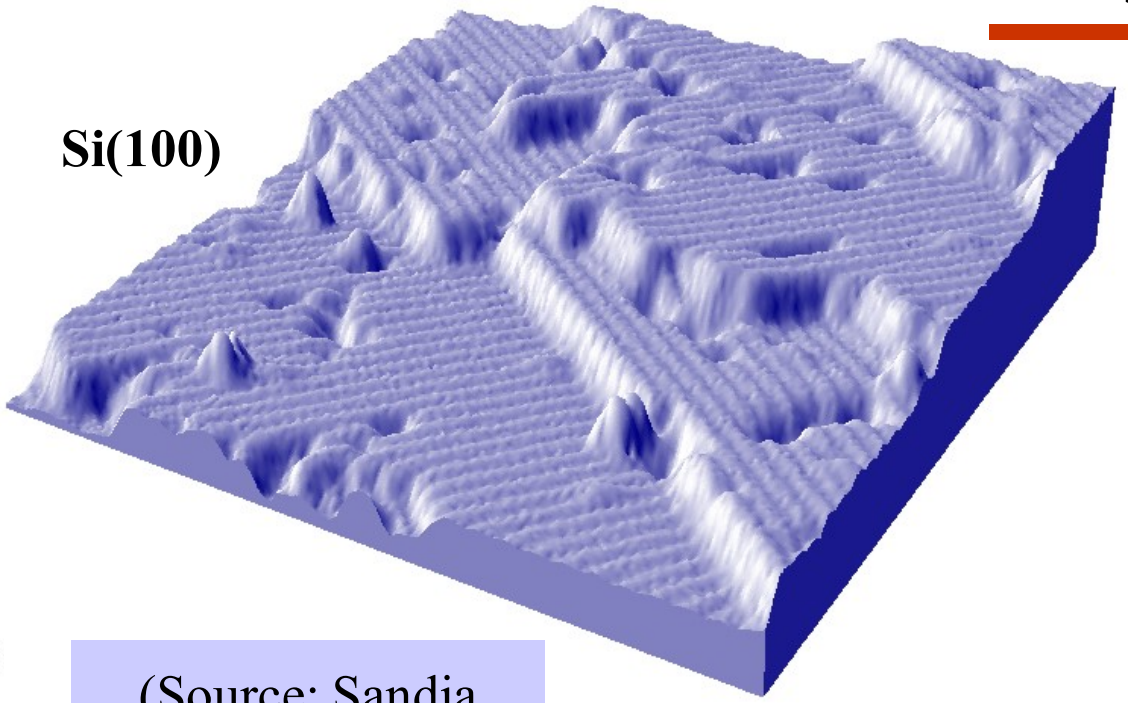
silicon



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

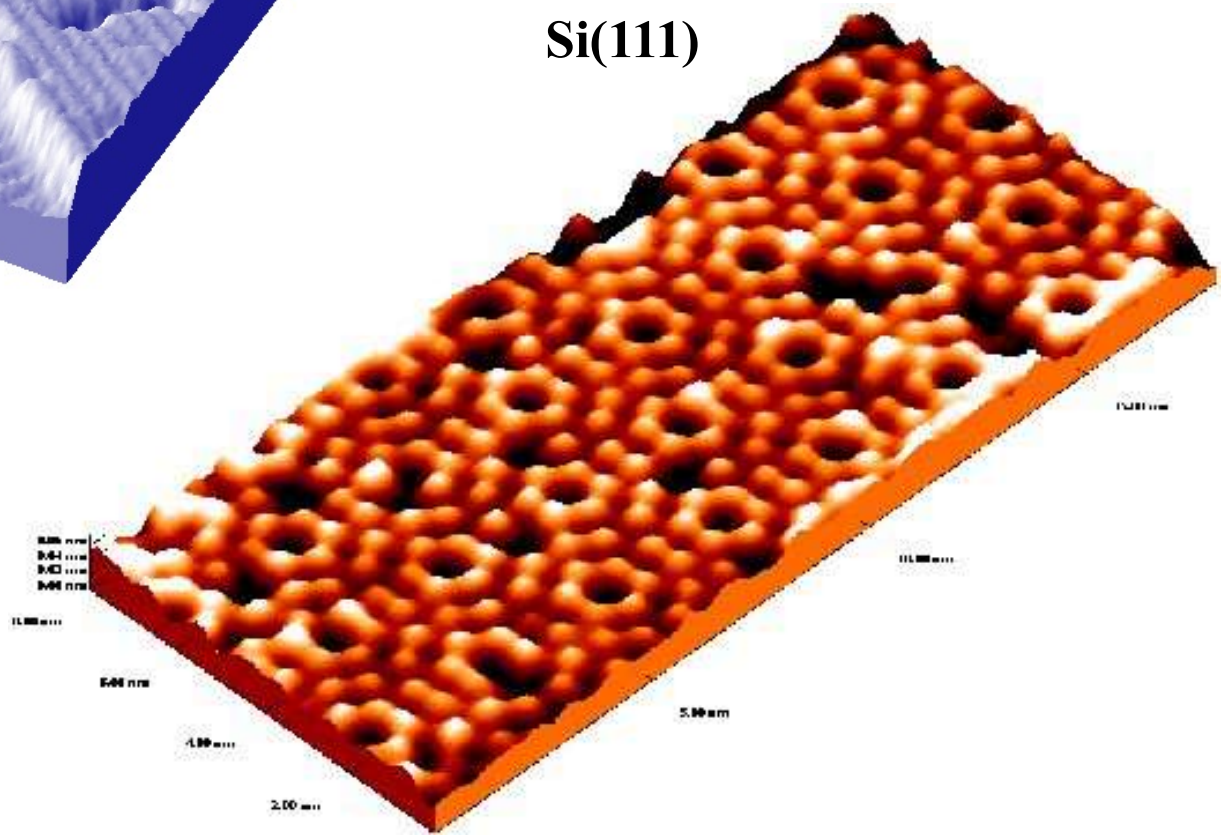
Silicon surfaces

Si(100)

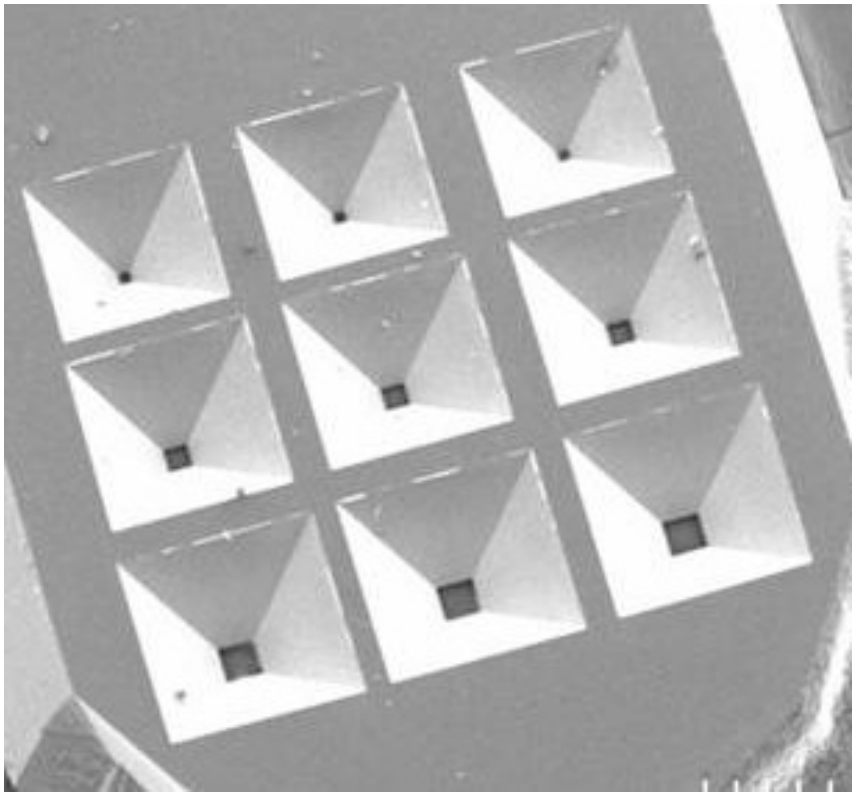


(Source: Sandia Nat.Labs.)

Si(111)



KOH etching of silicon



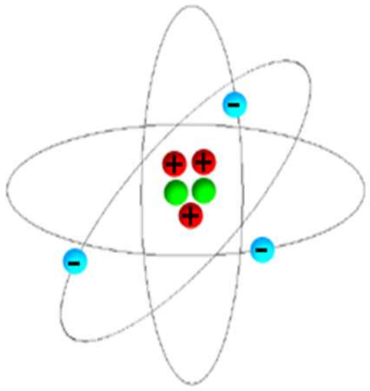
KOH etches Si {110} > {100} > {111}, producing a characteristic anisotropic V-etch, with sidewalls that form a 54.7° angle with the surface (35.3° from the normal).

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

Electrons in Crystals

Electrons

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

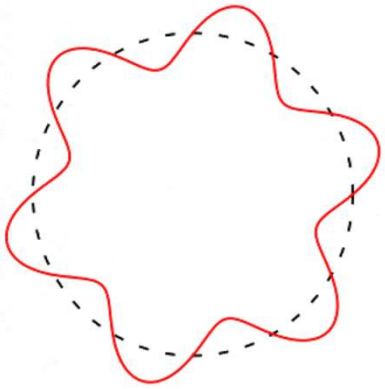


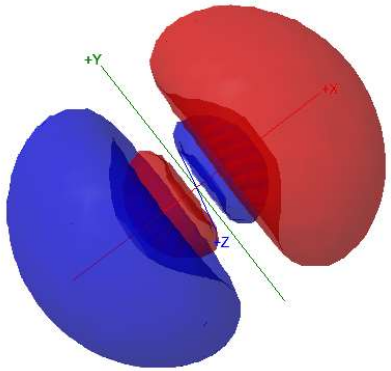
0.15 nm

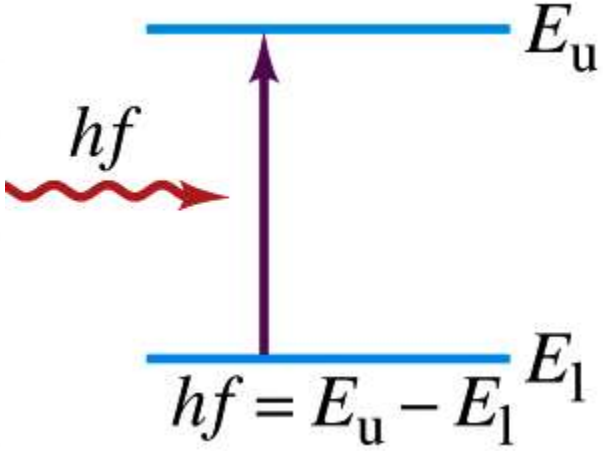
de aangegeven golflengten gelden in vacuüm

energie eV	*energie* eV	*hoofdquantum getal n =*	*golflengte* nm
14			
0	13,5950	∞	
	13,0560	5	
13	12,7497	4	
- 1			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

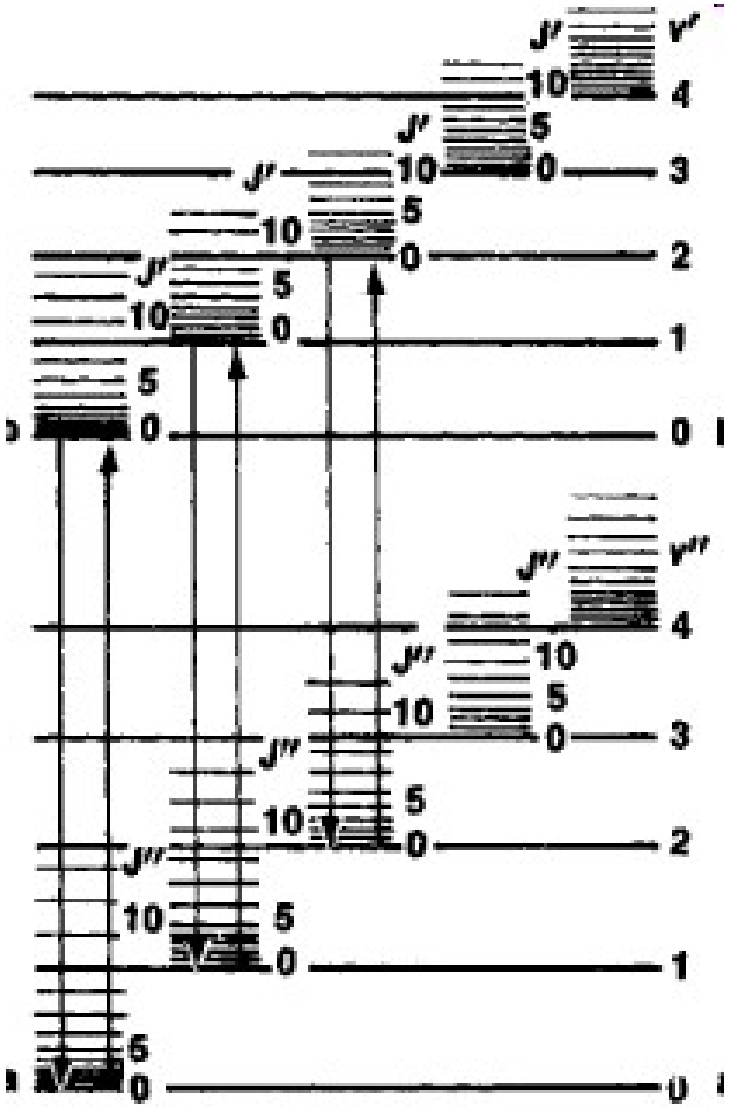
Fluorescent lamp

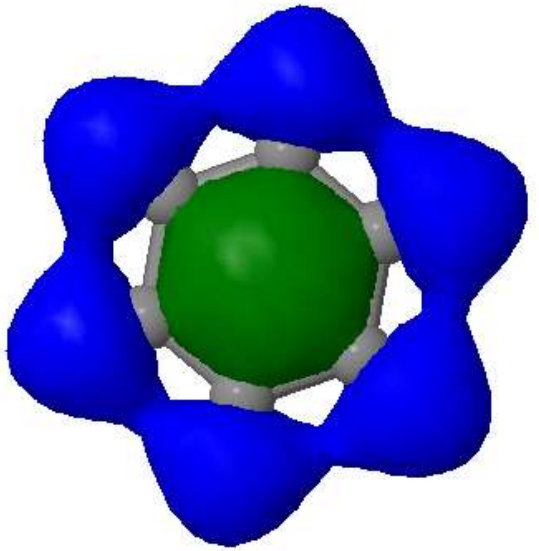


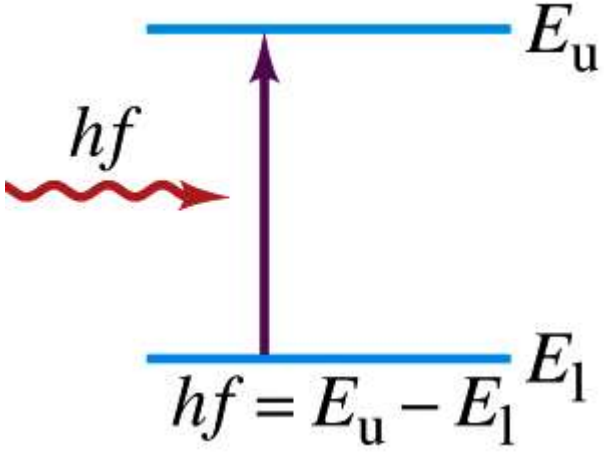




Molecular energy levels







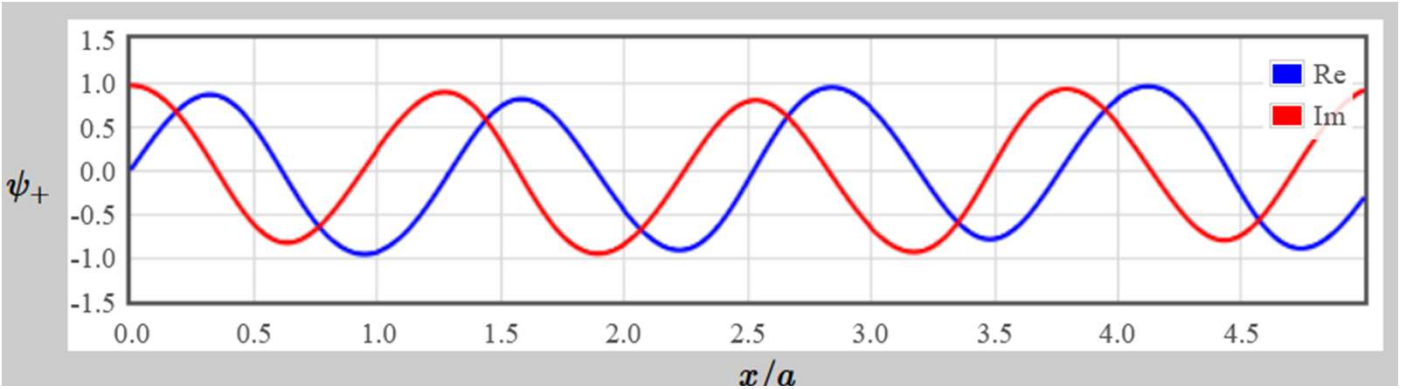
wave vector k

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

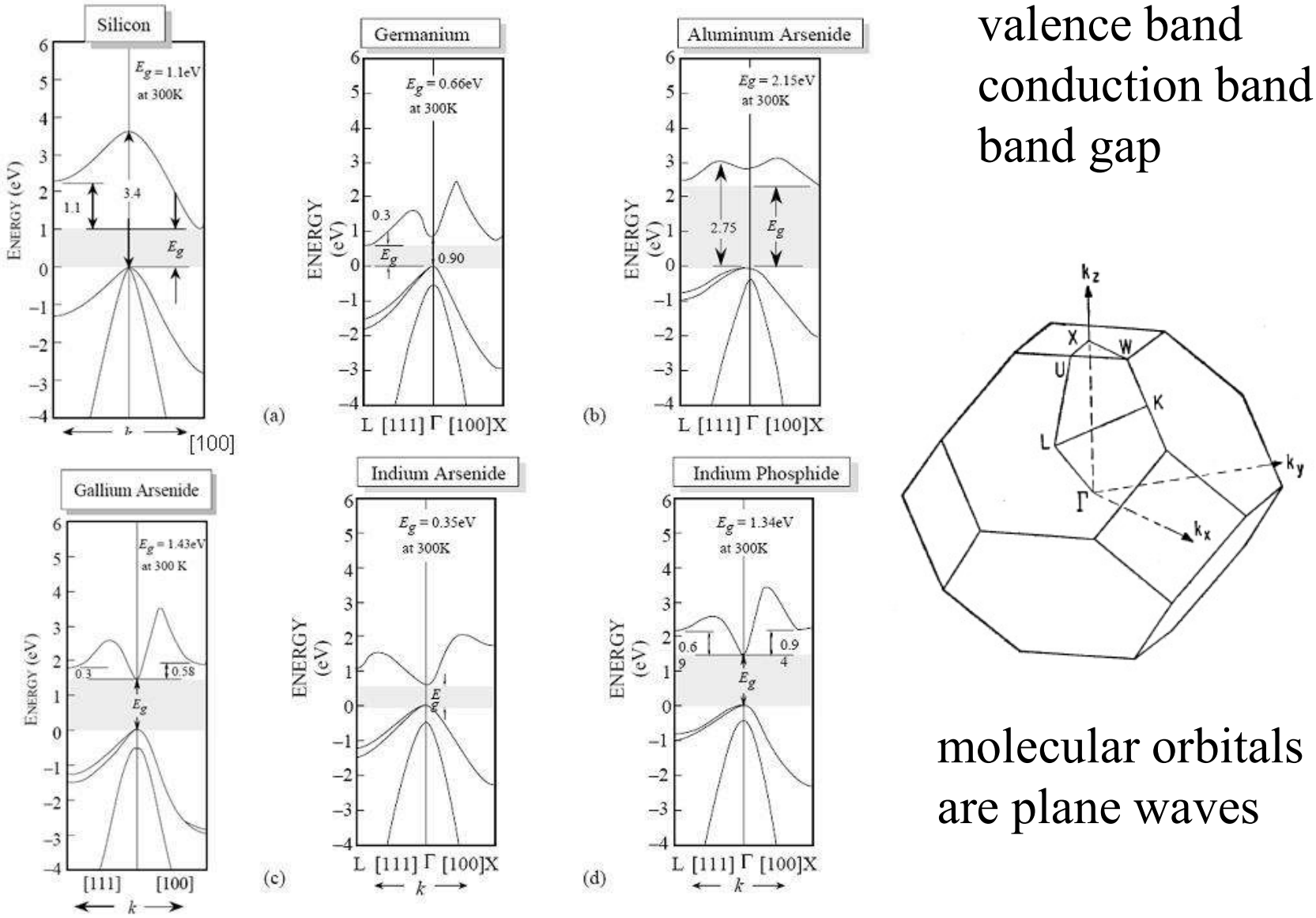
wavelength: $$\lambda = \frac{2\pi}{|\vec{k}|}$$

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

$$\psi = e^{ikx}u_k(x)$$



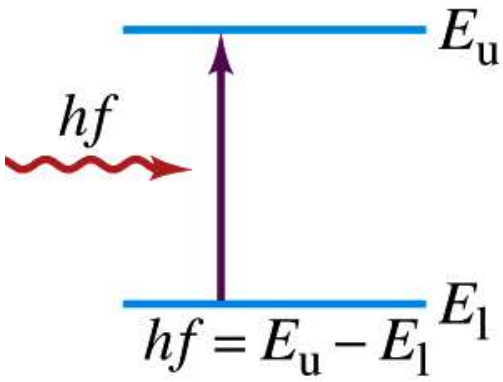
Semiconductors



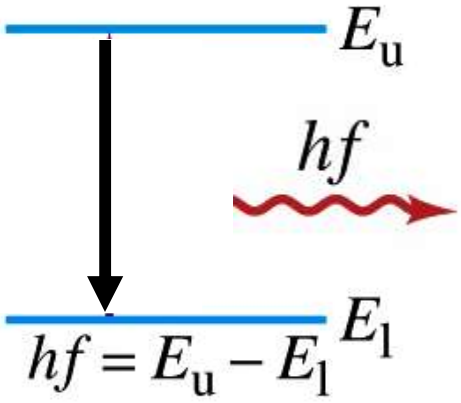
valence band
conduction band
band gap

molecular orbitals
are plane waves

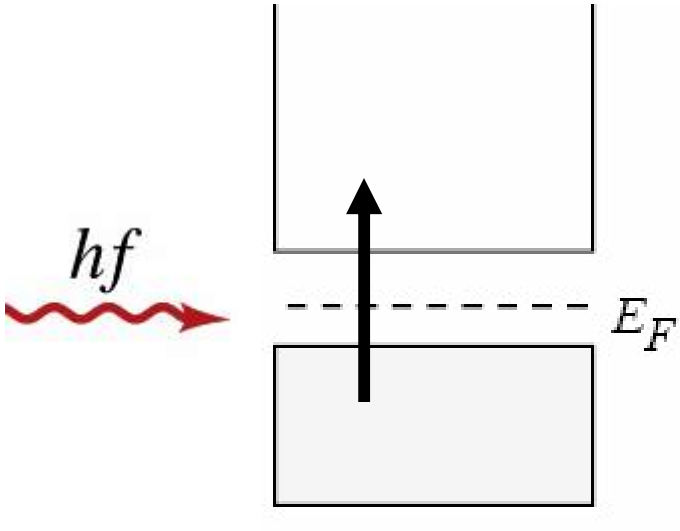
Absorption and emission of photons



absorption



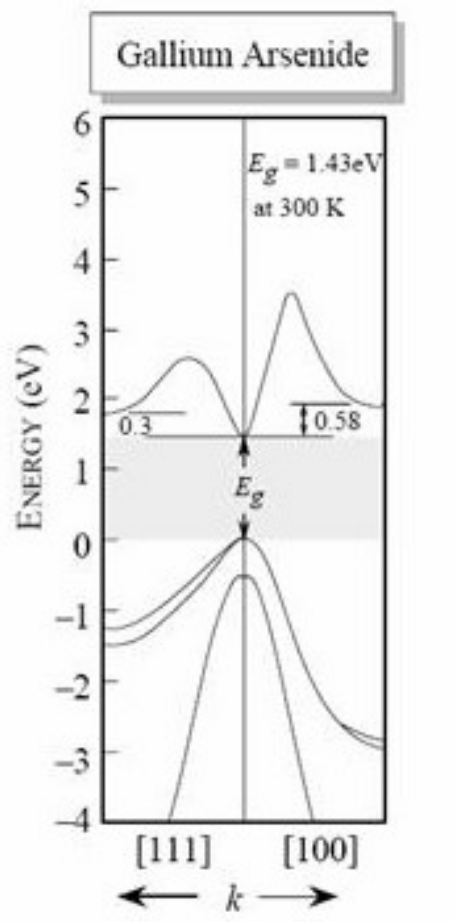
emission



semiconductor

$hf < E_g$ no absorption

What color light does a GaAs LED emit?



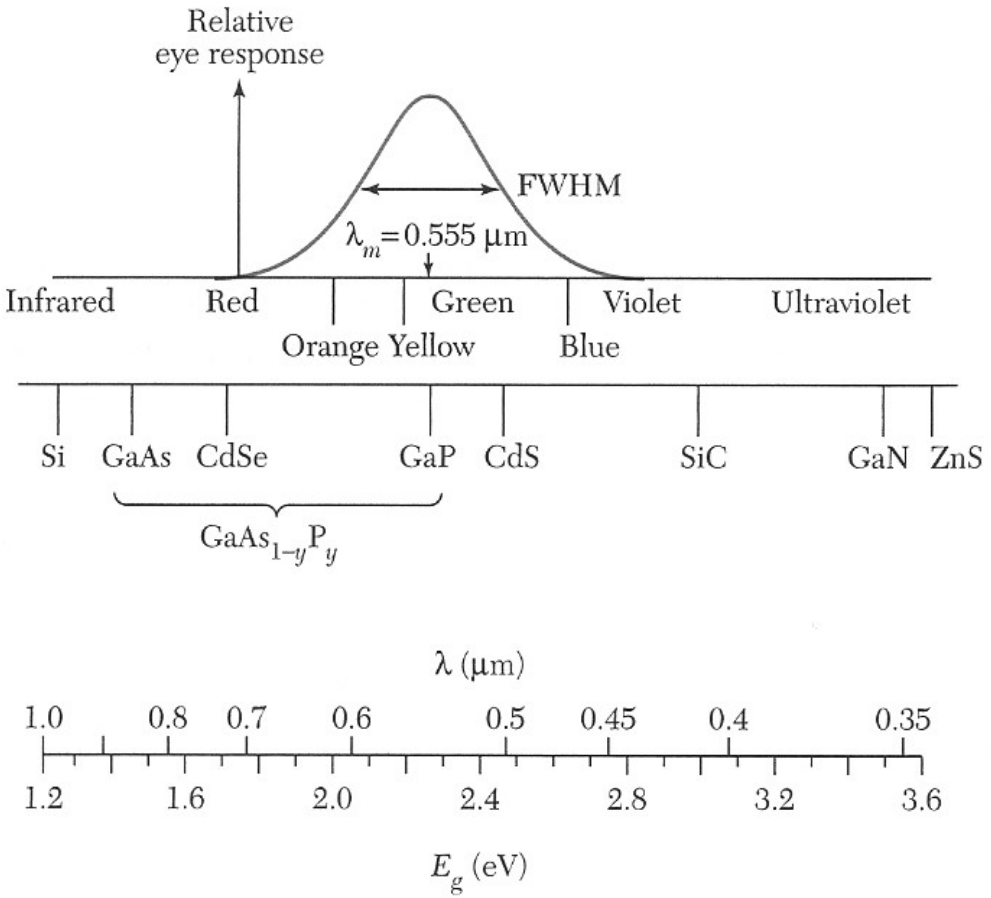
$$E = 1.6022 \times 10^{-19} \times 1.43 \text{ J} = hf = \frac{hc}{\lambda}$$

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

Light emitting diodes

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

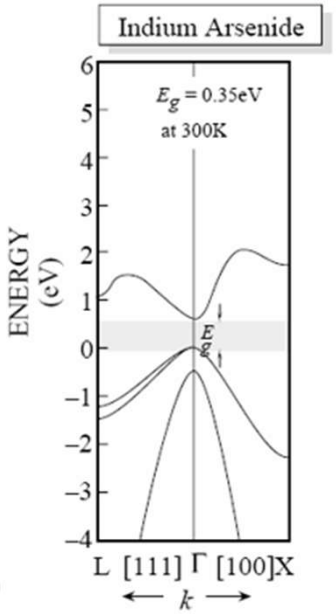
Material	Wavelength (nm)
InAsSbP/InAs	4200
InAs	3800
GaInAsP/GaSb	2000
GaSb	1800
$Ga_xIn_{1-x}As_{1-y}P_y$	1100-1600
$Ga_{0.47}In_{0.53}As$	1550
$Ga_{0.27}In_{0.73}As_{0.63}P_{0.37}$	1300
GaAs:Er,InP:Er	1540
Si:C	1300
GaAs:Yb,InP:Yb	1000
$Al_xGa_{1-x}As$:Si	650-940
GaAs:Si	940
$Al_{0.11}Ga_{0.89}As$:Si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



Direct and indirect band gaps

direct bandgap:
$\Delta k = 0$

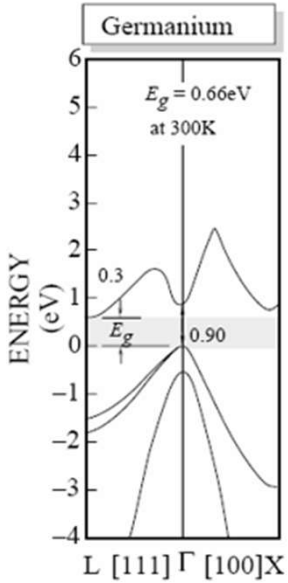
photons can be emitted



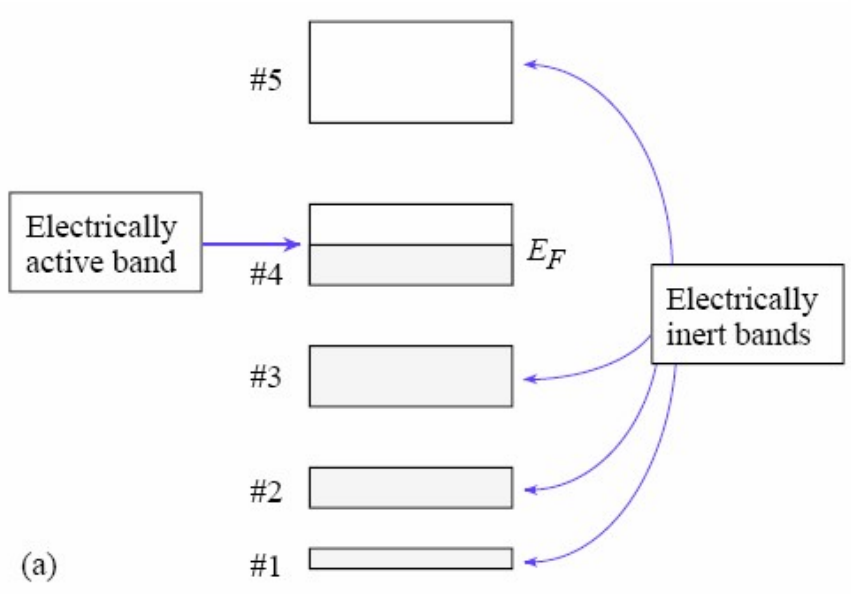
Momentum must be conserved when photons are absorbed or emitted.

indirect bandgap:
$\Delta k = 0$

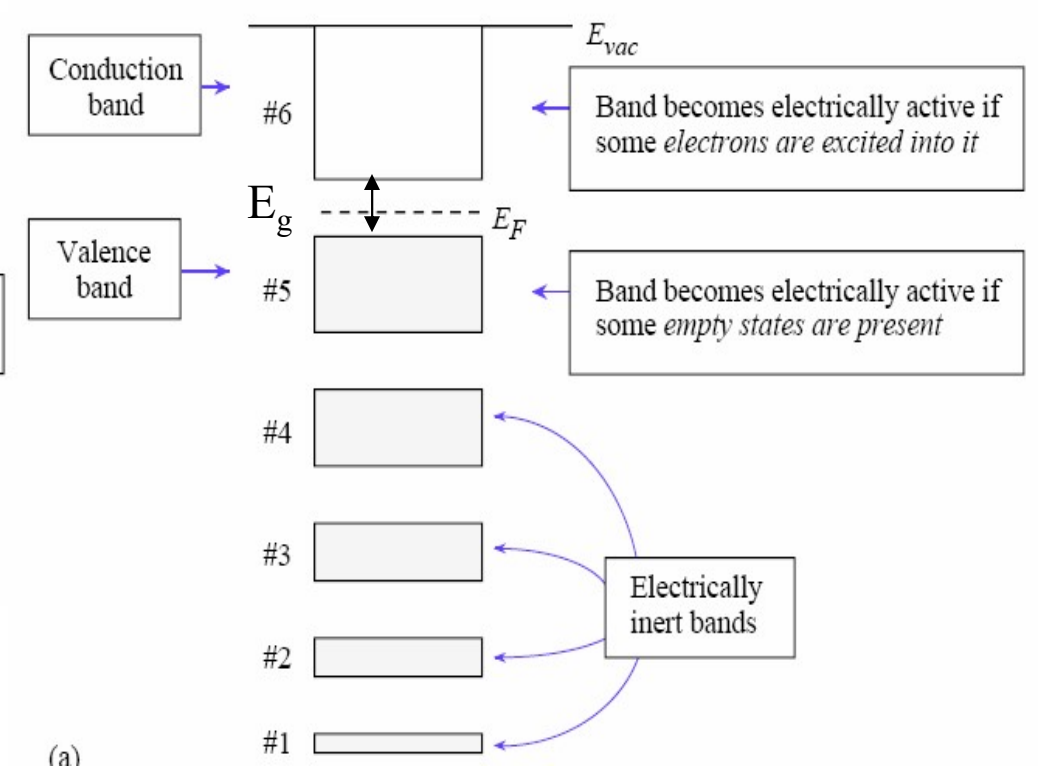
phonons are emitted



Metals, semiconductors, insulators



Metal



Semiconductor or insulator

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

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

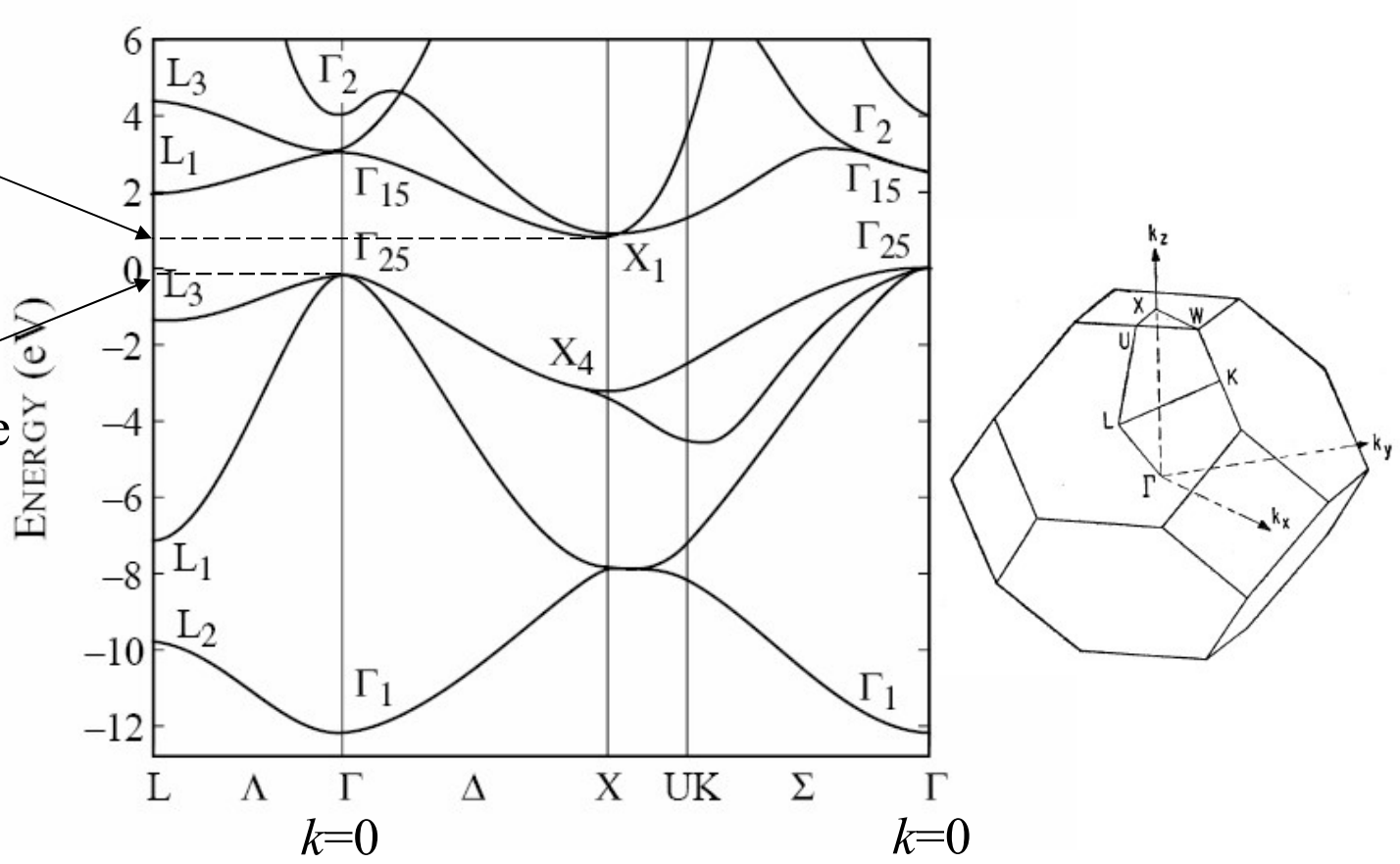
from: Singh

Silicon band structure

E_c = bottom of the conduction band

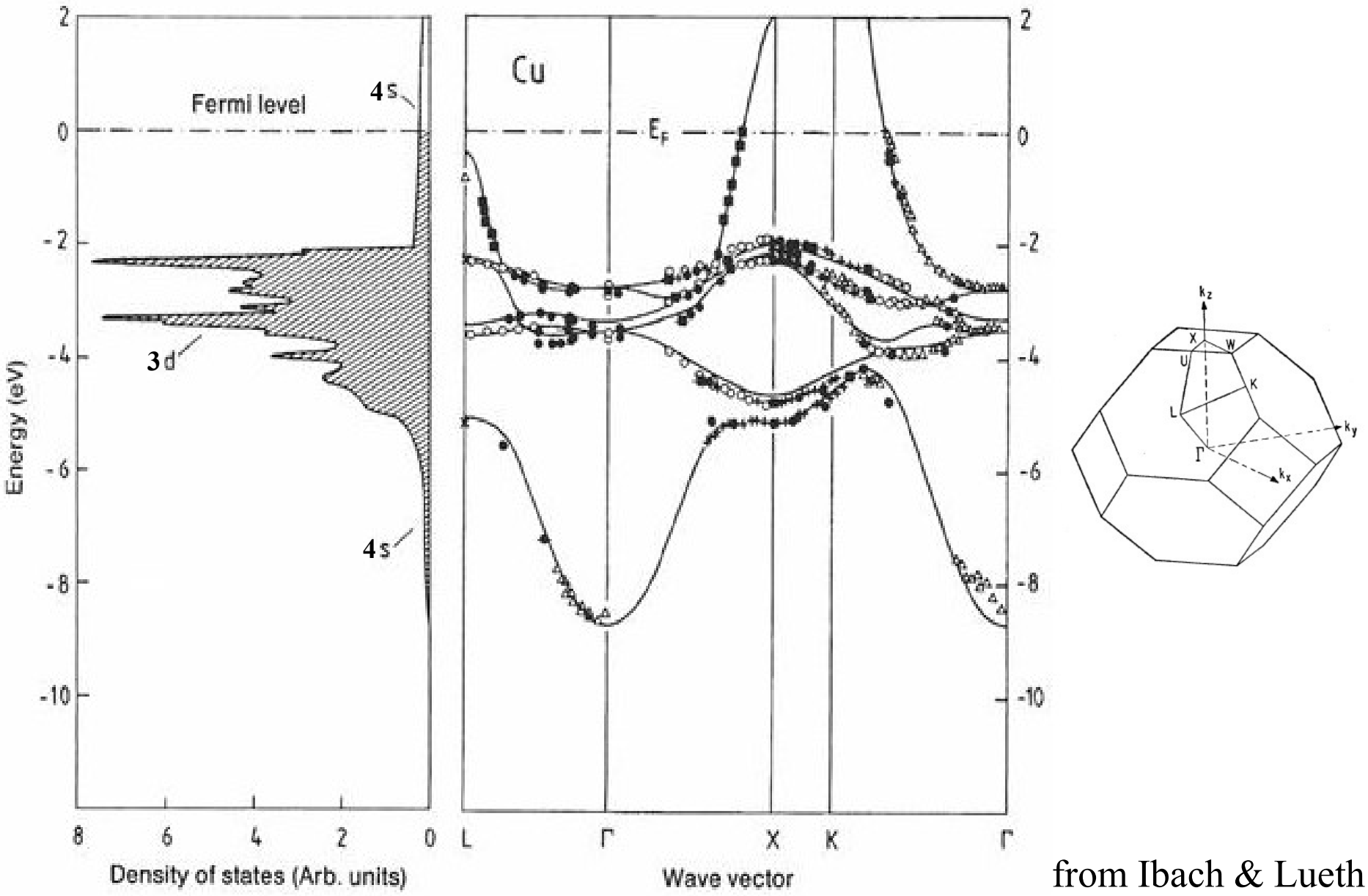
$E_g = E_c - E_v$

E_v = top of the valence band



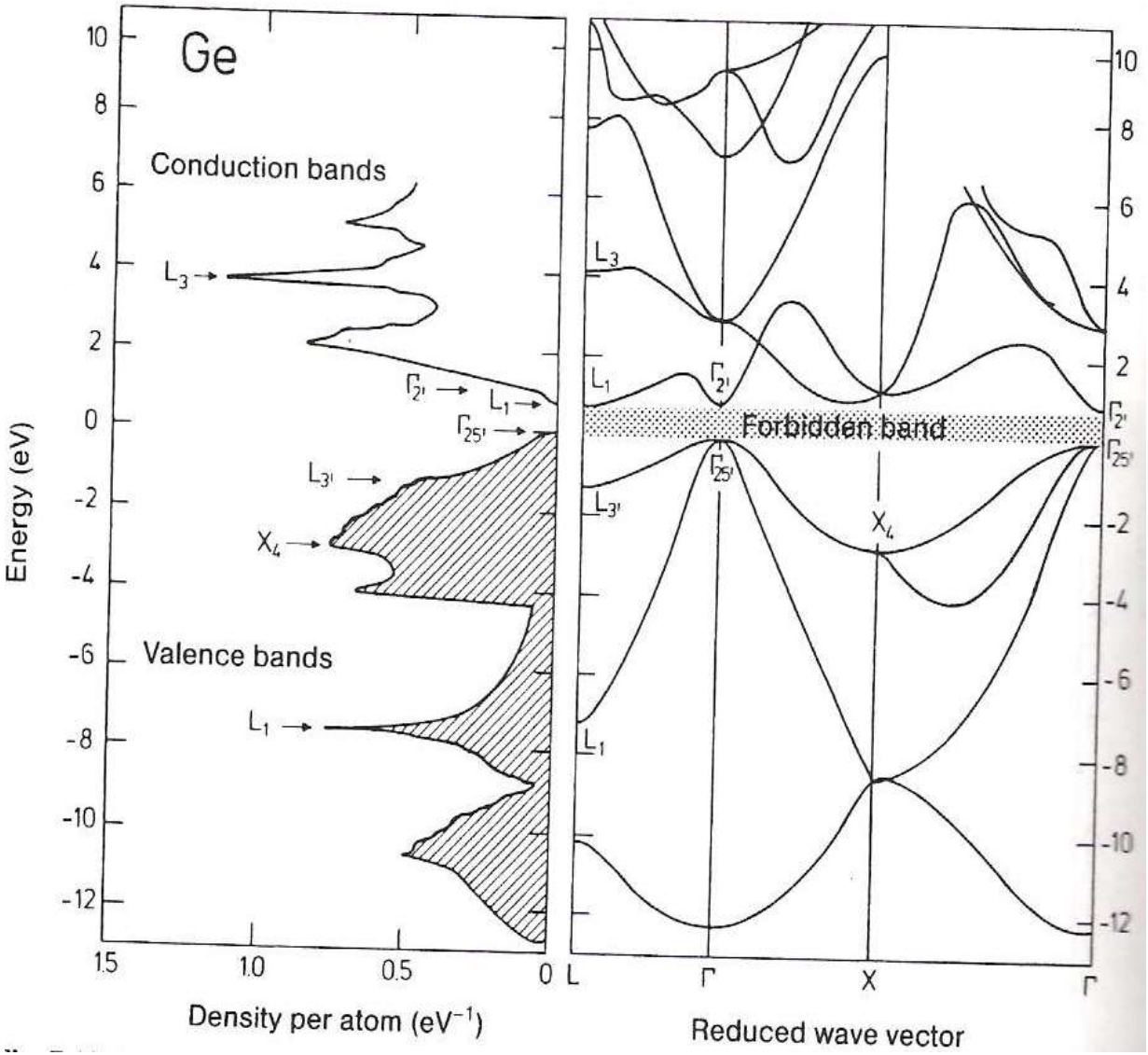
Electrons with energies in the gap are reflected out of the crystal.

Copper dispersion relation and density of states



from Ibach & Lueth

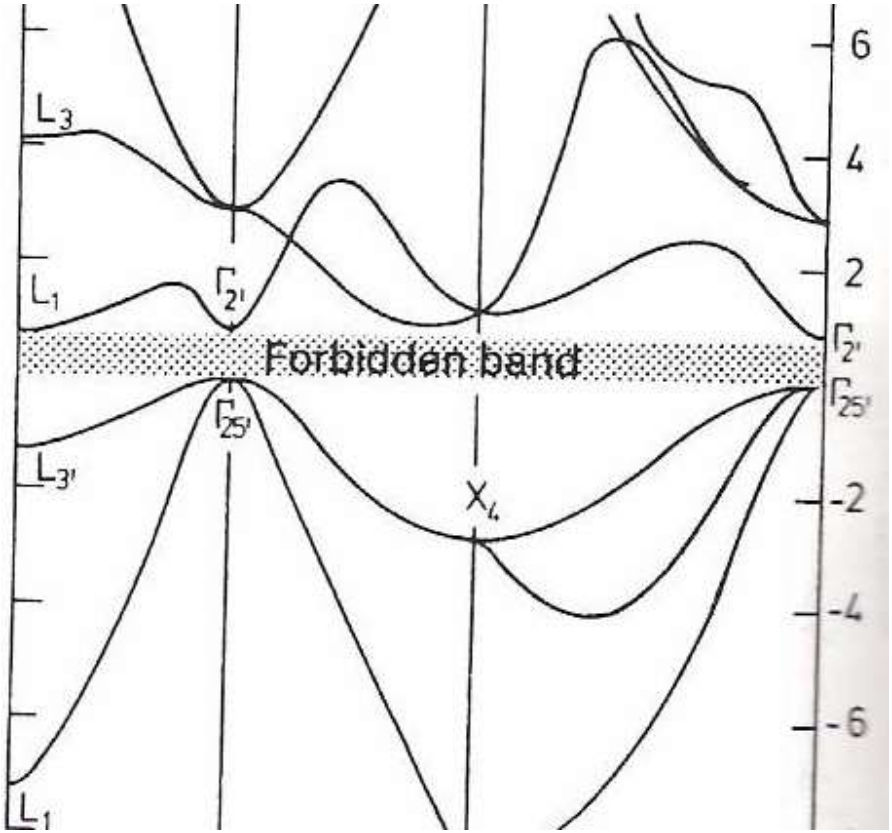
Germanium

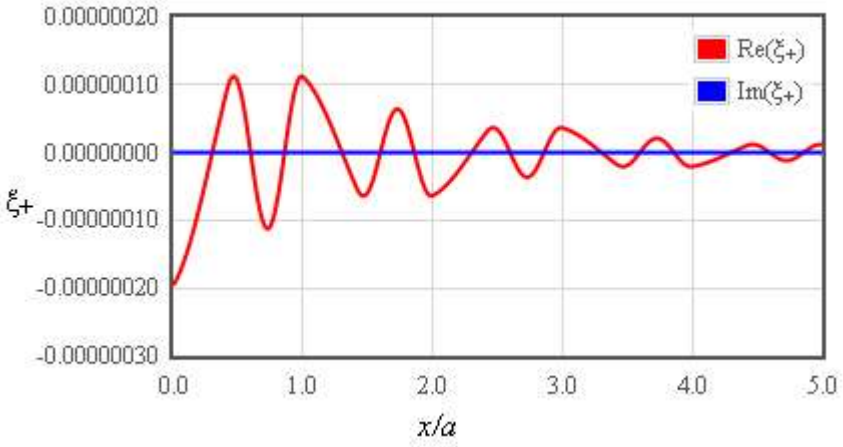


from Ibach & Lueth

Band gap

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



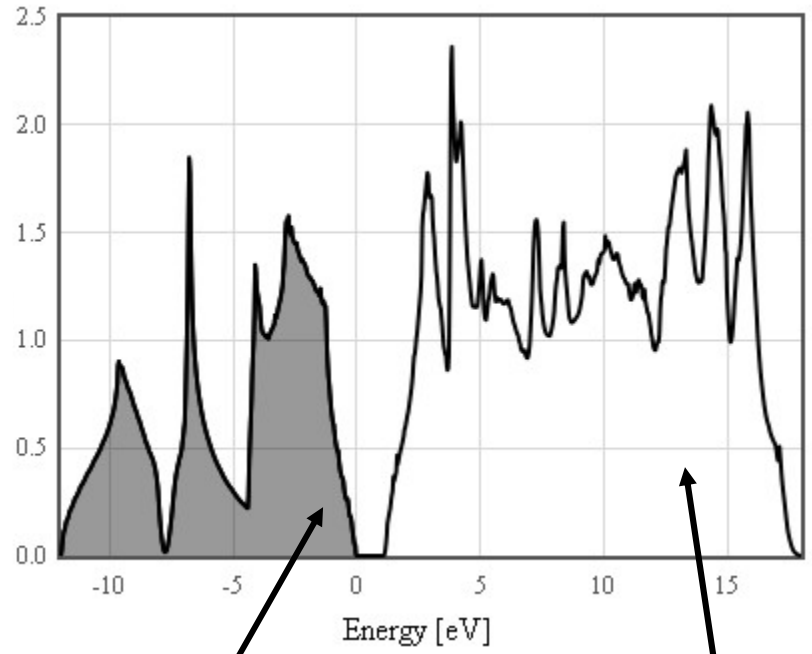


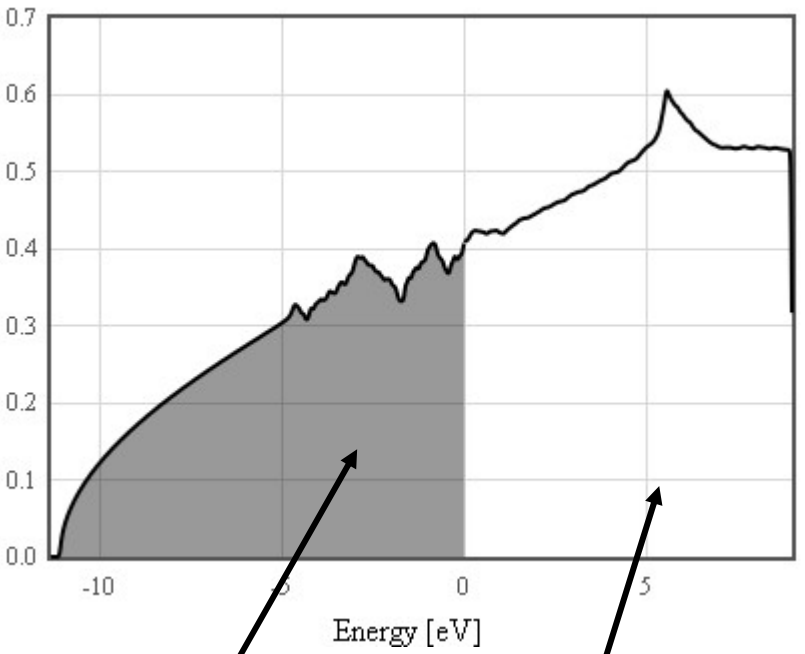
Density of states

Silicon

Aluminum

$D(E)$





filled states

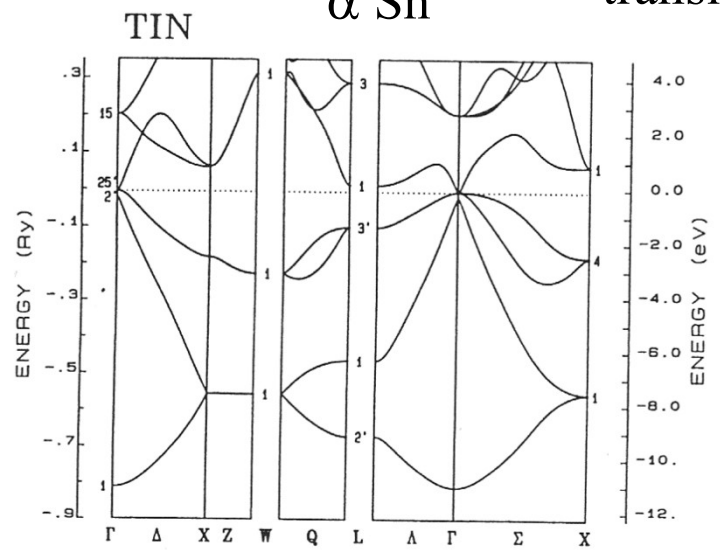
empty states

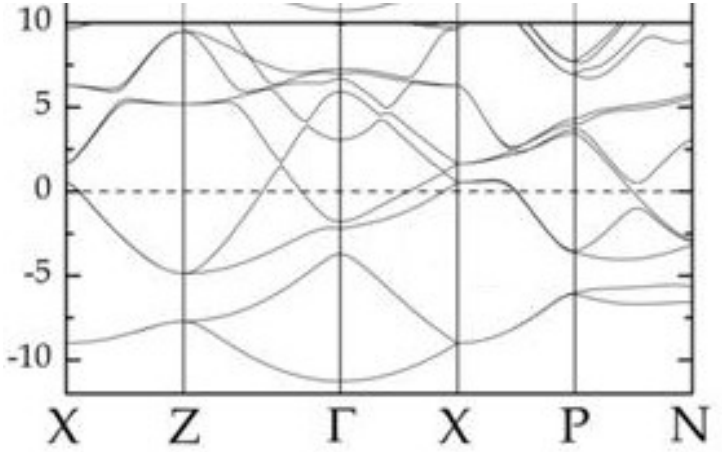
filled states

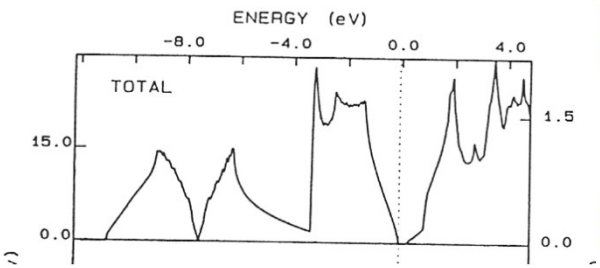
empty states

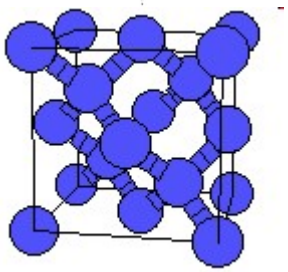
Structural phase transition in Sn

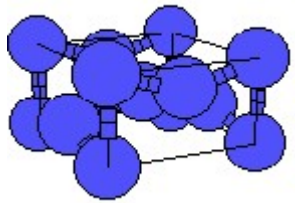
α Sn transition at 13 C metal β Sn







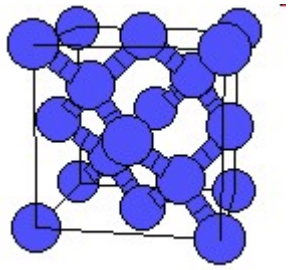




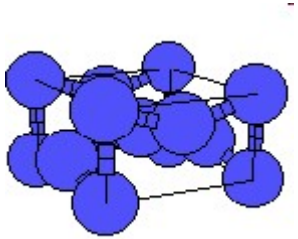
α-Sn, gray tin, diamond structure

β-Sn, white tin, tetragonal

Structural phase transitions

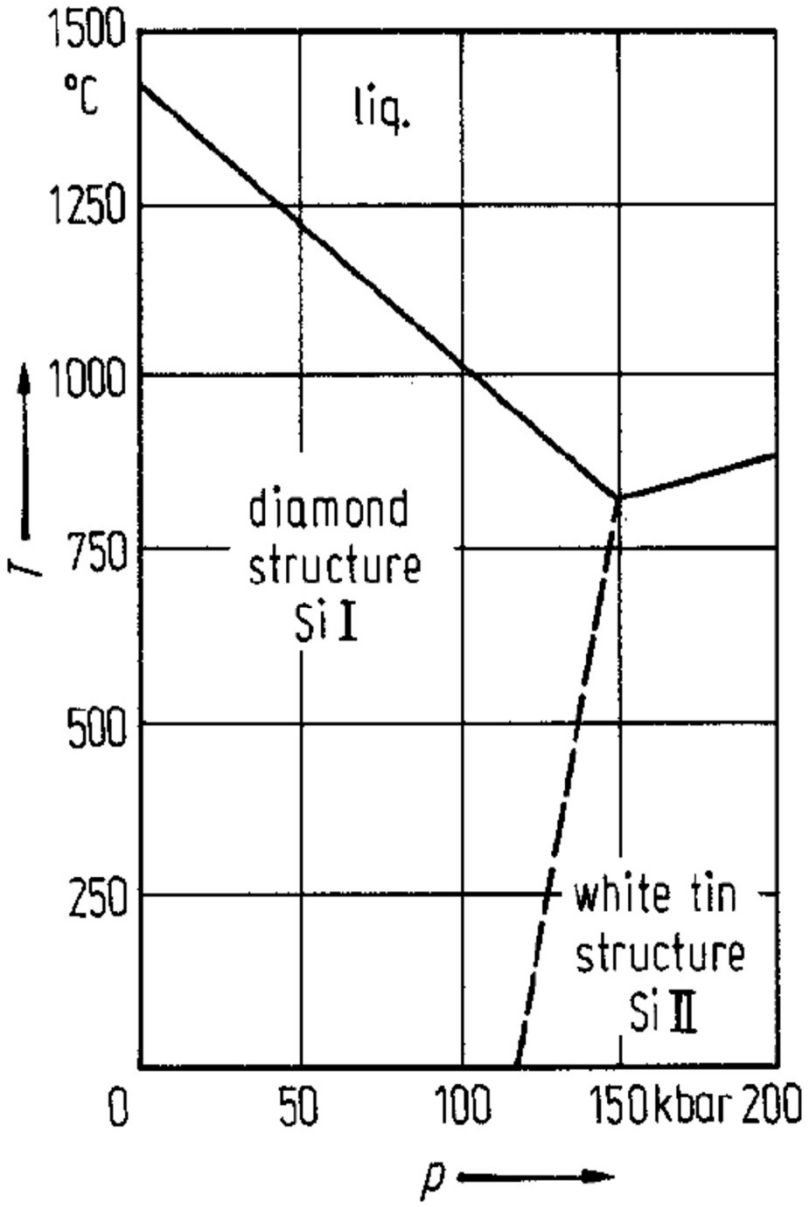


Si, diamond structure



Si II, β-Sn, tetragonal

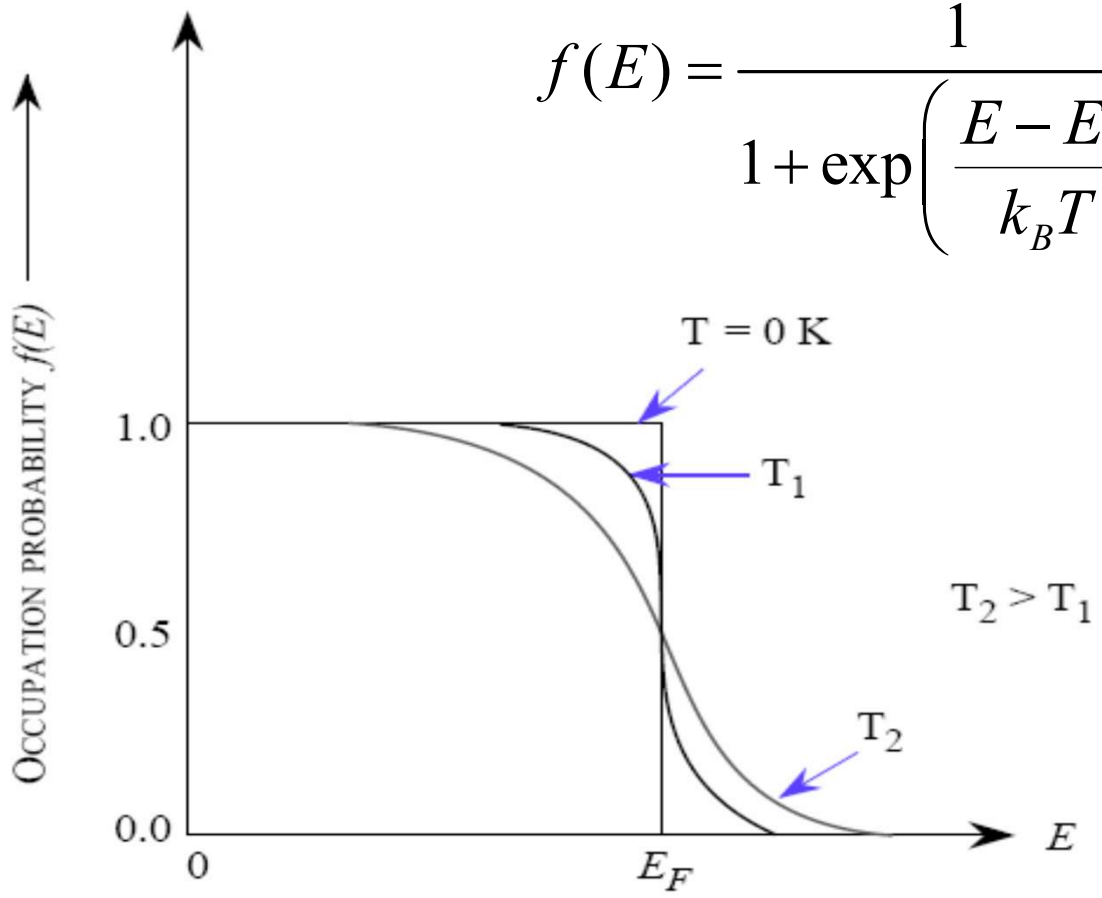
silicon makes a diamond to β-Sn transition under pressure



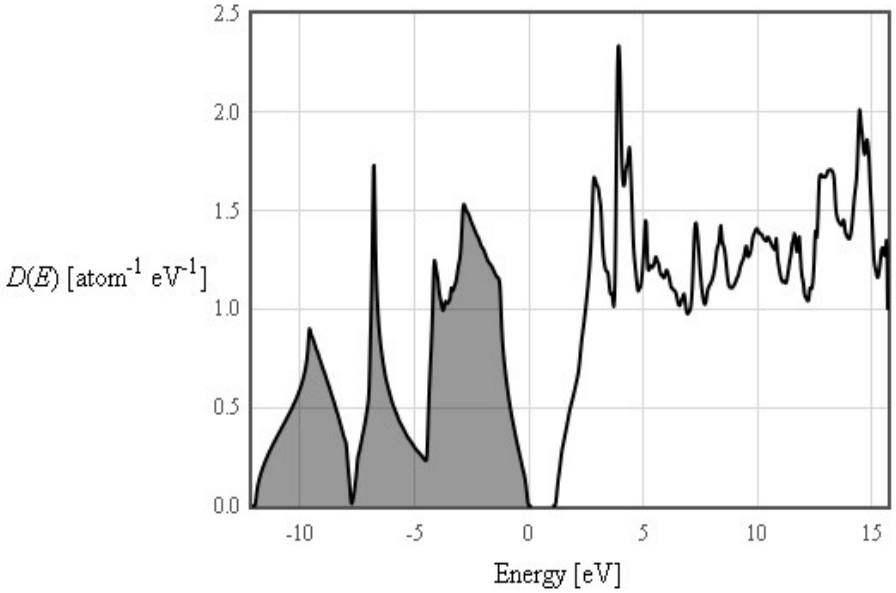
Fermi function

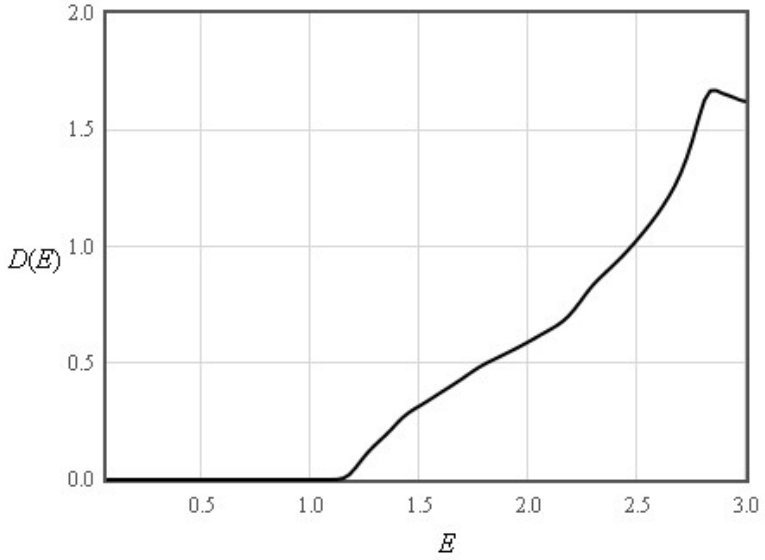
$f(E)$ is the probability that a state at energy E is occupied.

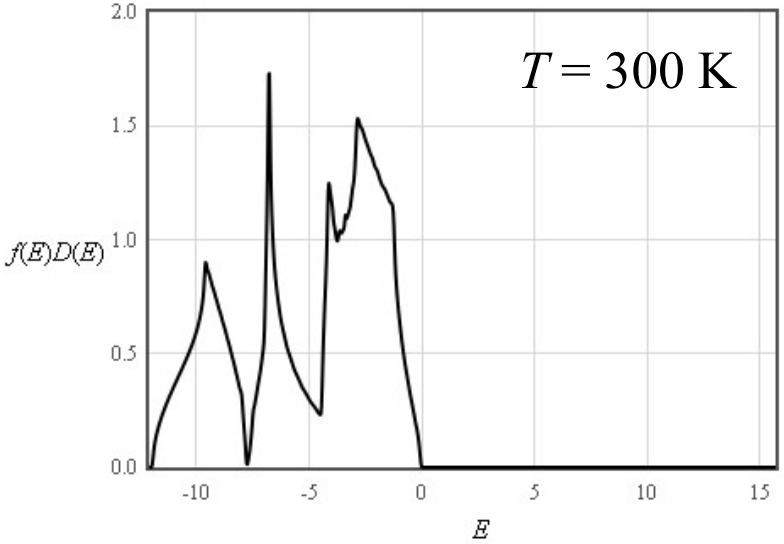
$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)}$$

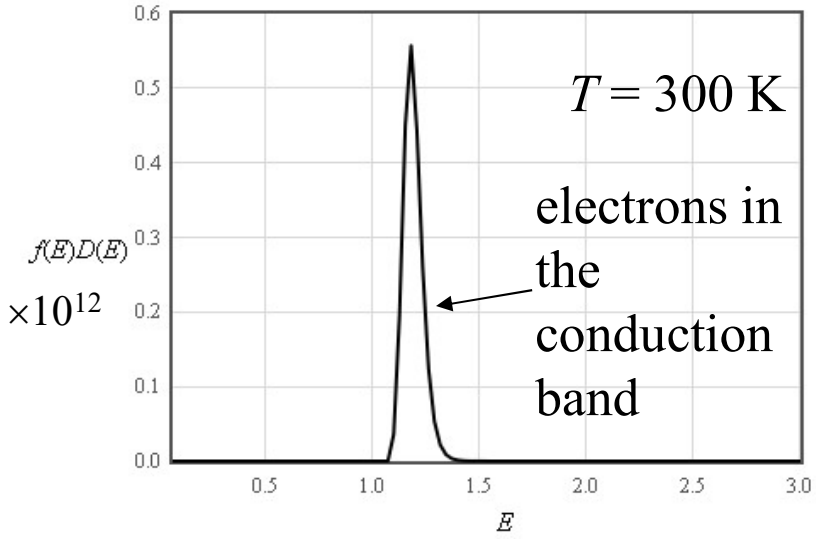


Silicon density of states









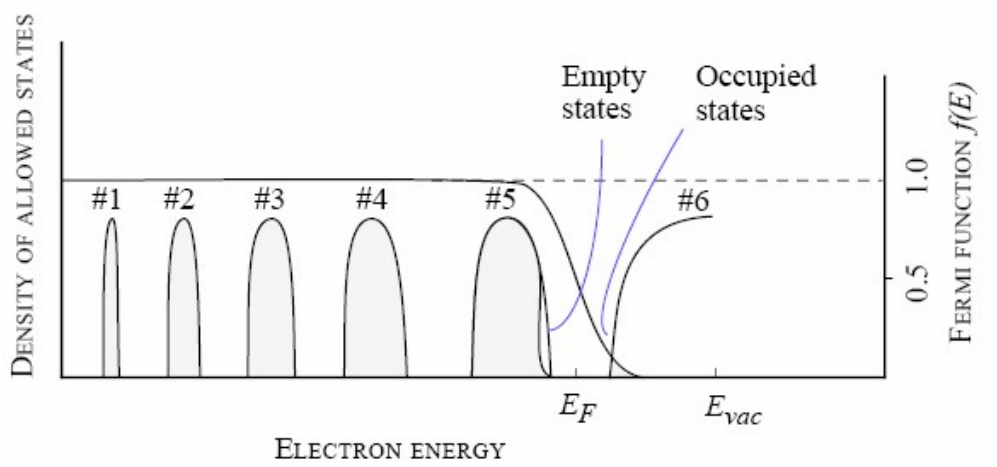
Fermi energy

The Fermi energy is implicitly defined as the energy that solves the following equation.

$$n = \int_{-\infty}^{\infty} D(E) f(E) dE$$

Here n is the electron density.

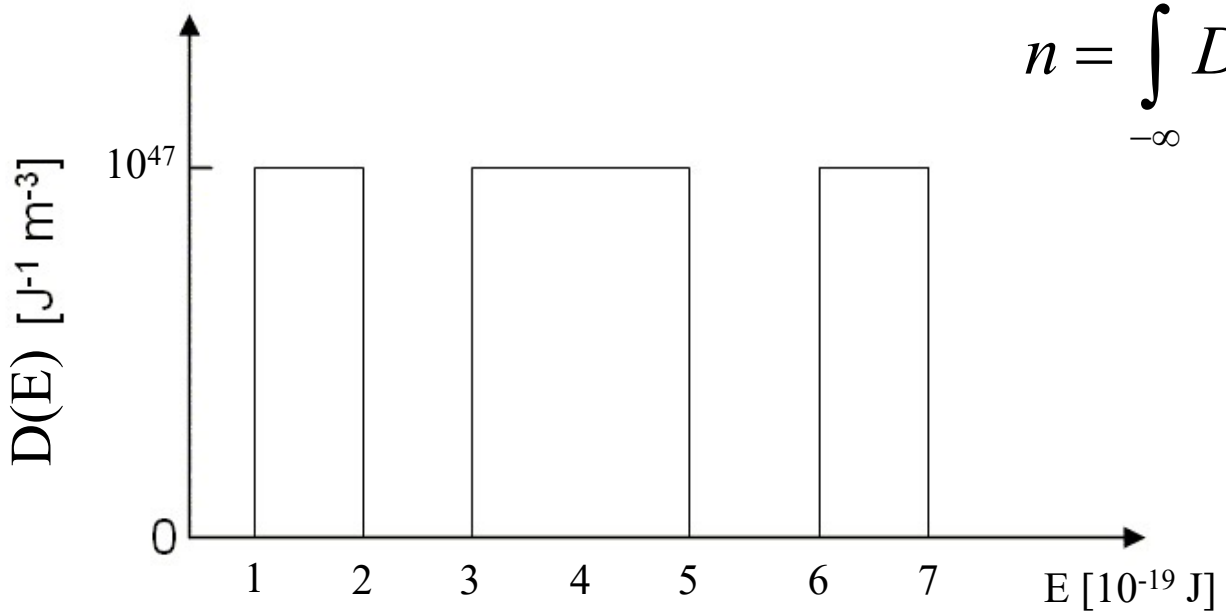
The density of states, the total number of electrons and the temperature are given. To find the Fermi energy, guess one and evaluate the integral. If n turns out too low, guess a higher E_F and if n turns out too high, guess a lower E_F.



Calculate the Fermi energy

The density of states for a particular material is given in the following figure.

$$n = \int_{-\infty}^{\infty} D(E) f(E) dE$$



$$n = 3 \times 10^{28}\ \mathrm{m}^{-3}$$

What is the Fermi energy at zero temperature? For a semiconductor, find the limiting value of the Fermi energy as the temperature approaches zero.

$E_f =$ _____ eV

What kind of material is this?

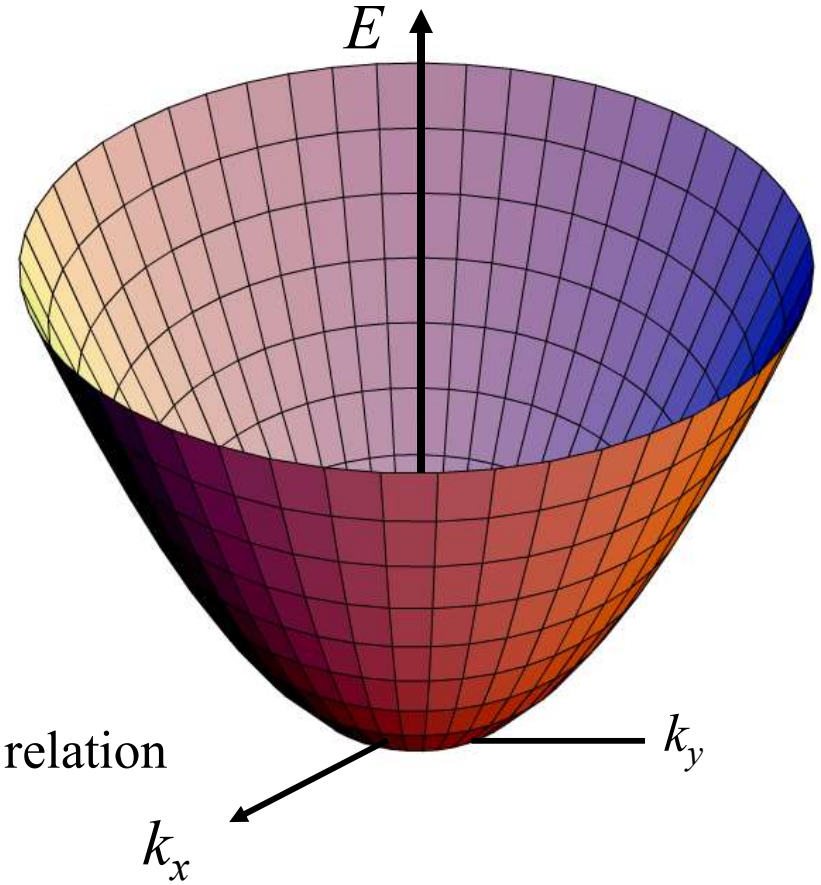
Metal

Intrinsic semiconductors

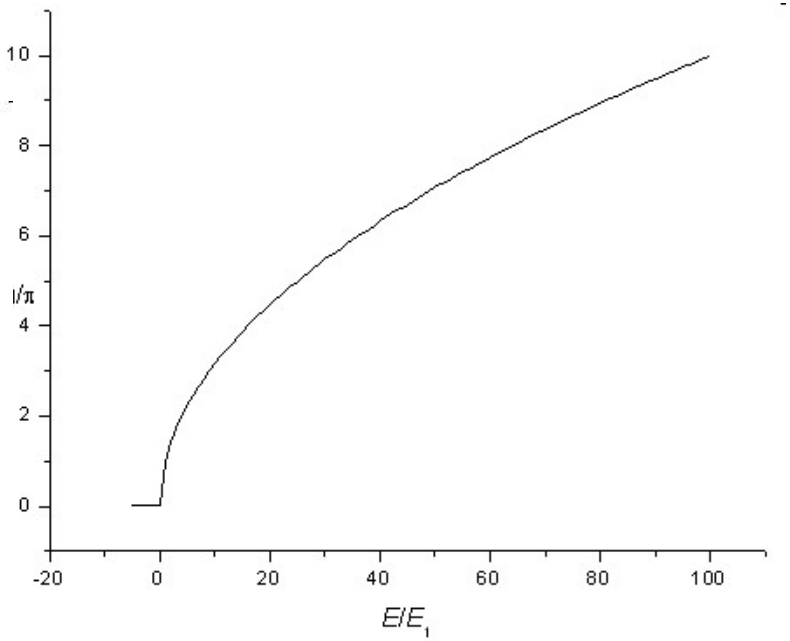
free electrons (simple model for a metal)

$$E(\vec{k}) = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) = \frac{p^2}{2m} = \tfrac{1}{2}mv^2$$

dispersion relation



3-d density of states



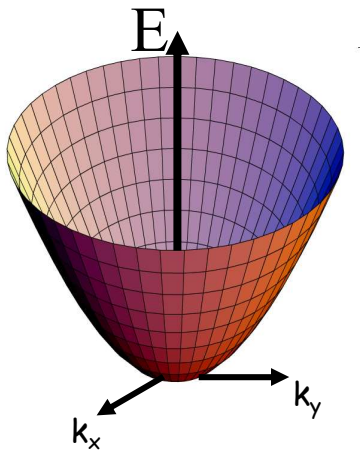
$$D(E) = \begin{cases} 0 & \text{for} \quad E < 0 \\ \dfrac{(2m)^{3/2}}{2\pi^2\hbar^3}\sqrt{E} & \text{for} \quad E > 0 \end{cases}$$

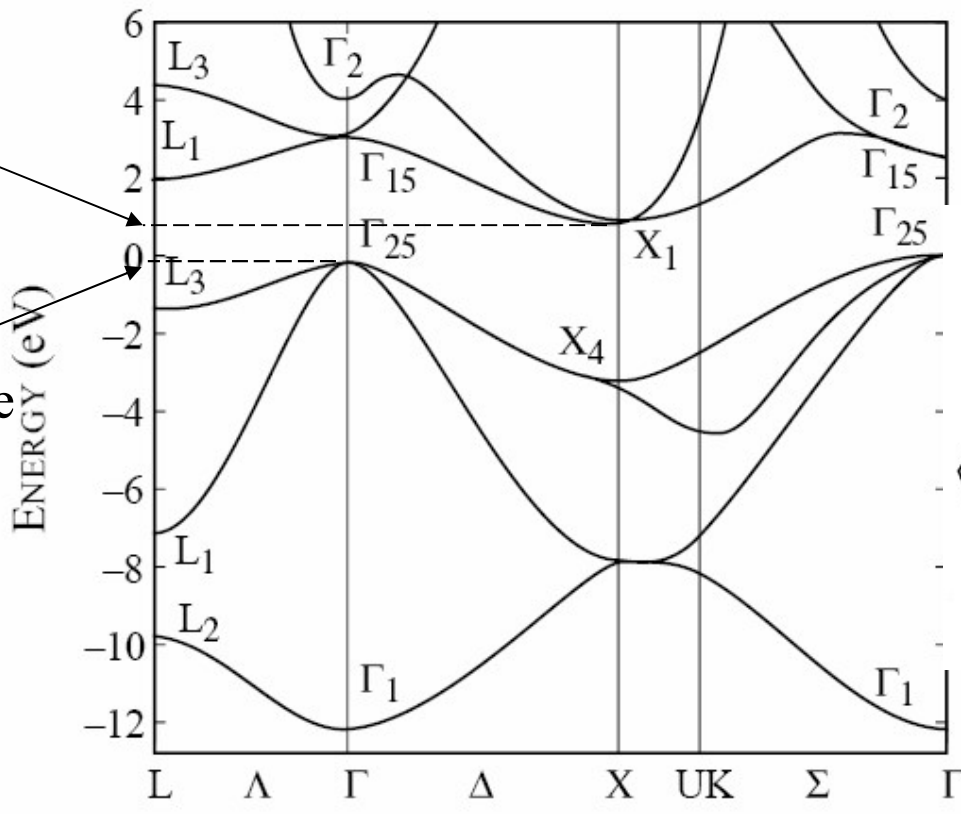
Silicon band structure

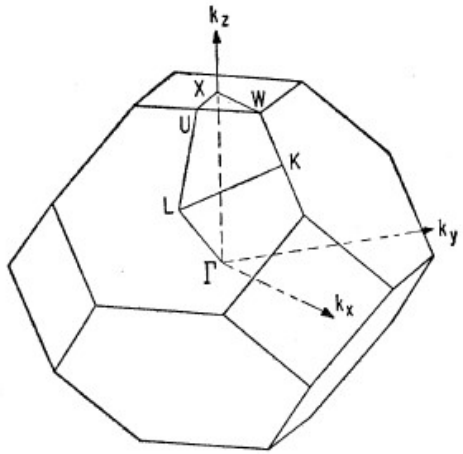
E_c = bottom of the conduction band

$E_g = E_c - E_v$

E_v = top of the valence band







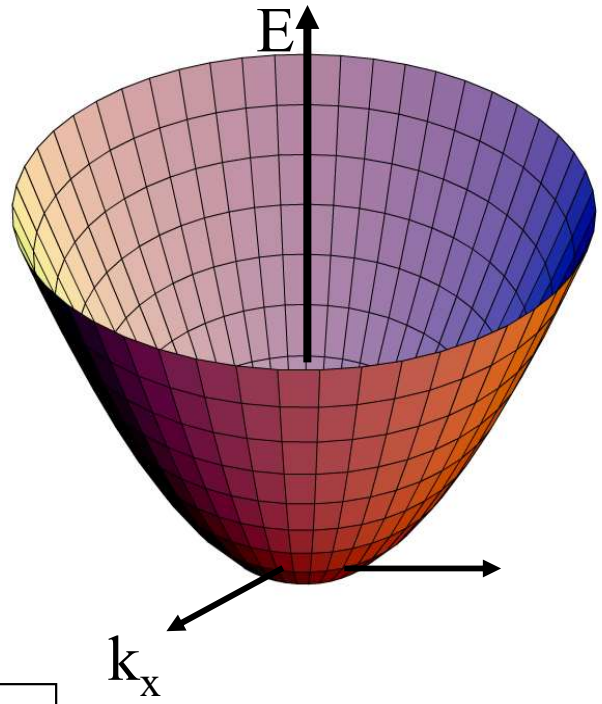
Near the bottom of the conduction band, the band structure looks like a parabola.

Effective mass

$$E(\vec{k}) = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) = \frac{p^2}{2m} = \tfrac{1}{2}mv^2$$

$$\frac{dE(\vec{k})}{dk_x} = \frac{\hbar^2 k_x}{m}$$

$$\frac{d^2E(\vec{k})}{dk_x^2} = \frac{\hbar^2}{m}$$



Effective mass

$$m_x^* = \frac{\hbar^2}{\dfrac{d^2E(\vec{k})}{dk_x^2}}$$

This effective mass is used to describe the response of electrons to external forces in the particle picture.

$$\vec{F} = -e\vec{E} = m^*\vec{a}$$