Institute of Solid State Physics

2

Semiconductor Crystals

Physics of semiconductor devices

Karin Zojer

October 8, 2025

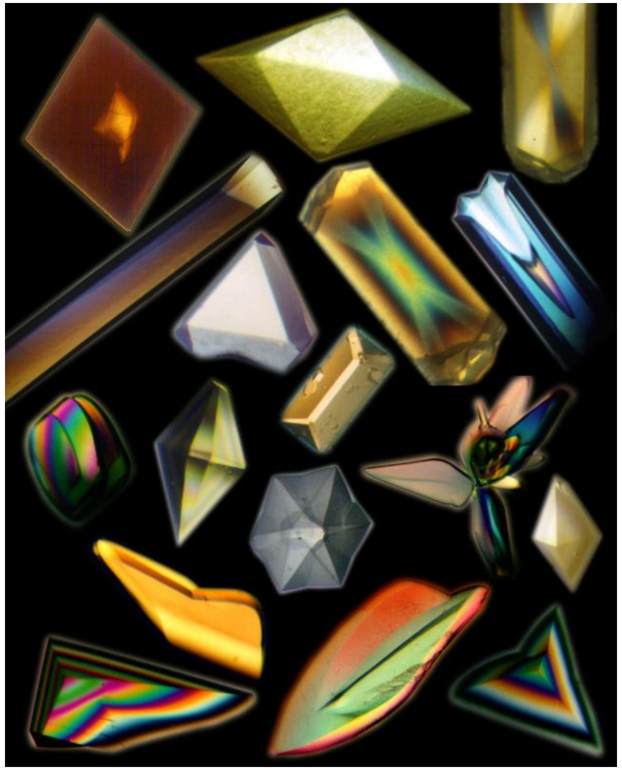
Crystal Structure

- atoms are arranged in a periodic pattern in a crystal.
- atomic arrangement affects the macroscopic properties of a material
- many important materials (silicon, steel) are crystals

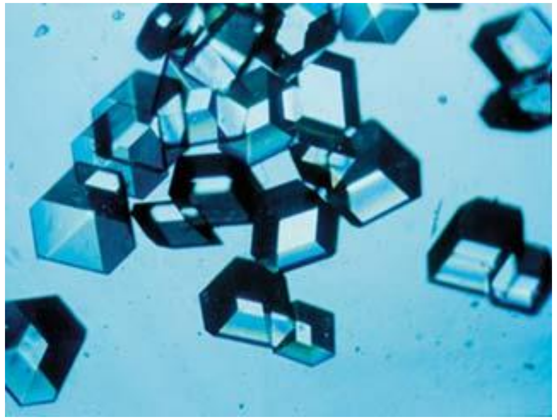
Gallium crystals

quartz

Crystal Structure



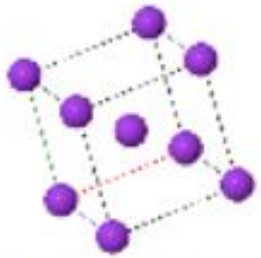
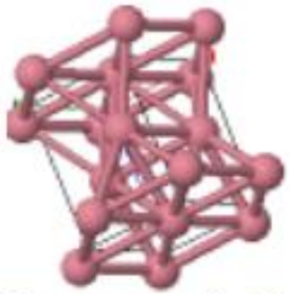
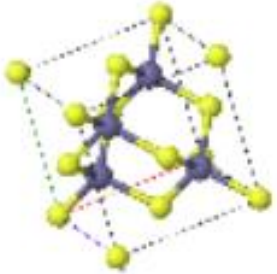
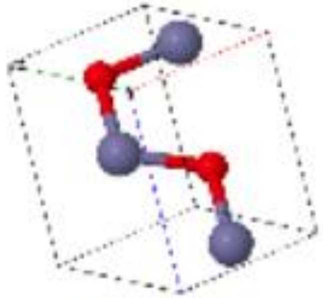
protein crystals



insulin crystals

NASA Marshall Space Flight Center (NASA-MSFC)

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 $h\vec{a}_1 + k\vec{a}_2 + l\vec{a}_3$

lattice vectors

always use integers for *h,k,l*

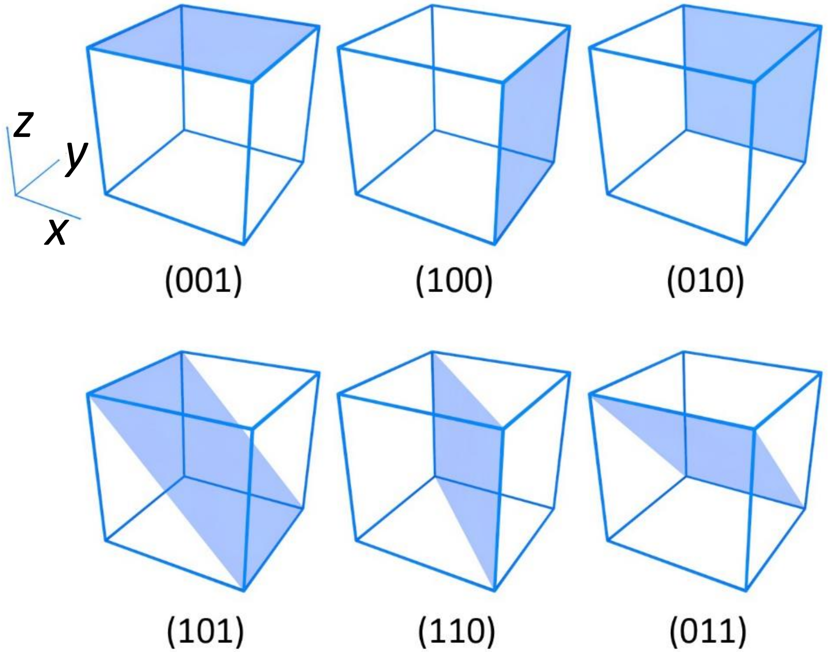
[ ] … specific **direction**

< > … family of equivalent **directions**

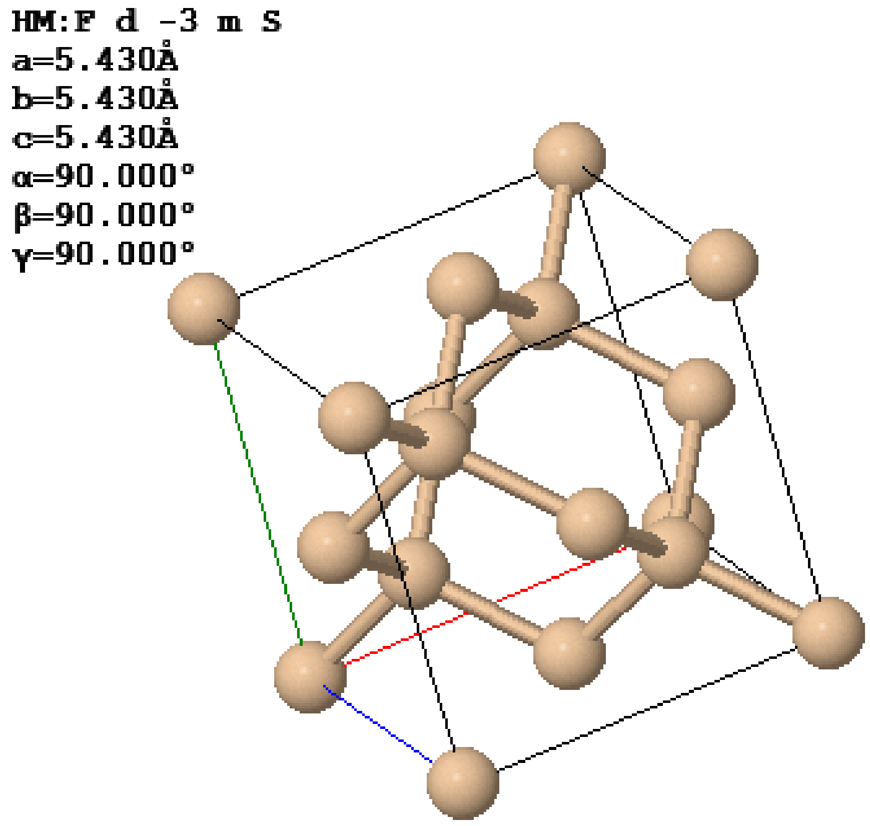
( ) … specific plane

{ } … family of equivalent planes

MOSFETs are made on {100} wafers



silicon



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: 1 K: 0 L: 0

show HKL plane | hide HKL plane

draw atoms in HKL plane

Thickness of HKL planes:

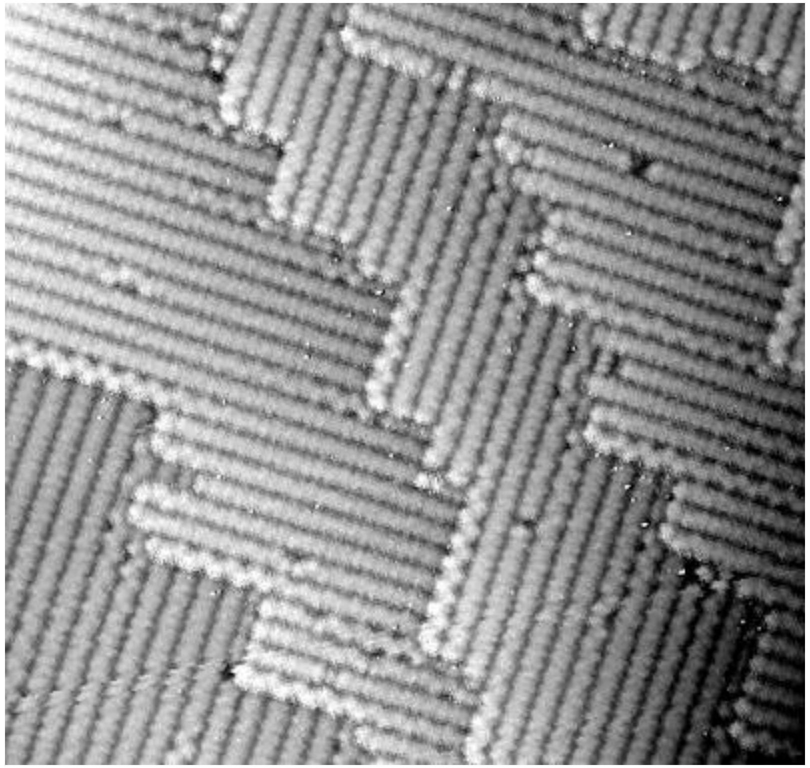
The conventional unit cell is a cube with sides of 0.543 nm. There are 8 atoms atoms in the conventional unit cell. (The image can be rotated with a mouse.)

JSmol

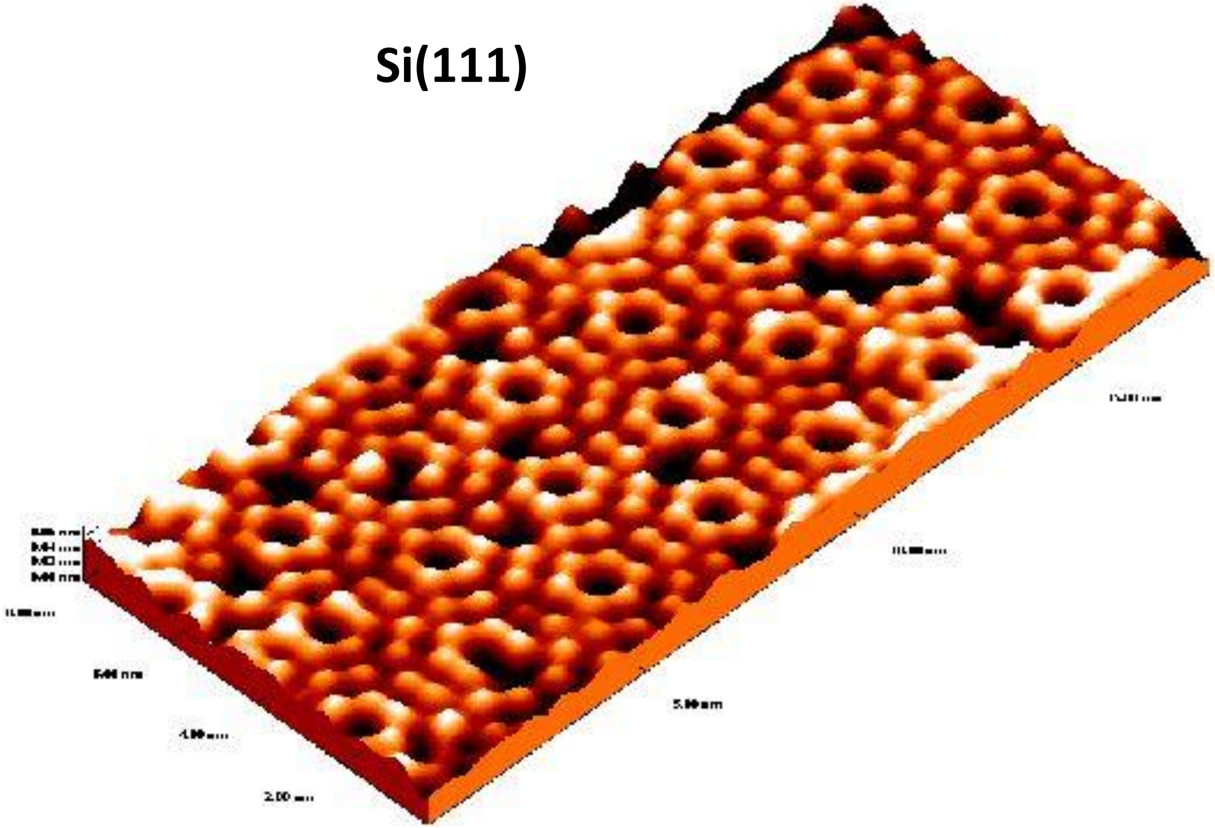
http://lampz.tugraz.at/~hadley/memm/materials/silicon/silicon.php

silicon surfaces

Si(100)



Si(111)



https://www.fz-juelich.de/en/pgi/pgi-3/groups/research/multi-tip-spm-instrument-development/stm-pictures

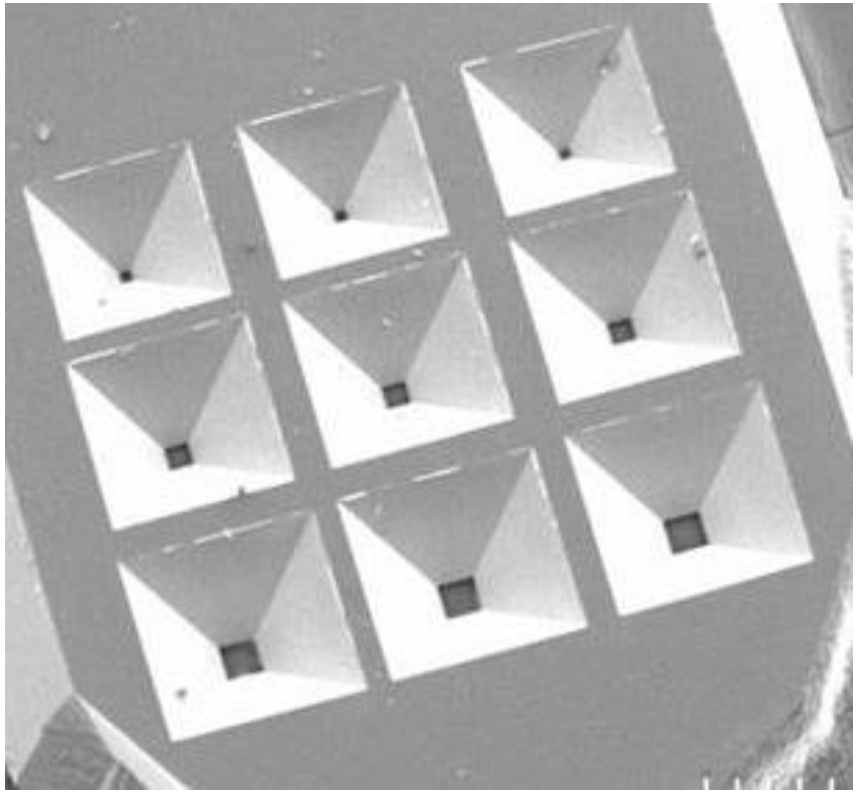
KOH etching of silicon

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).



{100} surface of Si wafer

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

3

Electrons in crystals

Physics of semiconductor devices

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Electrons

How electrons behave ?

How electrons behave in a crystal?

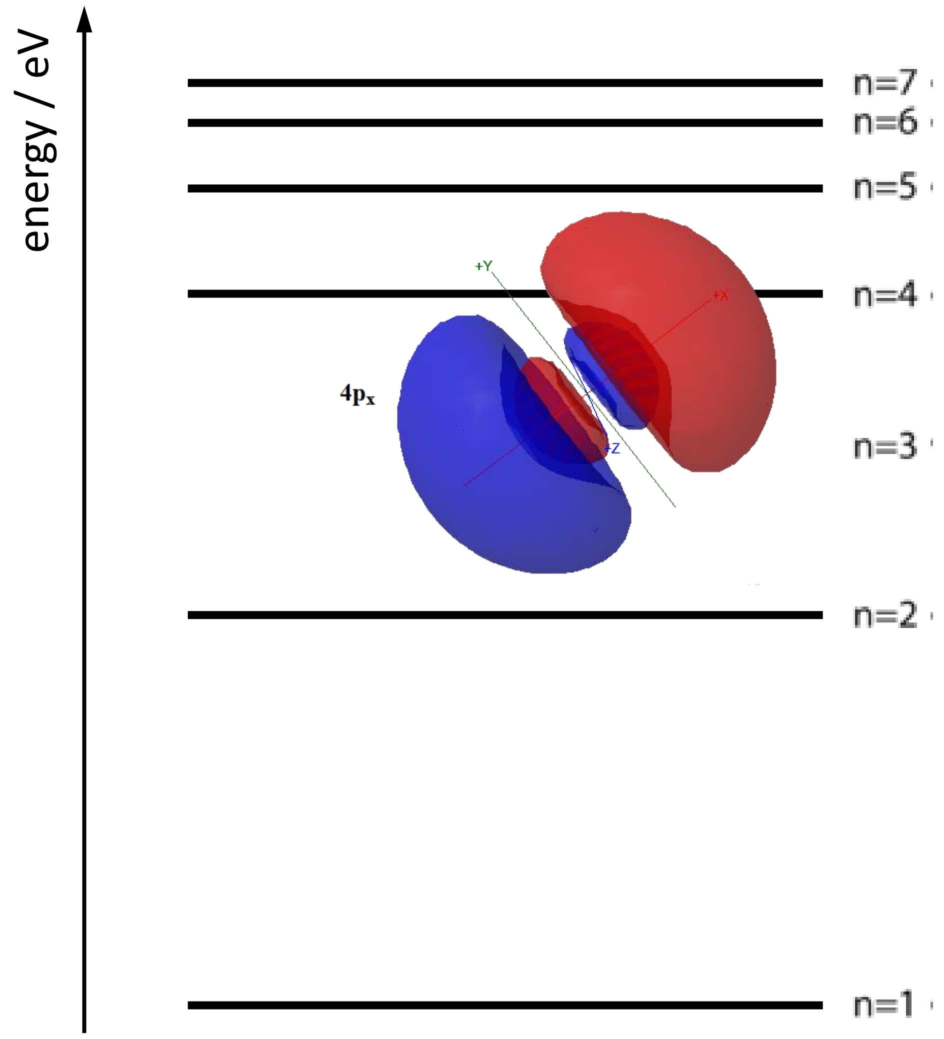
Charge = -1.6022×10^{-19} C

Mass = 9.11×10^{-31} kg

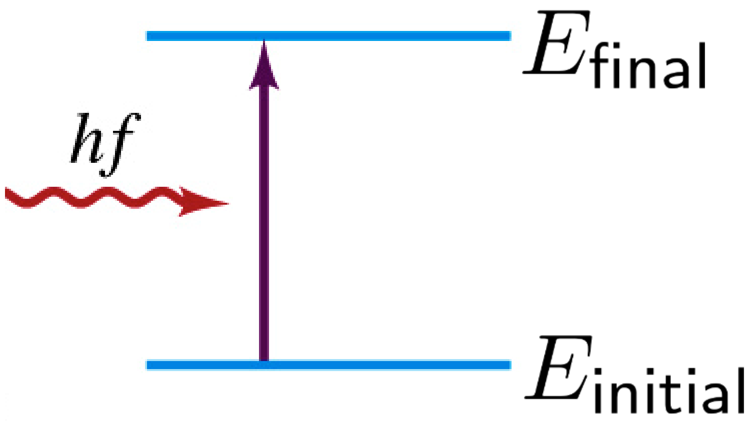
occupied space = ?

0.15 nm

Energy levels in atoms



Energy levels in atoms

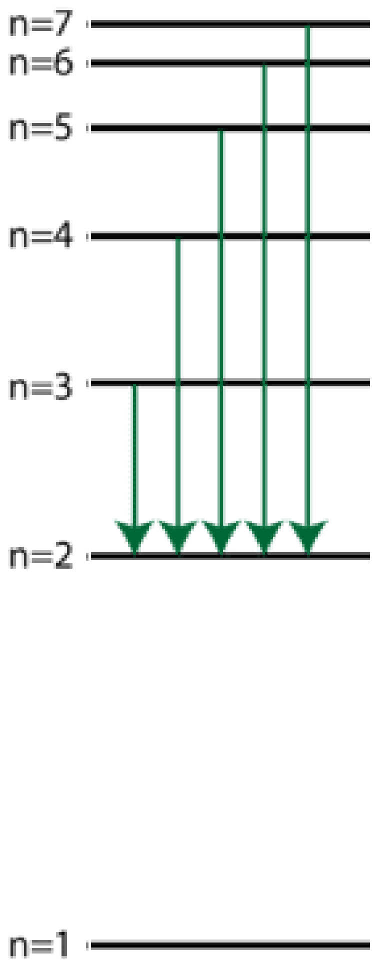


$$hf = E_{\text{final}} - E_{\text{initial}}$$

Fluoresce

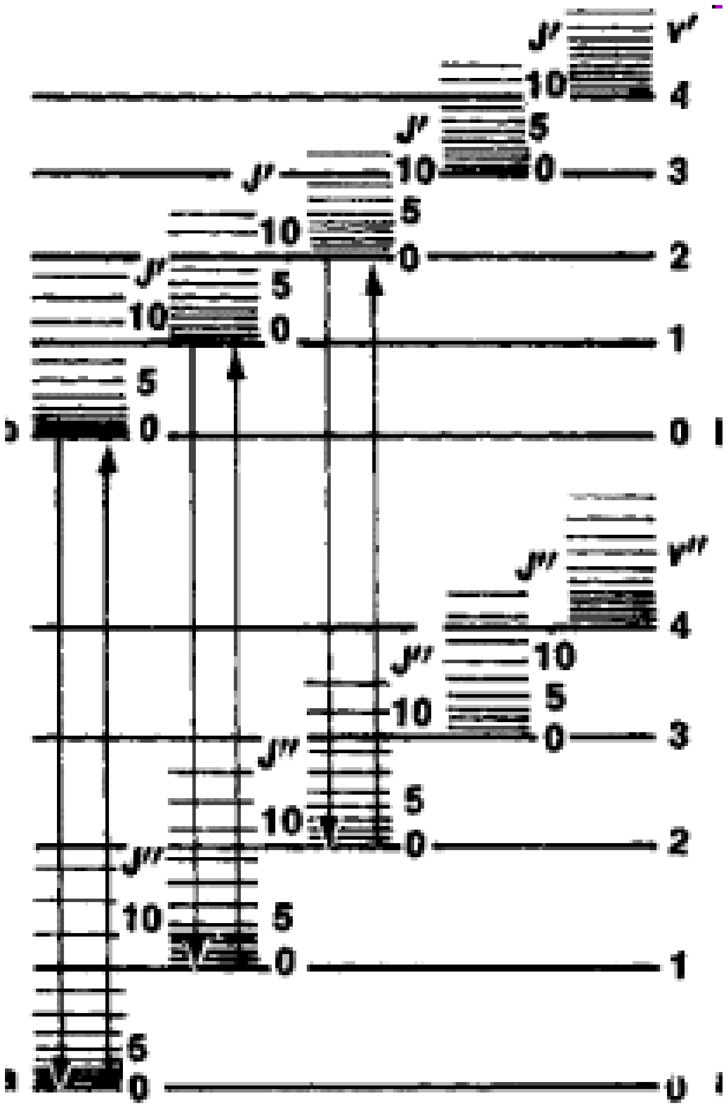
Hg

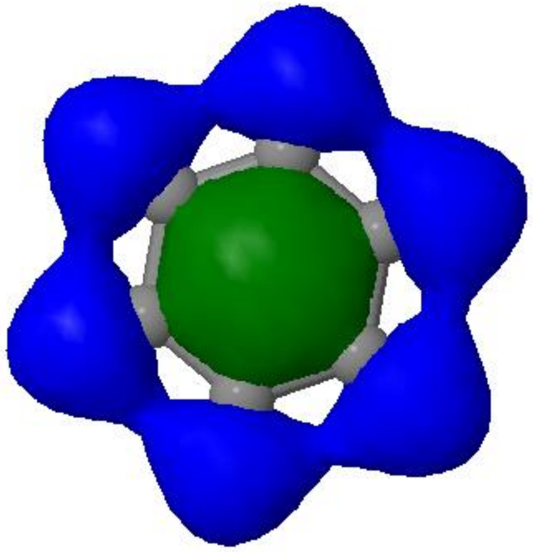
hydrogen atom



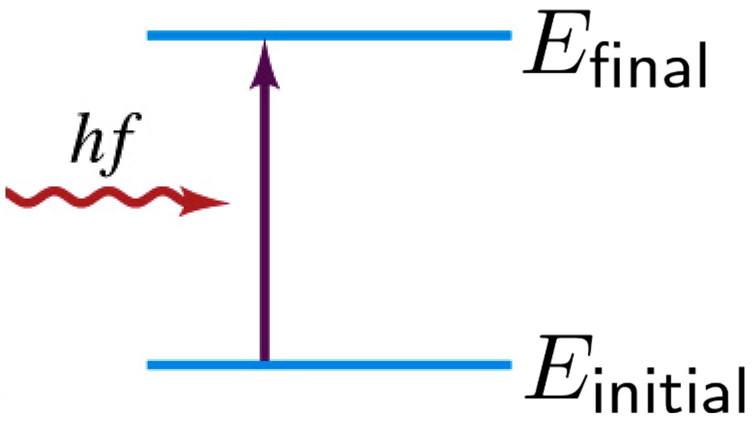
https://chem.libretexts.org/Bookshelves/Introductory_Chemistry/Introductory_Chemistry_(CK-12)/05%3A_Electr _ _Atoms/5.07%3A_Spectral_Lines_of_Atomic_Hydrogen

Molecular levels





valence electrons
spread across
molecule



$$hf = E_{\text{final}} - E_{\text{initial}}$$

wave vector k

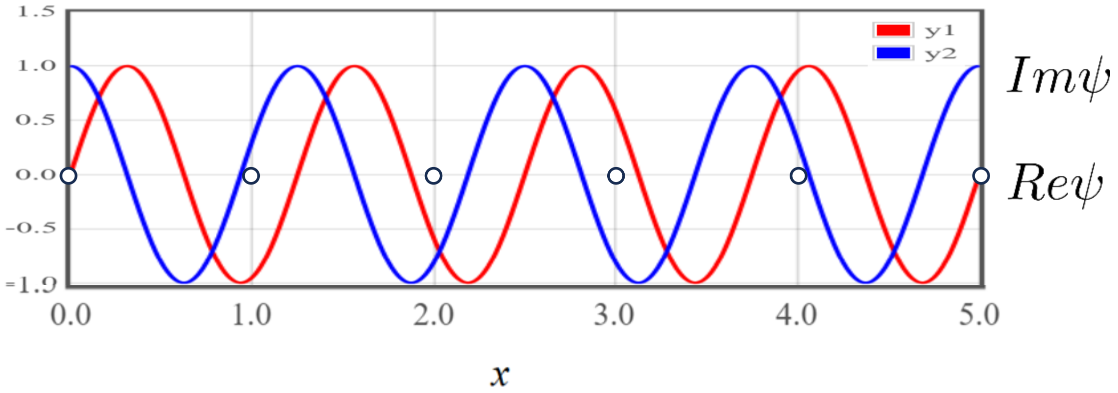
k-vector: $\vec{k}$, points in the direction a wave is propagating.

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

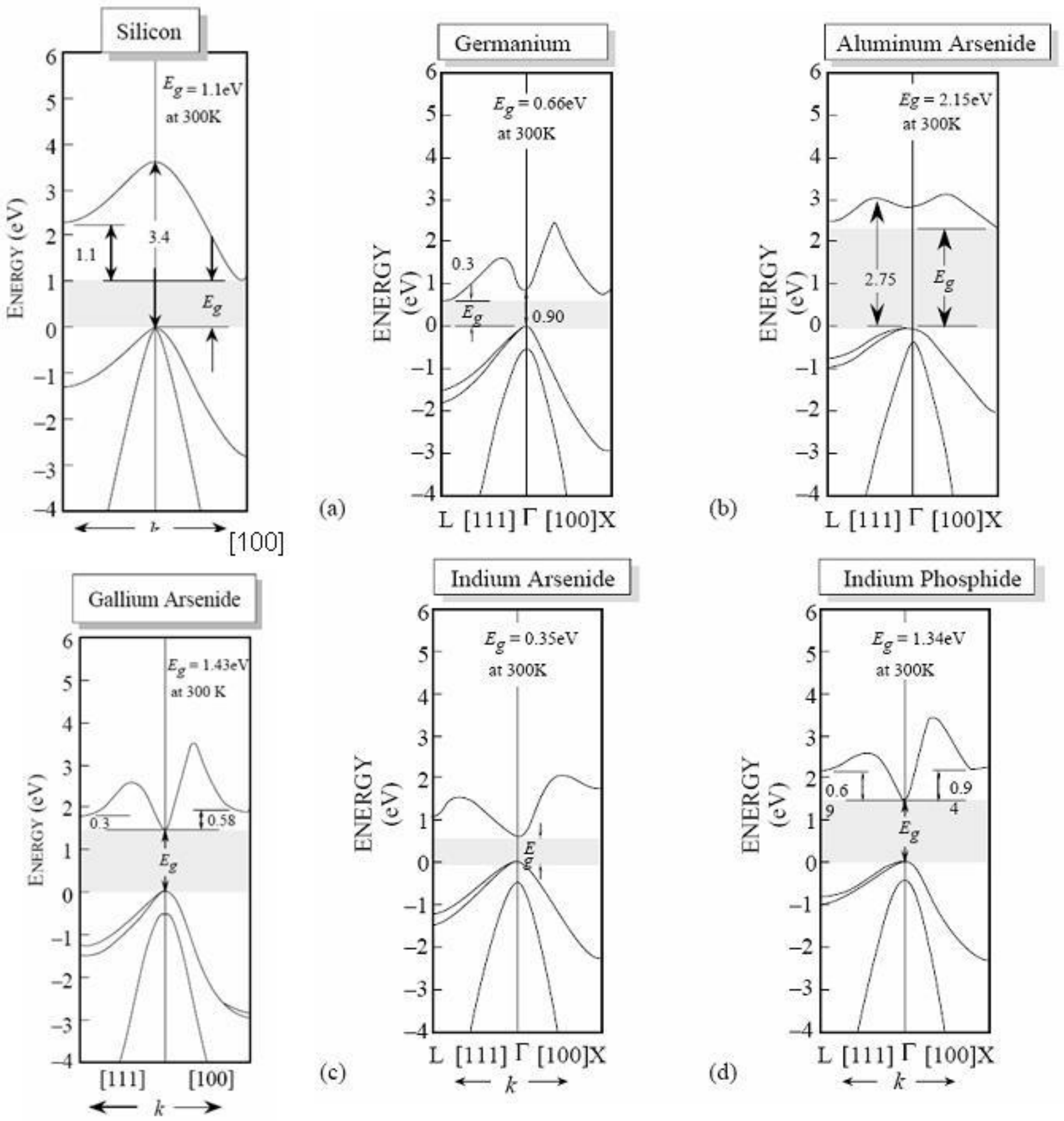
momentum: $$\vec{p} = \hbar\vec{k}$$

periodicity of the crystal lattice in that direction

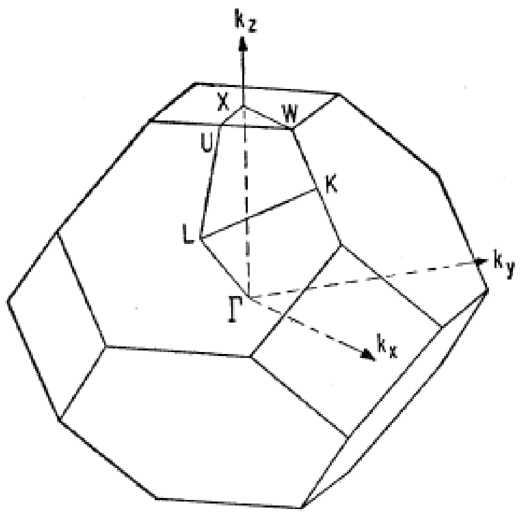
$$\psi = e^{ikx}u_k(x)$$



Semiconductors

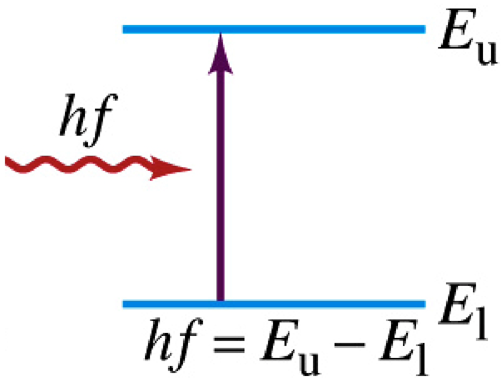


valence band
conduction band
band gap

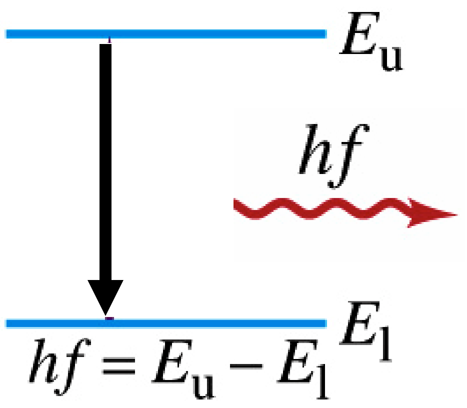


molecular orbitals
are plane waves

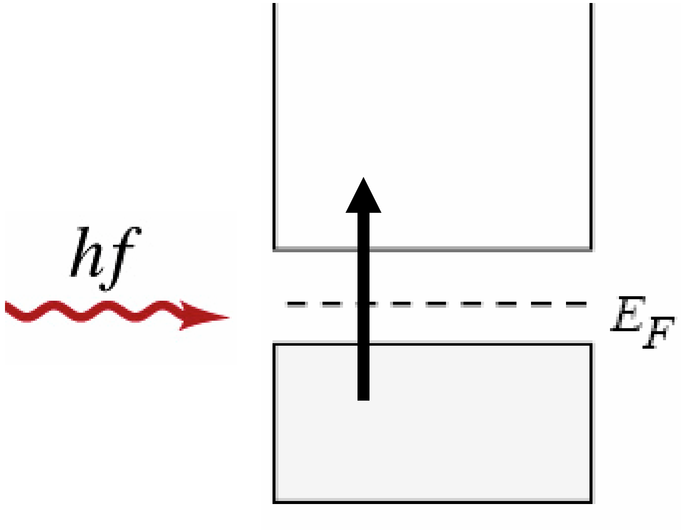
Absorption and emission of photons



absorption



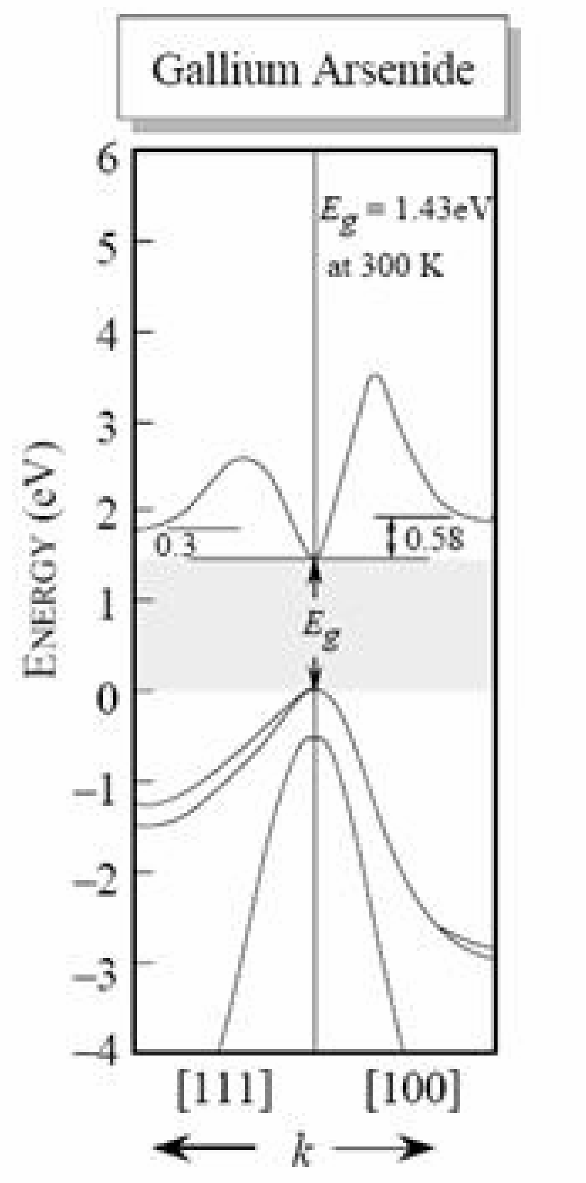
emission



semiconductor

$hf < E_g$ no absorption

What color light does a GaAs LED emit?



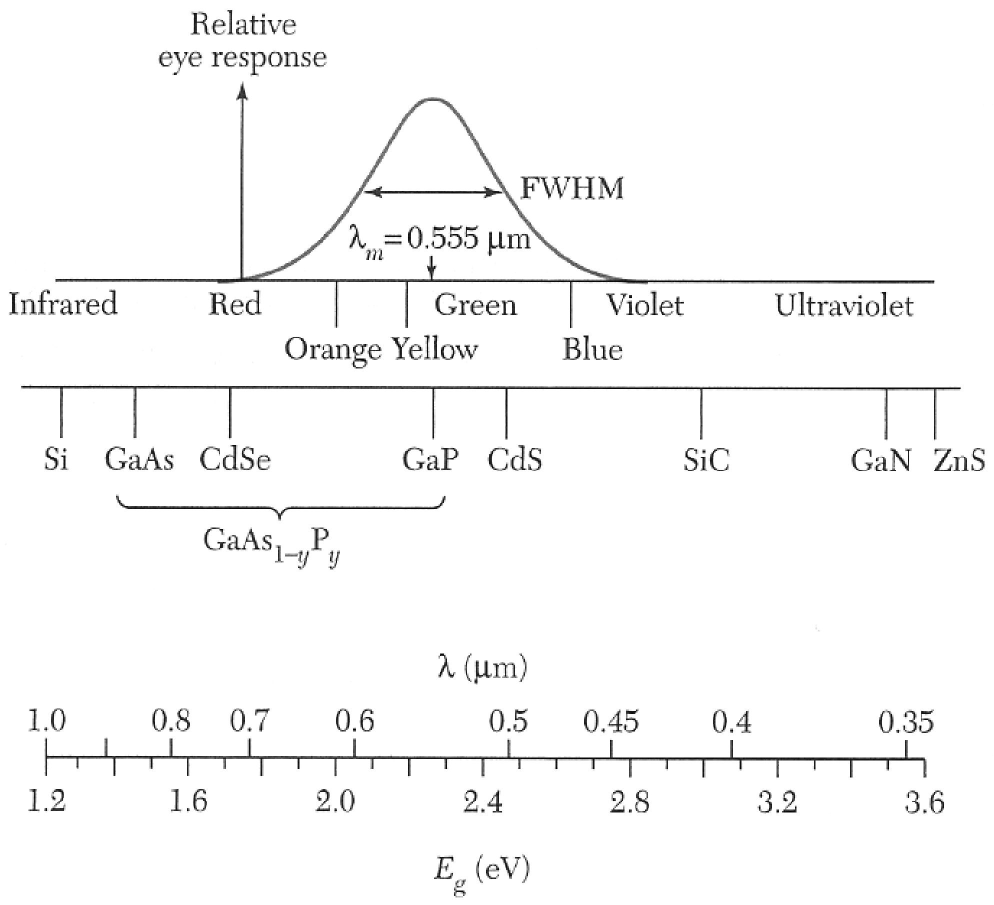
$$E = 1.6022 \times 10^{-19} \times 1.43 \text{ J} = hf = \frac{hc}{\lambda}$$

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

light emitting diodes

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

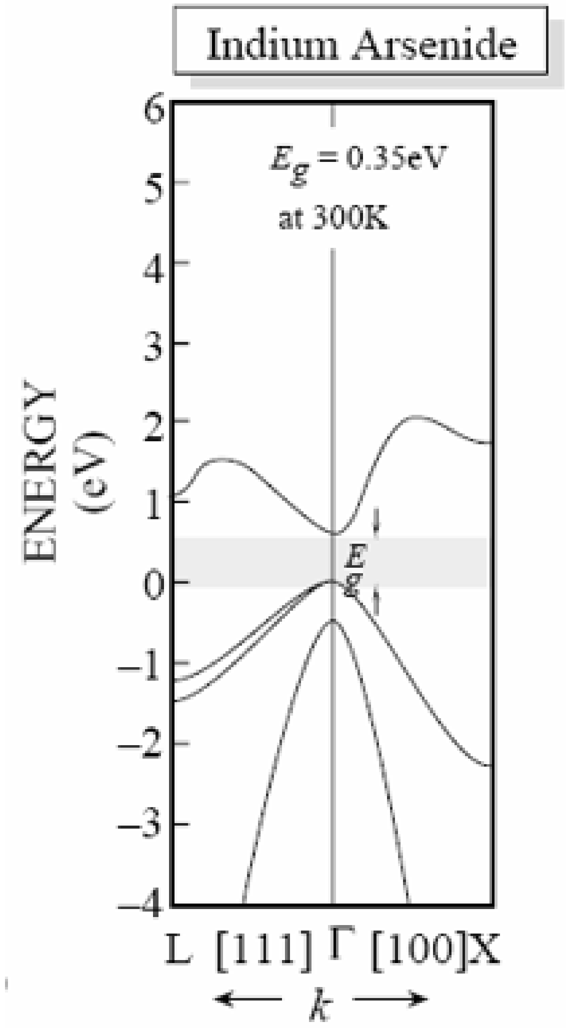
Material	Wavelength (nm)
InAsSbP/InAs	4200
InAs	3800
GaInAsP/GaSb	2000
GaSb	1800
$Ga_xIn_{1-x}As_{1-y}P_y$	1100-1600
$Ga_{0.47}In_{0.53}As$	1550
$Ga_{0.27}In_{0.73}As_{0.63}P_{0.37}$	1300
GaAs:Er,InP:Er	1540
Si:C	1300
GaAs:Yb,InP:Yb	1000
$Al_xGa_{1-x}As$:Si	650-940
GaAs:Si	940
$Al_{0.11}Ga_{0.89}As$:Si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

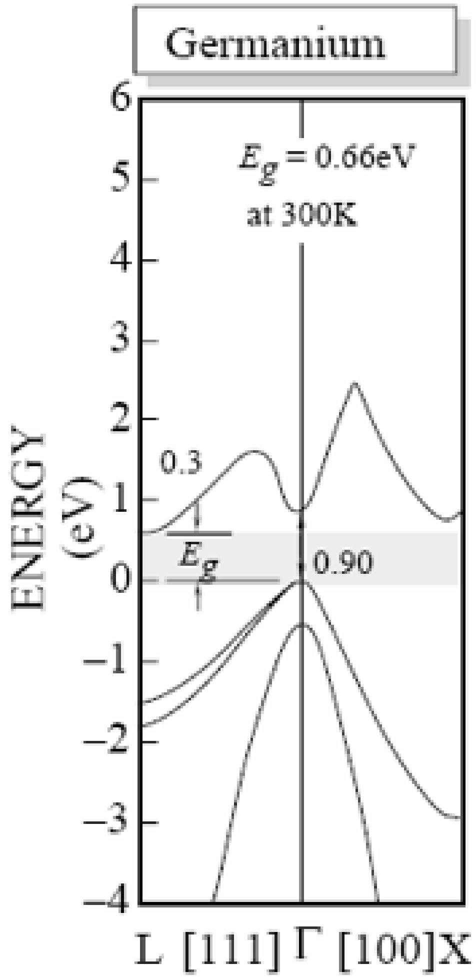
direct bandgap:
$\Delta k = 0$

photons can be emitted



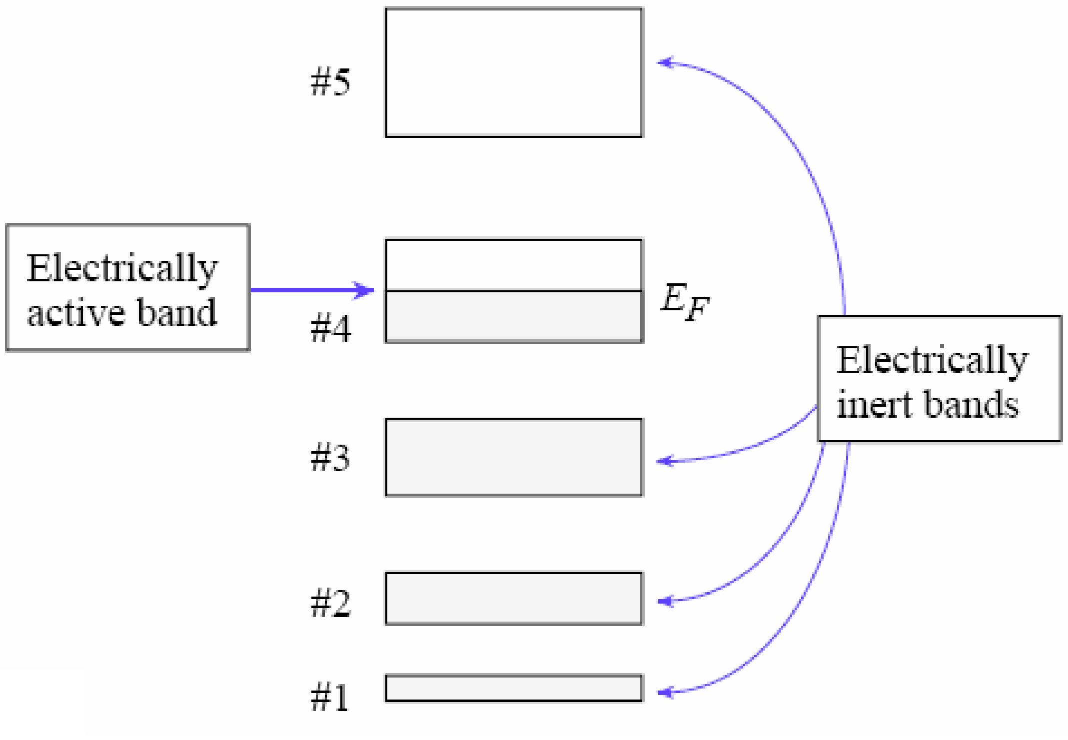
indirect bandgap:
$\Delta k \neq 0$

phonons are emitted

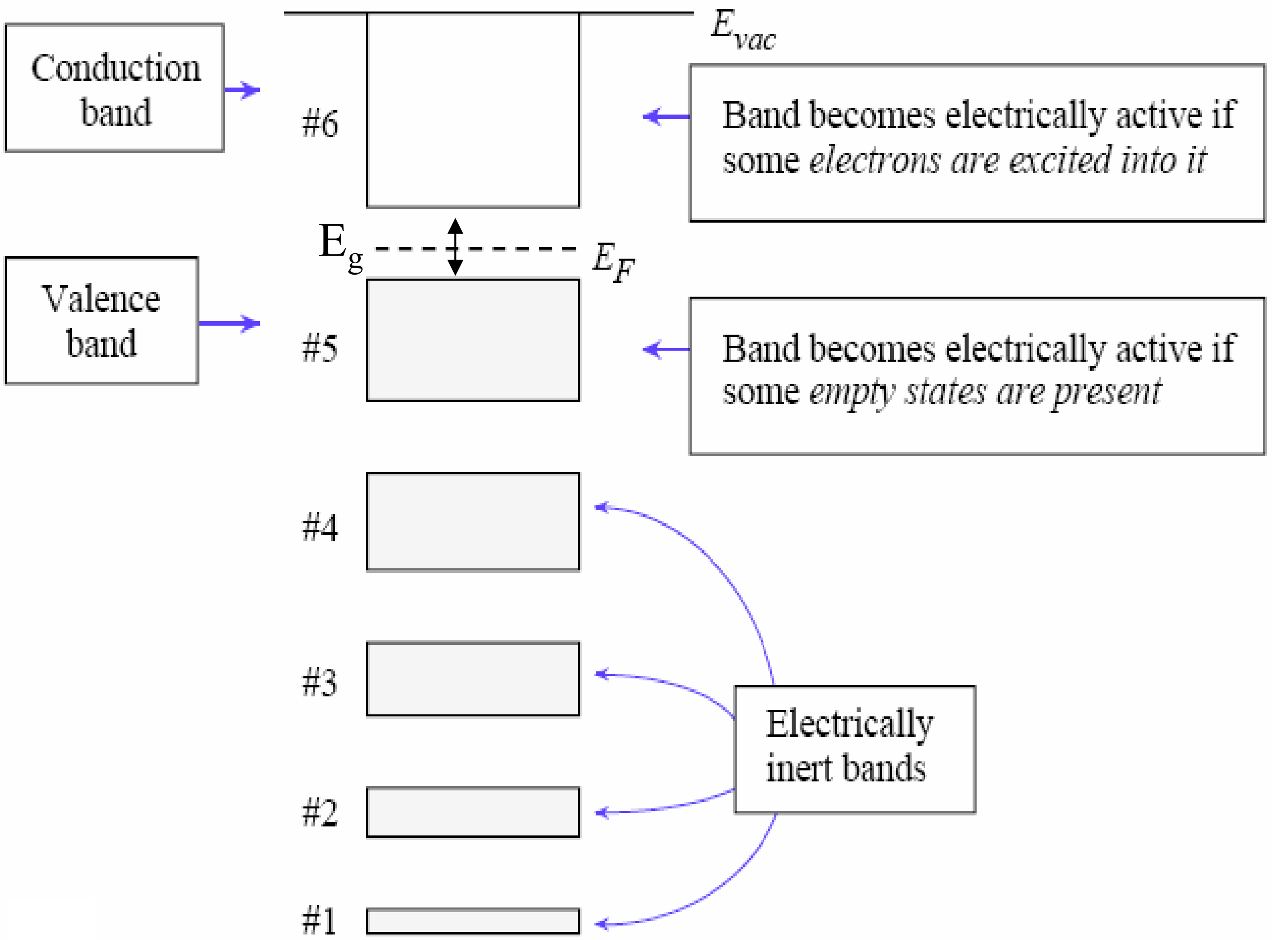


Momentum must be conserved when photons are absorbed or emitted.

Metals, semiconductors, insulators



Metal



Semiconductor or insulator

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

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

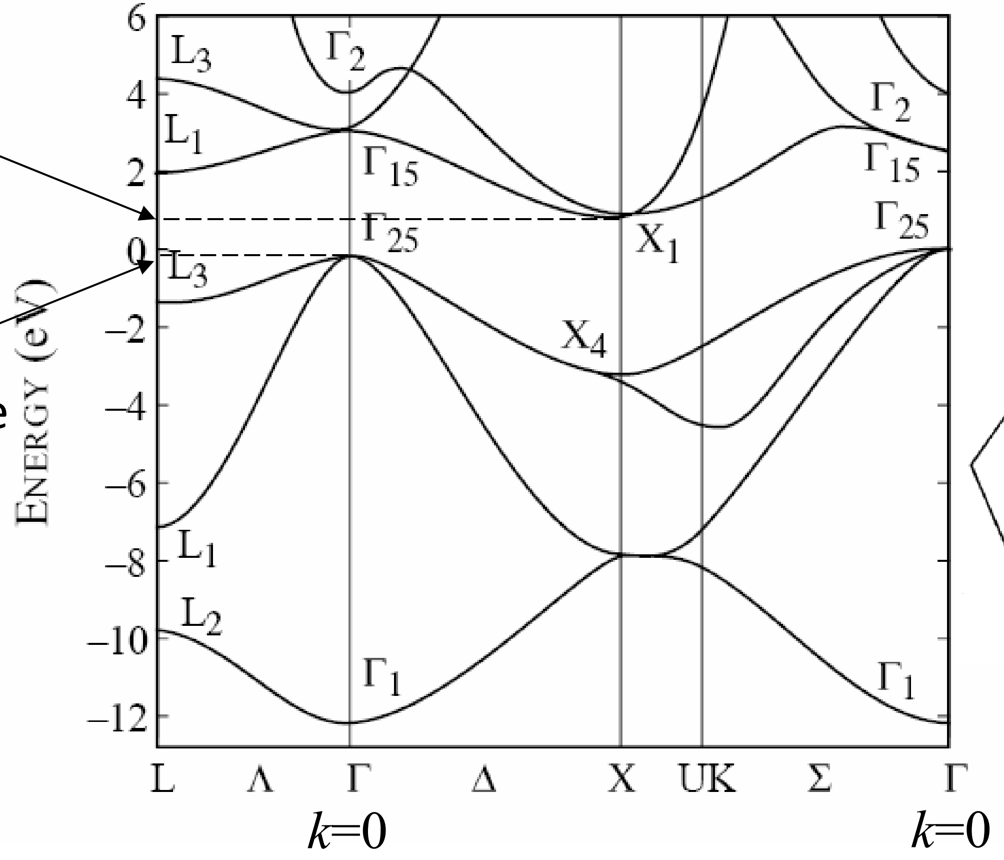
from: Singh

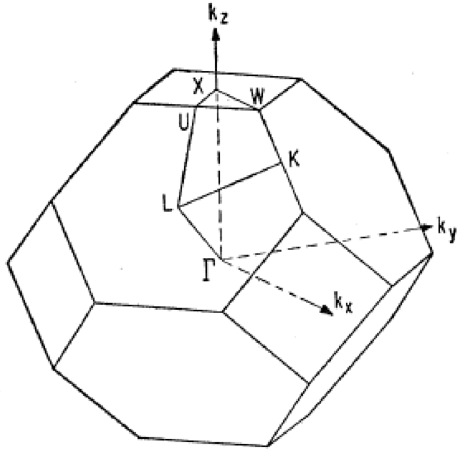
Silicon band structure

E_c = bottom of the conduction band

$E_g = E_c - E_v$

E_v = top of the valence band

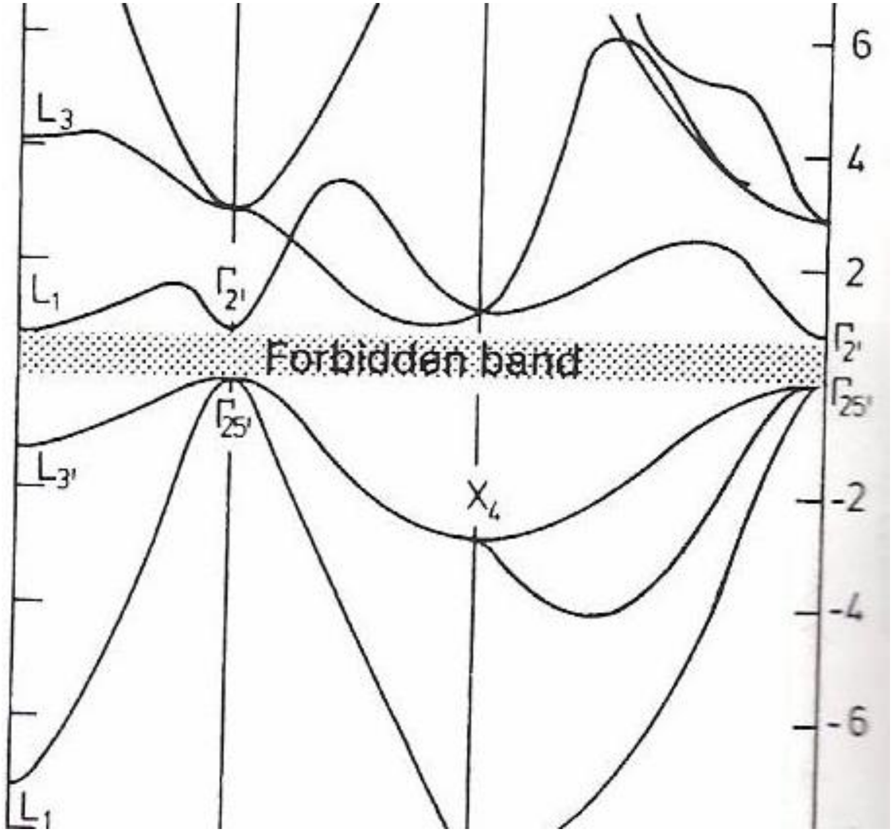


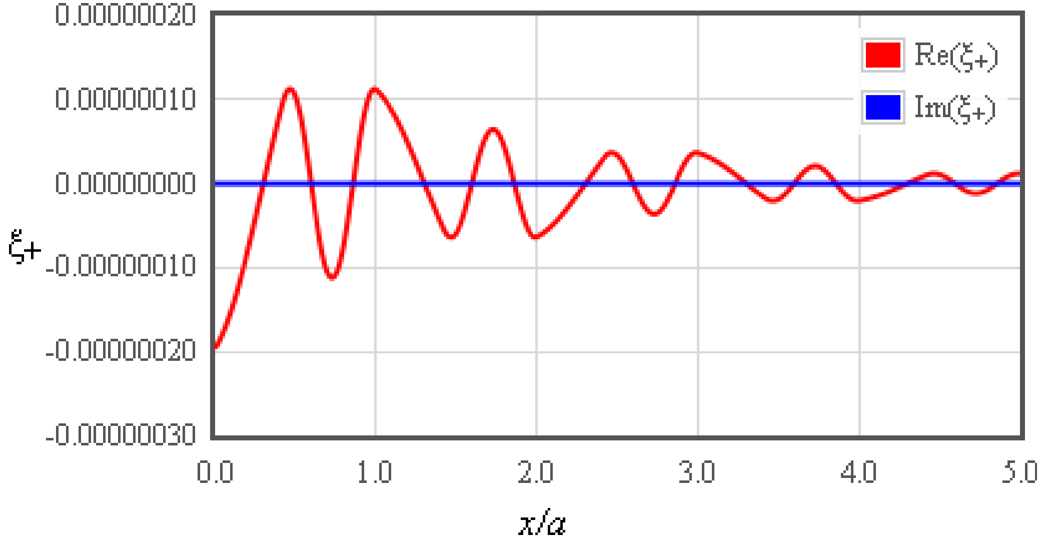


Electrons with energies in the gap are reflected out of the crystal.

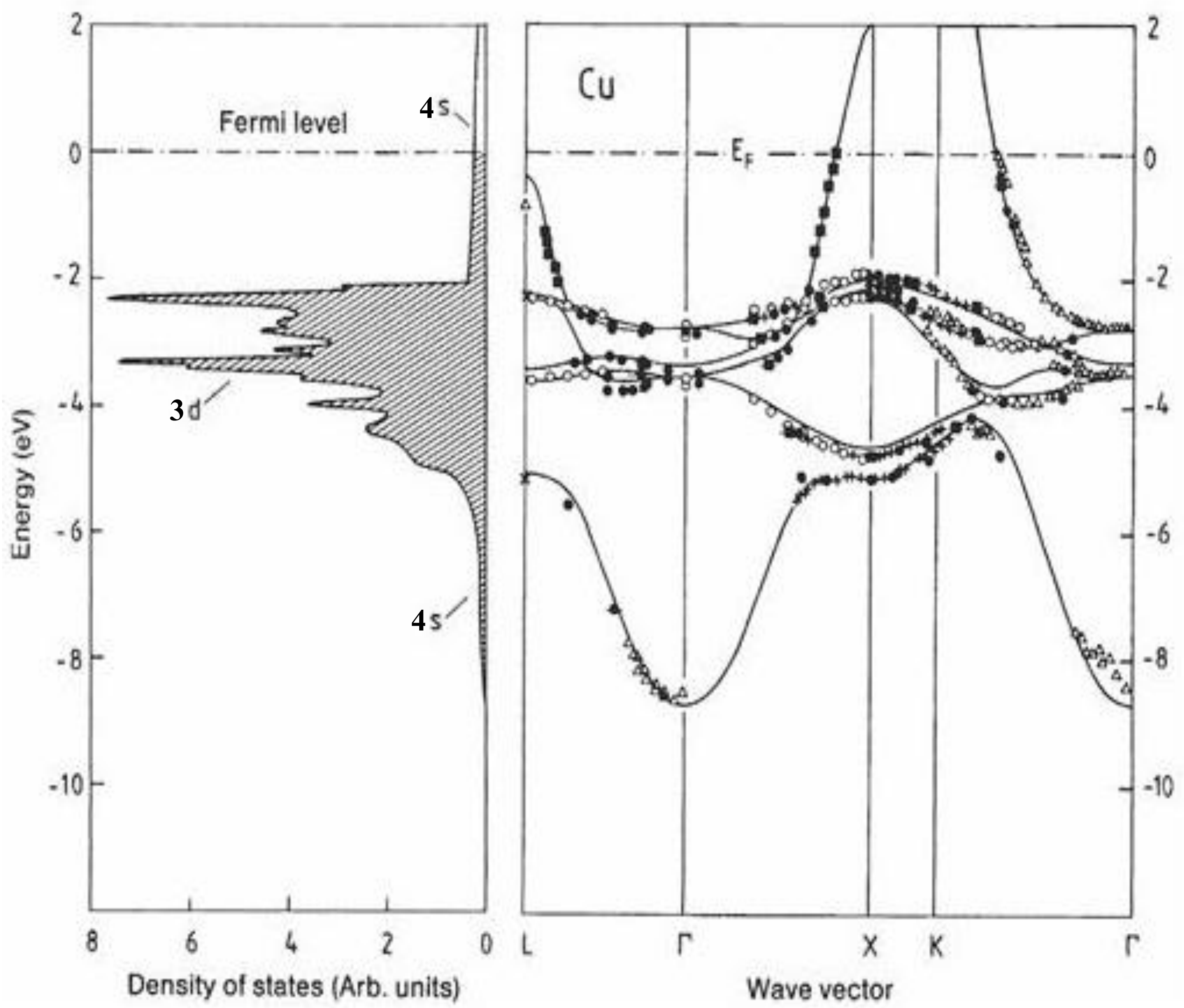
Band gap

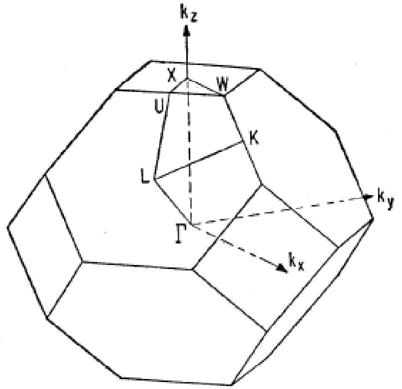
Electrons with energies in the gap are reflected out of the crystal.





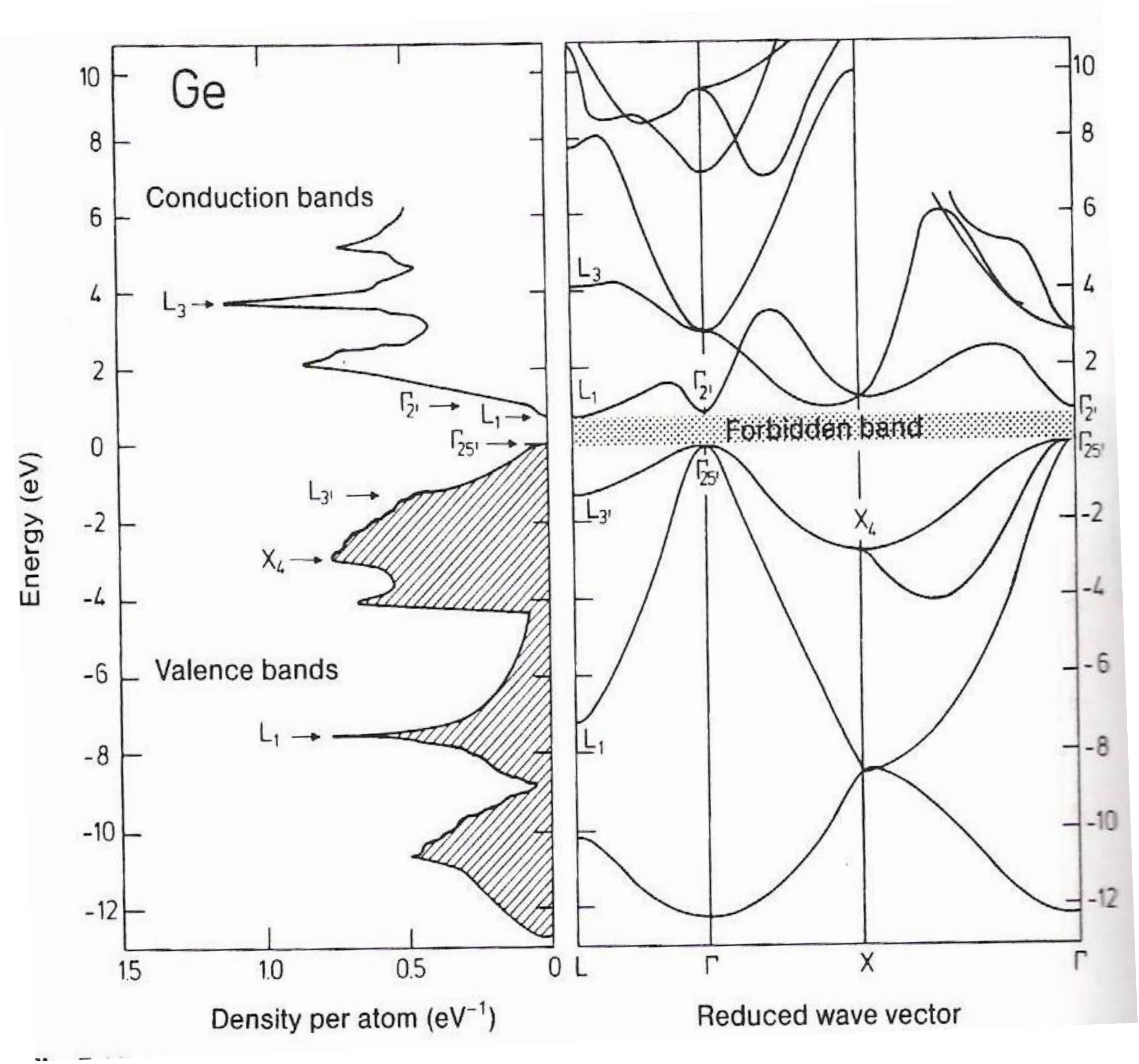
Copper: dispersion relation and density of states





from Ibach & Lueth

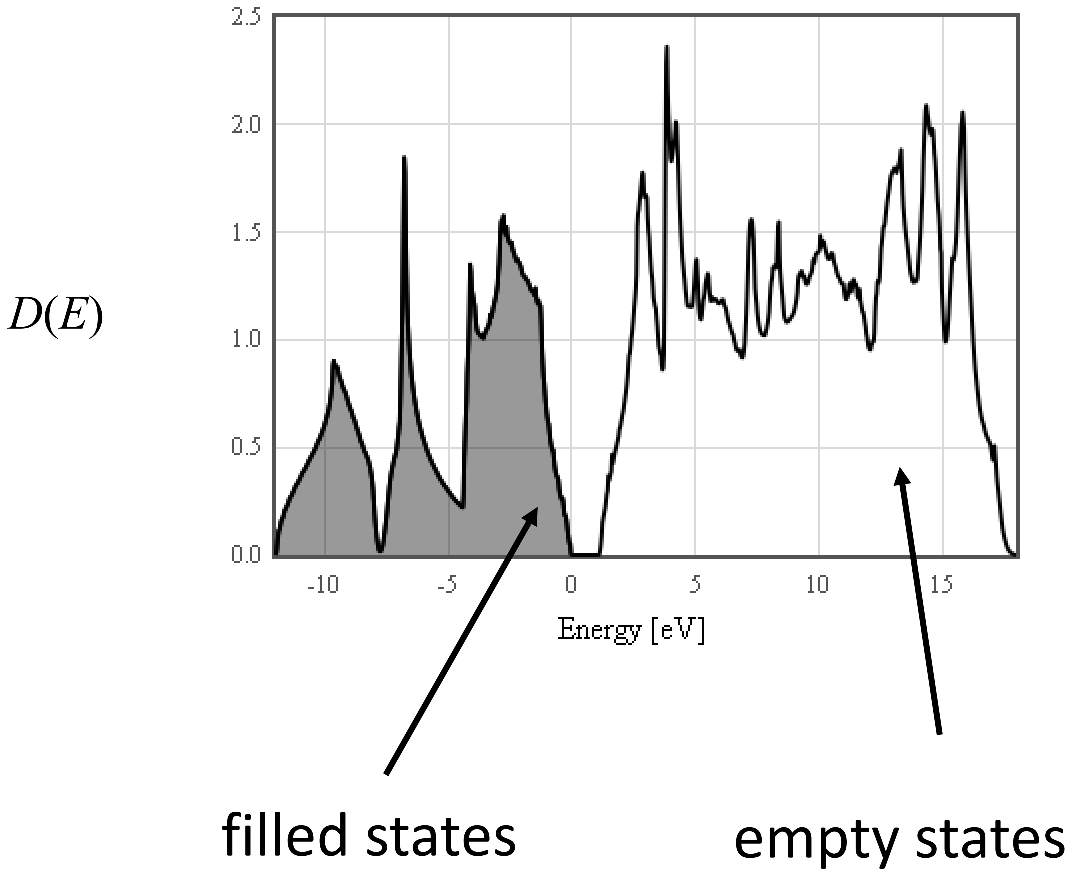
Germanium



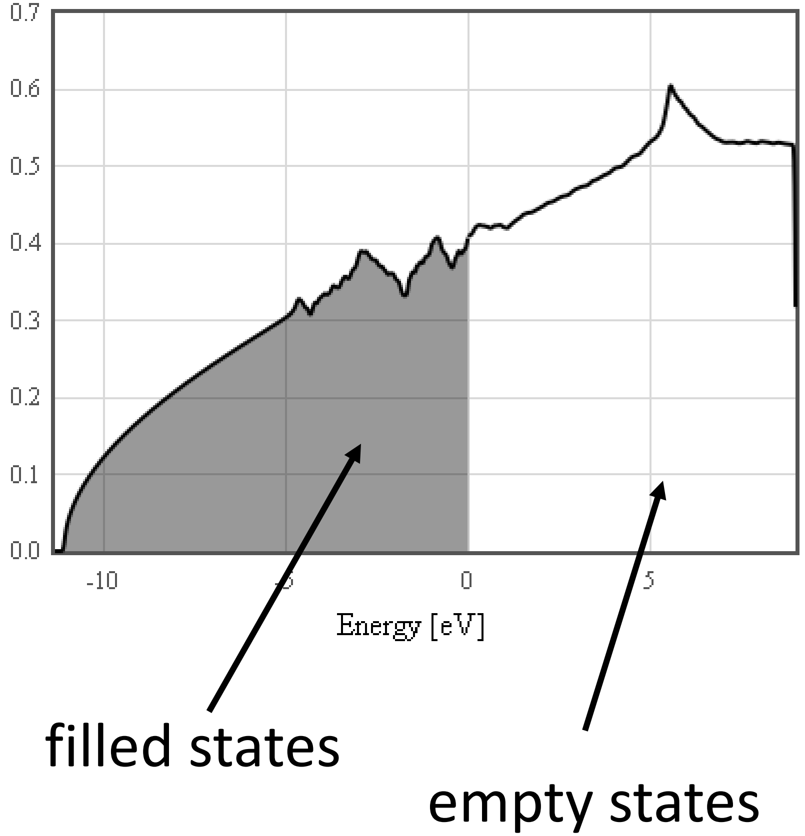
from Ibach & Lueth

Density of states

Silicon



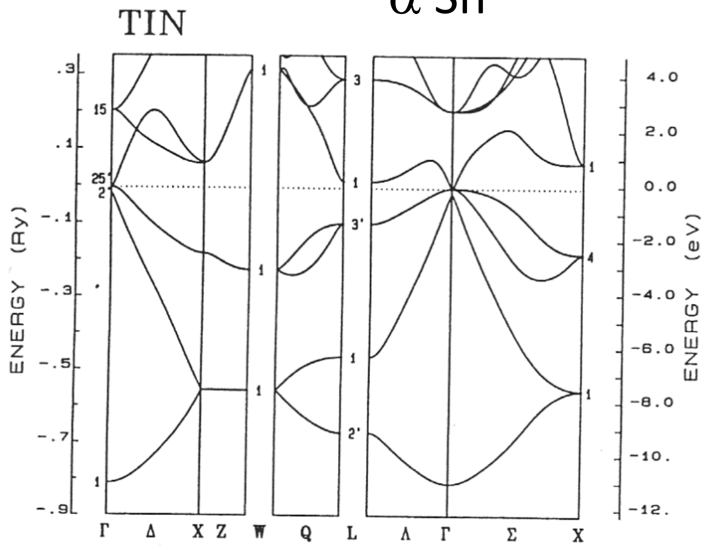
Aluminum

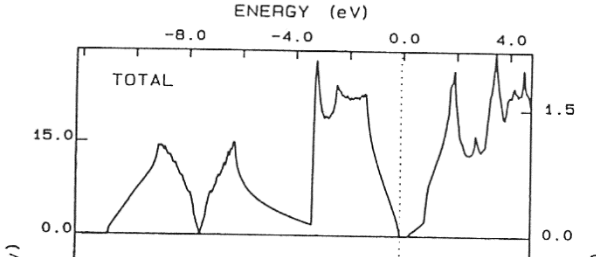


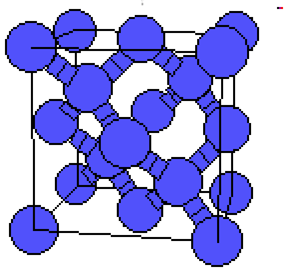
Structural phase transition in Sn

α Sn

transition at 13 C

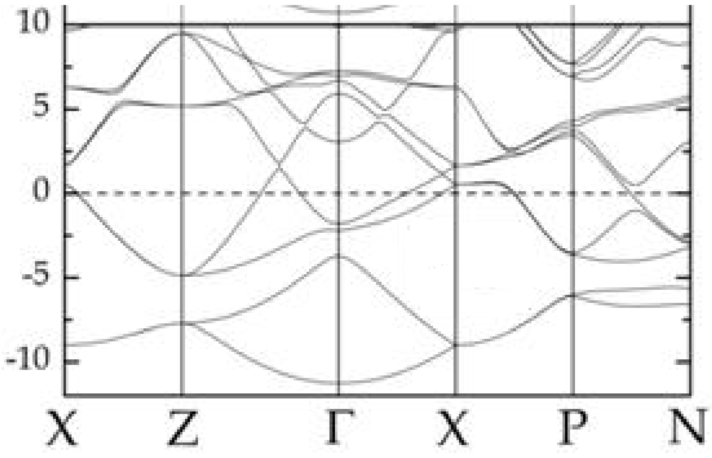


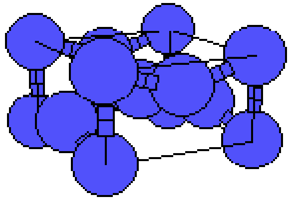




α-Sn, gray tin, diamond structure

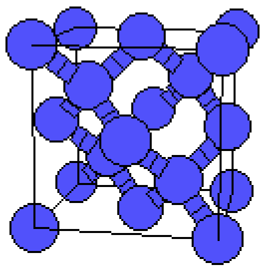
metal β Sn



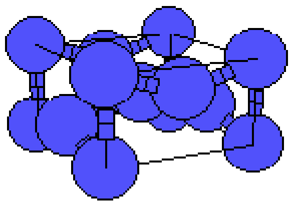


β-Sn, white tin, tetragonal

Structural phase transitions

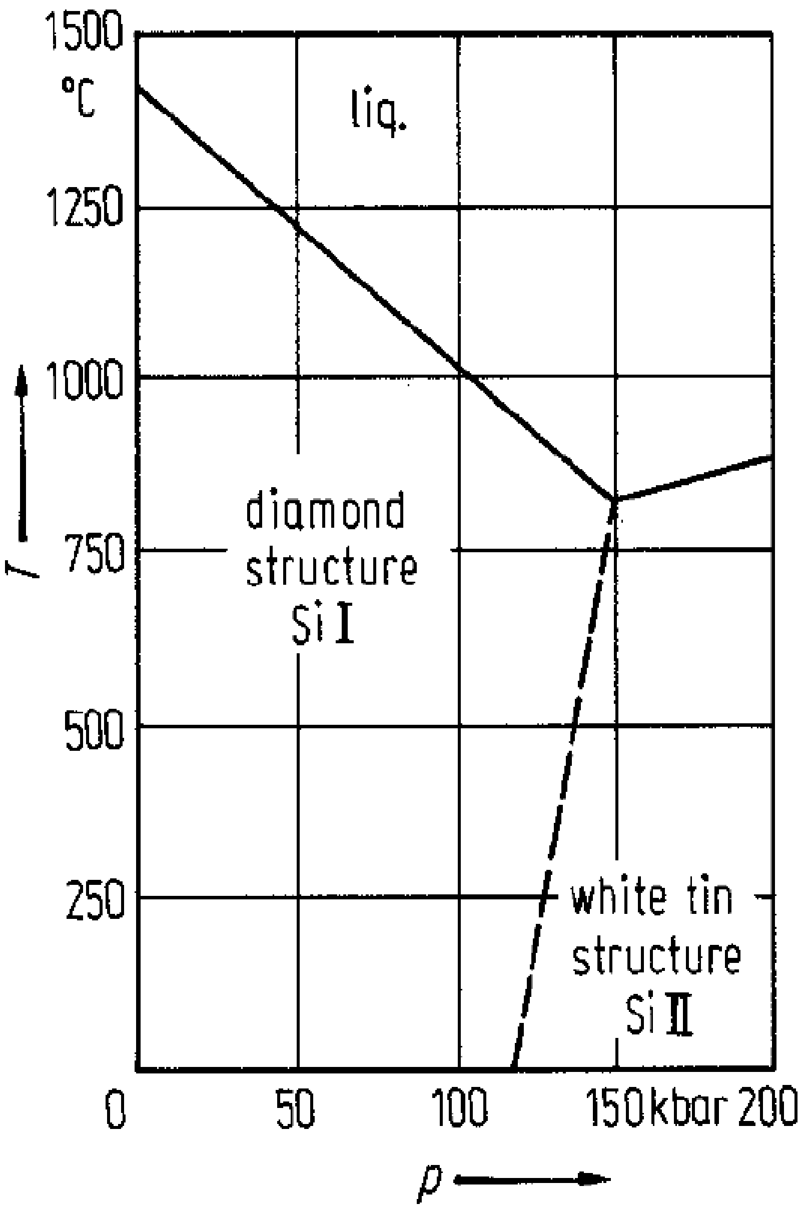


Si, diamond structure



Si II, β-Sn, tetragonal

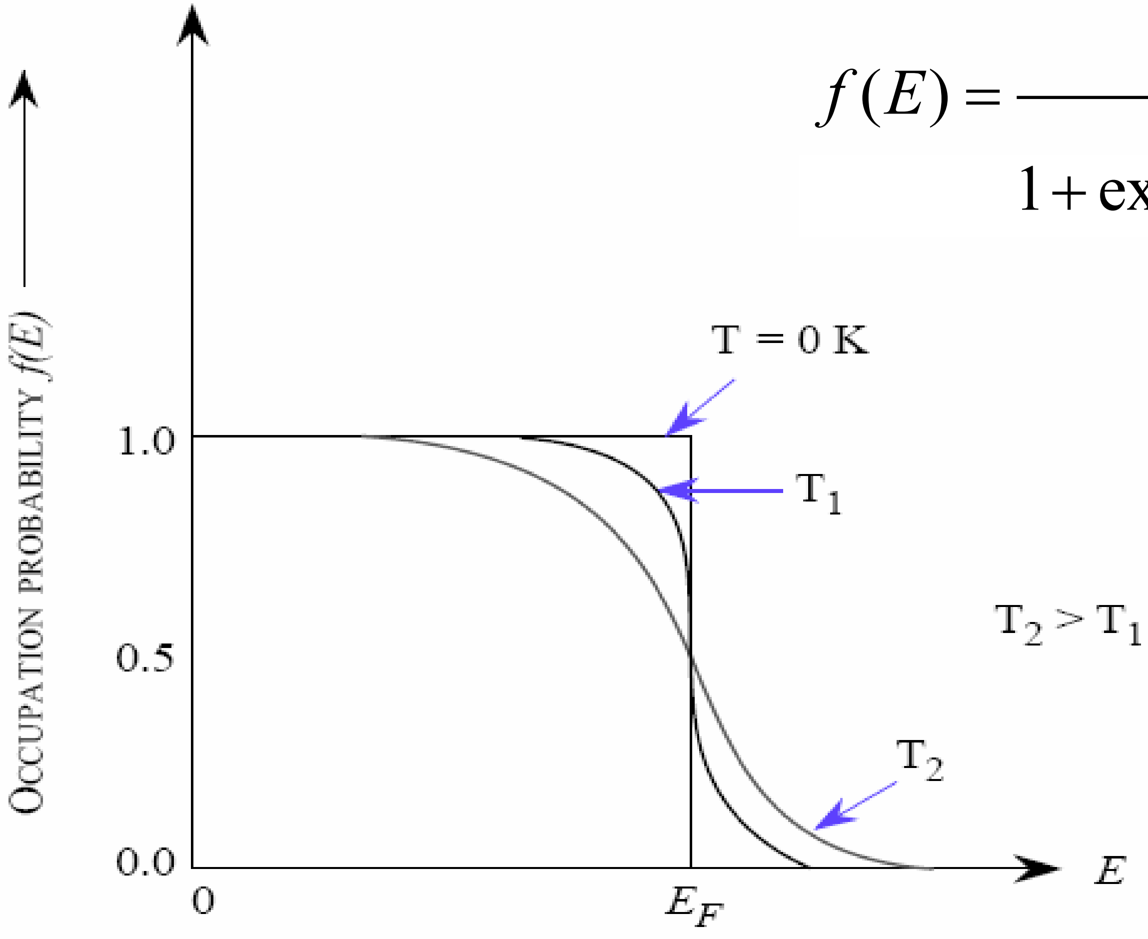
silicon makes a diamond to β-Sn transition <u>under pressure</u>



Fermi function

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

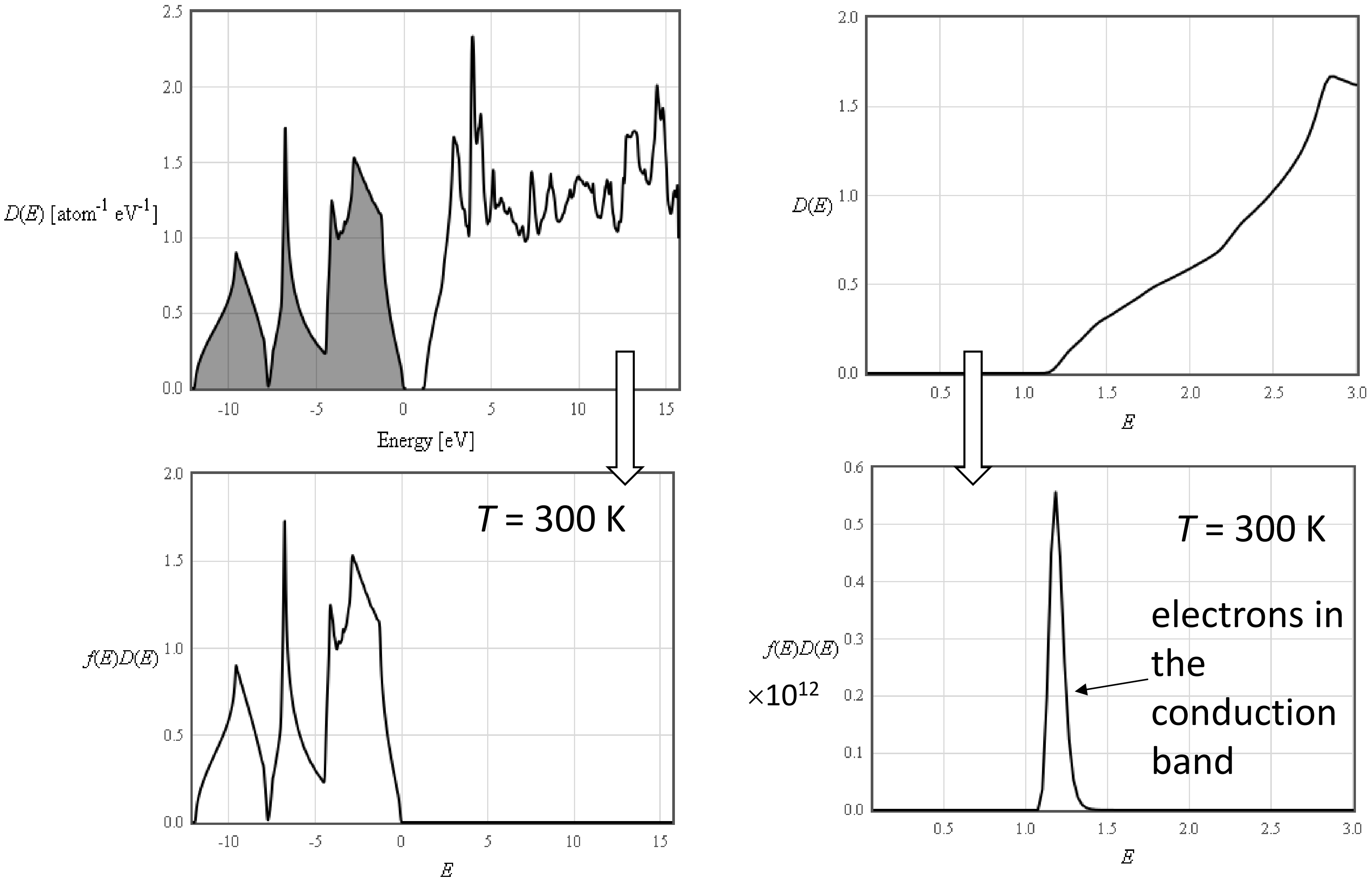
$$f(E) = \frac{1}{1 + \exp\left(\dfrac{E - E_F}{k_B T}\right)}$$



Silicon density of states

density of states

occupation



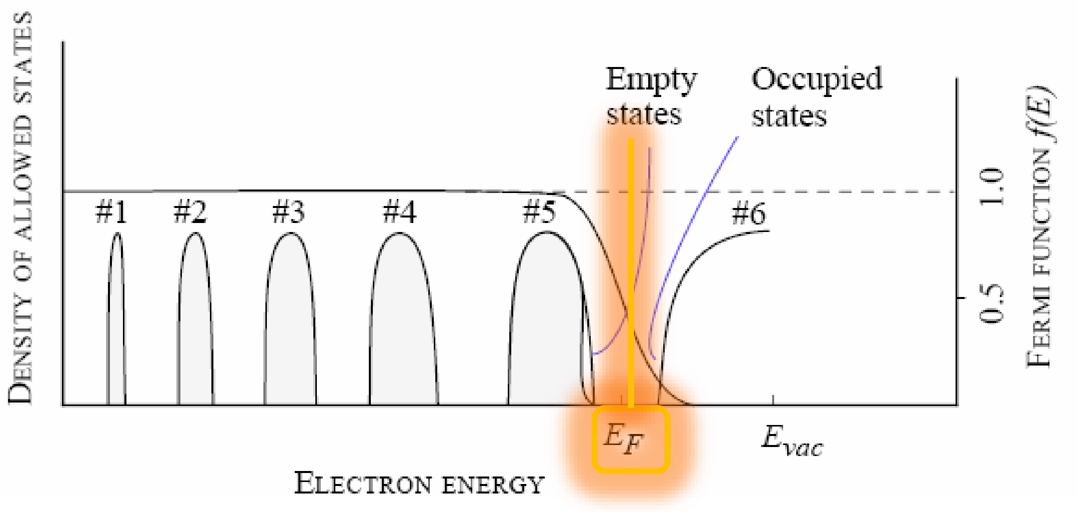
Fermi energy

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

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

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.



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Student: Not logged in

Physics of Semiconductor Devices

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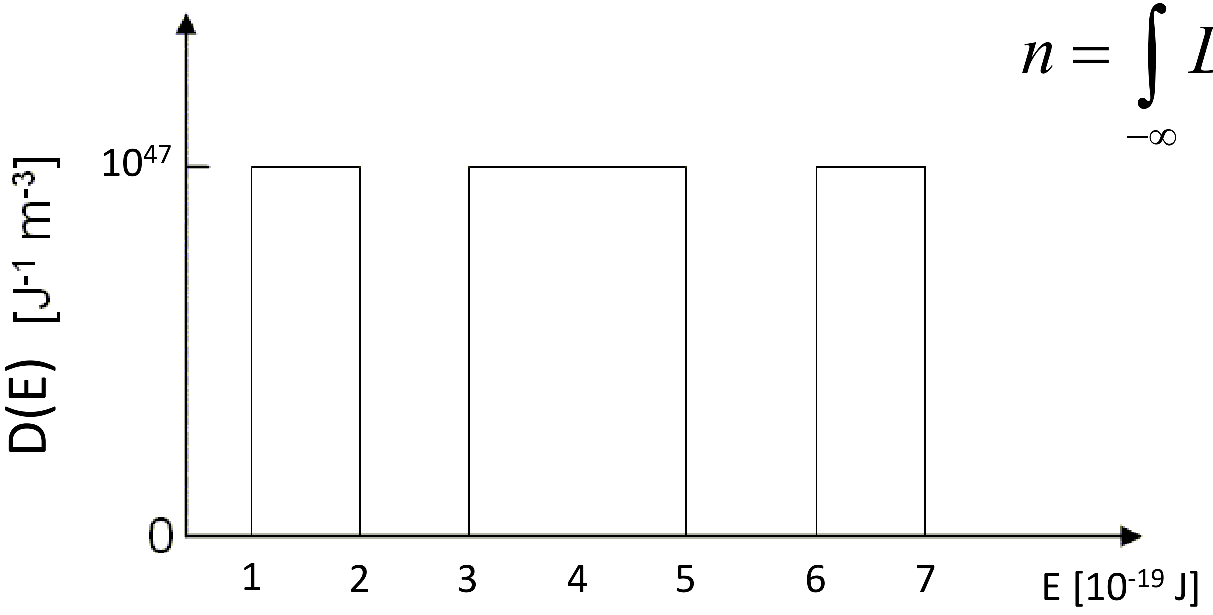
Calculate the Fermi energy

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



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

$n = 3\times10^{28}$ 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