

A SEMI-CONDUCTOR



inspired by
P. Y. Yu & M. Cardona,
Fundamentals of Semiconductors

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Semiconductor Crystals

Physics of semiconductor devices

Karin Zojer

October 14, 2026

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

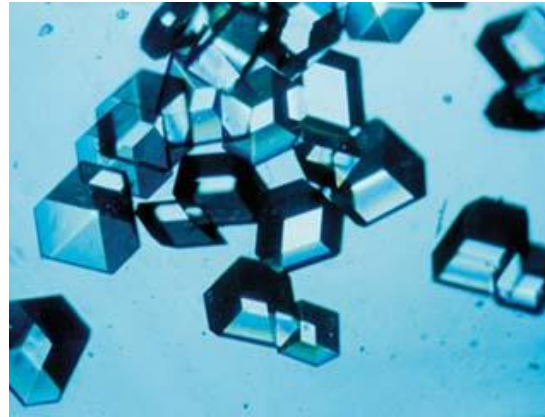


quartz

Crystal Structure

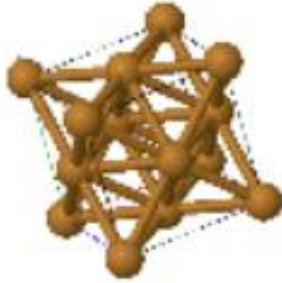


protein crystals



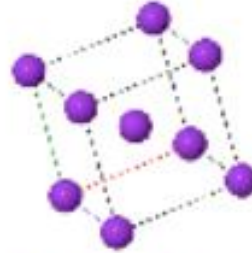
insulin crystals

Crystal Structures



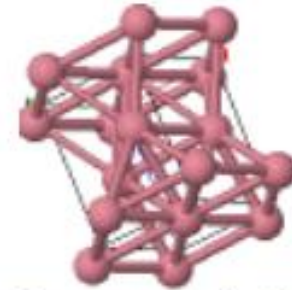
Face Centered
Cubic

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



Body Centered
Cubic

W, Cr, Fe, Mo, Ta



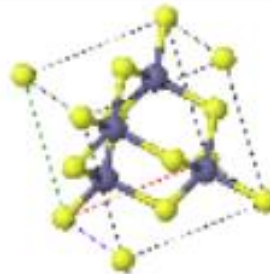
Hexagonal Close
Packed

Ti, Co, Zn, Zr



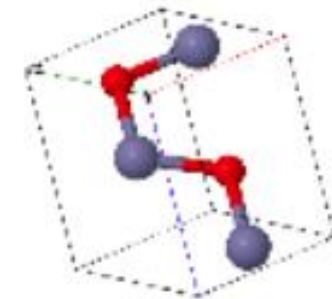
Diamond

C, Si, Ge, α -Sn



Zincblende

GaAs, InP, GaP, InAs,
AlAs



Wurtzite

ZnO, GaN, AlN, CdSe

Miller indices: Crystal planes

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

lattice vectors

always use integers for h, k, l

$[\]$... specific **direction**

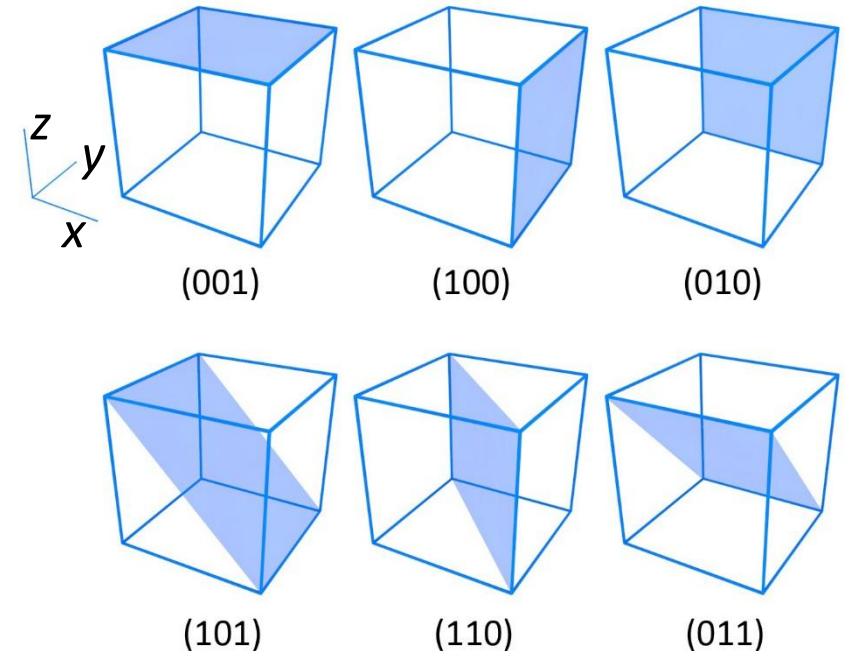
$\langle \rangle$... family of equivalent **directions**

$(\)$... specific plane

$\{ \}$... family of equivalent planes



MOSFETs are made on $\{100\}$ wafers



silicon

HM: $P \bar{3} m S$

$a=5.430\text{\AA}$

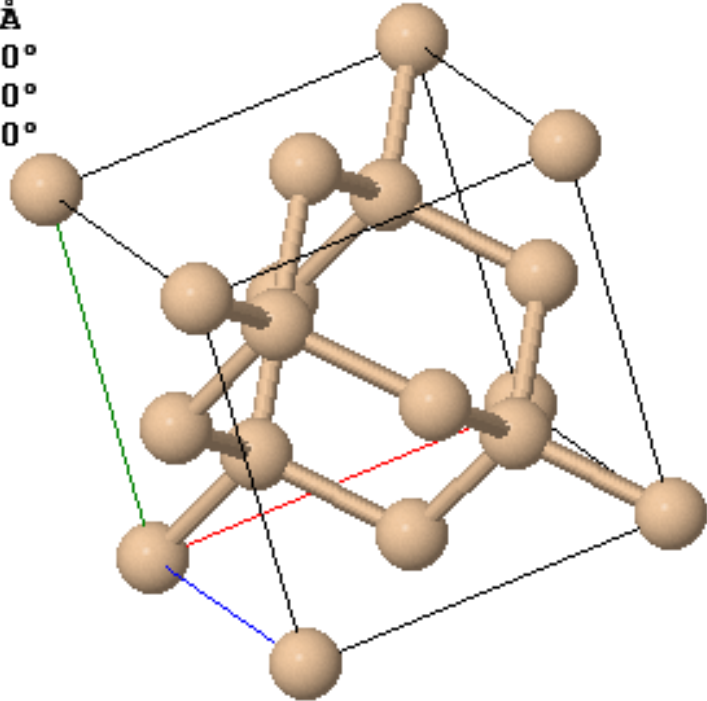
$b=5.430\text{\AA}$

$c=5.430\text{\AA}$

$\alpha=90.000^\circ$

$\beta=90.000^\circ$

$\gamma=90.000^\circ$



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: 1	K: 0	L: 0
show HKL plane	hide HKL plane	
draw atoms in HKL plane		
Thickness of HKL planes:		

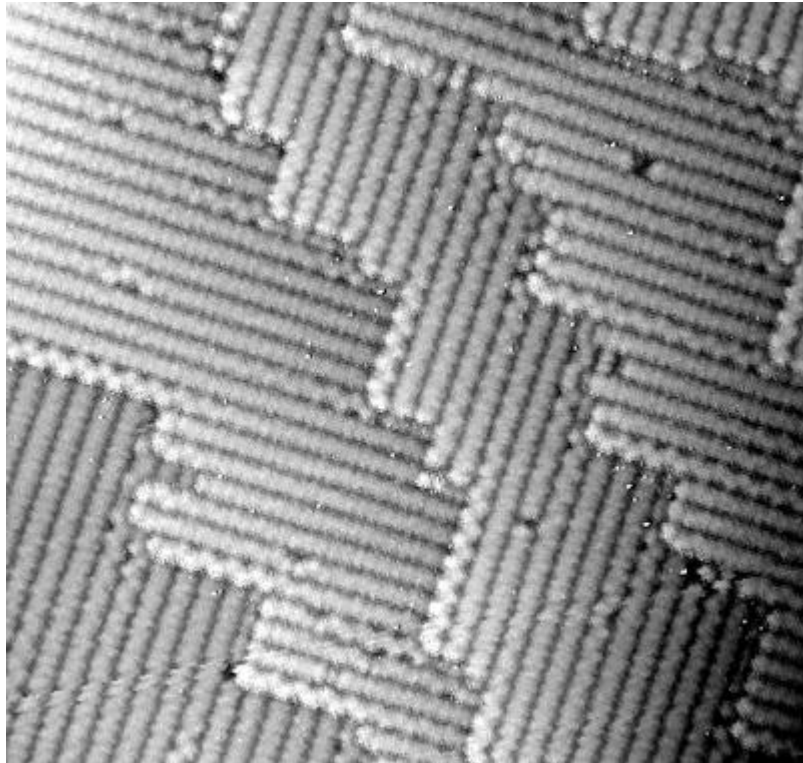
The conventional unit cell is a cube with sides of 0.543 nm. There are 8 atoms in the conventional unit cell. (The image can be rotated with a mouse.)

JSmol

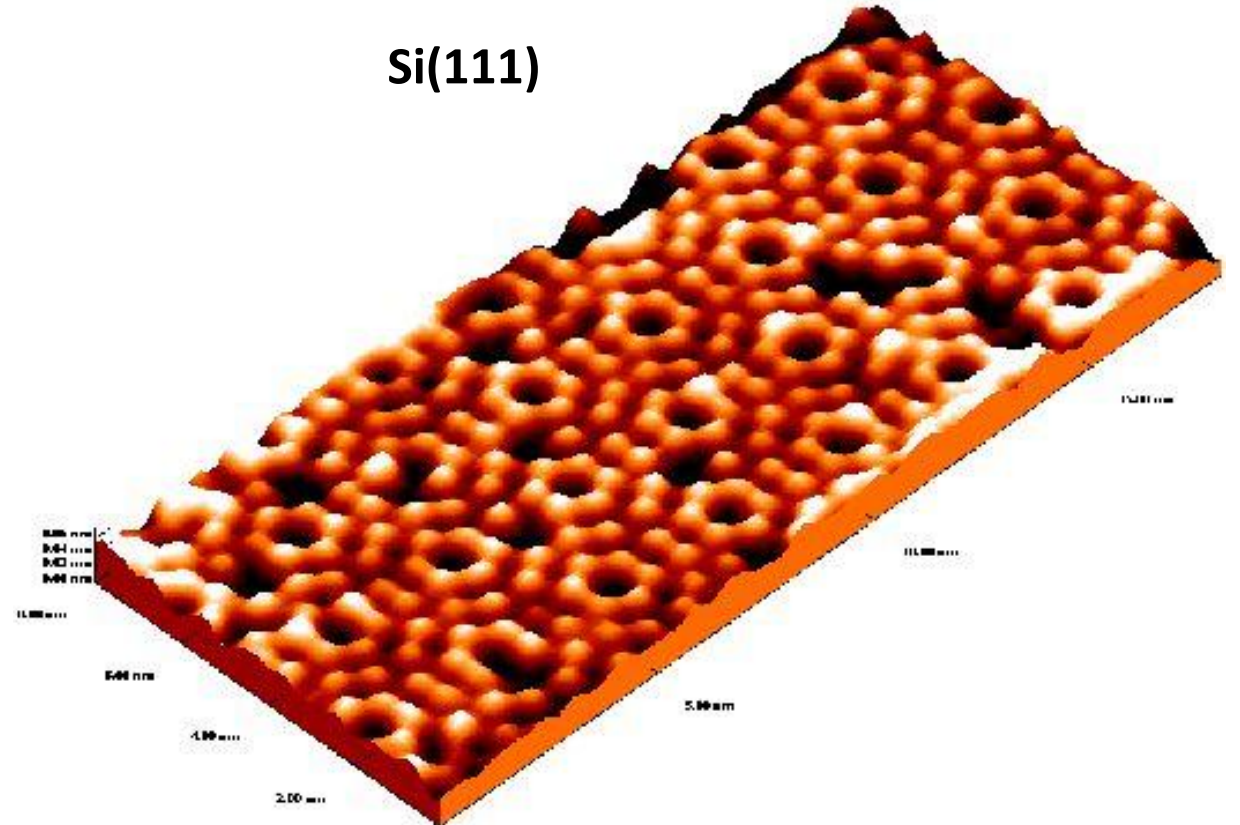
<http://lampz.tugraz.at/~hadley/memm/materials/silicon/silicon.php>

silicon surfaces

Si(100)

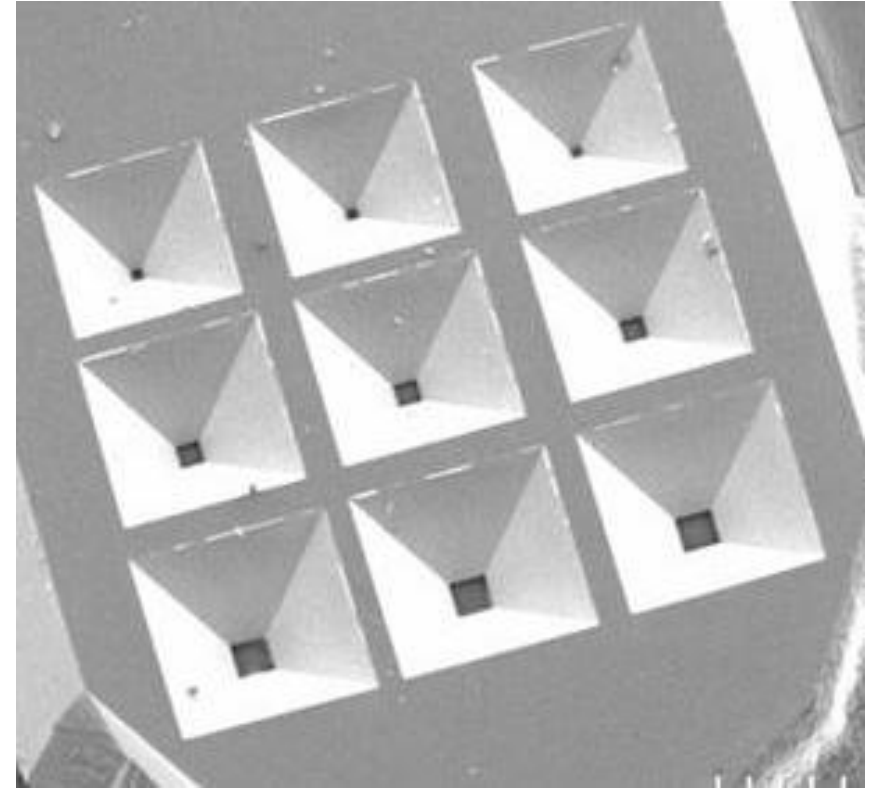


Si(111)



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

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Electrons in crystals

Physics of semiconductor devices

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Electrons

How electrons behave ?

How electrons behave in a crystal?

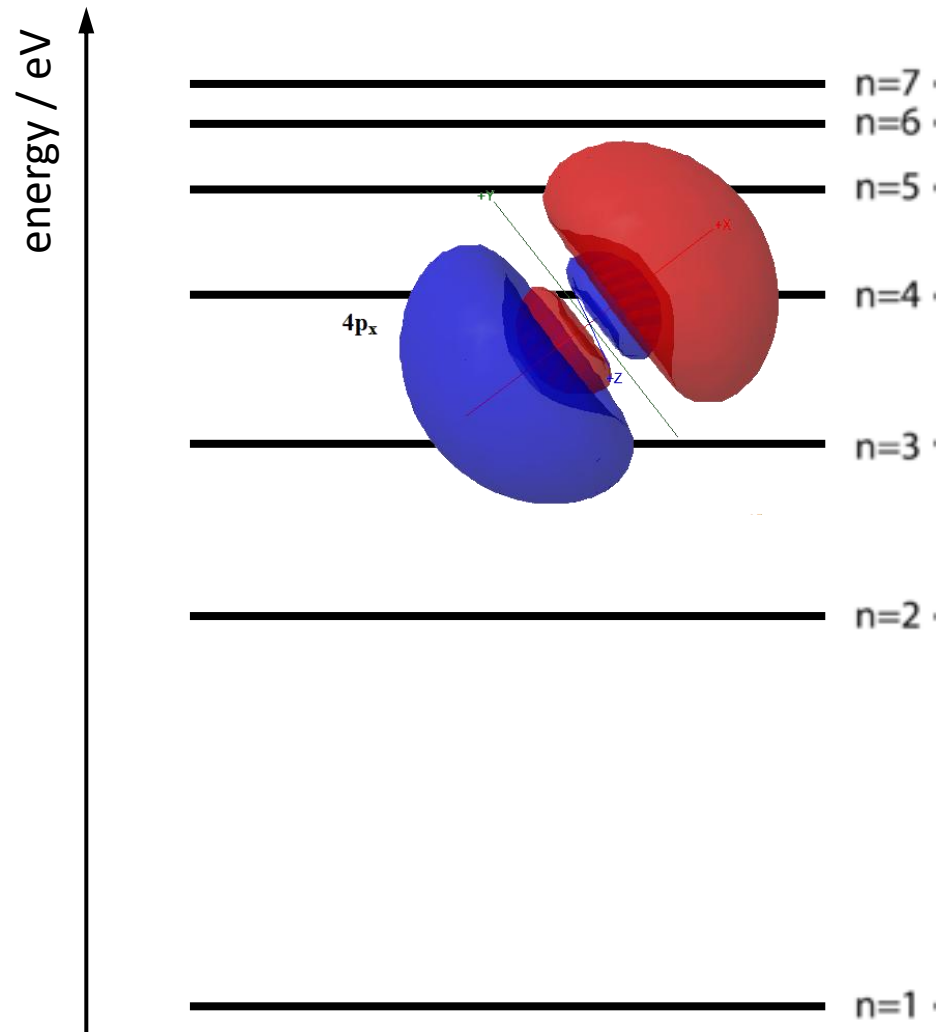
Charge = -1.6022×10^{-19} C

Mass = 9.11×10^{-31} kg

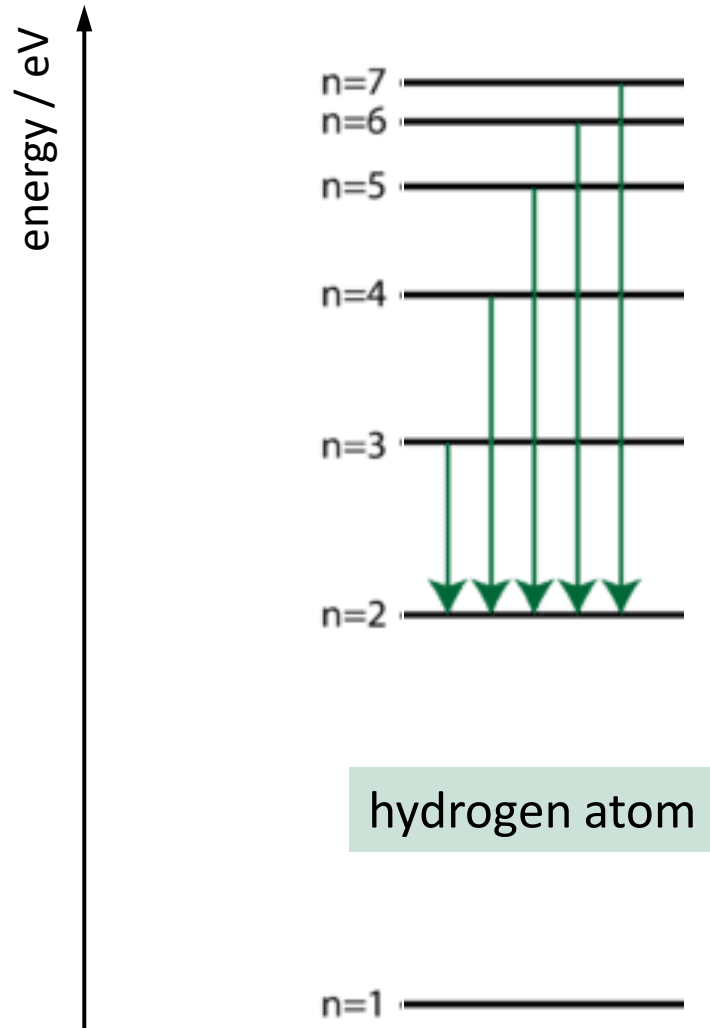
occupied space = ?


0.15 nm

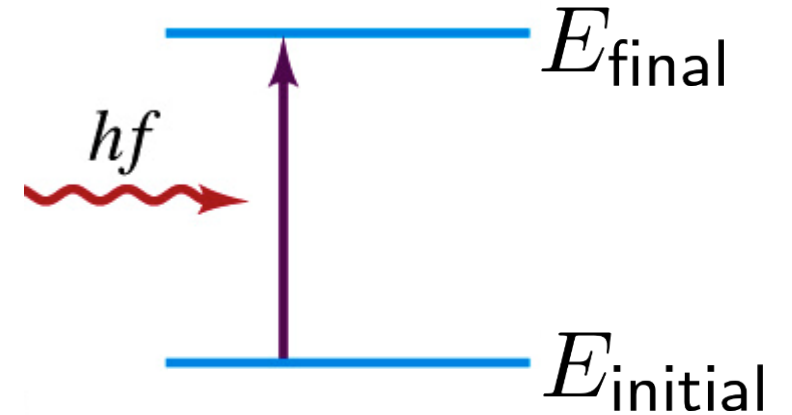
Energy levels in atoms



Energy levels in atoms

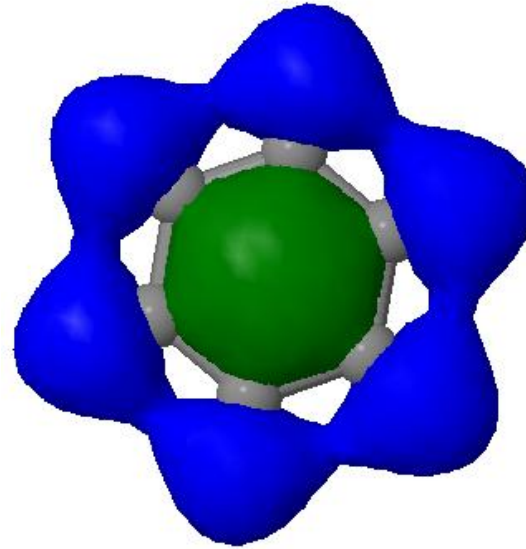
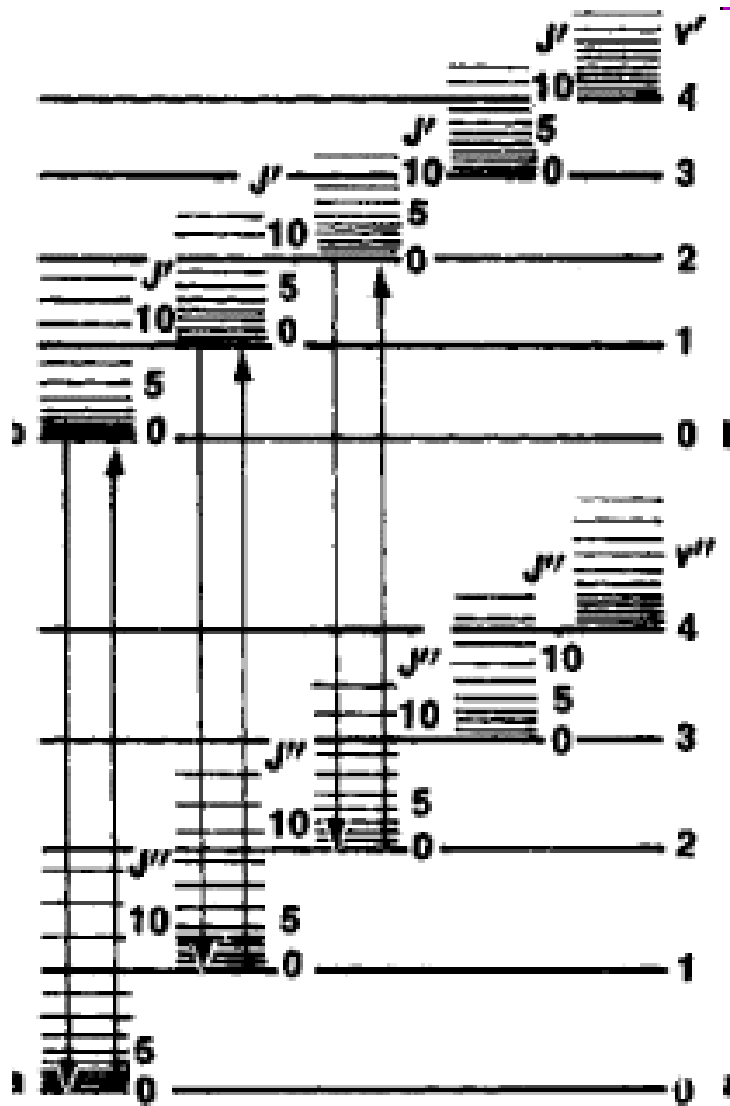


fluorescent lamp

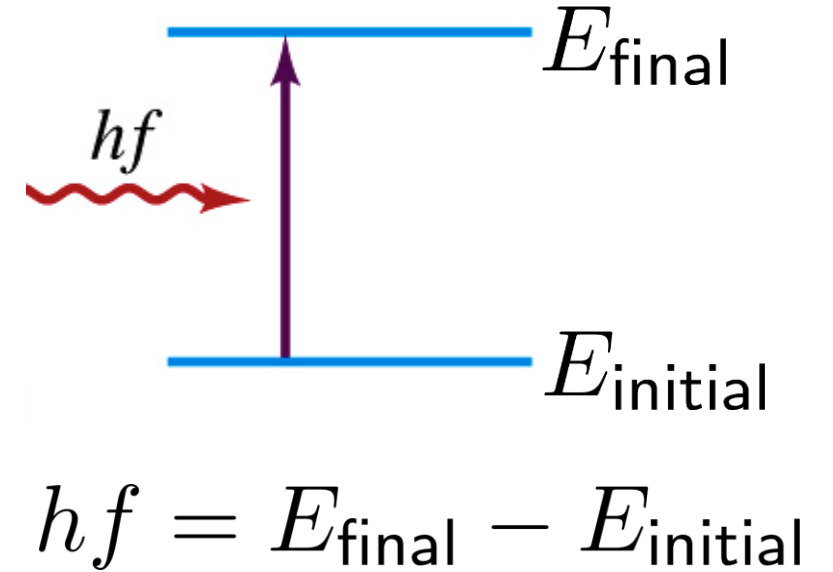


$$hf = E_{\text{final}} - E_{\text{initial}}$$

Molecular levels



valence electrons
spread across
molecule



wave vector k

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

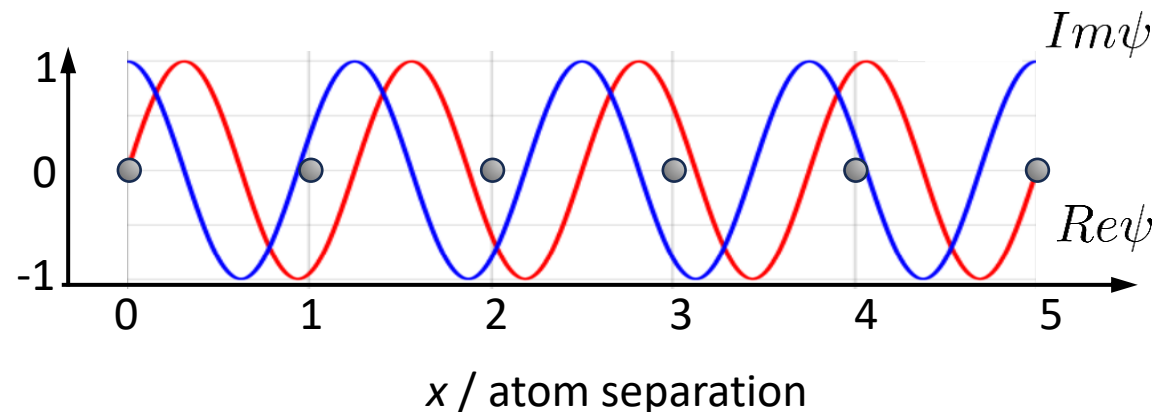
wavelength: $\lambda = \frac{2\pi}{|\vec{k}|}$



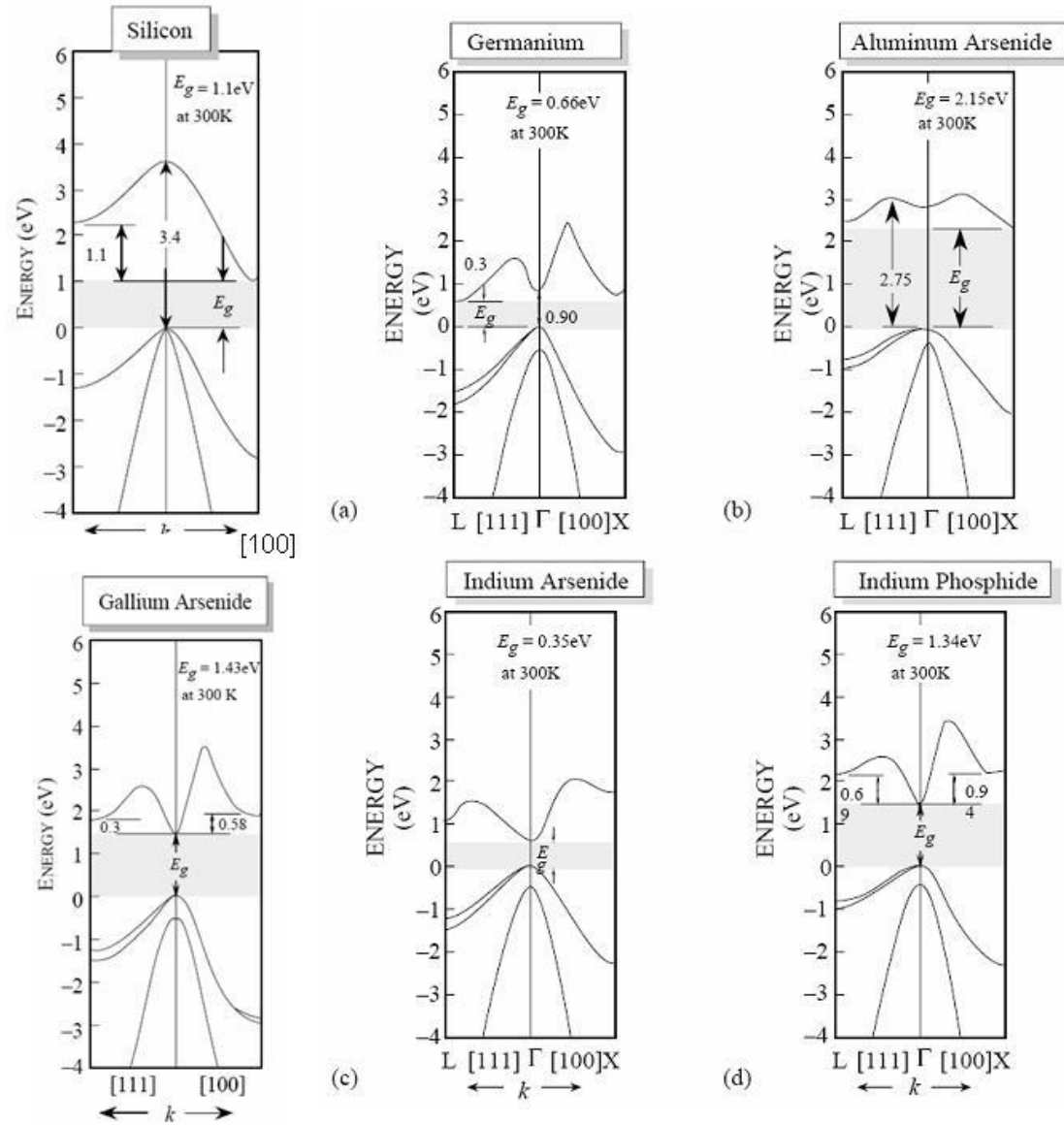
periodicity of the crystal
lattice in that direction

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

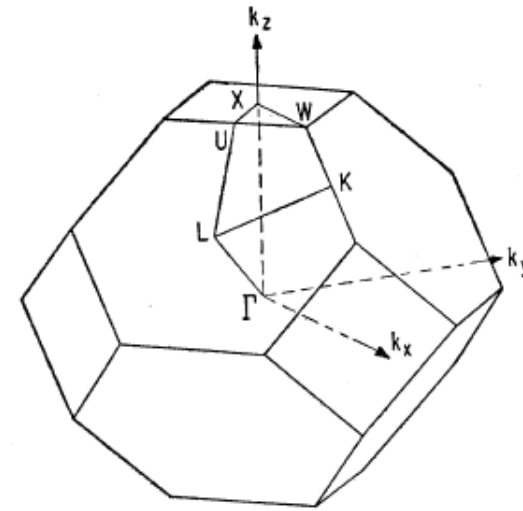
$$\psi = e^{ikx} u_k(x)$$



Semiconductors



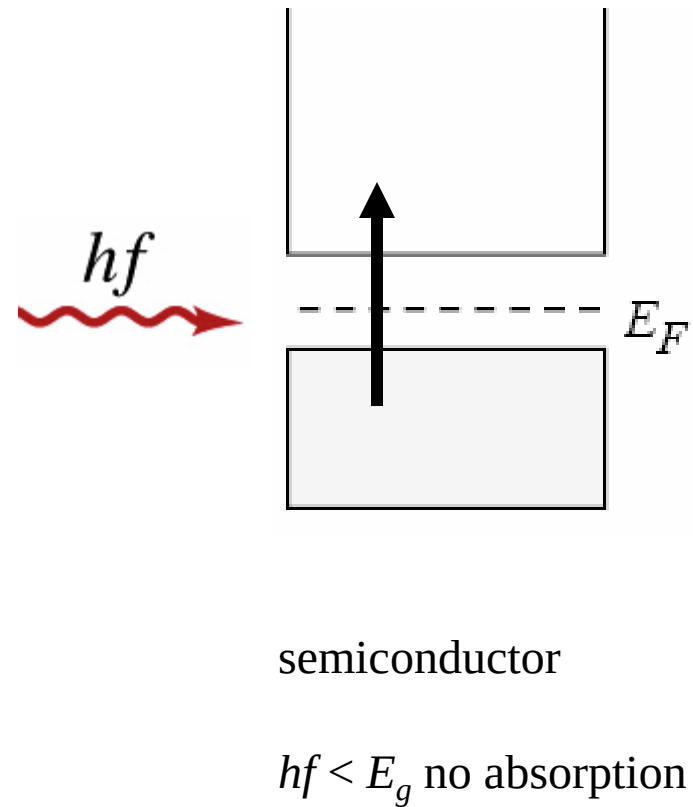
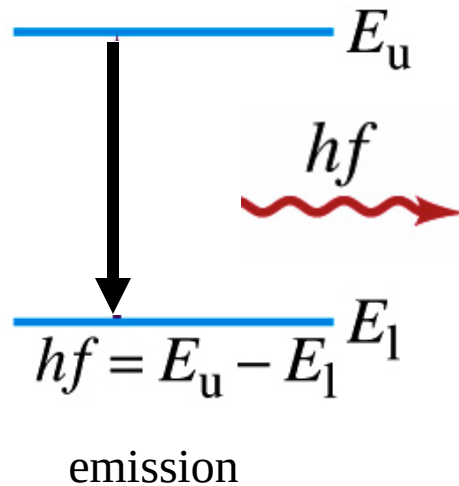
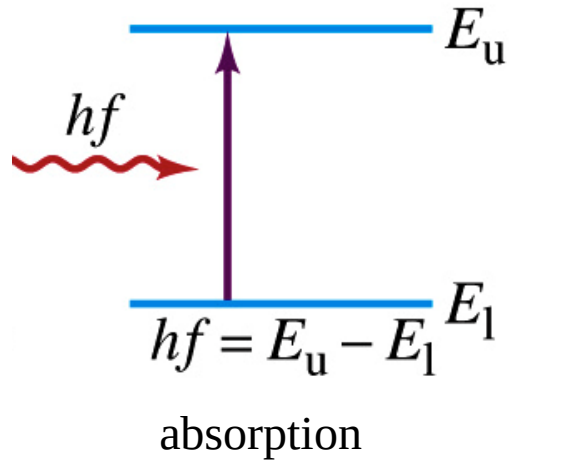
**valence band
conduction band
band gap**



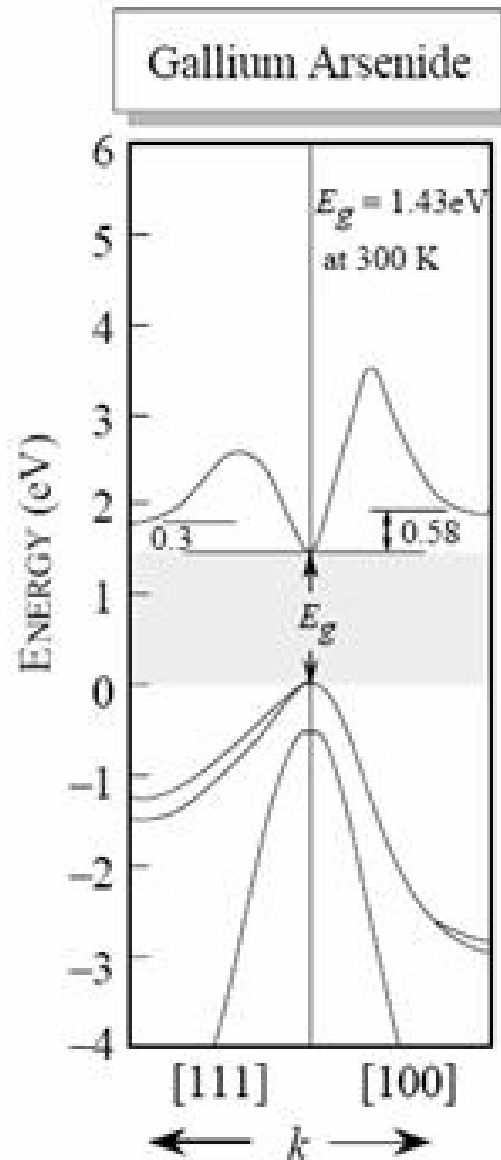
**molecular orbitals
are plane waves**



Absorption and emission of photons



What color light does a GaAs LED emit?



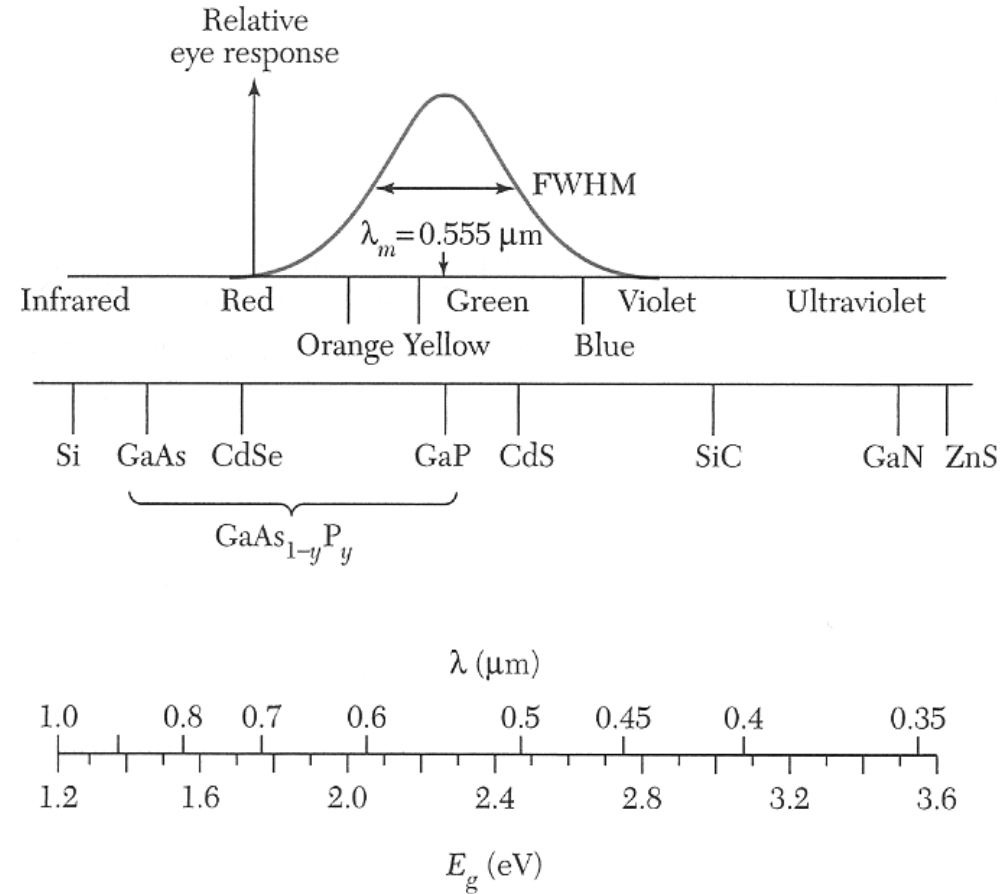
$$E = 1.6022 \times 10^{-19} \times 1.43 \text{ J} = hf = \frac{hc}{\lambda}$$

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

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
$\text{Ga}_x\text{In}_{1-x}\text{As}_{1-y}\text{P}_y$	1100-1600
$\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$	1550
$\text{Ga}_{0.27}\text{In}_{0.73}\text{As}_{0.63}\text{P}_{0.37}$	1300
GaAs:Er, InP:Er	1540
Si:C	1300
GaAs:Yb, InP:Yb	1000
$\text{Al}_x\text{Ga}_{1-x}\text{As:Si}$	650-940
GaAs:Si	940
$\text{Al}_{0.11}\text{Ga}_{0.89}\text{As:Si}$	830
$\text{Al}_{0.4}\text{Ga}_{0.6}\text{As:Si}$	650
$\text{GaAs}_{0.6}\text{P}_{0.4}$	660
$\text{GaAs}_{0.4}\text{P}_{0.6}$	620
$\text{GaAs}_{0.15}\text{P}_{0.85}$	590
$(\text{Al}_x\text{Ga}_{1-x})_{0.5}\text{In}_{0.5}\text{P}$	655
GaP	690
GaP:N	550-570
$\text{Ga}_x\text{In}_{1-x}\text{N}$	340,430,590
SiC	400-460
BN	260,310,490

light emitting diodes

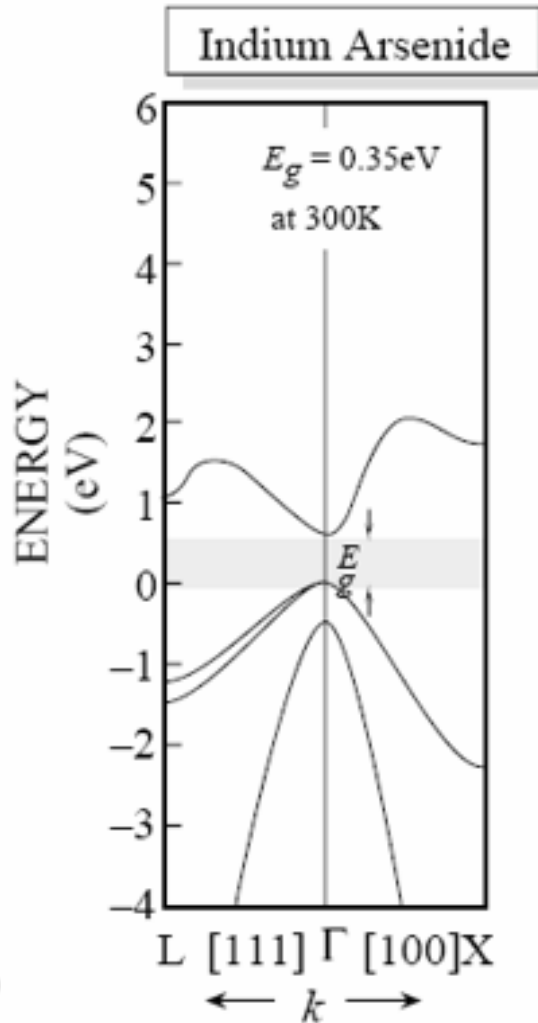


direct and indirect band gaps

direct bandgap:

$$\Delta k = 0$$

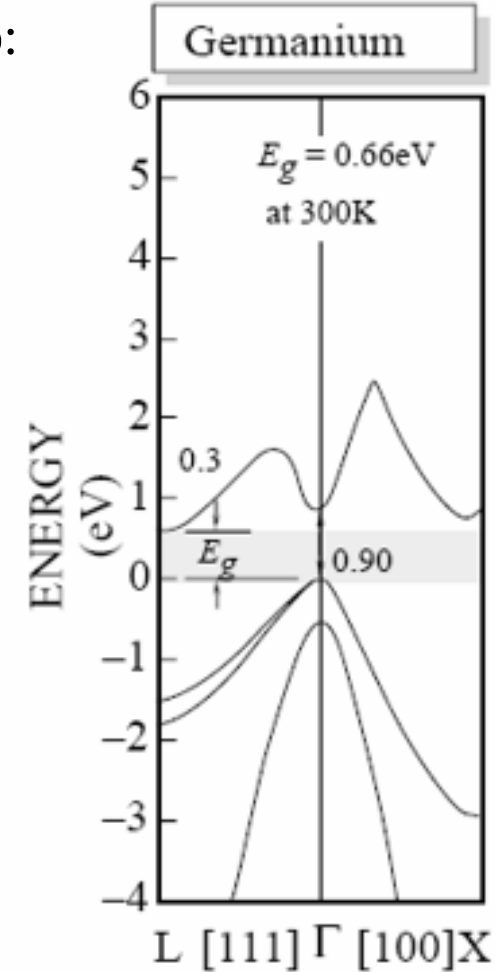
photons can be emitted



indirect bandgap:

$$\Delta k \neq 0$$

phonons are emitted



Momentum must be conserved when photons are absorbed or emitted.

3

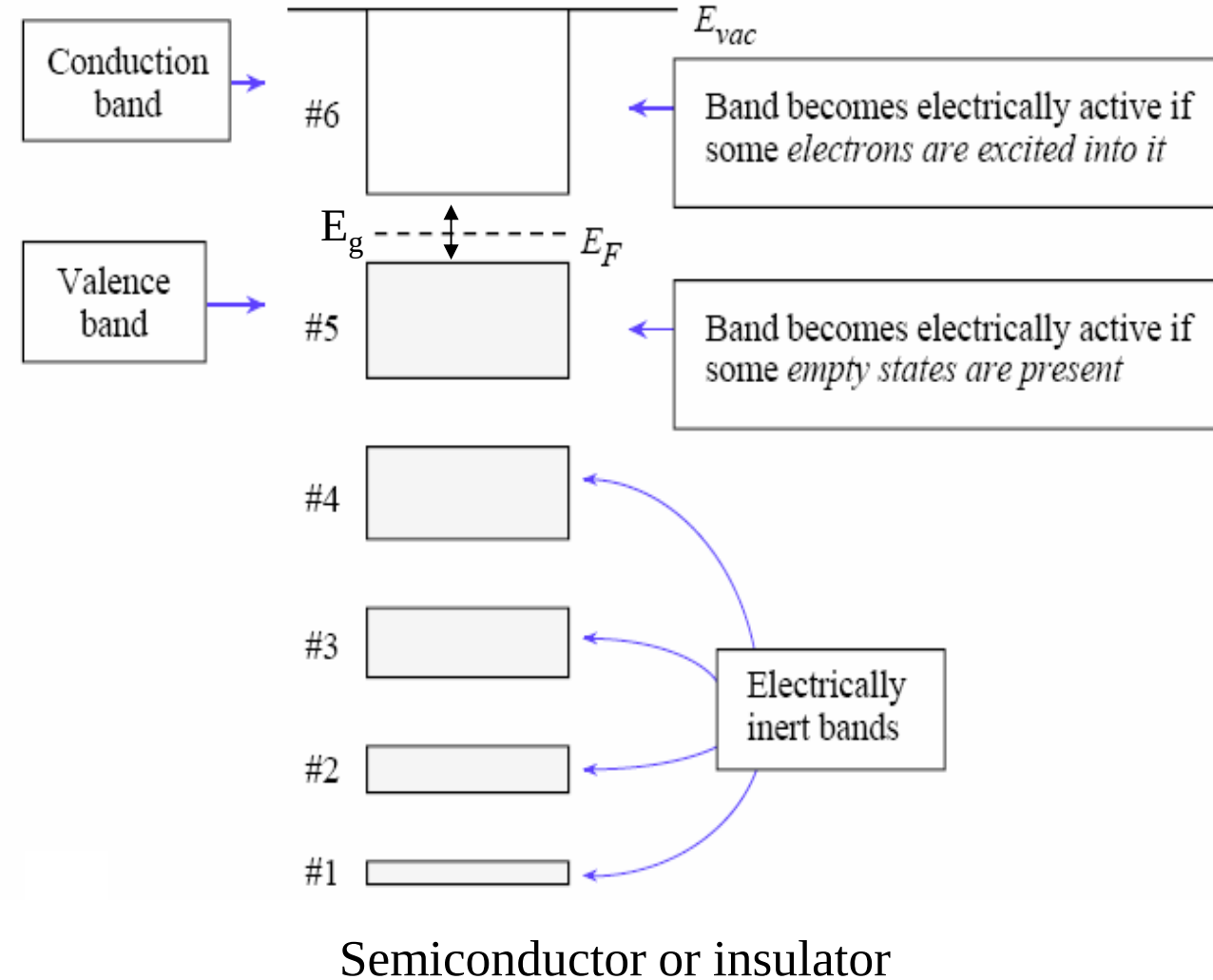
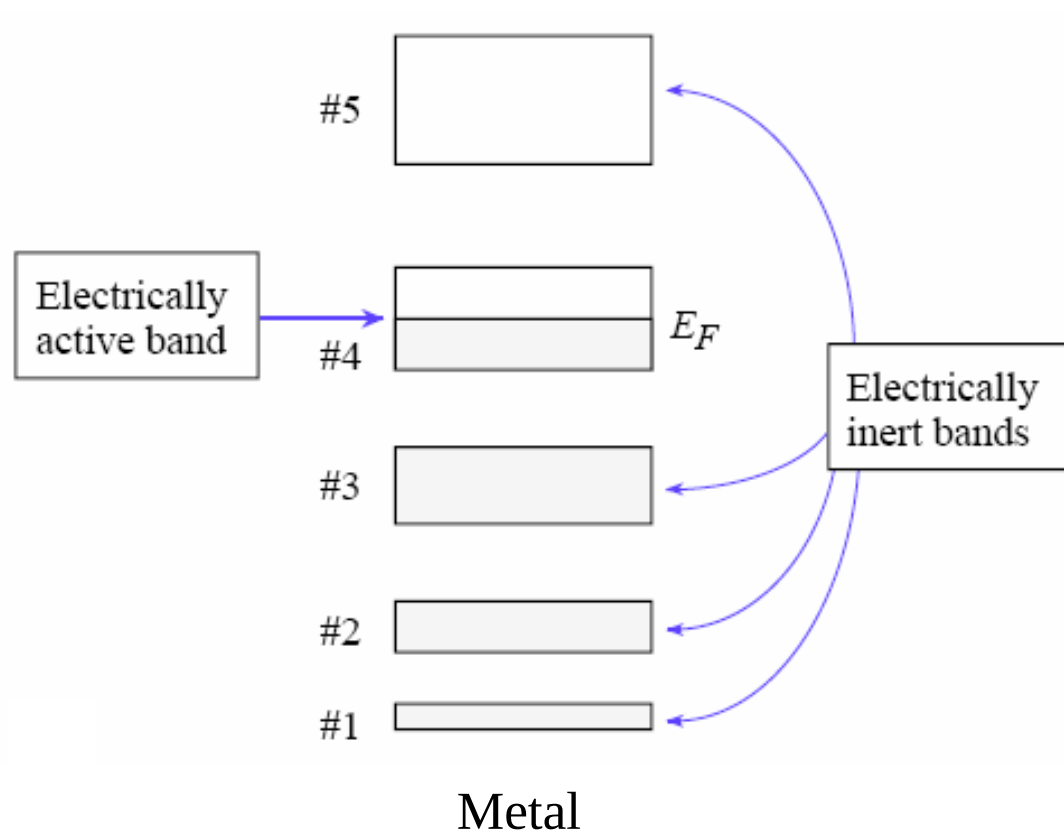
Electrons in crystals (part 2)

Physics of semiconductor devices

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Metals, semiconductors, insulators

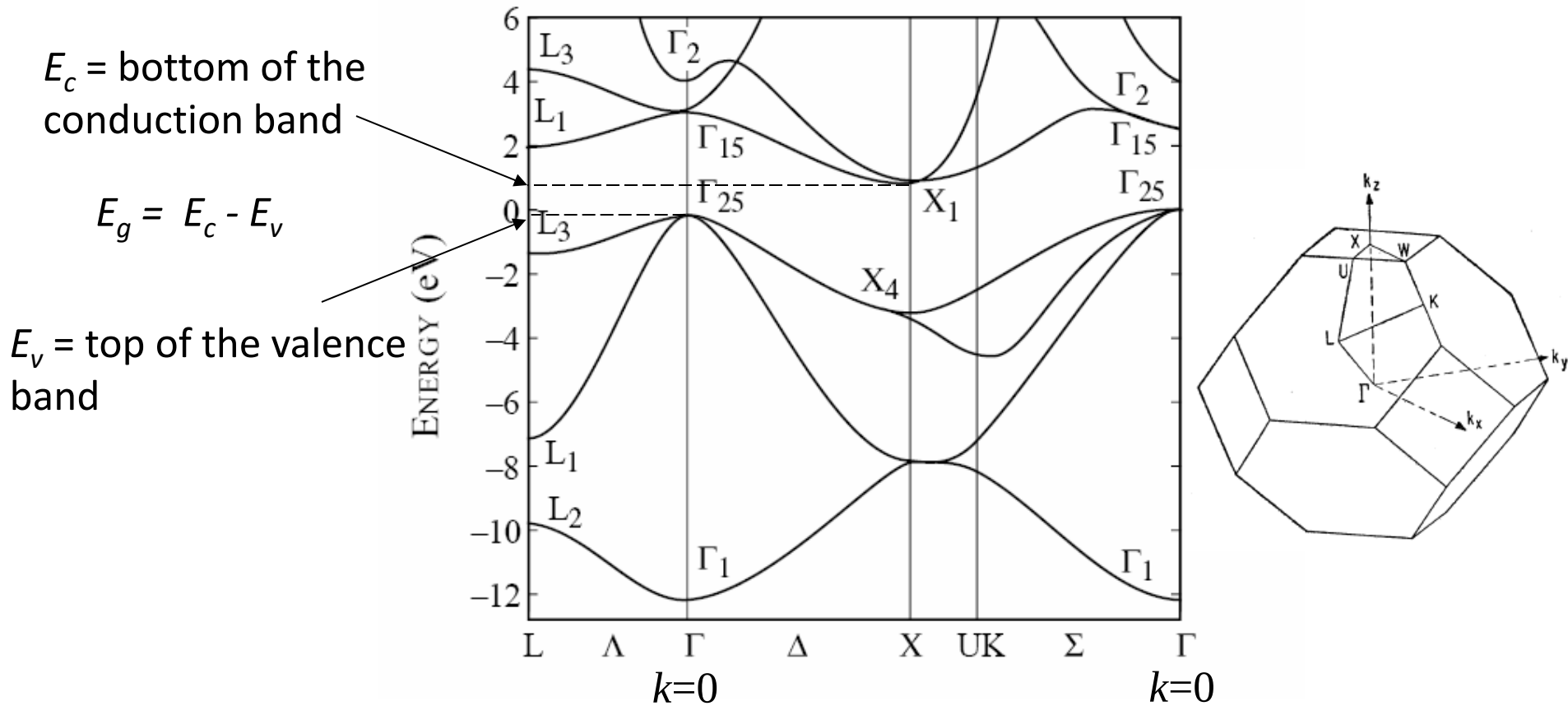


from: Singh

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

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

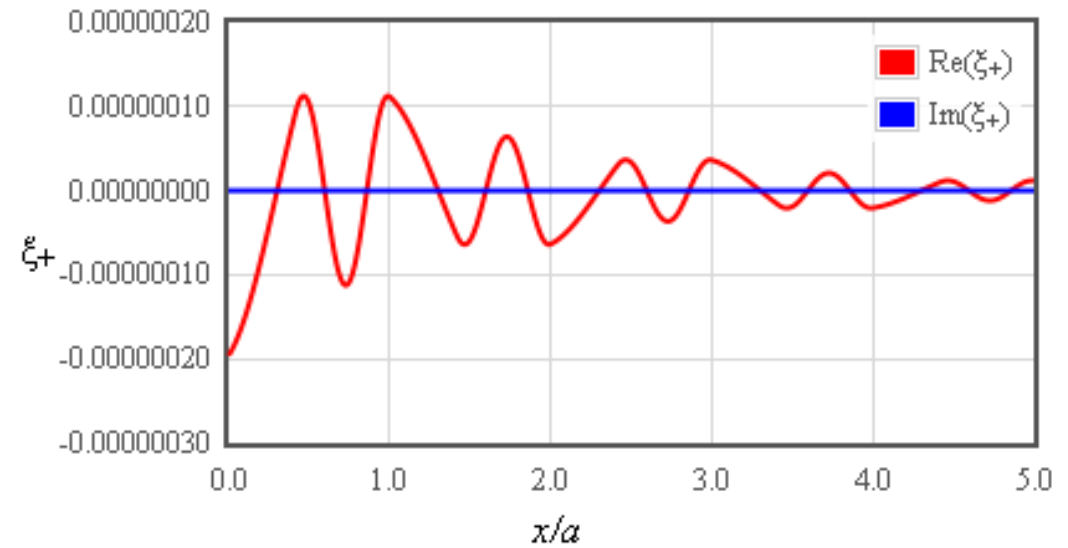
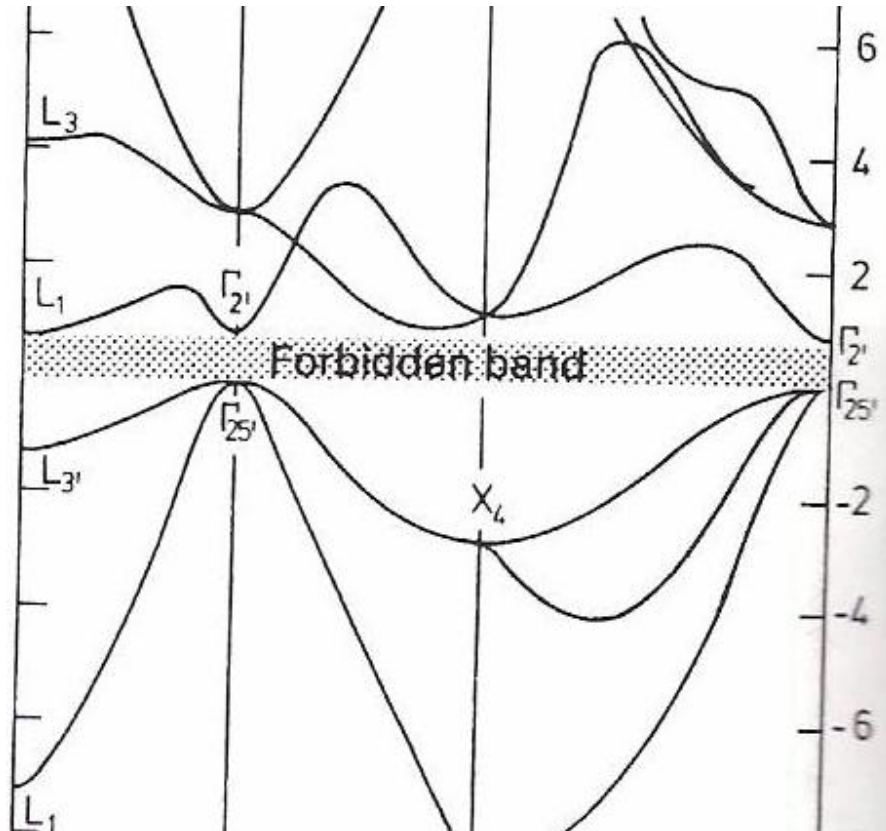
Silicon band structure



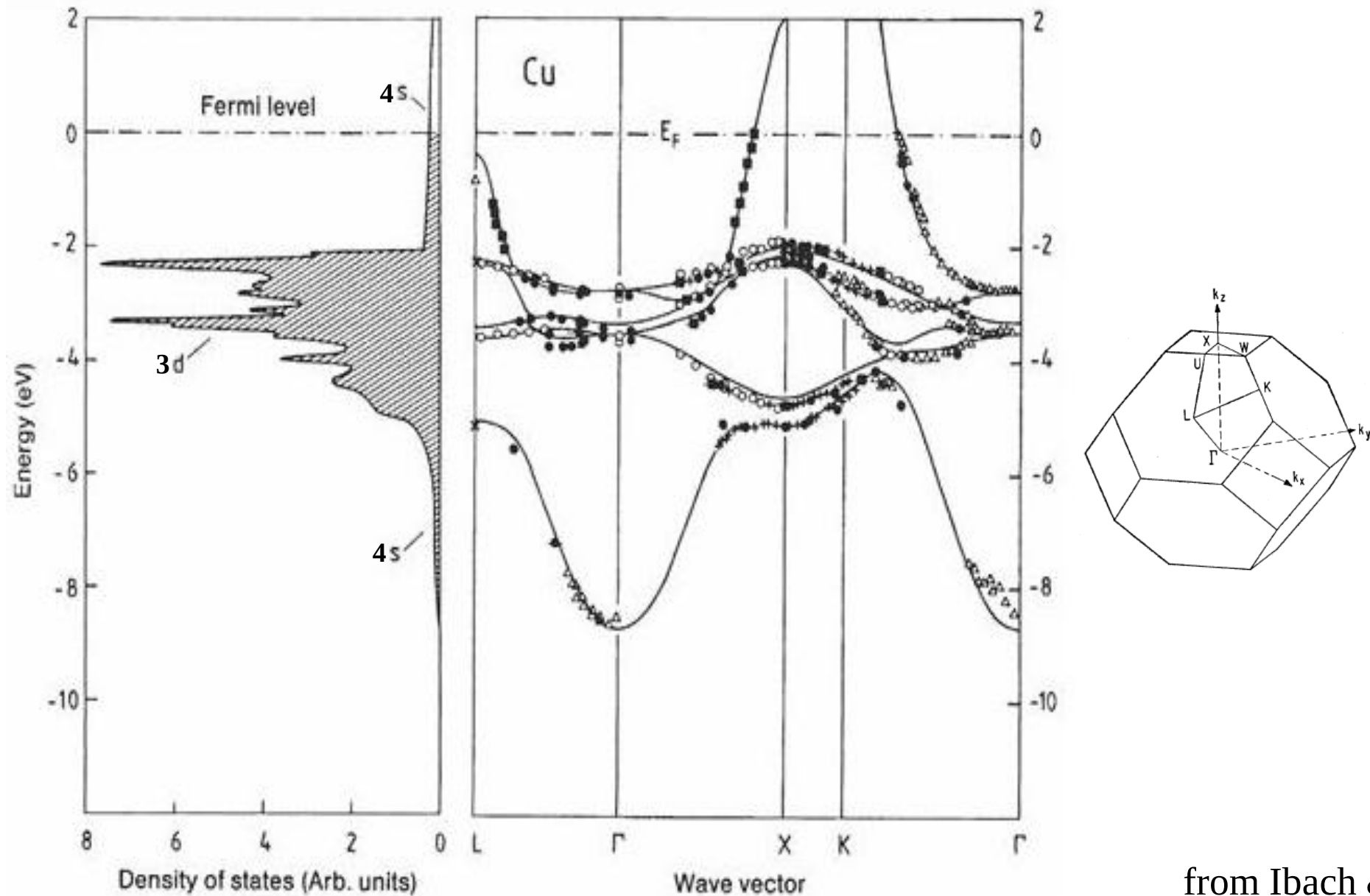
Electrons with energies in the gap are reflected out of the crystal.

Band gap

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

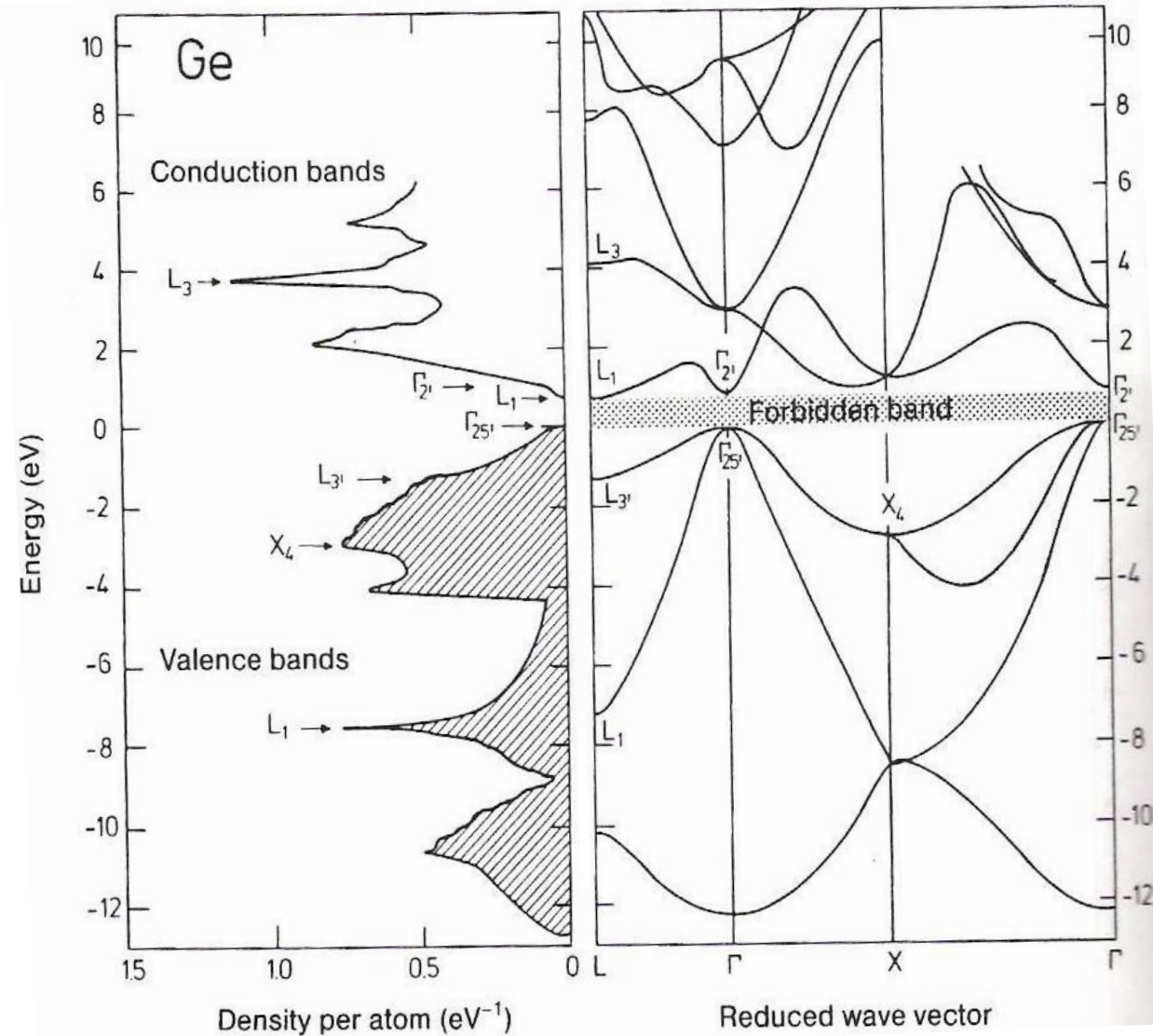


Copper: dispersion relation and density of states



from Ibach & Lueth

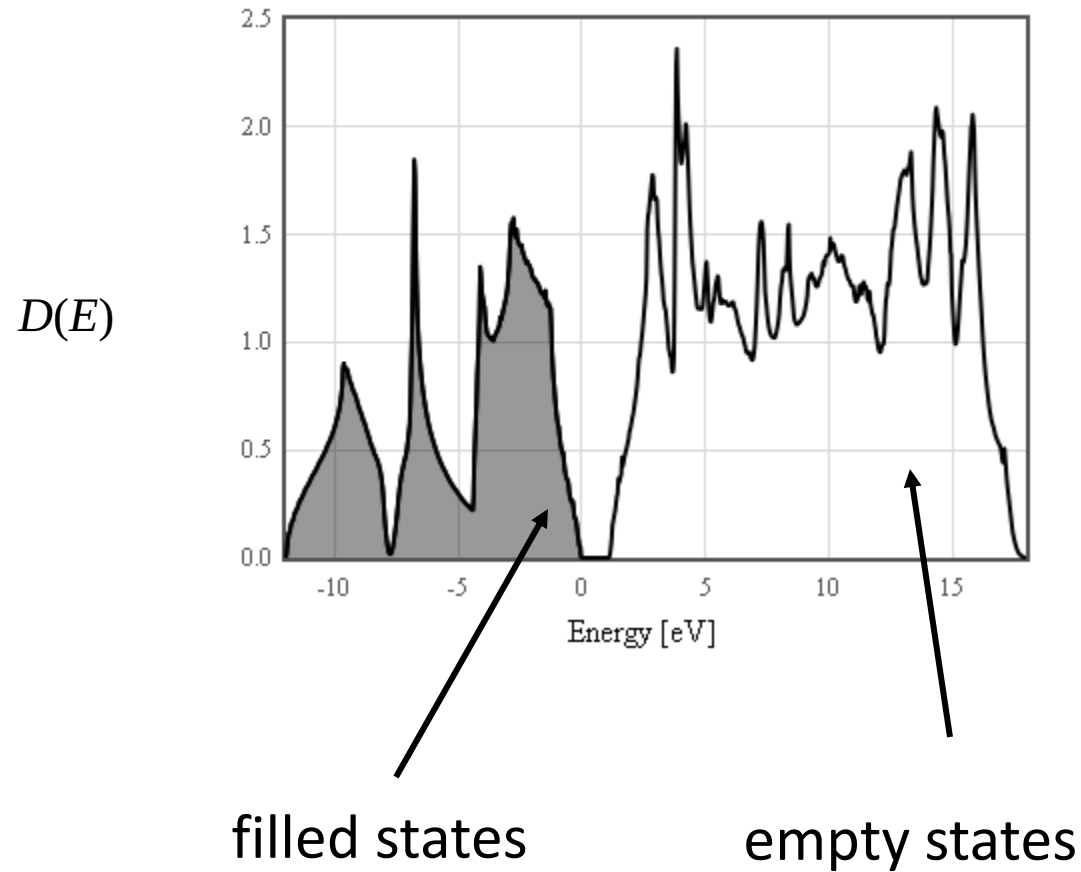
Germanium



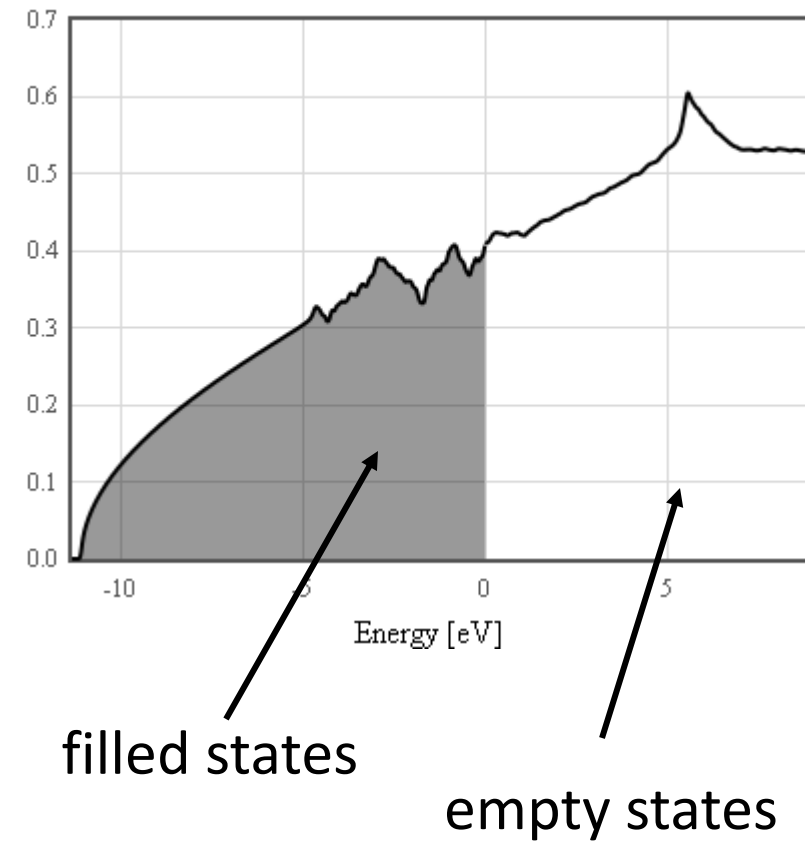
from Ibach & Lueth

Density of states

Silicon

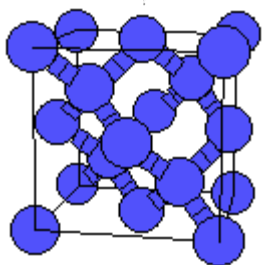
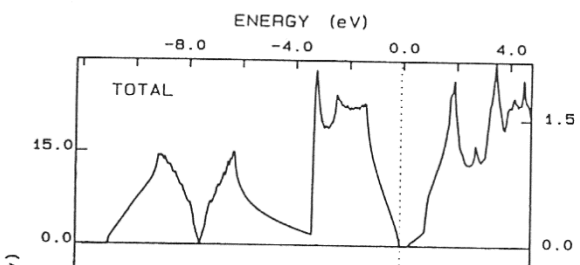
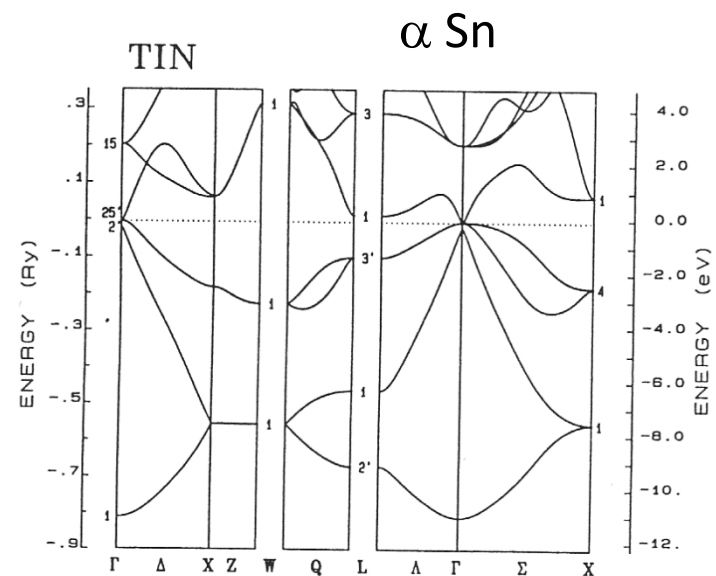


Aluminum

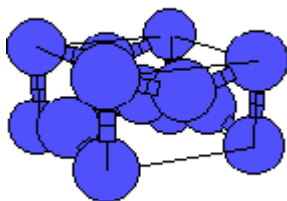
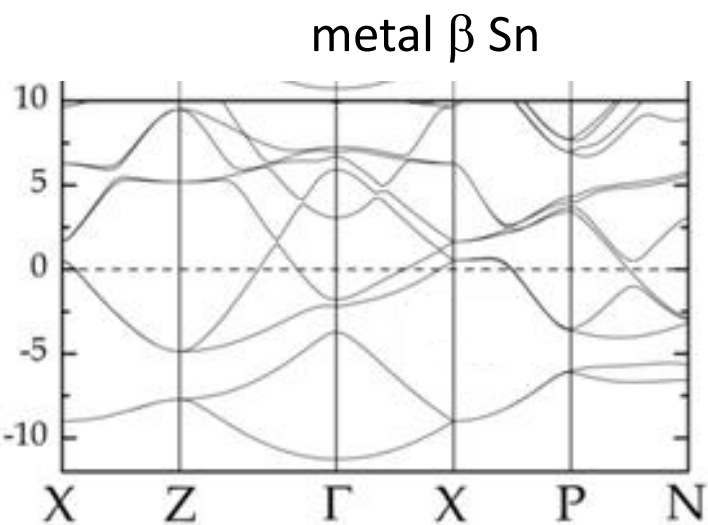


Structural phase transition in Sn

transition at 13 C

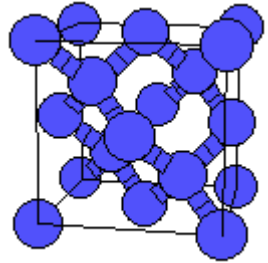


α -Sn, gray tin, diamond structure

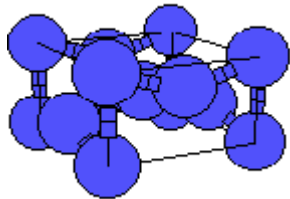


β -Sn, white tin, tetragonal

Structural phase transitions

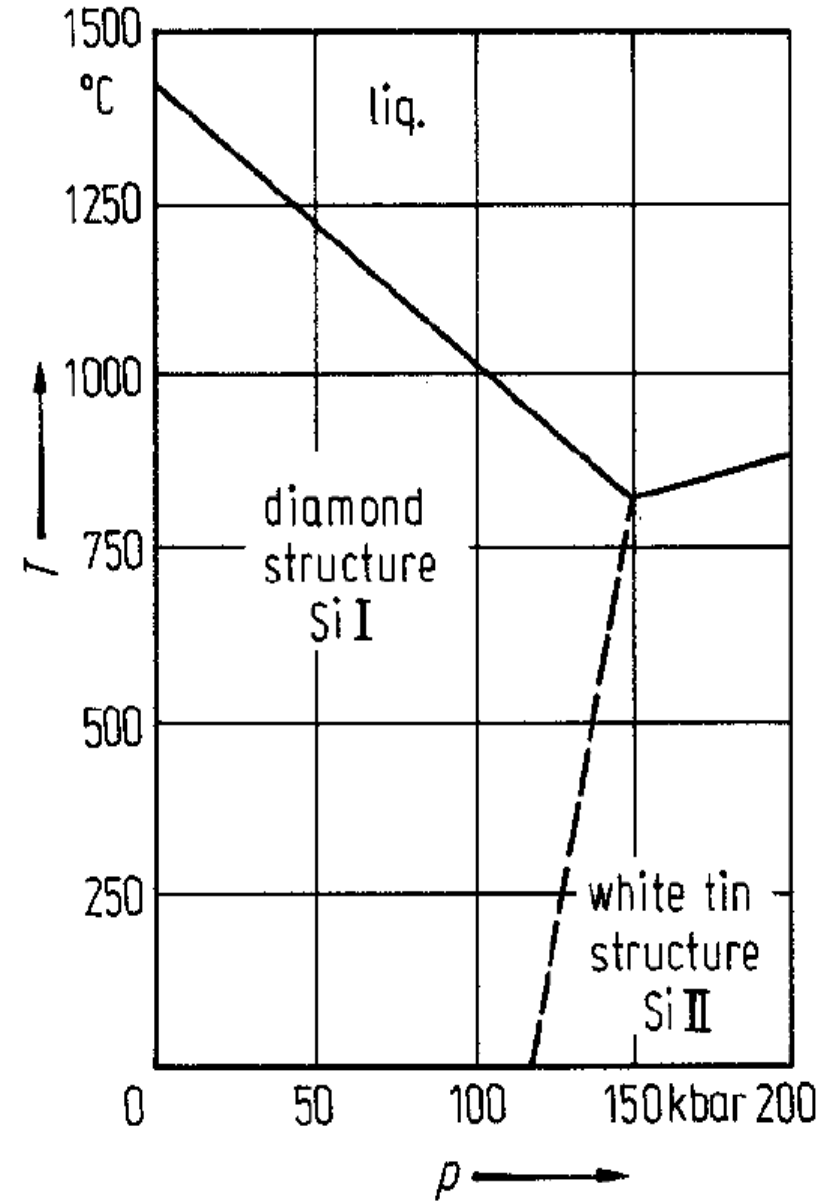


Si, diamond structure



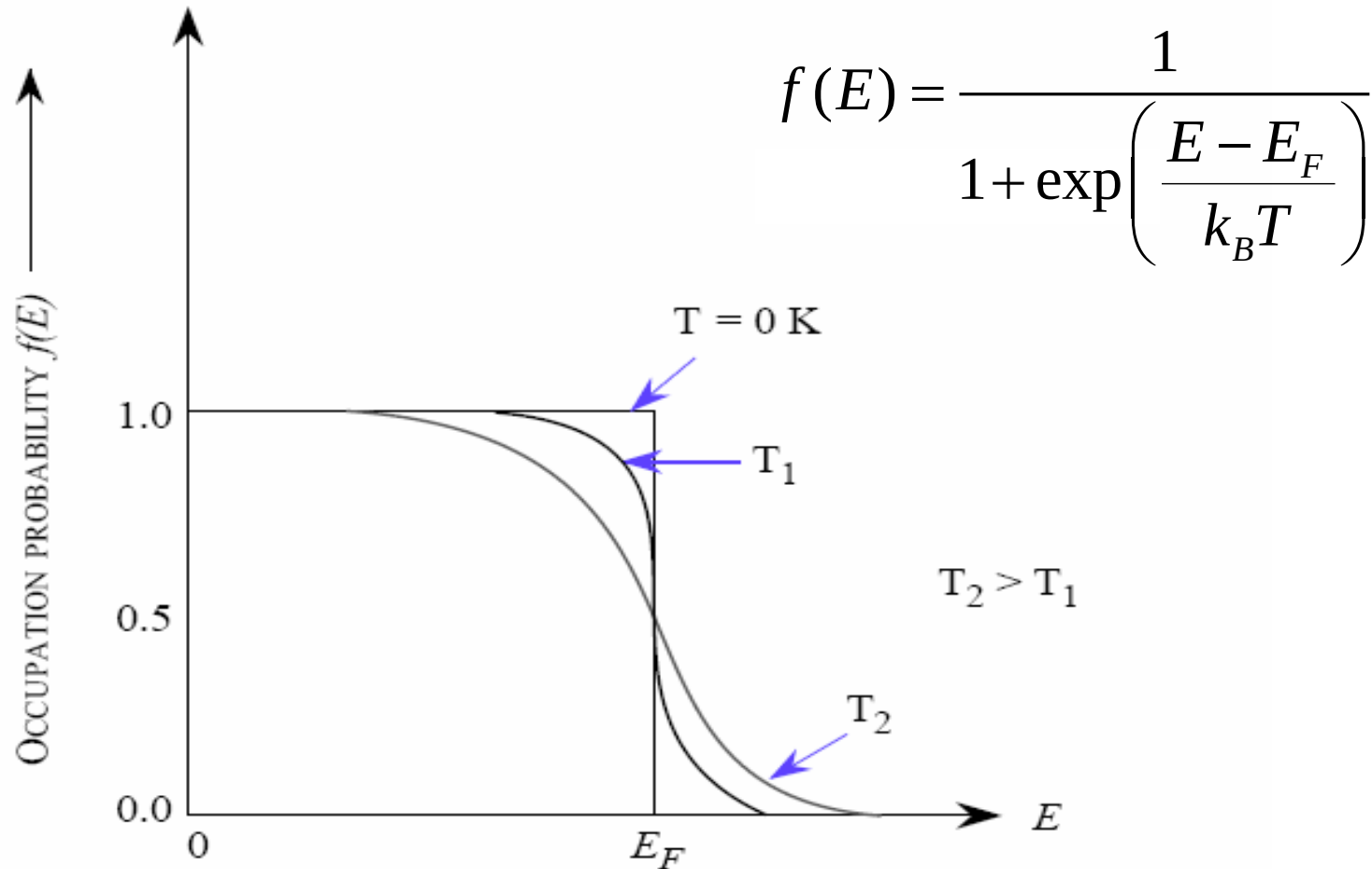
Si II, β -Sn, tetragonal

silicon makes a diamond to β -Sn transition under pressure



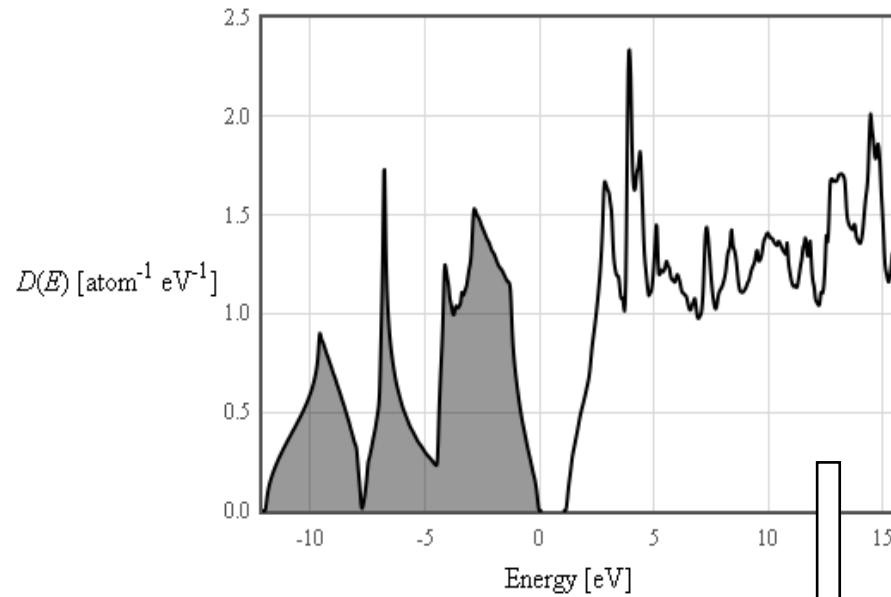
Fermi function

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

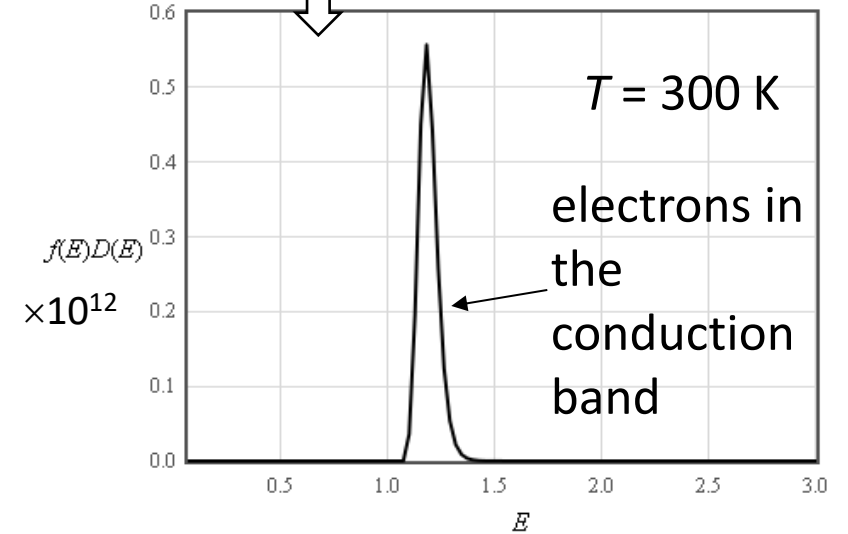
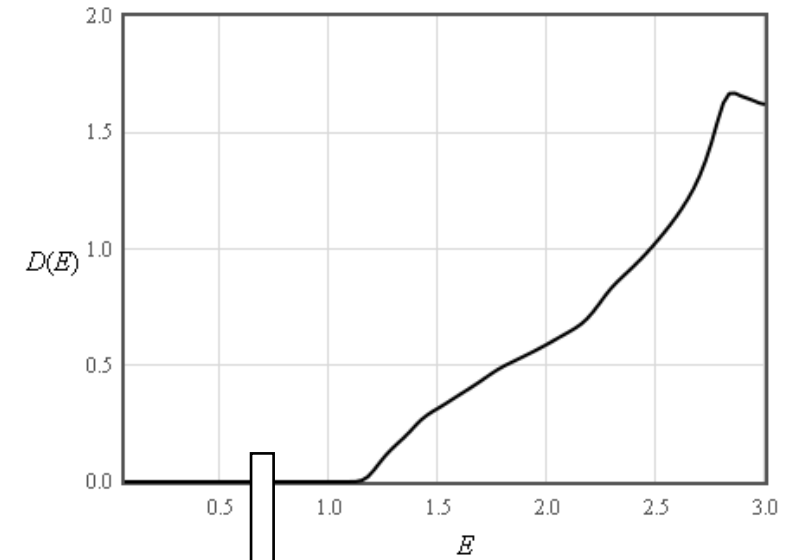
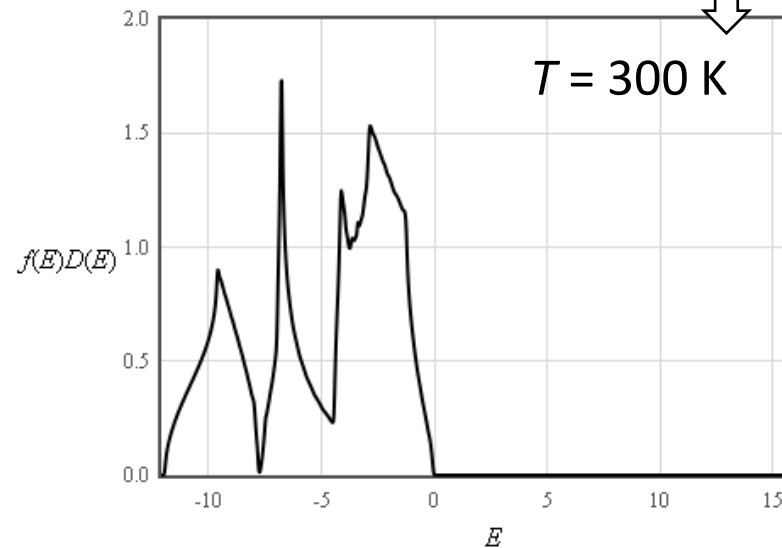


Silicon density of states

density of states



occupation

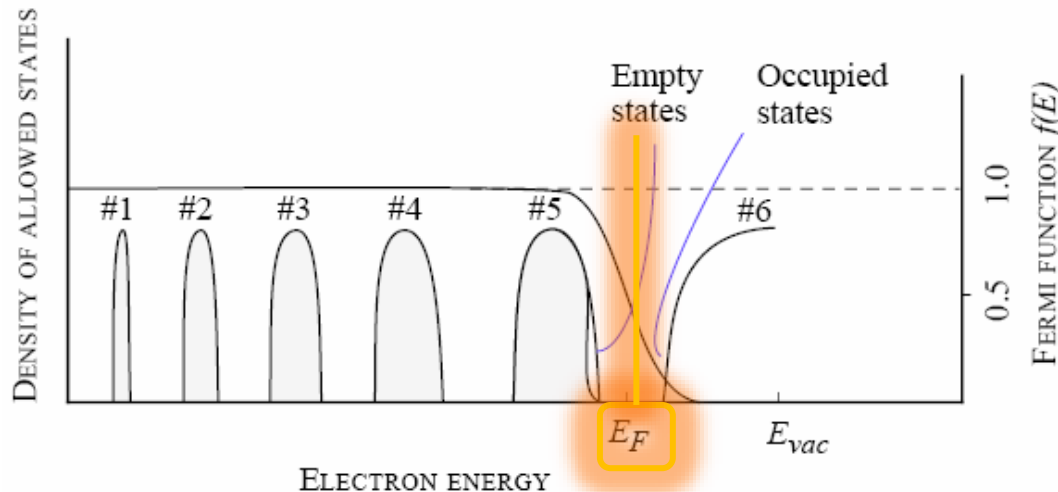


Fermi energy

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

$$n = \int_{-\infty}^{\infty} D(E) f(E; T, E_F) dE \quad n \text{ is the electron density}$$

- 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 .

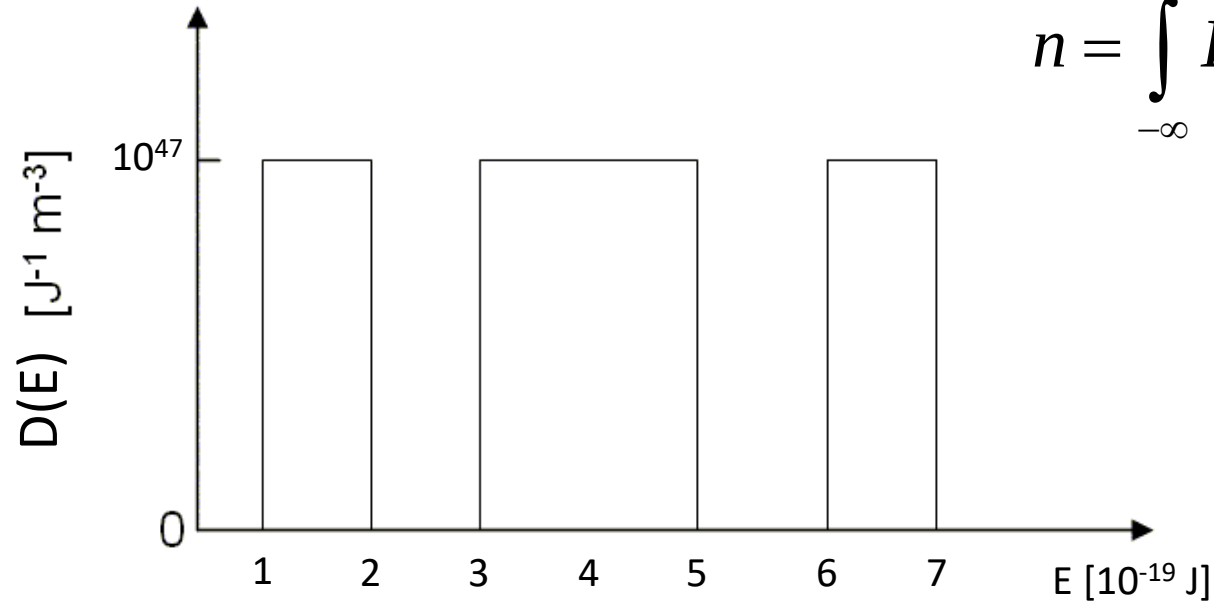


D

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Calculate the Fermi energy

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



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

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

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?