24. Semiconductors

June 21, 2018

Thermal conductivity

$$\vec{j}_U = \bar{E}\vec{j}$$

Average particle energy

$$u = \bar{E}n$$

internal energy density

$$\vec{j}_U = -\bar{E}D\nabla n = -D\nabla u$$

$$\vec{j}_U = -D\frac{du}{dT}\nabla T = -Dc_v\nabla T$$

$$\vec{j}_U = -K\nabla T$$

Thermal conductivity

$$K = Dc_v$$

$$K \to 0 \quad \text{as} \quad T \to 0$$

Wiedemann - Franz law

$$\frac{K}{\sigma} = \frac{Dc_v}{ne\mu}$$

Einstein relation: $D = \frac{\mu k_B T}{e}$

Dulong - Petit: $c_v = 3nk_B$

$$\frac{K}{\sigma} = \frac{3k_B^2}{e^2} T$$

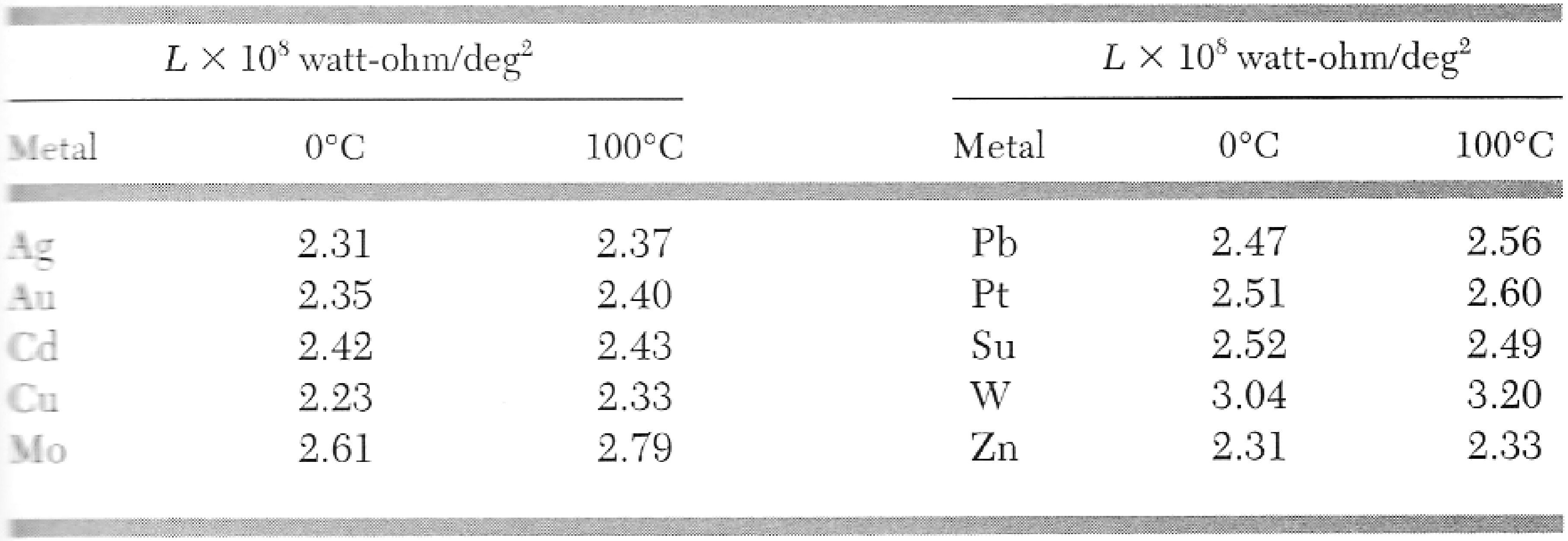
Wiedemann Franz law $L = \frac{K_{el}}{\sigma T} = 2.22 \times 10^{-8} \quad \mathrm{W\ \Omega / K^2}$

Lorentz number

Lorenz number

$$L = \frac{K_{el}}{\sigma T} = 2.22 \times 10^{-8} \qquad \mathrm{W\,\Omega / K^2}$$

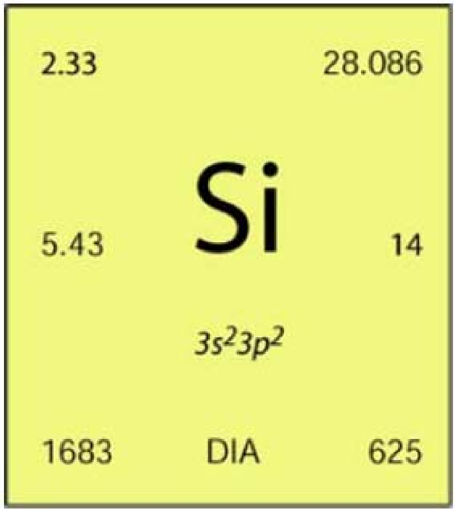
Table 5 Experimental Lorenz numbers



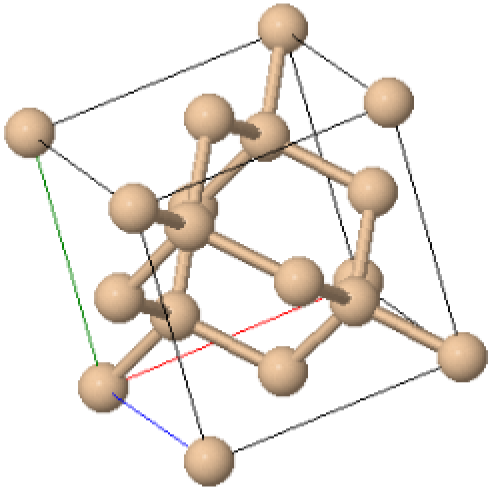
	$L \times 10^8$ watt-ohm/deg^2			$L \times 10^8$ watt-ohm/deg^2	
Metal	0°C	100°C	Metal	0°C	100°C
Ag	2.31	2.37	Pb	2.47	2.56
Au	2.35	2.40	Pt	2.51	2.60
Cd	2.42	2.43	Su	2.52	2.49
Cu	2.23	2.33	W	3.04	3.20
Mo	2.61	2.79	Zn	2.31	2.33

At low temperatures the classical predictions for the thermal and electrical conductivities are too high but their ratio is correct. Only the electrons within $k_B T$ of the Fermi surface contribute.

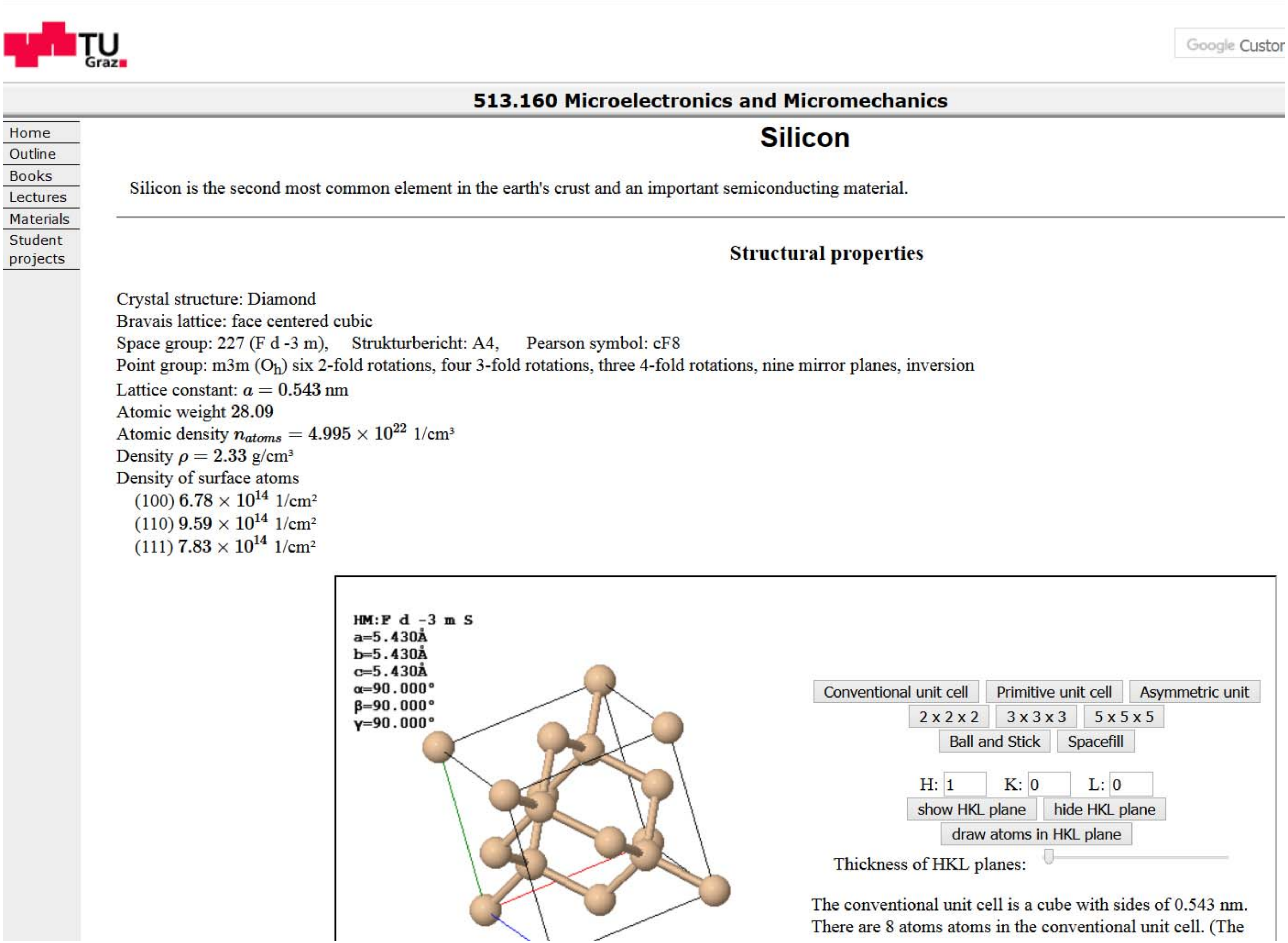
Silicon



- Important semiconducting material
- 2nd most common element on earths crust (rocks, sand, glass, concrete)
- Often doped with other elements
- Oxide SiO_2 is a good insulator



silicon crystal = diamond crystal structure



513.160 Microelectronics and Micromechanics

Silicon

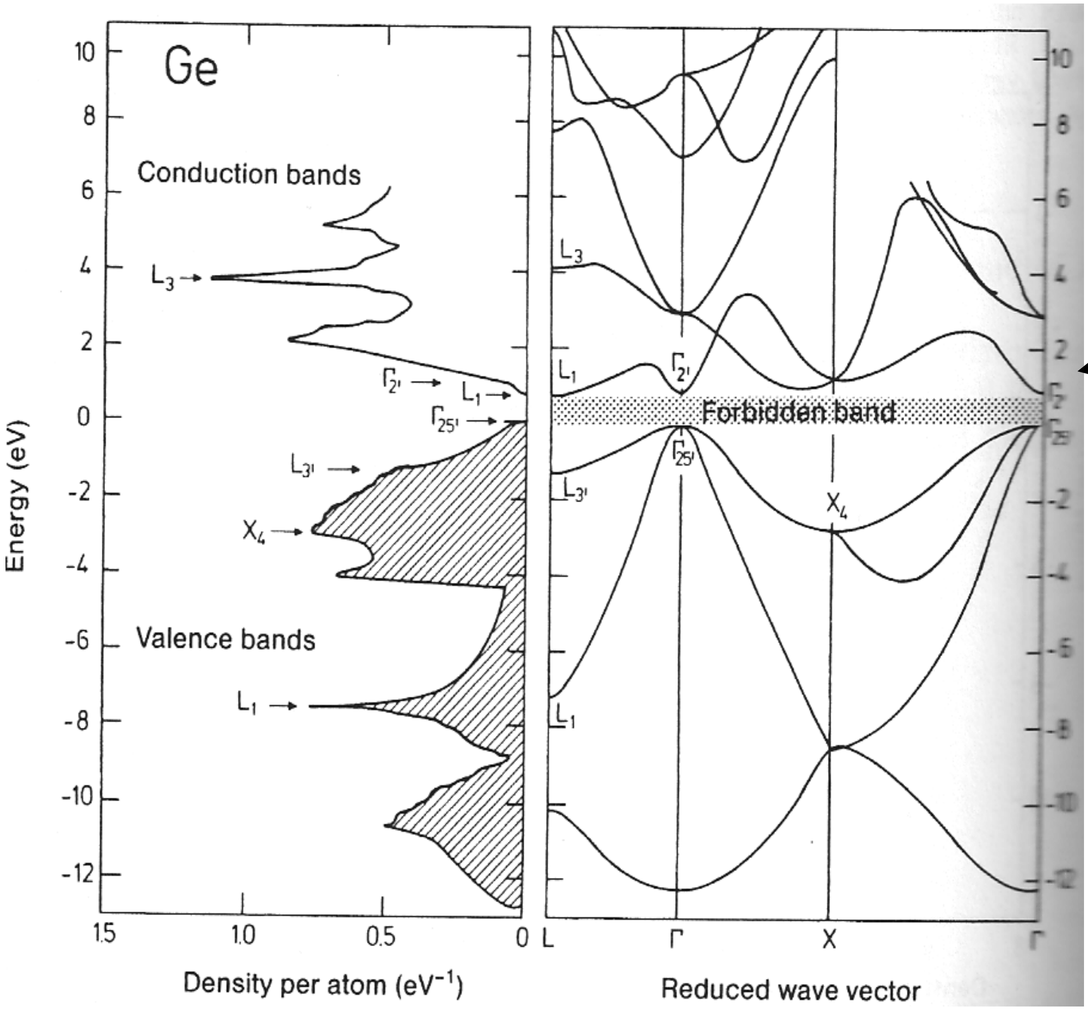
Silicon is the second most common element in the earth's crust and an important semiconducting material.

Structural properties

Crystal structure: Diamond
Bravais lattice: face centered cubic
Space group: 227 (F d -3 m), Strukturbericht: A4, Pearson symbol: cF8
Point group: m3m (O_h) six 2-fold rotations, four 3-fold rotations, three 4-fold rotations, nine mirror planes, inversion
Lattice constant: $a = 0.543$ nm
Atomic weight 28.09
Atomic density $n_{atoms} = 4.995 \times 10^{22}$ 1/cm³
Density $\rho = 2.33$ g/cm³
Density of surface atoms
(100) 6.78×10^{14} 1/cm²
(110) 9.59×10^{14} 1/cm²
(111) 7.83×10^{14} 1/cm²

The conventional unit cell is a cube with sides of 0.543 nm. There are 8 atoms atoms in the conventional unit cell. (The

Semiconductors



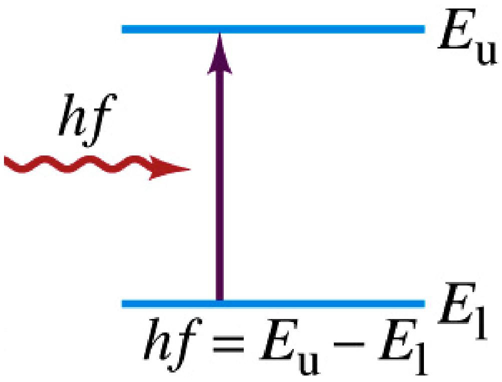
Conduction band

Valence band

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

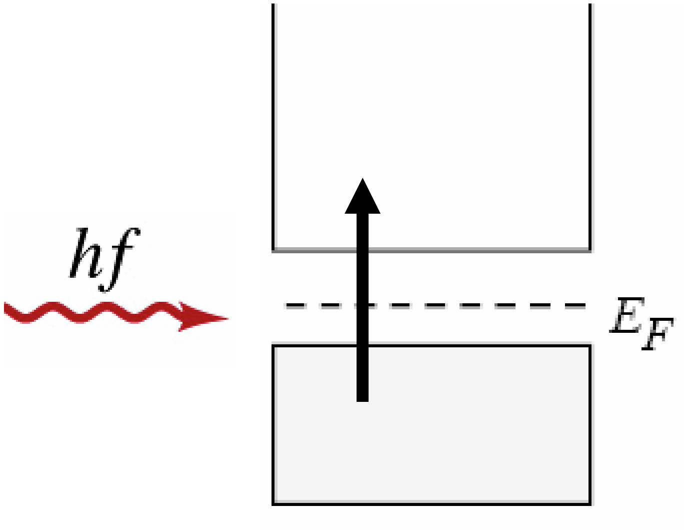
From Ibach & Lueth

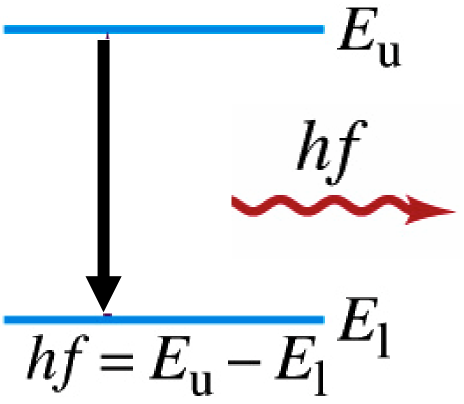
Absorption and emission of photons



$$hf = E_u - E_l$$

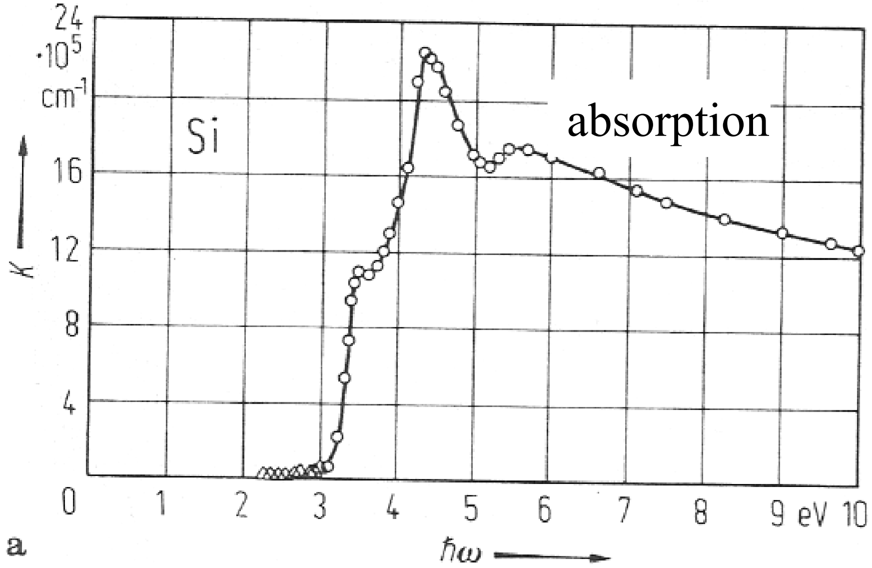
absorption



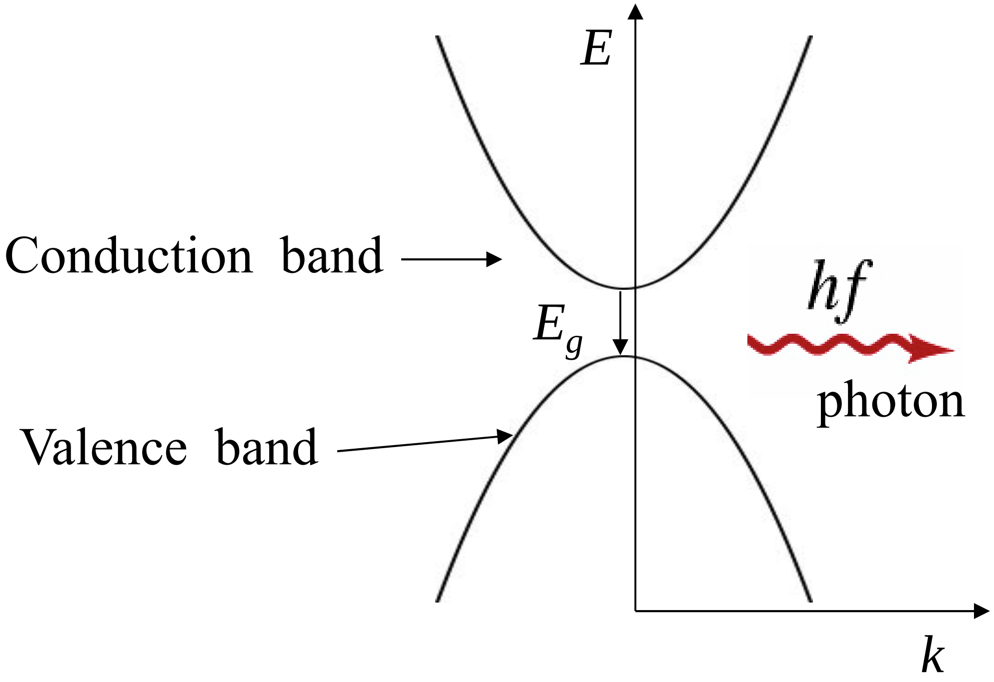


$$hf = E_u - E_l$$

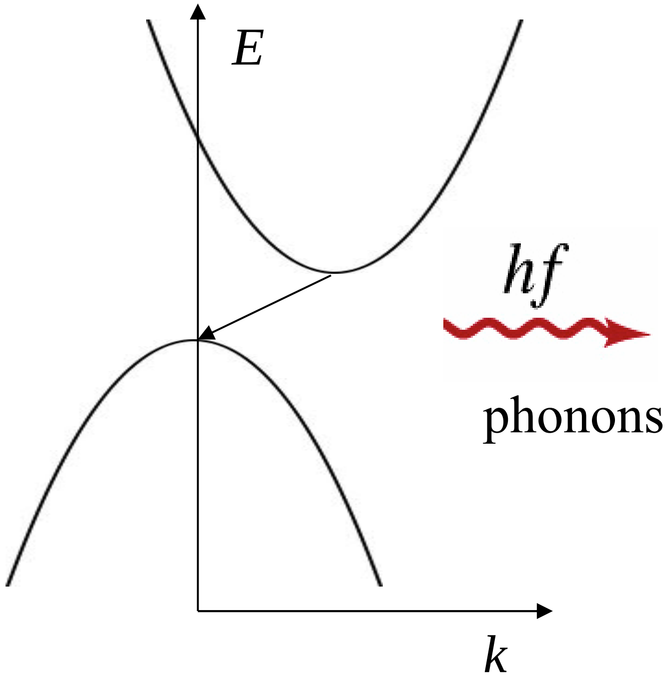
emission



Direct and indirect band gaps



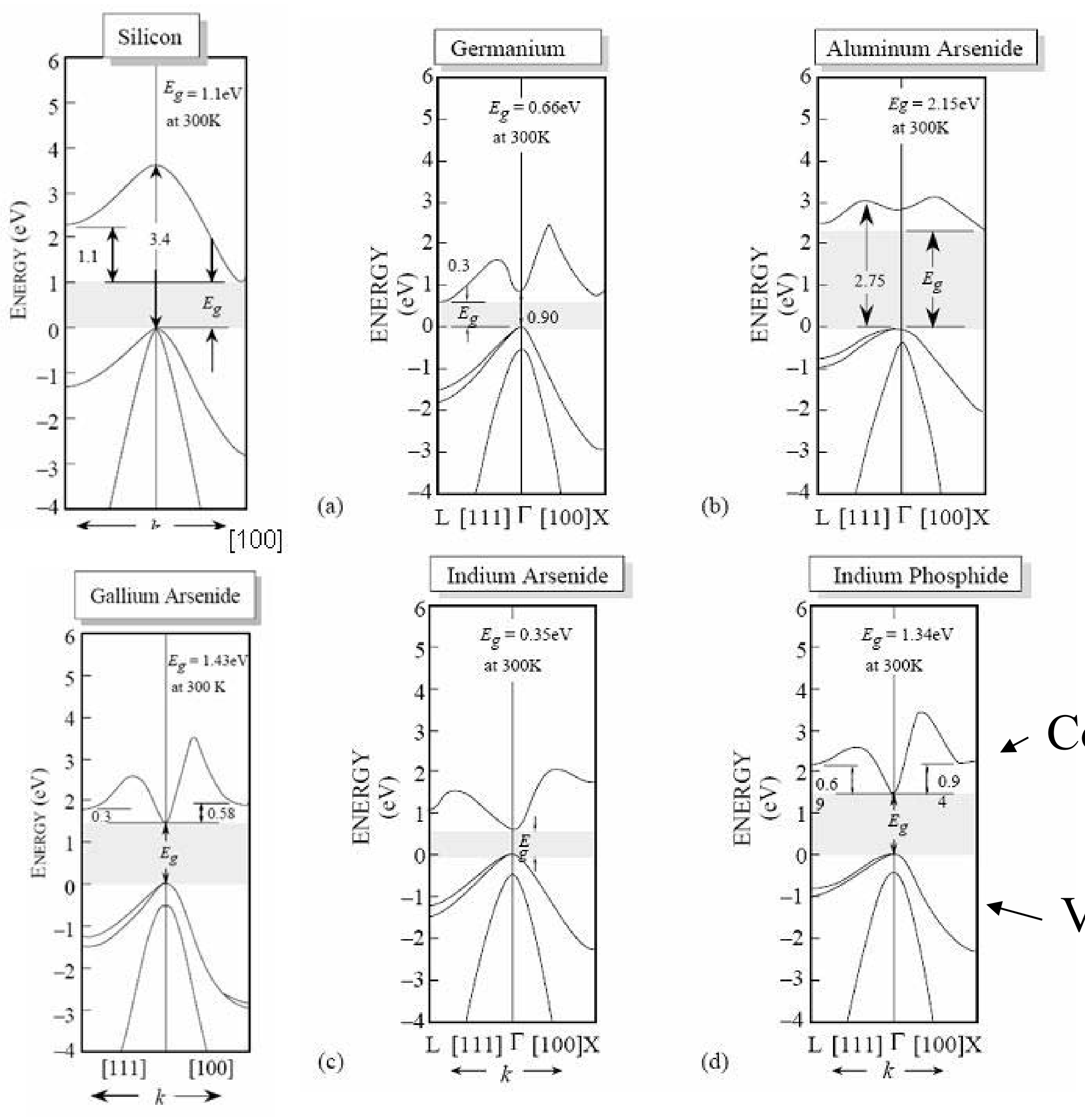
Direct bandgap

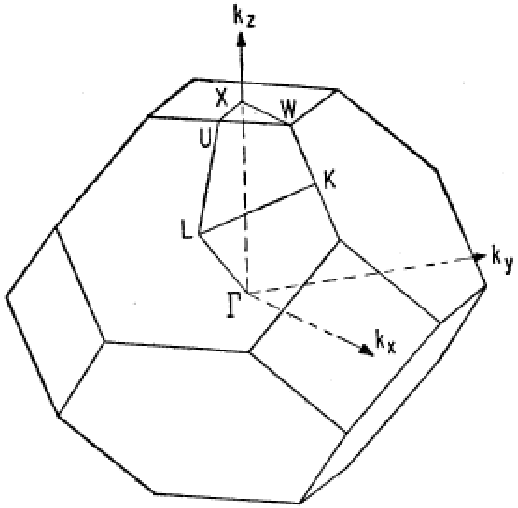


Indirect bandgap

Direct bandgap semiconductors are used for optoelectronics

Semiconductors





Conduction band

Valence band

Light emitting diodes

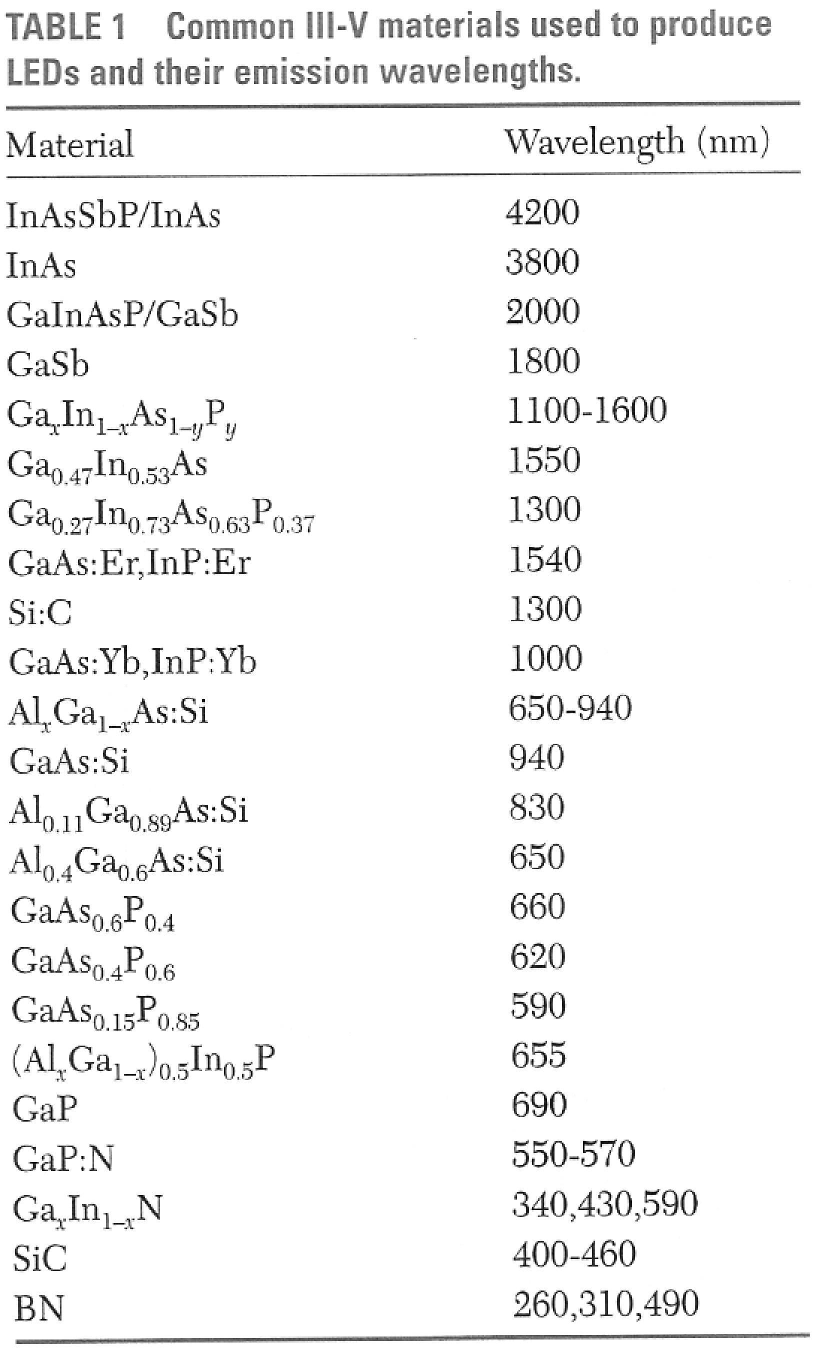
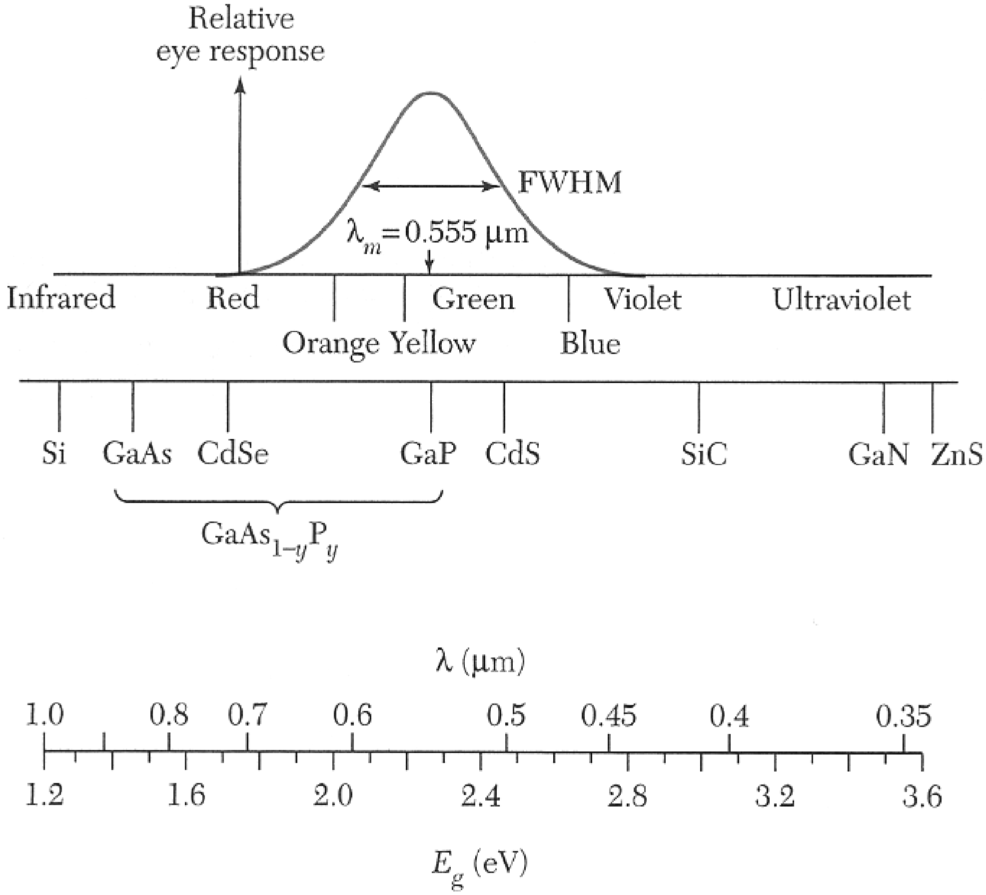
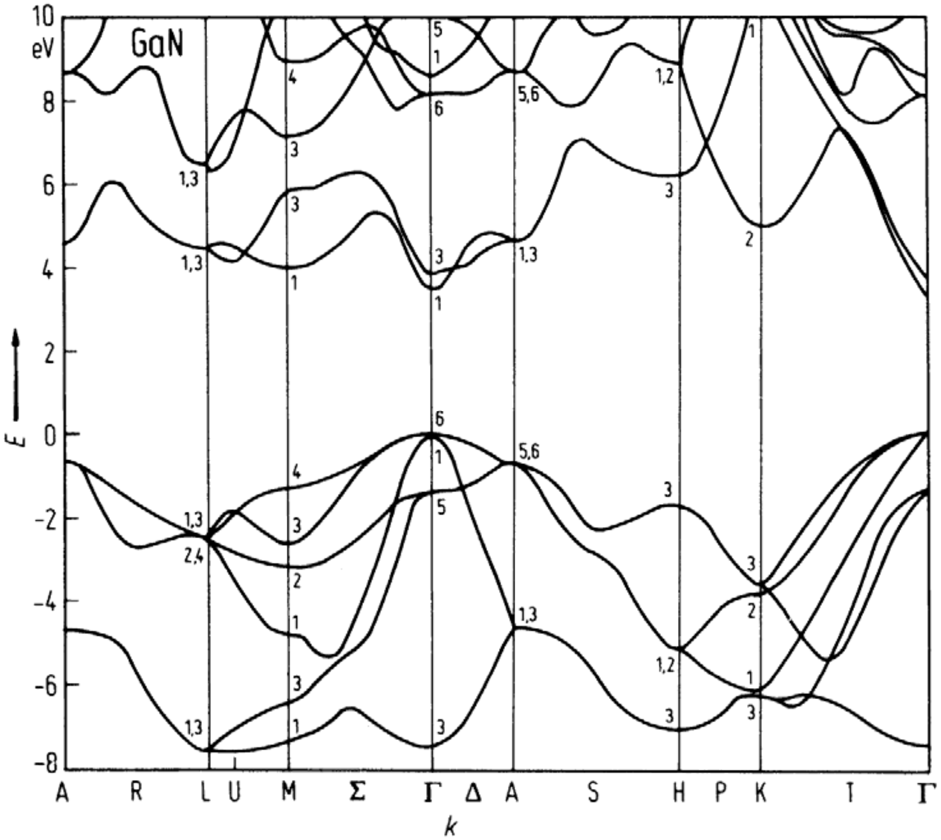


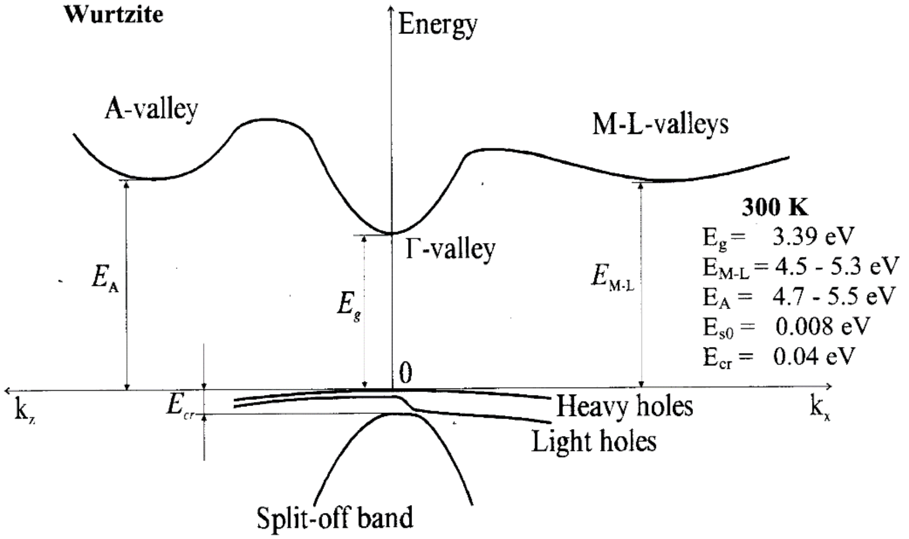
TABLE 1 **Common III-V materials used to produce LEDs and their emission wavelengths.**

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



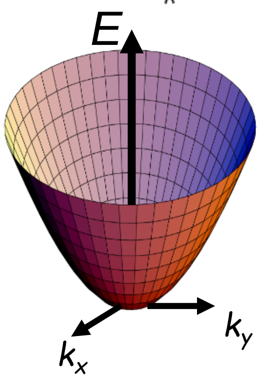
GaN

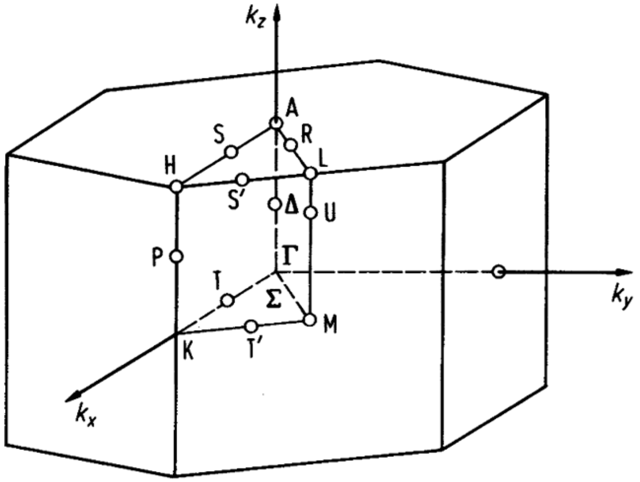




300 K

E_g = 3.39 eV
$E_{M\text{-}L}$ = 4.5 - 5.3 eV
E_A = 4.7 - 5.5 eV
E_{s0} = 0.008 eV
E_{cr} = 0.04 eV

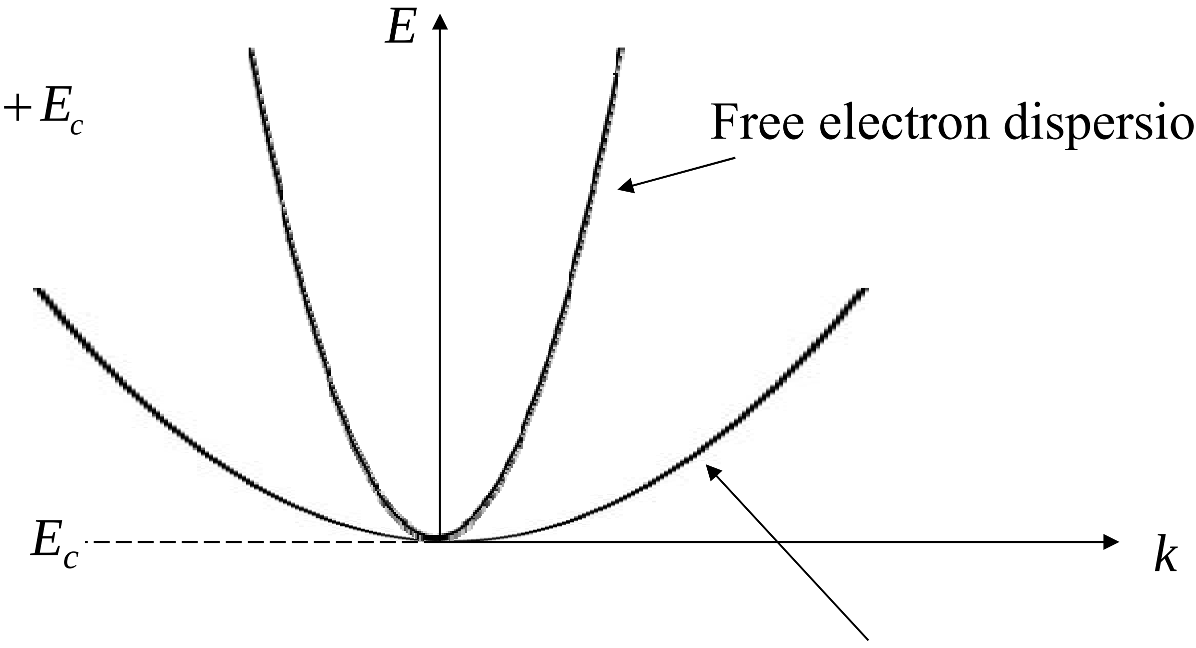




1st Brillioun zone of hcp

Conduction band minimum

$$E = \frac{\hbar^2 \left(\vec{k}-\vec{k}_0\right)^2}{2m^*} + E_c$$

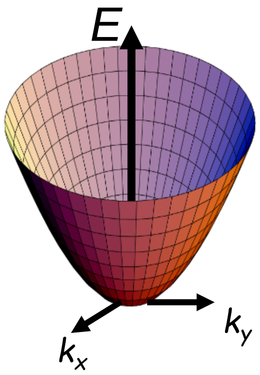


Free electron dispersion relation

Minimum of the conduction band

Near the conduction band minimum, the bands are approximately parabolic.

Effective mass



$$E = \frac{\hbar^2\left(\vec{k}-\vec{k}_0\right)^2}{2m^*} + E_c$$

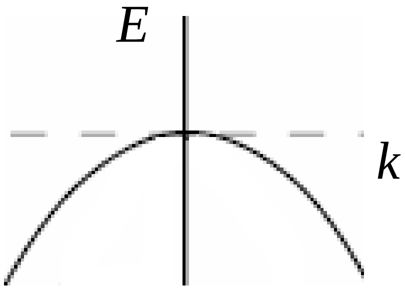
The parabola at the bottom of the conduction band does not have the same curvature as the free-electron dispersion relation. We define an effective mass to characterize the conduction band minimum.

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

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

Top of the valence band

In the valence band, the effective mass is negative.



$$m^* = \frac{\hbar^2}{\frac{d^2E(\vec{k})}{dk_x^2}} < 0$$

Charge carriers in the valence band are positively charged holes.

m^*_h = effective mass of holes

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

Holes

A completely filled band does not contribute to the current.

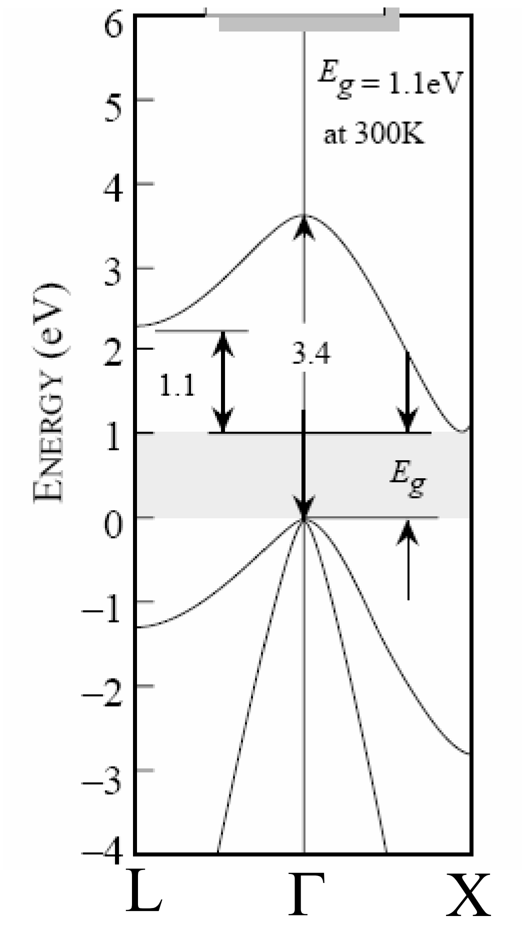
$$\vec{j} = \int_{\text{filled states}} -e\vec{v}(\vec{k})D(\vec{k})\, f(\vec{k})d\vec{k}$$

$$= \int_{\text{band}} -e\vec{v}(\vec{k})D(\vec{k})\, f(\vec{k})d\vec{k} - \int_{\text{empty states}} -e\vec{v}(\vec{k})D(\vec{k})\, f(\vec{k})d\vec{k}$$

$$= \int_{\text{empty states}} e\vec{v}(\vec{k})D(\vec{k})\, f(\vec{k})d\vec{k}$$

Holes have a positive charge and a positive mass.

Effective Mass



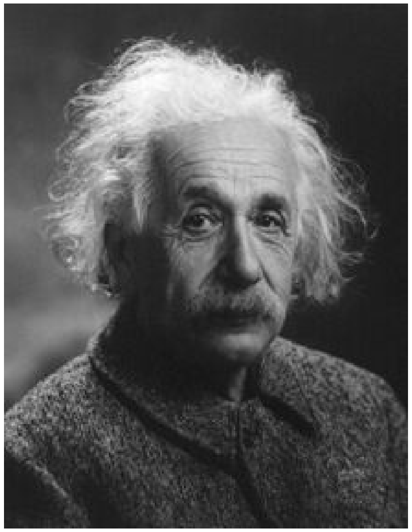
$$E = \frac{\hbar^2 \left(\vec{k} - \vec{k}_0\right)^2}{2m^*} + E_c$$

$$m_e^* = \frac{\hbar^2}{\dfrac{d^2E}{dk_x^2}}$$

$$E = \frac{-\hbar^2 \left(\vec{k} - \vec{k}_0\right)^2}{2m^*} + E_v$$

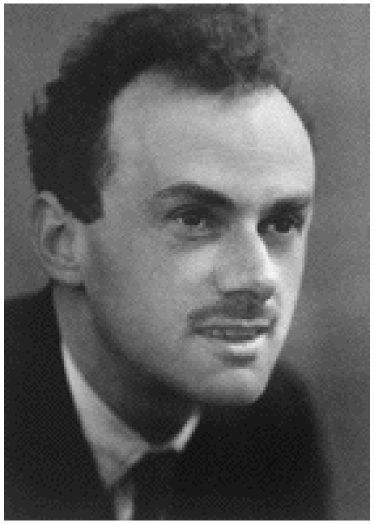
$$m_h^* = \frac{-\hbar^2}{\dfrac{d^2E}{dk_x^2}}$$

Holes



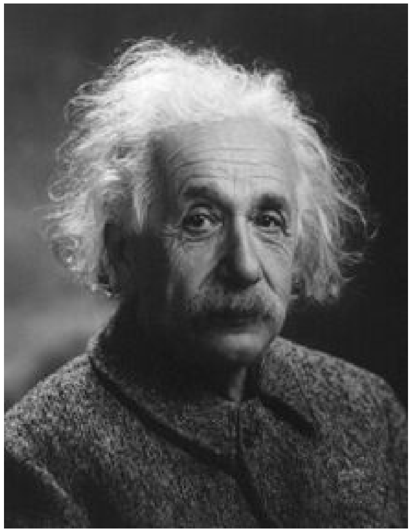
Albert Einstein

Erwin Schrödinger



Paul Adrien Maurice Dirac

Holes



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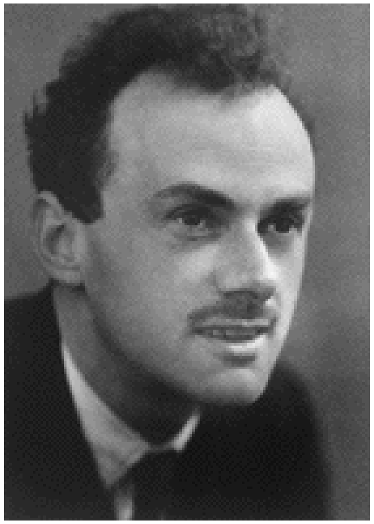


Paul Adrien Maurice Dirac

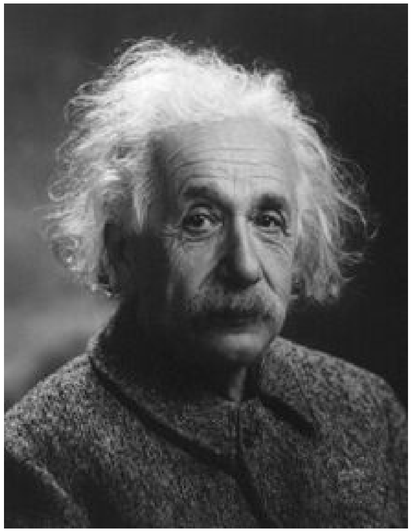
$$\frac{d^2u}{dt^2} = c^2 \frac{d^2u}{dx^2}$$

Wave equation

$$\frac{du}{dt} = k \frac{d^2u}{dx^2}$$

Heat equation

Holes



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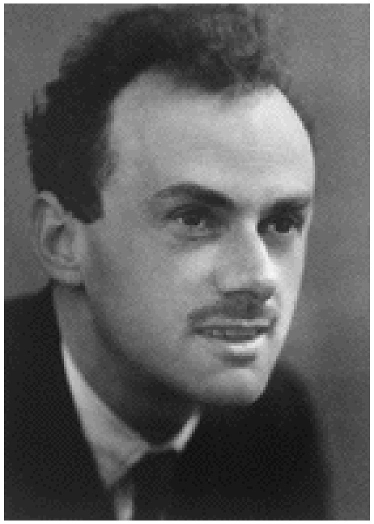

Paul Adrien Maurice Dirac

$$\left(\beta mc^2+\sum_{j=1}^{3}\alpha_j p_j c\right)\psi = i\hbar\frac{\partial\psi}{\partial t}$$

Dirac equation