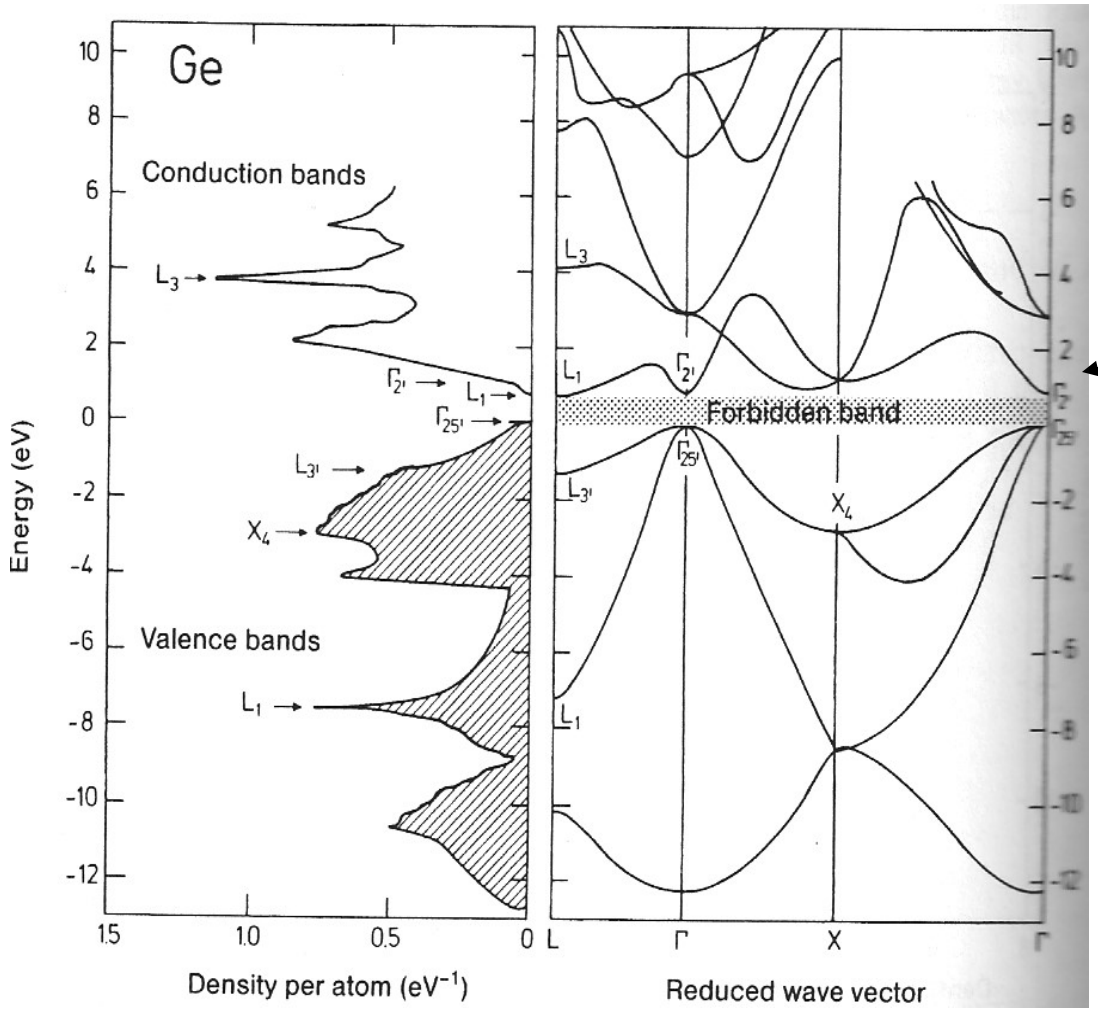
Semiconductors



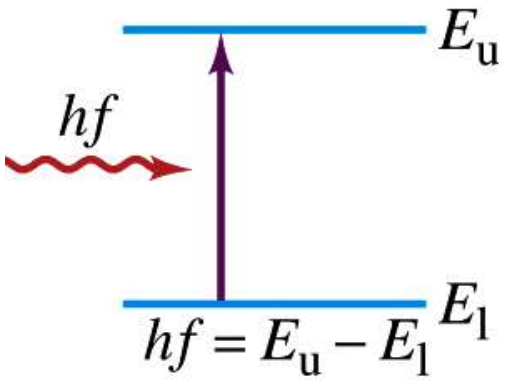
Conduction band

Valence band

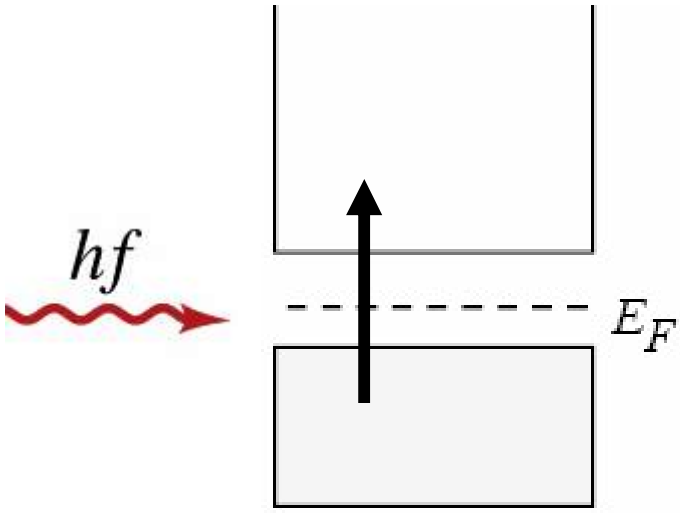
$$n = \int_{-\infty}^{\infty} D(E) f(E) dE$$

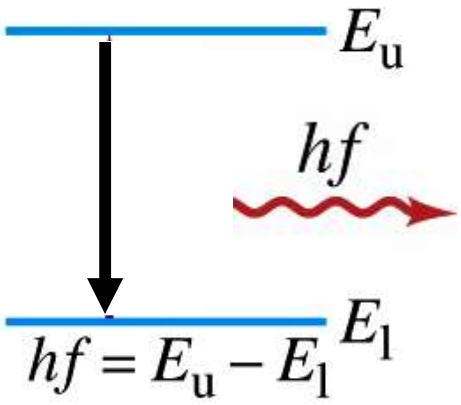
From Ibach & Lueth

Absorption and emission of photons

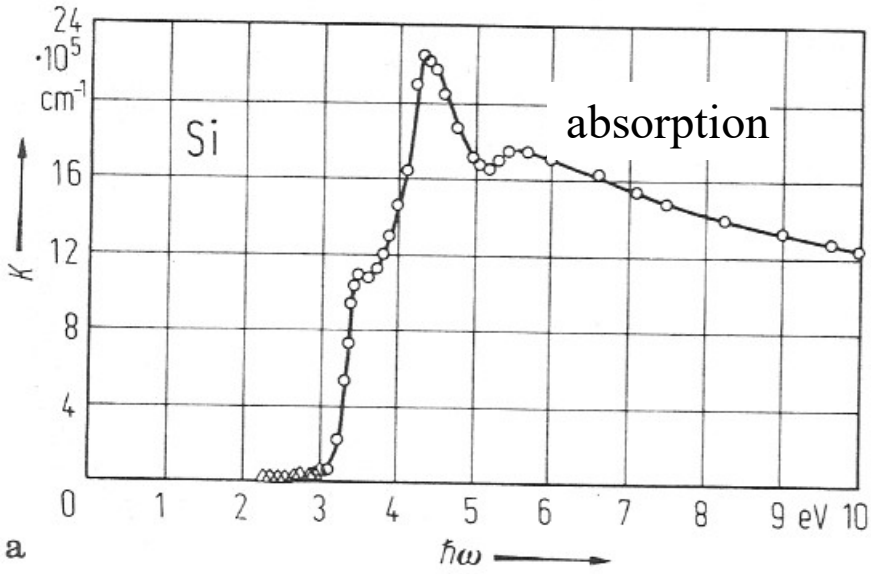


absorption

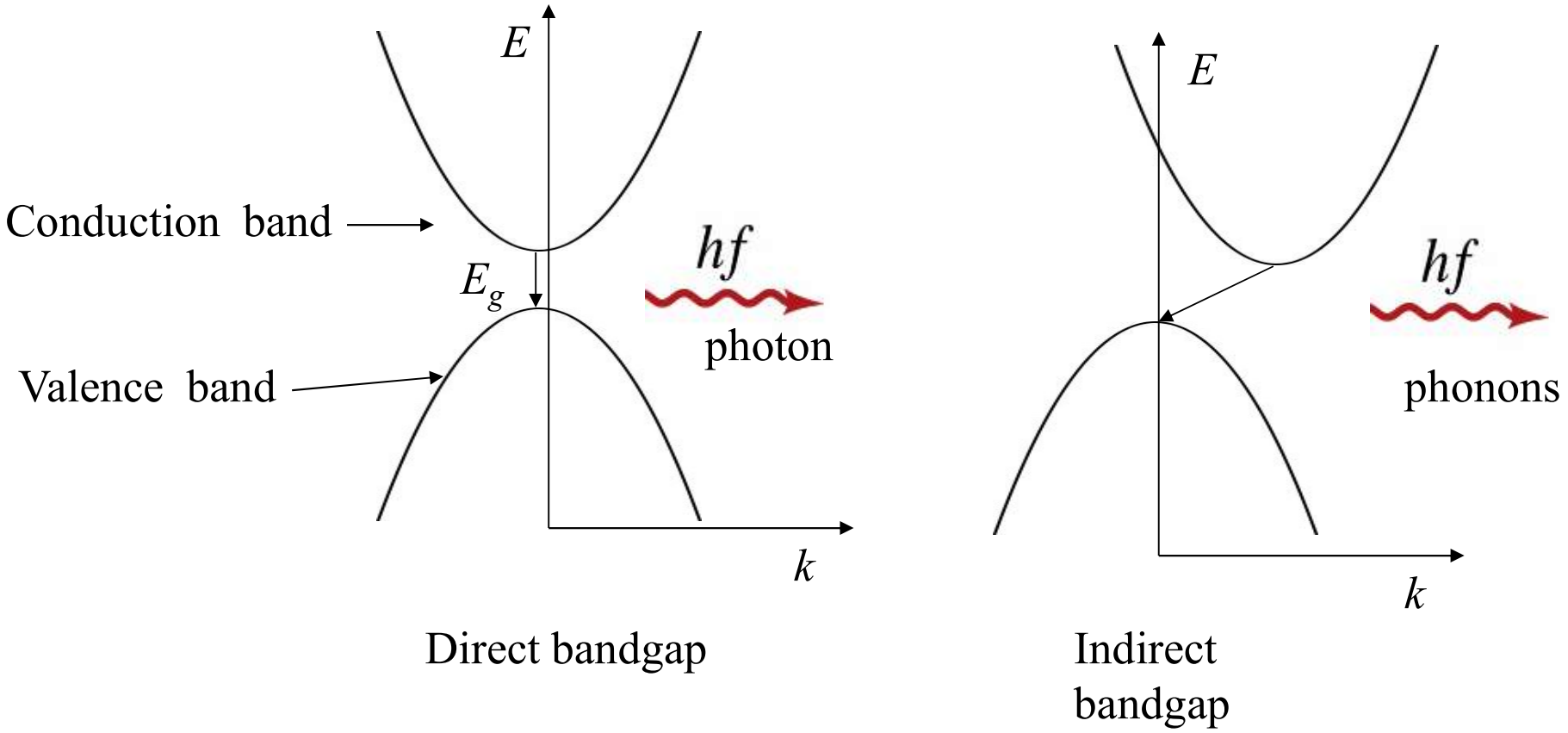




emission

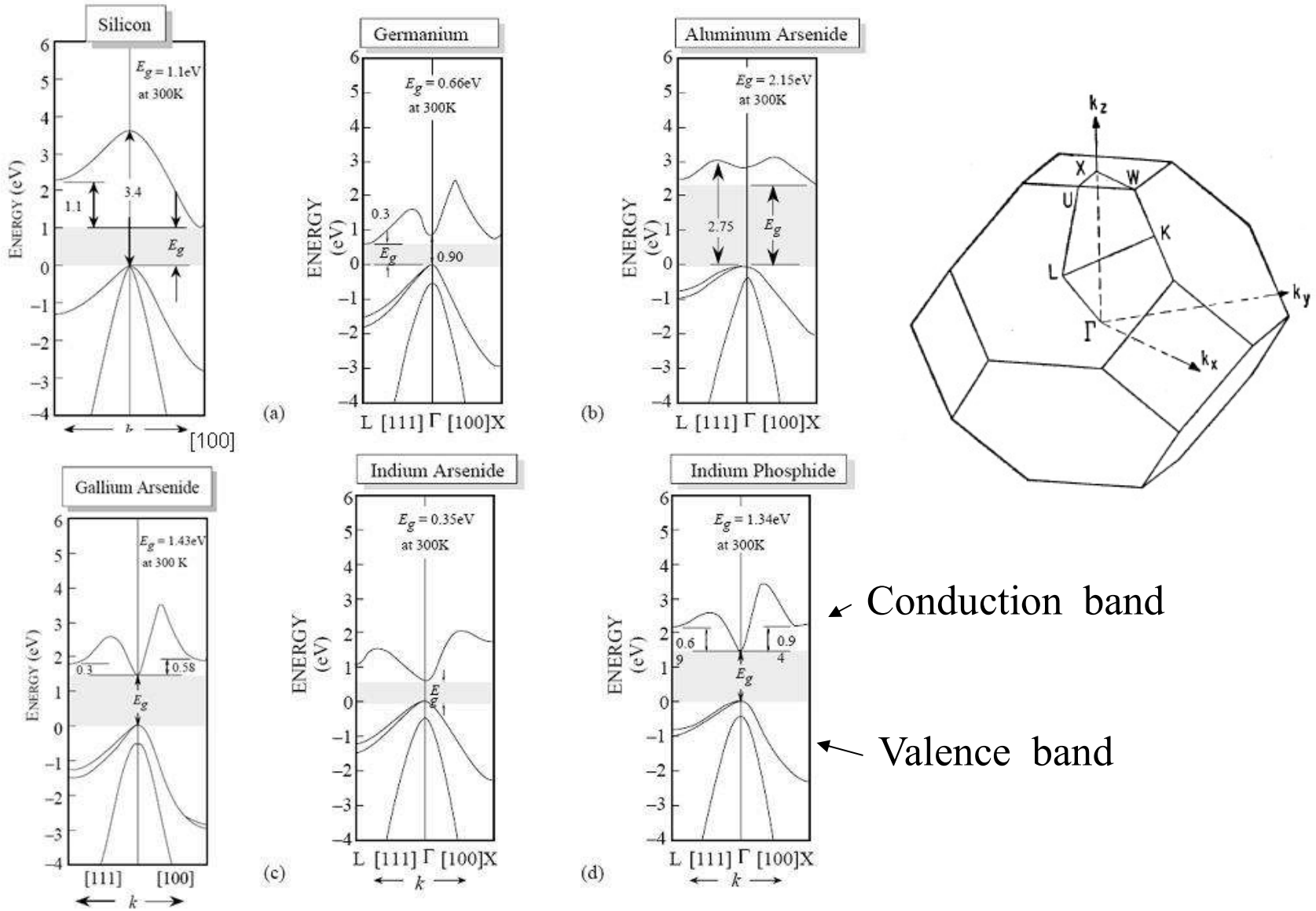


Direct and indirect band gaps



Direct bandgap semiconductors are used for optoelectronics

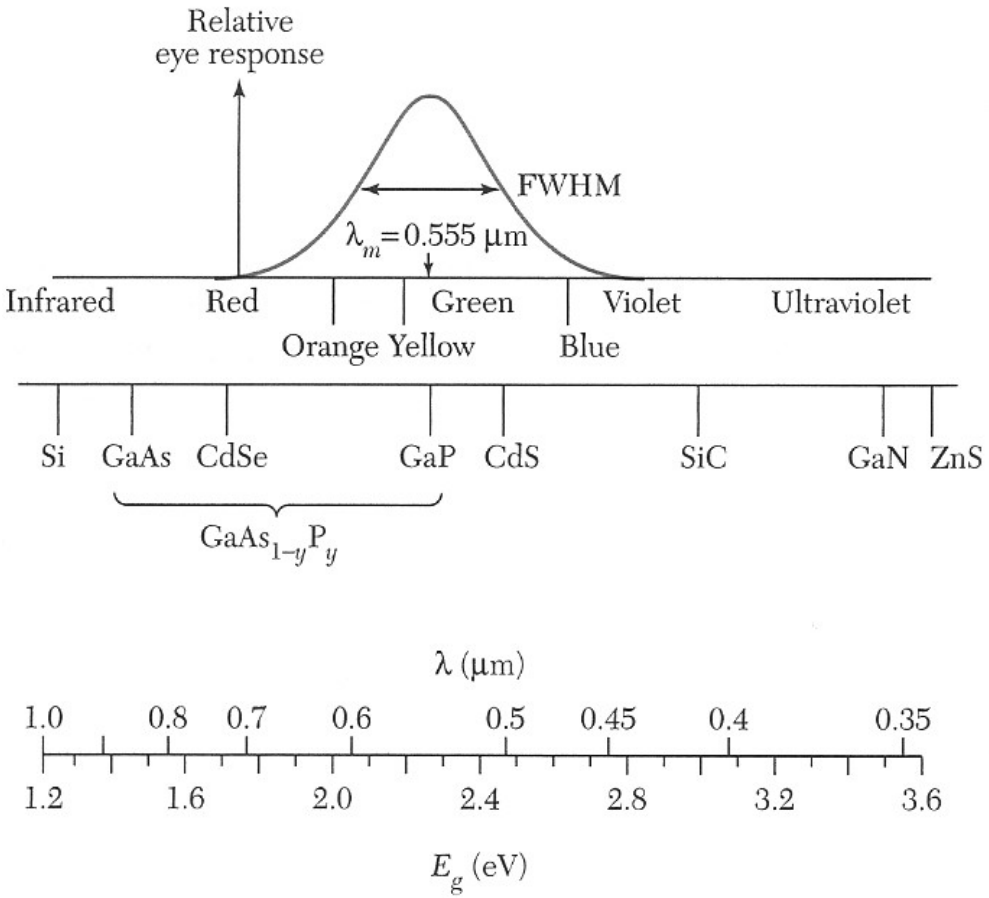
Semiconductors



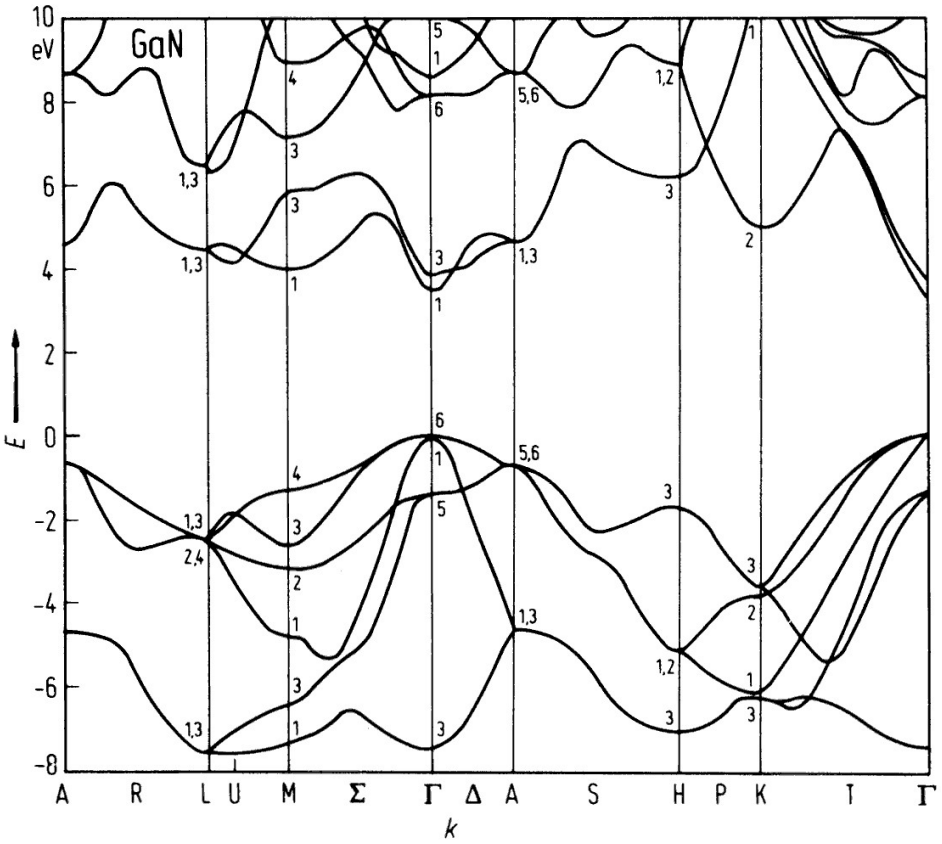
Light emitting diodes

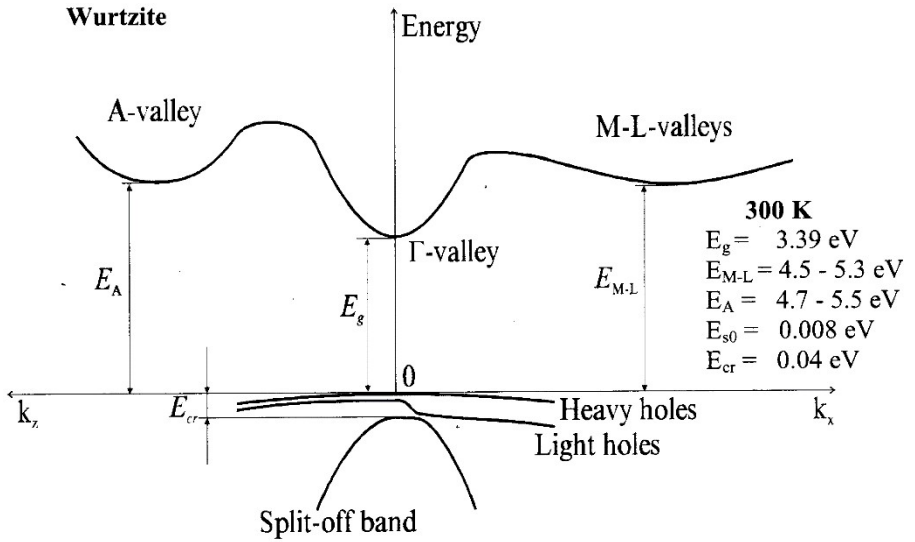
TABLE 1 Common III-V materials used to produce LEDs and their emission wavelengths.

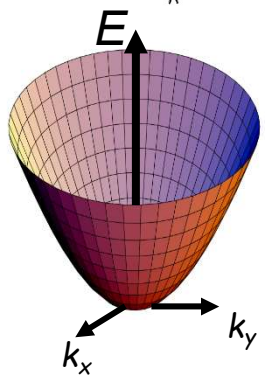
Material	Wavelength (nm)
InAsSbP/InAs	4200
InAs	3800
GaInAsP/GaSb	2000
GaSb	1800
$Ga_xIn_{1-x}As_{1-y}P_y$	1100-1600
$Ga_{0.47}In_{0.53}As$	1550
$Ga_{0.27}In_{0.73}As_{0.63}P_{0.37}$	1300
GaAs:Er,InP:Er	1540
Si:C	1300
GaAs:Yb,InP:Yb	1000
$Al_xGa_{1-x}As$:Si	650-940
GaAs:Si	940
$Al_{0.11}Ga_{0.89}As$:Si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

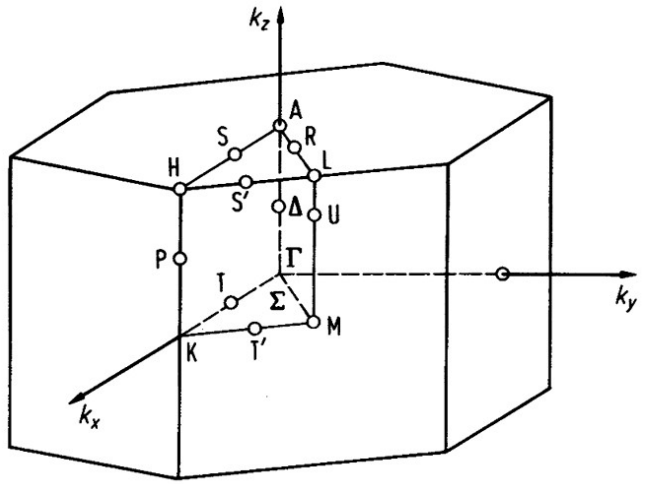


GaN





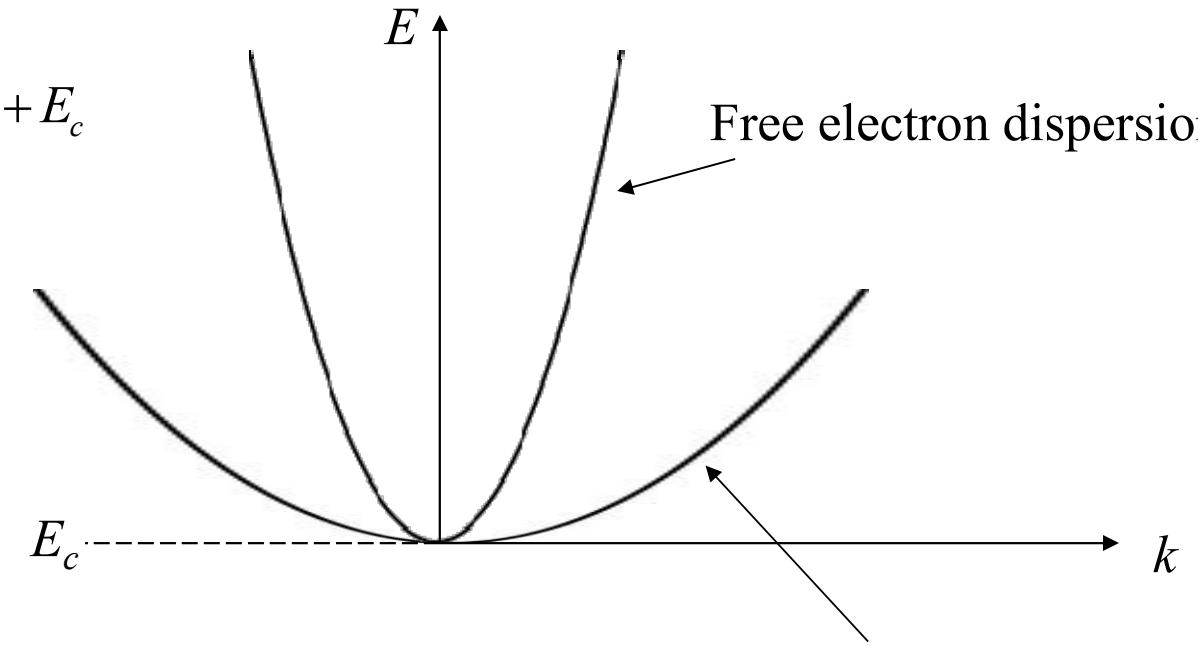




1st Brillioun zone of hcp

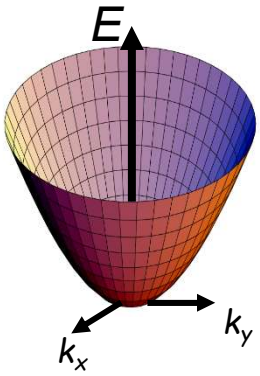
Conduction band minimum

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



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

Effective mass



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

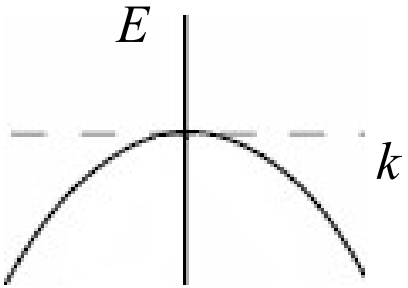
The parabola at the bottom of the conduction band does not have the same curvature as the free-electron dispersion relation. We define an effective mass to characterize the conduction band minimum.

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

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.

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

m^*_h = effective mass of holes

Holes

A completely filled band does not contribute to the current.

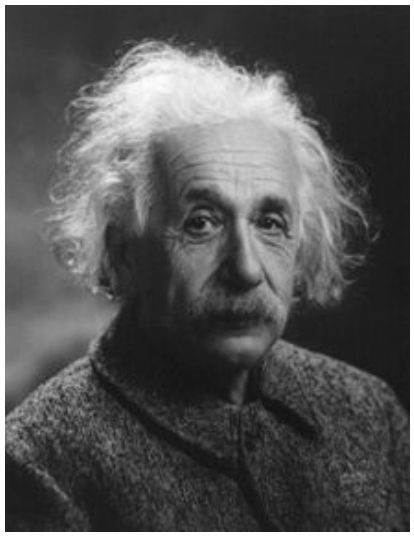
$$\vec{j} = \int_{\text{filled states}} -e\vec{v}(\vec{k})D(\vec{k})f(\vec{k})d\vec{k}$$

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

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

Holes have a positive charge and a positive mass.

Holes

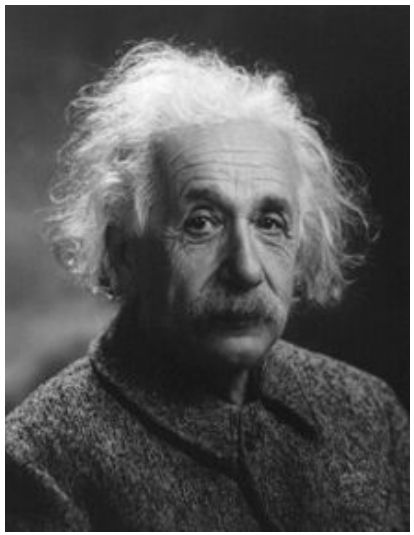


Albert Einstein

Erwin Schrödinger

Paul Adrien Maurice Dirac

Holes



Albert Einstein

Erwin Schrödinger

Paul Adrien Maurice Dirac

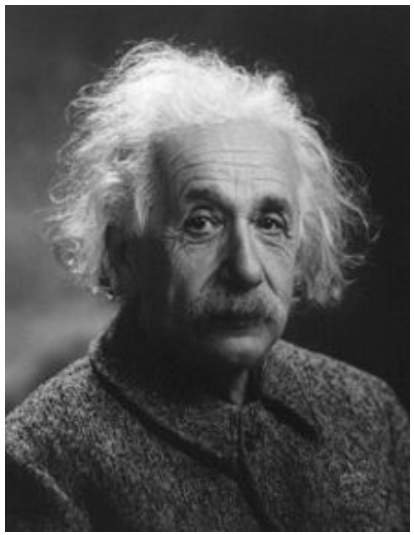
$$\frac{d^2u}{dt^2} = c^2 \frac{d^2u}{dx^2}$$

Wave equation

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

Heat equation

Holes



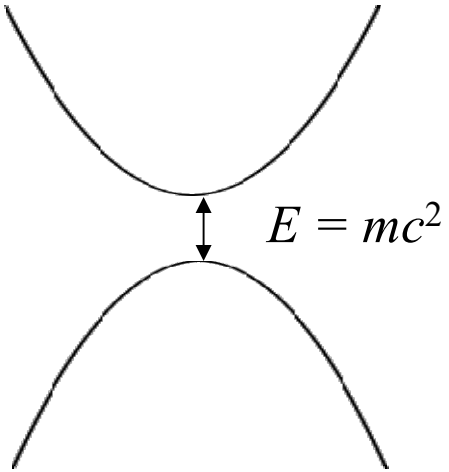
Albert Einstein

Erwin Schrödinger

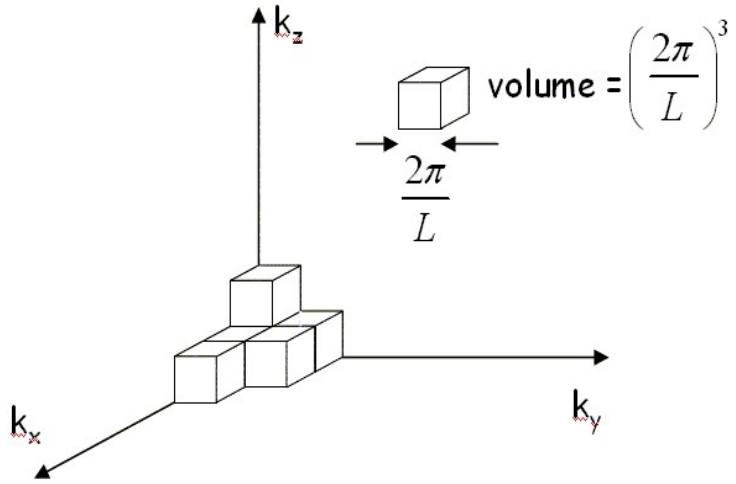
Paul Adrien Maurice Dirac

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

Dirac equation



Free particles in 3-d

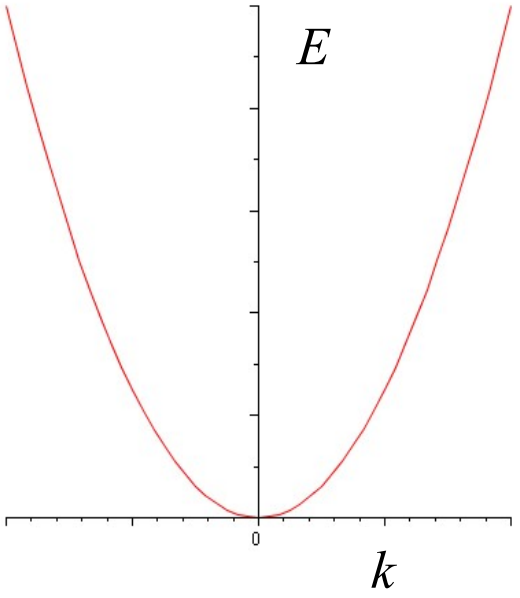


$$k_x, k_y, k_z = \ldots, \frac{-4\pi}{L}, \frac{-2\pi}{L}, 0, \frac{2\pi}{L}, \frac{4\pi}{L}, \ldots$$

Density of states

$$D(k) = \frac{k^2}{\pi^2}$$

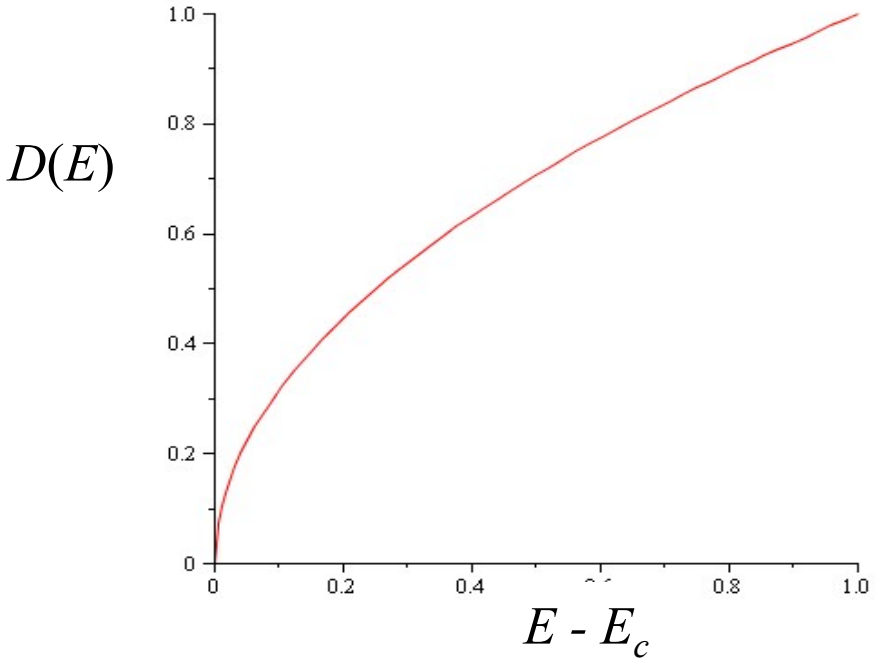
$$E = \frac{\hbar^2 k^2}{2m}$$



$$\frac{dk}{dE} = \frac{1}{2\hbar}\sqrt{\frac{2m}{E}}$$

$$D(E) = D(k)\frac{dk}{dE} = \frac{(2m)^{\frac{3}{2}}}{2\pi^2\hbar^3}\sqrt{E}$$

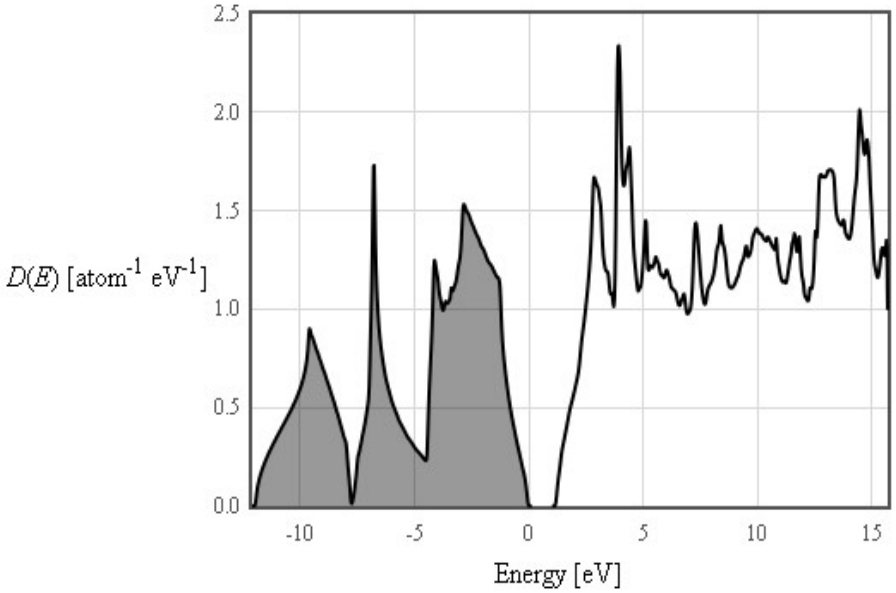
Electron density of states at the bottom of the conduction band

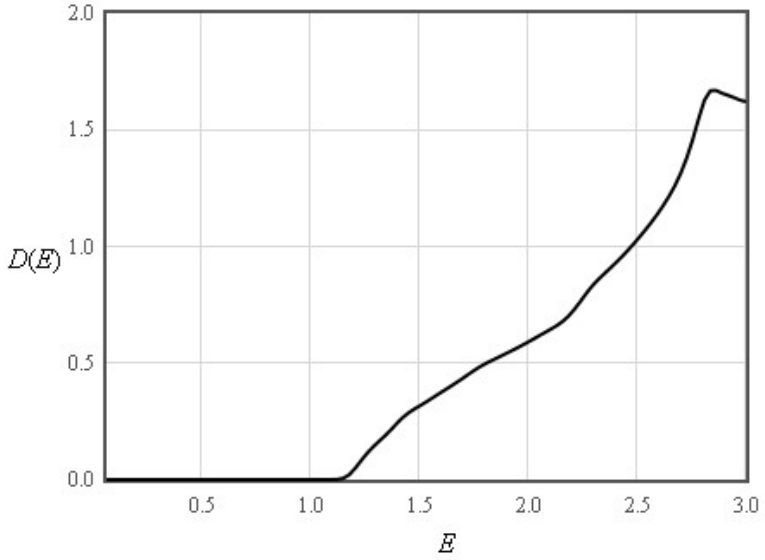


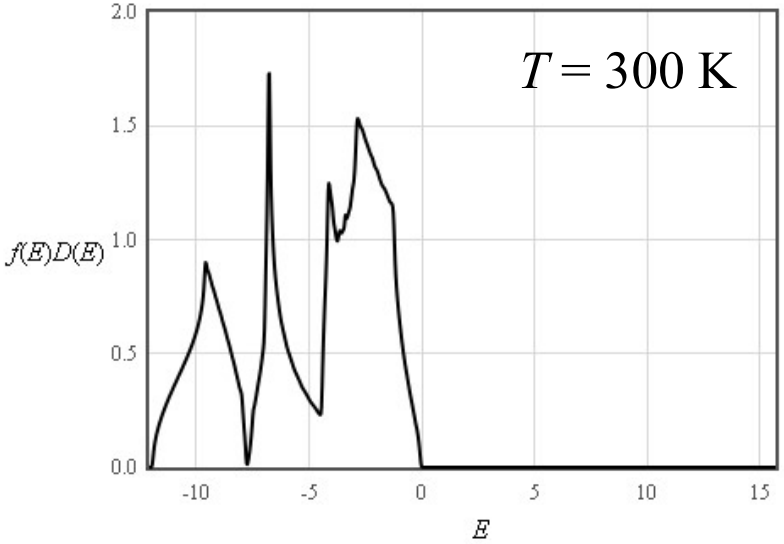
$$D(E) = D(k)\frac{dk}{dE} = \frac{\left(2m^*\right)^{\frac{3}{2}}}{2\pi^2\hbar^3}\sqrt{E - E_c}$$

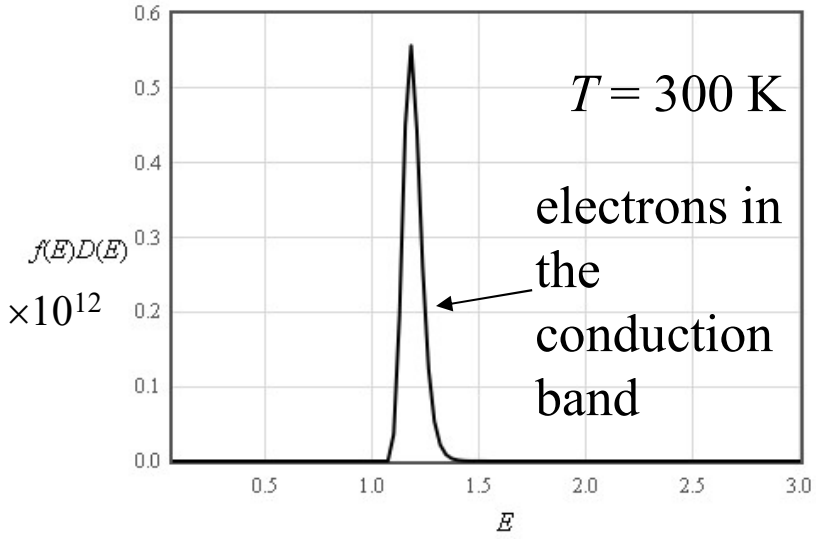
The free electron density of states is modified by the effective mass.

Silicon density of states



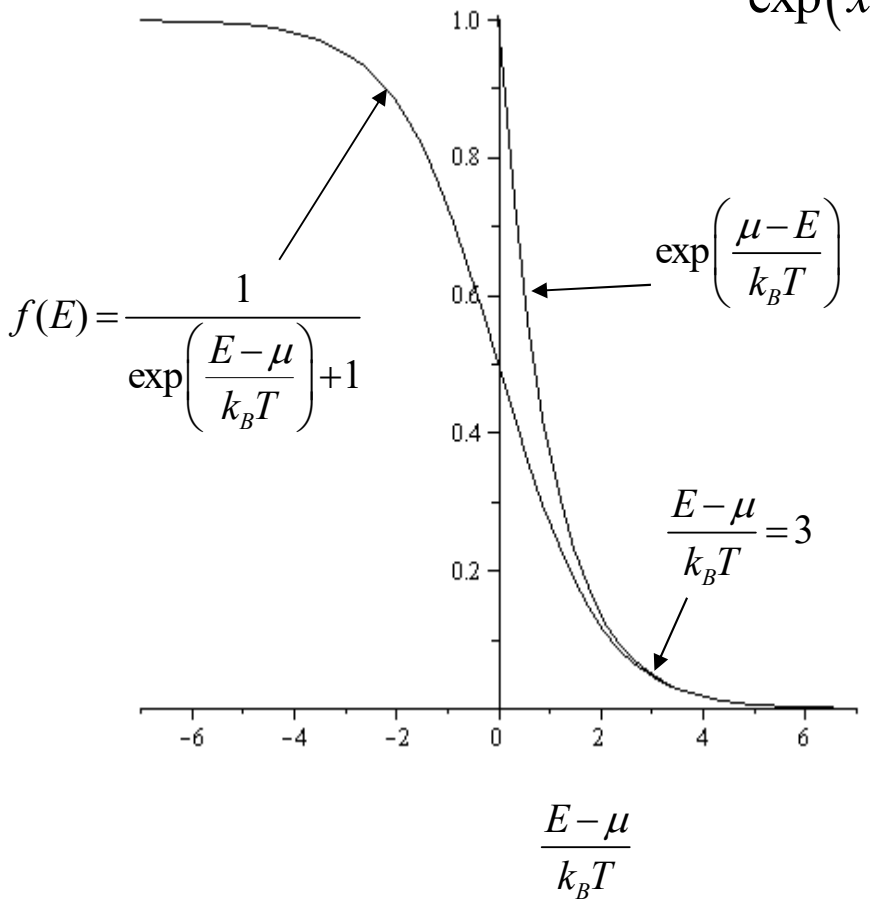






Boltzmann approximation

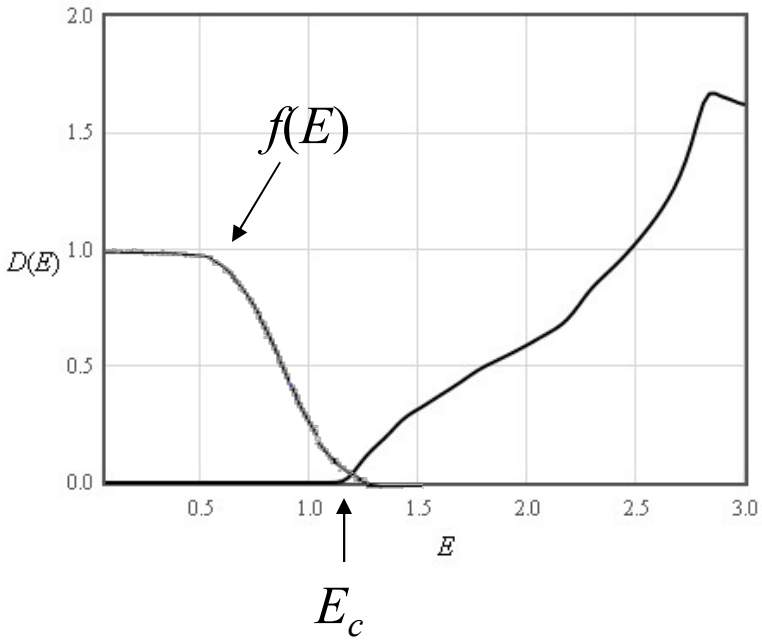
$$\frac{1}{\exp(x)+1} \approx \exp(-x) \quad \text{for } x > 3$$



Density of electrons in the conduction band

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

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



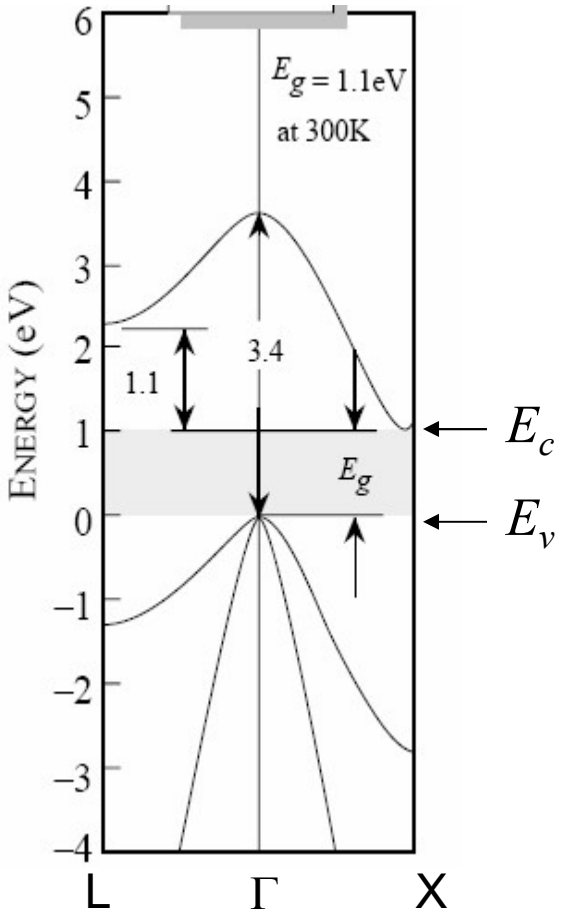
for $\frac{E-\mu}{k_B T} > 3$ $\qquad f(E) \approx \exp\left(\frac{\mu-E}{k_B T}\right)$ Boltzmann approximation

$$n \approx \frac{\pi}{2}\left(\frac{2m^*}{\hbar^2\pi^2}\right)^{3/2} \int_{E_c}^{\infty} \exp\left(\frac{\mu-E}{k_B T}\right)\sqrt{E-E_c}\,dE = \frac{\pi}{2}\left(\frac{2m^* k_B T}{\hbar^2\pi^2}\right)^{3/2} \exp\left(\frac{\mu-E_c}{k_B T}\right)\int_0^{\infty} \exp(-x)\sqrt{x}\,dx$$

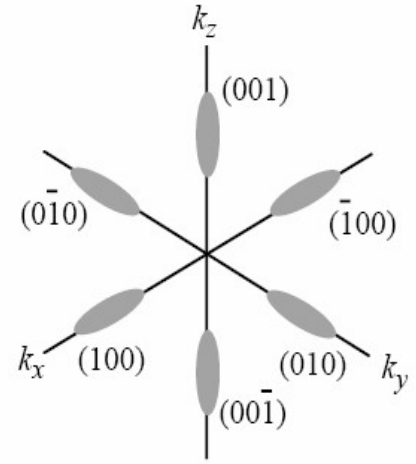
$$x = \frac{E-E_c}{k_B T} \qquad \int_0^{\infty} \sqrt{x} e^{-x} dx = \frac{\sqrt{\pi}}{2}$$

$$n \approx 2\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)^{3/2} \exp\left(\frac{\mu-E_c}{k_B T}\right) = N_c(T) \exp\left(\frac{\mu-E_c}{k_B T}\right)$$

Density of electrons in the conduction band



$$n = 2\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T}\right)$$

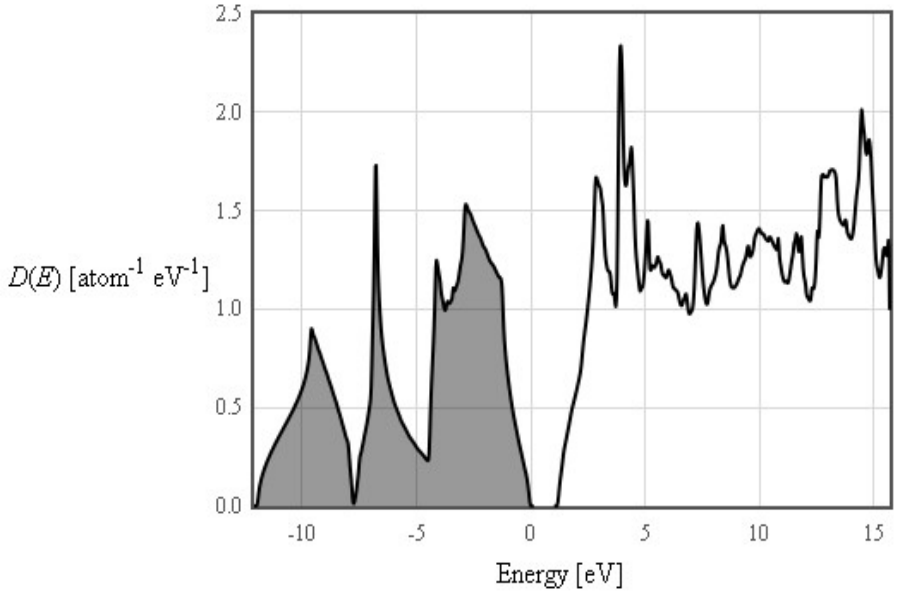


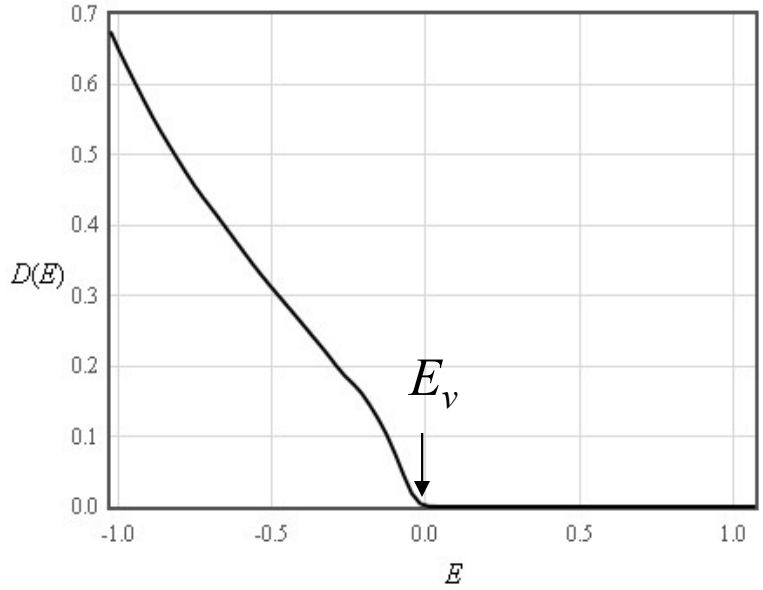
$$n = N_c\left(\frac{T}{300}\right)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T}\right)$$

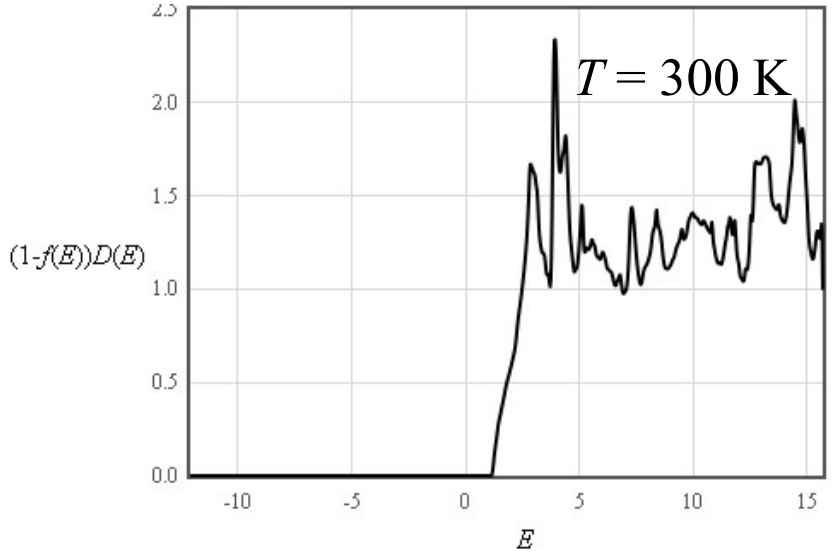
N_c = effective density of states in conduction band

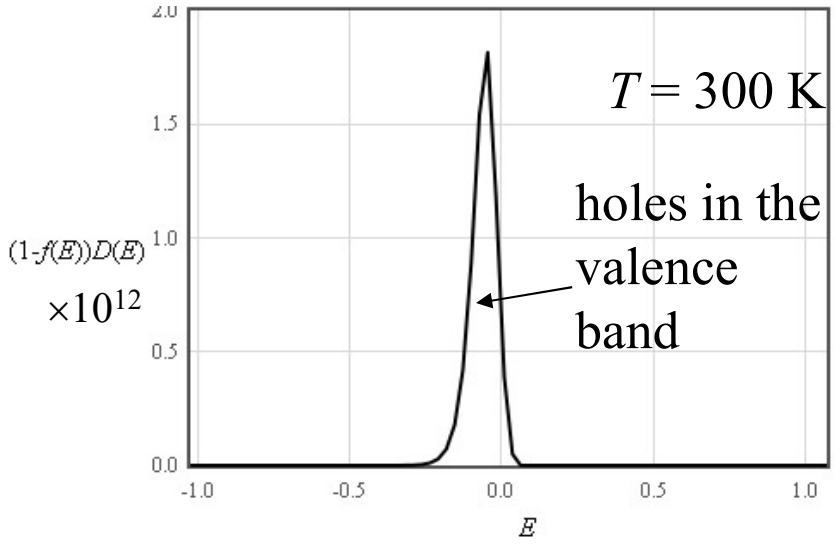
Properties	Si	Ge	GaAs
Bandgap E_g	1.12 eV	0.66 eV	1.424 eV
Effective density of states in conduction band (300 K) N_c	2.78×10^{25} m^{-3}	1.04×10^{25} m^{-3}	4.45×10^{23} m^{-3}

Silicon density of states



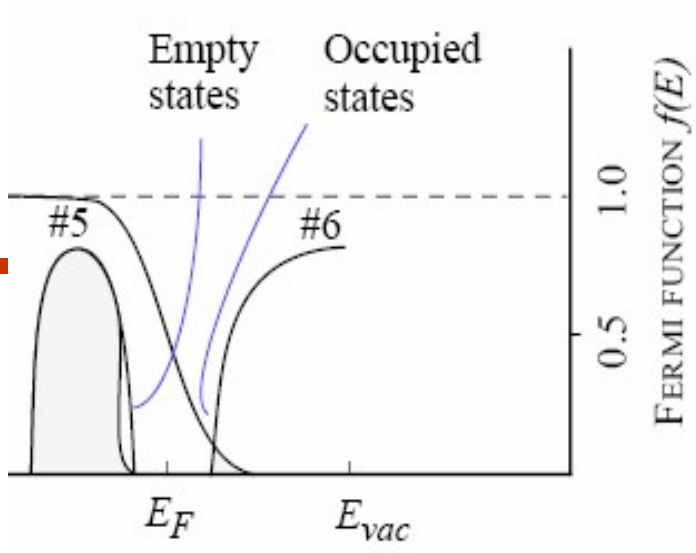






Density of holes in the valence band

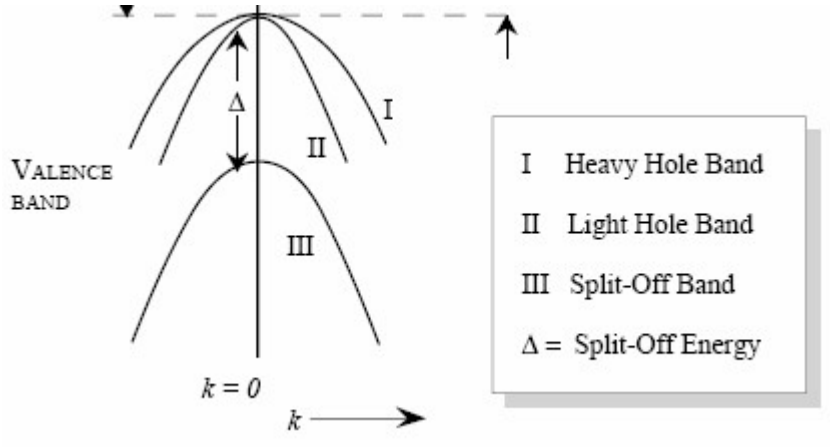
$$p = \int_{-\infty}^{E_v} D(E)\left(1 - f(E)\right) dE$$



for $\frac{E-\mu}{k_B T} < -3$ $\qquad 1 - f(E) \approx \exp\left(\frac{E-\mu}{k_B T}\right)$ $\qquad$ Boltzmann approximation

$$p \approx \frac{\pi}{2}\left(\frac{2m^*}{\hbar^2\pi^2}\right)^{3/2} \int_{-\infty}^{E_v} \exp\left(\frac{E-\mu}{k_B T}\right)\sqrt{E_v - E}\, dE = 2\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)^{3/2} \exp\left(\frac{E_v - \mu_c}{k_B T}\right) = N_v(T)\exp\left(\frac{E_v - \mu}{k_B T}\right)$$

Density of electrons in the conduction band
Density of holes in the valence band



$$n = N_c \left(\frac{T}{300} \right)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T} \right)$$

$$p = N_v \left(\frac{T}{300} \right)^{3/2} \exp\left(\frac{E_v - \mu}{k_B T} \right)$$

Properties	Si	Ge	GaAs
Bandgap E_g	1.12 eV	0.66 eV	1.424 eV
Effective density of states in conduction band (300 K) N_c	2.78×10^{25} m^{-3}	1.04×10^{25} m^{-3}	4.45×10^{23} m^{-3}
Effective density of states in valence band (300 K) N_v	9.84×10^{24} m^{-3}	6.0×10^{24} m^{-3}	7.72×10^{24} m^{-3}
Effective mass electrons m^*/m_0	$m_l^* = 0.98$ $m_t^* = 0.19$	$m_l^* = 1.64$ $m_t^* = 0.082$	$m^* = 0.067$
Effective mass holes m^*/m_0	$m_{lh}^* = 0.16$ $m_{hh}^* = 0.49$	$m_{lh}^* = 0.044$ $m_{hh}^* = 0.28$	$m_{lh}^* = 0.082$ $m_{hh}^* = 0.45$
Crystal structure	diamond	diamond	zincblende
Density	2.328 g/cm³	5.3267 g/cm³	5.32 g/cm³
Atoms/m³	5.0×10^{28}	4.42×10^{28}	4.42×10^{28}

Semiconductors

density of electrons in the conduction band

$$n = N_c \left(\frac{T}{300} \right)^{\frac{3}{2}} \exp\left(\frac{\mu - E_c}{k_B T} \right)$$

effective density of states in the conduction band at 300 K

density of holes in the valence band

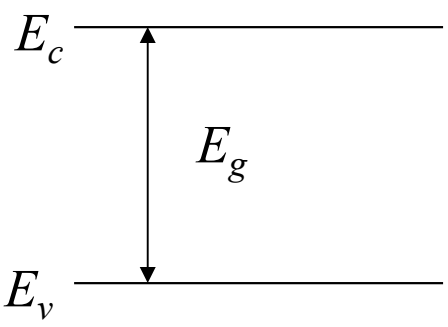
$$p = N_v \left(\frac{T}{300} \right)^{\frac{3}{2}} \exp\left(\frac{E_v - \mu}{k_B T} \right)$$

effective density of states in the valence band at 300 K

Law of mass action

$$np = N_c \exp\left(\frac{\mu - E_c}{k_B T}\right) N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

$$np = N_c N_v \exp\left(\frac{-E_g}{k_B T}\right)$$

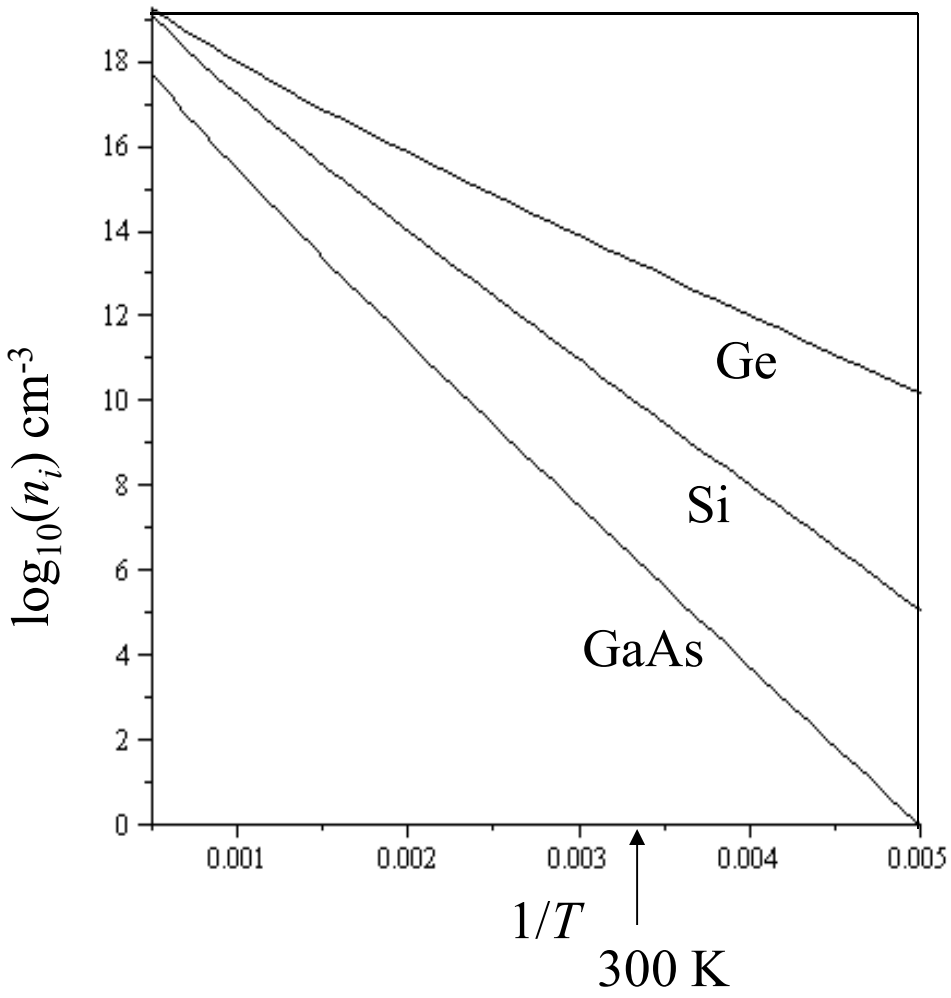


For intrinsic semiconductors (no impurities)

$$n = p = n_i = \sqrt{N_c N_v} \exp\left(\frac{-E_g}{2k_B T}\right)$$

intrinsic carrier density

Intrinsic carrier concentration



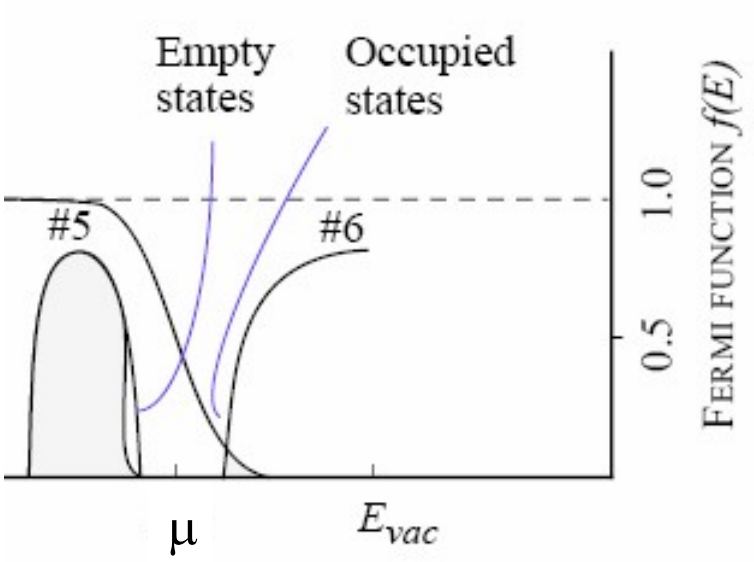
$$n_i = \sqrt{N_v N_c \left(\frac{T}{300}\right)^3} \exp\left(-\frac{E_g}{2k_B T}\right)$$

$\sim 5 \times 10^{22}$ atoms/cm^3

Chemical potential of an intrinsic semiconductor

$$n = p = N_c \exp\left(\frac{\mu - E_c}{k_B T}\right) = N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

$$\exp\left(\frac{\mu - E_c - E_v + \mu}{k_B T}\right) = \frac{N_v}{N_c}$$



$$\frac{2\mu}{k_B T} = \frac{E_c + E_v}{k_B T} + \ln\left(\frac{N_v}{N_c}\right)$$

$$\boxed{\mu = \frac{E_c + E_v}{2} + \frac{k_B T}{2} \ln\left(\frac{N_v}{N_c}\right)}$$

E_c ——————

μ ----------

E_v ——————

Properties	Si	Ge	GaAs
Bandgap E_g	1.12 eV	0.66 eV	1.424 eV
Effective density of states in conduction band (300 K) N_c	2.78×10^{25} m^{-3}	1.04×10^{25} m^{-3}	4.45×10^{23} m^{-3}
Effective density of states in valence band (300 K) N_v	9.84×10^{24} m^{-3}	6.0×10^{24} m^{-3}	7.72×10^{24} m^{-3}

Boltzmann approximation

The table below gives the contribution of electrons in intrinsic semiconductors and insulators to some thermodynamic quantities. These results where calculated in the Boltzmann approximation where it is assumed that the chemical potential lies in the band gap more than $3k_BT$ from the band edge. The electronic contribution to the thermodynamic quantities are usually much smaller than the contribution of the phonons and thus the electronic components are often simply ignored.

	1-d	2-d	3-d
Density of states	$D(E)=\begin{cases}\frac{1}{\hbar\pi}\sqrt{\frac{2m_h^*}{(E_v-E)}} & E<E_v\\ 0 & E_v<E<E_c\\ \frac{1}{\hbar\pi}\sqrt{\frac{2m_e^*}{(E-E_c)}} & E>E_c\end{cases}$ J^{-1} m^{-1}	$D(E)=\begin{cases}\frac{m_h^*}{\hbar^2\pi}H(E_v-E) & E<E_v\\ 0 & E_v<E<E_c\\ \frac{m_e^*}{\hbar^2\pi}H(E-E_c) & E>E_c\end{cases}$ J^{-1} m^{-2} $H(x)=0$ for $x<0$ and $H(x)=1$ for $x>0$	$D(E)=\begin{cases}\frac{\left(2m_h^*\right)^{\frac{3}{2}}}{2\pi^2\hbar^3}\sqrt{E_v-E} & E<\\ 0 & E_v<E<E_\\ \frac{\left(2m_e^*\right)^{\frac{3}{2}}}{2\pi^2\hbar^3}\sqrt{E-E_c} & E>\end{cases}$
Density of electrons in the conduction band $n=\int_{E_c}^{\infty}D(E)f(E)dE$	$n=\sqrt{\frac{m_e^*k_BT}{\hbar^2\pi}}\exp\left(\frac{\mu-E_c}{k_BT}\right)$ m^{-1}	$n=\frac{m_e^*k_BT}{\hbar^2\pi}\exp\left(\frac{\mu-E_c}{k_BT}\right)$ m^{-2}	$n=\frac{1}{\sqrt{2}}\left(\frac{m_e^*k_BT}{\pi\hbar^2}\right)^{3/2}\exp\left(\frac{\mu-E}{k_BT}\right.$
Density of holes in the valence band $p=\int_{-\infty}^{E_v}D(E)(1-f(E))dE$	$p=\sqrt{\frac{m_h^*k_BT}{\hbar^2\pi}}\exp\left(\frac{E_v-\mu}{k_BT}\right)$ m^{-1}	$p=\frac{m_h^*k_BT}{\hbar^2\pi}\exp\left(\frac{E_v-\mu}{k_BT}\right)$ m^{-2}	$p=\frac{1}{\sqrt{2}}\left(\frac{m_h^*k_BT}{\pi\hbar^2}\right)^{3/2}\exp\left(\frac{E_v-}{k_BT}\right.$
Law of mass action	$np=\frac{k_BT}{\hbar^2\pi}\sqrt{m_e^*m_h^*}\exp\left(\frac{-E_g}{k_BT}\right)$ m^{-2}	$np=\left(\frac{k_BT}{\pi\hbar^2}\right)^2m_e^*m_h^*\exp\left(\frac{-E_g}{k_BT}\right)$ m^{-4}	$np=\frac{1}{2}\left(\frac{k_BT}{\pi\hbar^2}\right)^3\left(m_e^*m_h^*\right)^{3/2}\exp\left(\frac{-}{k_B}\right.$
Intrisic carrier density $n_i=\sqrt{np}$	$n_i=\sqrt{\frac{k_BT}{\hbar^2\pi}}\left(m_e^*m_h^*\right)^{1/4}\exp\left(\frac{-E_g}{2k_BT}\right)$ m^{-1}	$n_i=\frac{k_BT}{\pi\hbar^2}\sqrt{m_e^*m_h^*}\exp\left(\frac{-E_g}{2k_BT}\right)$ m^{-2}	$n_i=\frac{1}{\sqrt{2}}\left(\frac{k_BT}{\pi\hbar^2}\right)^{3/2}\left(m_e^*m_h^*\right)^{3/4}\exp\left(\frac{-}{2}\right.$
Chemical potential Set $n=p$, solve for μ	$\mu=\frac{E_v+E_c}{2}-\frac{k_BT}{4}\ln\left(\frac{m_e^*}{m_h^*}\right)$ J	$\mu=\frac{E_v+E_c}{2}-\frac{k_BT}{2}\ln\left(\frac{m_e^*}{m_h^*}\right)$ J	$\mu=\frac{E_v+E_c}{2}-\frac{3}{4}k_BT\ln\left(\frac{m_e^*}{m_h^*}\right.$
Internal energy density $u=\int_{-\infty}^{\infty}ED(E)f(E)dE$	$u=u(T=0)+\sqrt{\frac{2k_BT}{\hbar^2\pi}}\left(m_e^*m_h^*\right)^{1/4}\exp\left(\frac{-E_g}{2k_BT}\right)\left(E_g+k_BT\right)$ J m^{-1}	$u=u(T=0)+\frac{k_BT}{\hbar^2\pi}\sqrt{m_e^*m_h^*}\exp\left(\frac{-E_g}{2k_BT}\right)\left(E_g+2k_BT\right)$ J m^{-2}	$u=u(T=0)+\frac{\sqrt{2\pi}}{2\pi^2\hbar^3}\left(m_e^*m_h^*\right)^{3/4}\exp\left(\frac{-E_g}{2k_BT}\right)\left(k_B\right.$
Helmholtz free energy $f=u-Ts$	$f=u(T=0)-2\sqrt{\frac{2k_B}{\hbar^2\pi}}\left(m_e^*m_h^*\right)^{1/4}\exp\left(\frac{-E_g}{2k_BT}\right)k_BT^{3/2}$ J m^{-1}	$f=u(T=0)-\frac{2\sqrt{m_e^*m_h^*}}{\hbar^2\pi}k_B^2T^2\exp\left(\frac{-E_g}{2k_BT}\right)$ J m^{-2}	$f=u(T=0)-\frac{\sqrt{2\pi}}{\pi^2\hbar^3}\left(m_e^*m_h^*\right)^{3/4}\left(k_BT\right)^{5/2}$ e
Specific heat $C_v=\left(\frac{\partial u}{\partial T}\right)_{V=const}$	$C_v=\sqrt{\frac{2k_B}{\hbar^2\pi}}\left(m_e^*m_h^*\right)^{1/4}\exp\left(\frac{-E_g}{2k_BT}\right)\left(\frac{E_g^2\sqrt{T}}{2k_BT^2}+\frac{E_g}{\sqrt{T}}+\frac{3k_B\sqrt{T}}{2}\right)$ J K^{-1} m^{-1}	$C_v=\frac{\sqrt{m_e^*m_h^*}}{\hbar^2\pi}\exp\left(\frac{-E_g}{2k_BT}\right)\left(\frac{E_g^2}{2T}+2k_BE_g+4k_B^2T\right)$ J K^{-1} m^{-2}	$C_v=\frac{\sqrt{2\pi}}{2\pi^2\hbar^3}\left(m_e^*m_h^*\right)^{3/4}\exp\left(\frac{-E_g}{2k_BT}\right)\left(k_BT\right)^{3/2}\left(\frac{15}{2}k_B\right.$
Entropy $s=\int\frac{C_v}{T}dT$	$s=\sqrt{\frac{2k_B}{\hbar^2\pi}}\left(m_e^*m_h^*\right)^{1/4}\exp\left(\frac{-E_g}{2k_BT}\right)\left(\frac{E_g}{\sqrt{T}}+3k_B\sqrt{T}\right)$ J K^{-1} m^{-1}	$s=\frac{\sqrt{m_e^*m_h^*}}{\hbar^2\pi}\exp\left(\frac{-E_g}{2k_BT}\right)\left(k_BE_g+4k_B^2T\right)$ J K^{-1} m^{-2}	$s=\frac{\sqrt{2\pi}}{2\pi^2\hbar^3}\left(m_e^*m_h^*\right)^{3/4}\exp\left(\frac{-E_g}{2k_BT}\right)\left(k_BT\right)^{3/2}\left($

Intrinsic semiconductors

In the Boltzmann approximation, the density of states of a semiconductor is,

$$D(E) = \begin{cases} \frac{(2m_h^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{E_v - E}, & \text{if } E < E_v \\ 0, & \text{if } E_v < E < E_c \\ \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{E - E_c}, & \text{if } E_c < E \end{cases}$$

Here m_e^* and m_h^* are the 'density of states effective masses' for electrons and holes. Usually in the literature, effective density of states at 300 K is given instead of the 'density of states effective masses'. The relationship between the two is,

$$m_h^* = \frac{\pi\hbar^2}{300k_B}\left(\sqrt{2}N_v(300)\right)^{2/3}$$

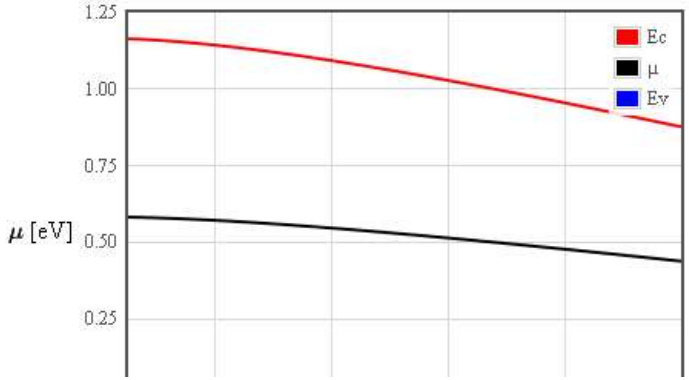
$$m_e^* = \frac{\pi\hbar^2}{300k_B}\left(\sqrt{2}N_c(300)\right)^{2/3}$$

In an intrinsic semiconductor, the density of electrons equals the density of holes, $n = p = n_i = \sqrt{N_c\left(\frac{T}{300}\right)^{3/2} N_v\left(\frac{T}{300}\right)^{3/2}}\exp\left(\frac{-E_g}{2k_BT}\right)$.

By setting the concentration of electrons equal to the concentration of holes, it is possible to solve for the chemical potential. The bandgap of most semiconductors is temperature dependent. The form below lets you input the temperature dependance of the bandgap. The bandgaps for some semiconductors can be loaded into the form with the buttons on the right.

$$n = N_c(300)\left(\frac{T}{300}\right)^{3/2}\exp\left(\frac{\mu - E_c}{k_BT}\right) = p = N_v(300)\left(\frac{T}{300}\right)^{3/2}\exp\left(\frac{E_v - \mu}{k_BT}\right).$$

$$\mu = \frac{E_v + E_c}{2} + k_BT\ln\left(\frac{N_v(300)}{N_c(300)}\right).$$



$N_c(300\text{ K}) =$ 2.78E19 1/cm³

$N_v(300\text{ K}) =$ 9.84E18 1/cm³

$E_g =$ 1.166-4.73E-4*T*T/(T+636) eV

$T_1 =$ 50 K

$T_2 =$ 1000 K

Replot

Semiconductor

Si Ge GaAs

http://lamp.tu-graz.ac.at/~hadley/ss1/semiconductors/intrinsic.php