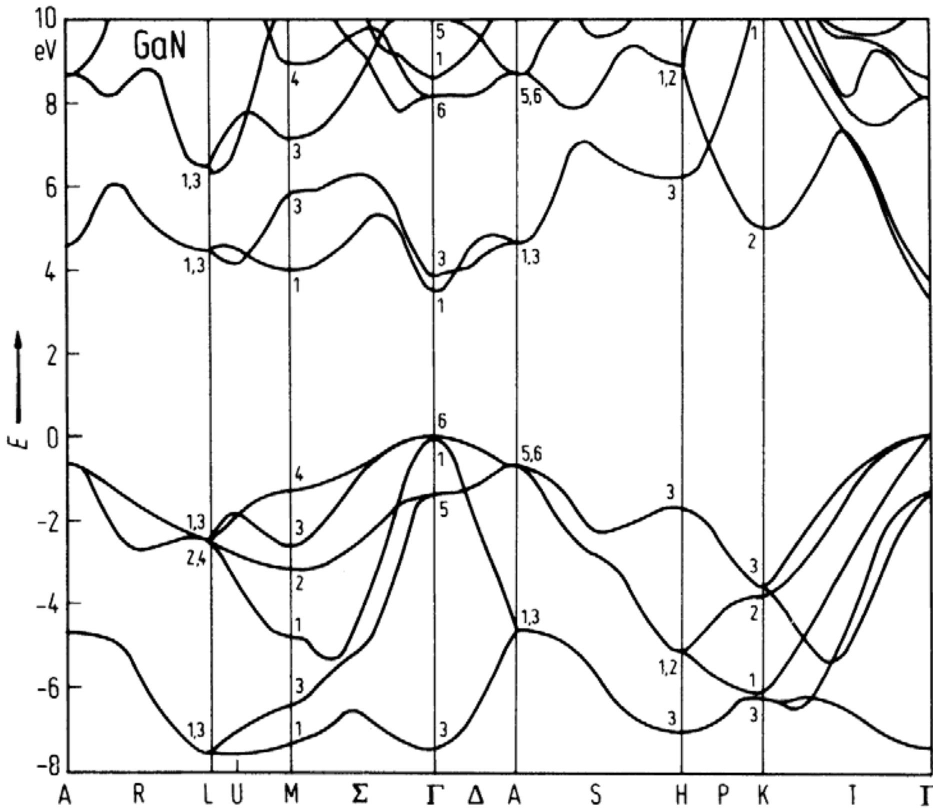
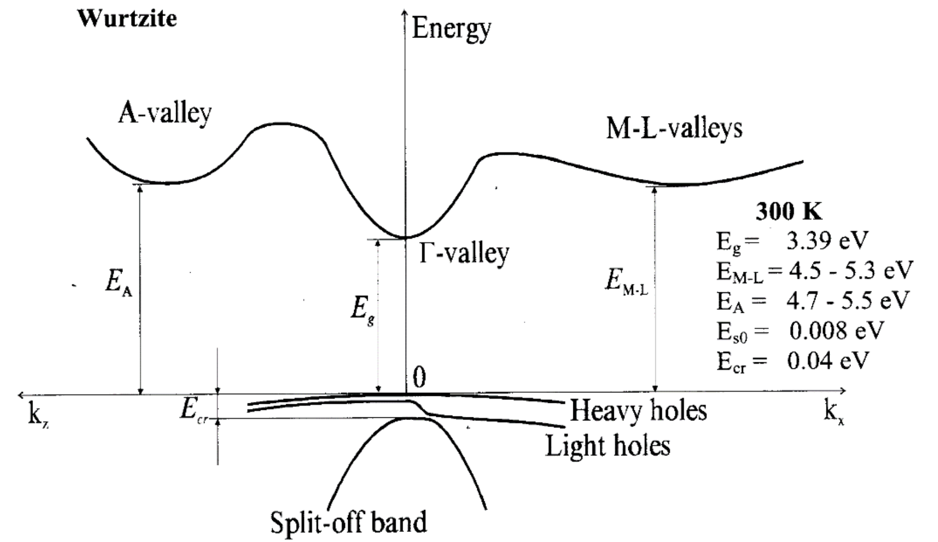
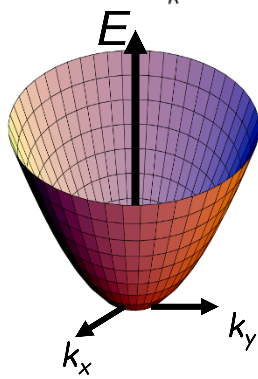
25. Semiconductors

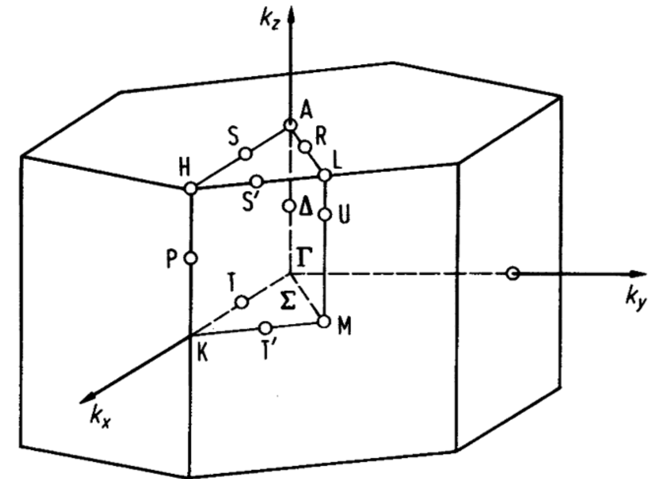
June 26, 2018

GaN









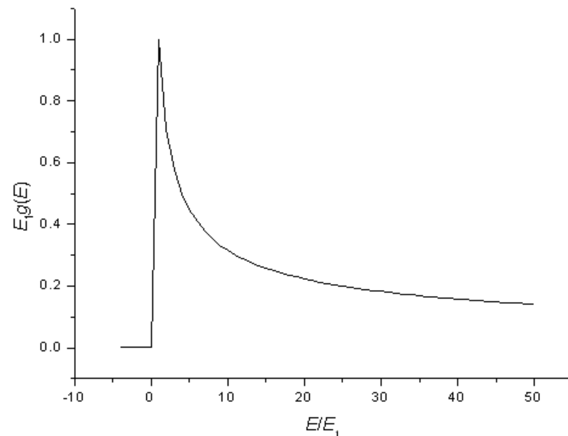
1st Brillioun zone of hcp

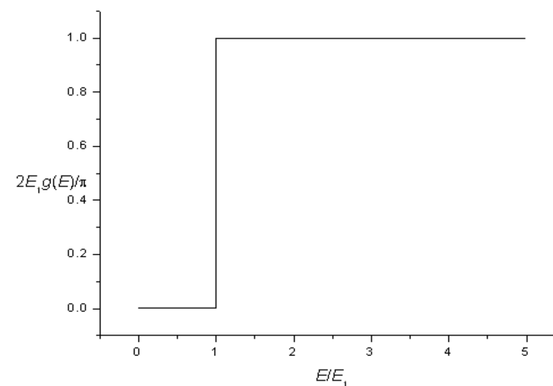
Free electron Fermi gas

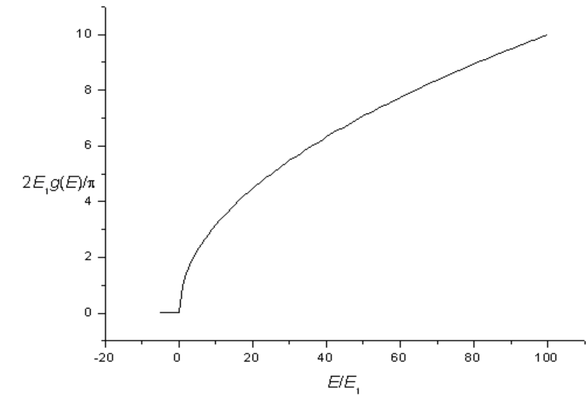
1 - d $$D(E) = \sqrt{\frac{2m}{\hbar^2 \pi^2 E}} = \frac{n}{2\sqrt{E_F E}} \quad \text{J}^{-1}\text{m}^{-1}$$

2 - d $$D(E) = \frac{m}{\hbar^2 \pi} = \frac{n}{E_F} \quad \text{J}^{-1}\text{m}^{-2}$$

3 - d $$D(E) = \frac{\pi}{2}\left(\frac{2m}{\hbar^2 \pi^2}\right)^{3/2}\sqrt{E} = \frac{3n}{2E_F^{3/2}}\sqrt{E} \quad \text{J}^{-1}\text{m}^{-3}$$



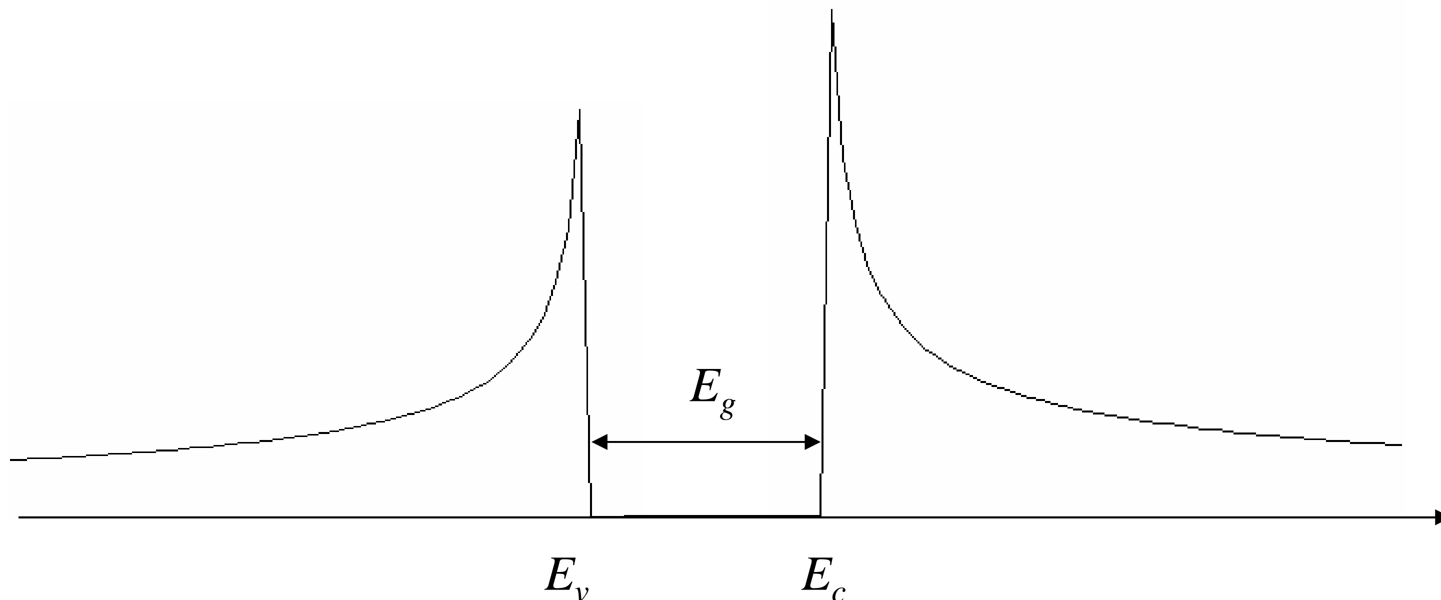




Semiconductors and insulators - 1d

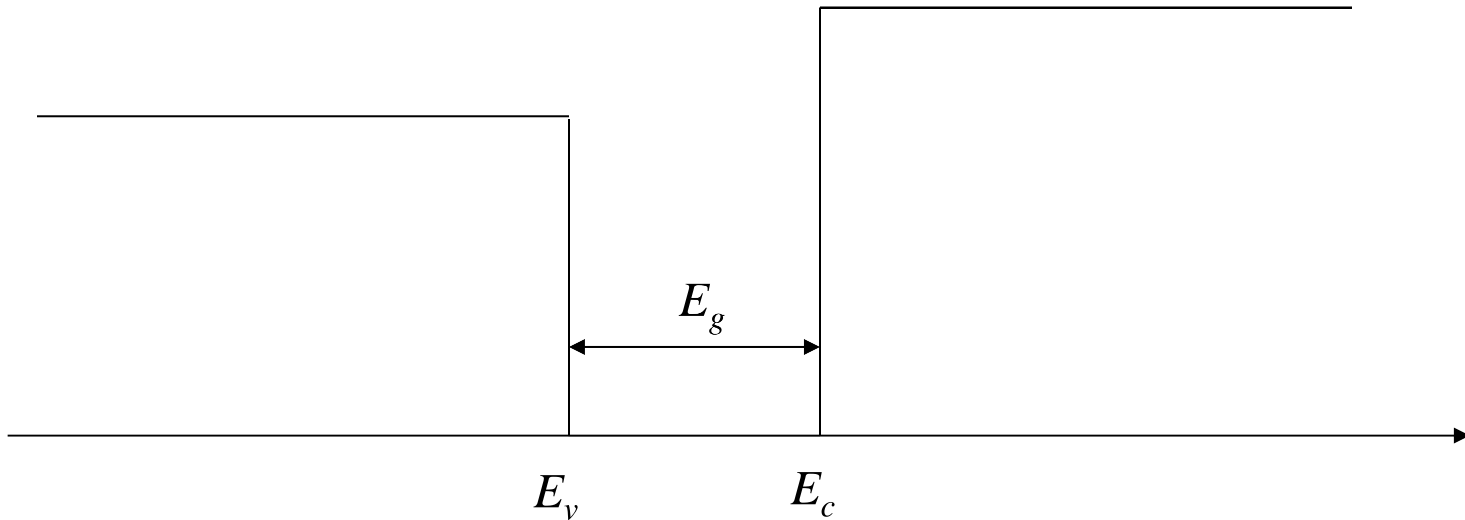
$$E = \frac{\hbar^2 (\vec{k} - \vec{k}_0)^2}{2m^*}$$

$$D(E) = \begin{cases} \dfrac{D_c}{\sqrt{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \dfrac{D_v}{\sqrt{(E - E_c)}} & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$



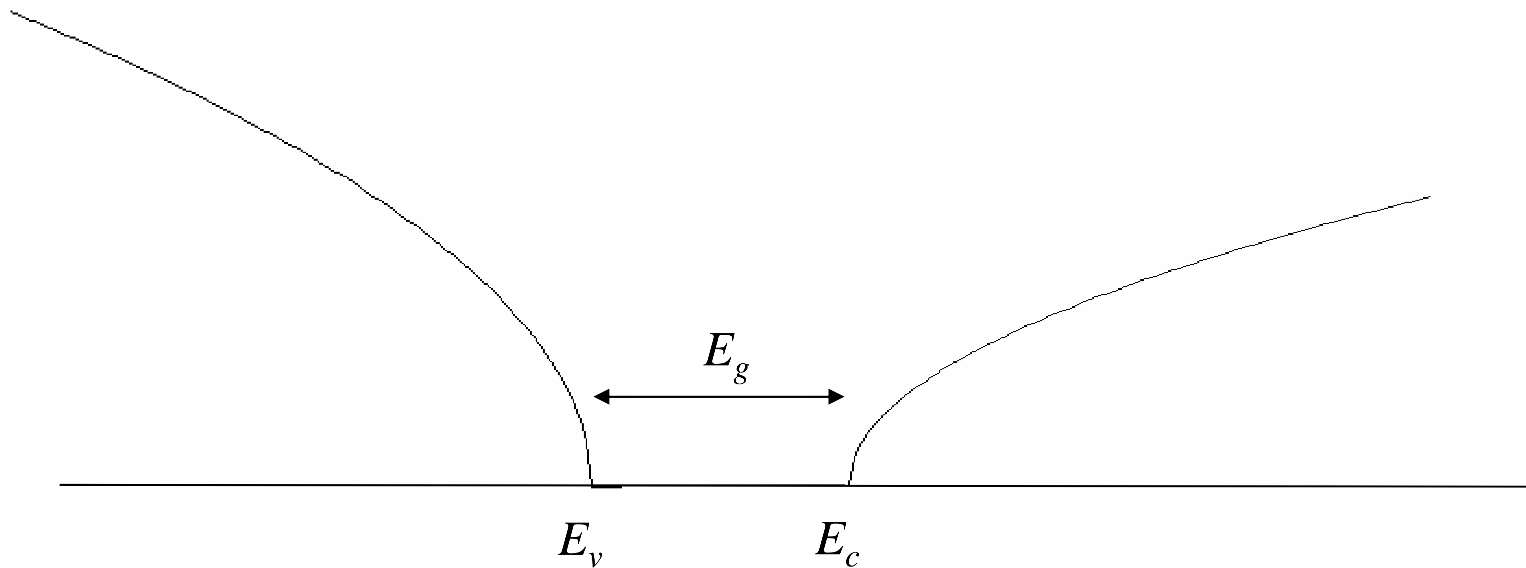
Semiconductors and insulators - 2d

$$D(E) = \begin{cases} D_c & E < E_v \\ 0 & E_v < E < E_c \\ D_v & E_c < E \end{cases} \quad \mathrm{J^{-1}m^{-3}}$$

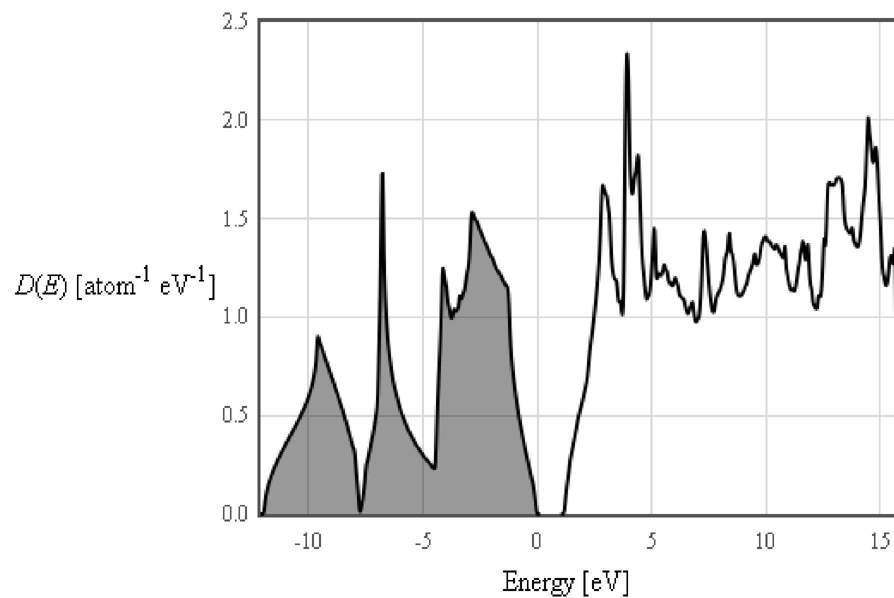


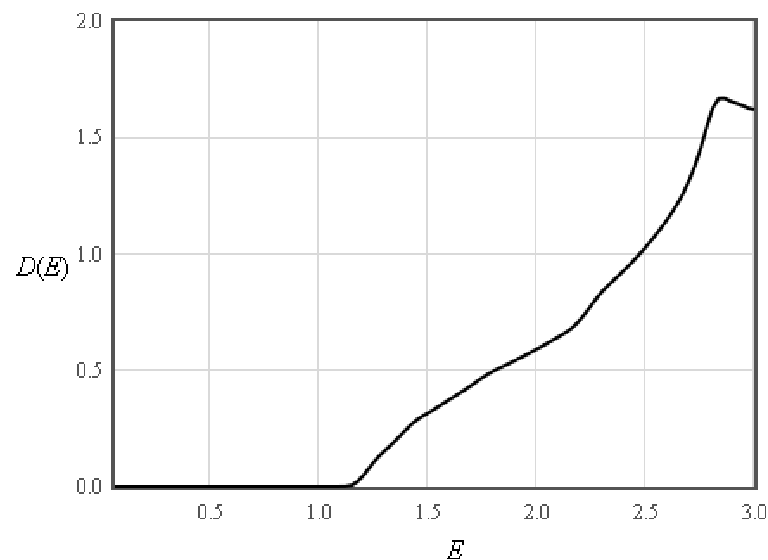
Semiconductors and insulators - 3d

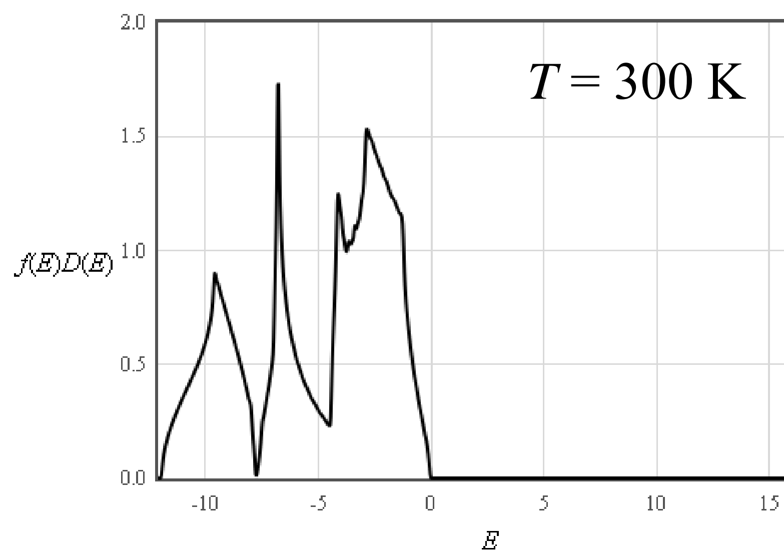
$$D(E) = \begin{cases} D_c\sqrt{E_v - E} & E < E_v \\ 0 & E_v < E < E_c \\ D_v\sqrt{E - E_c} & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$

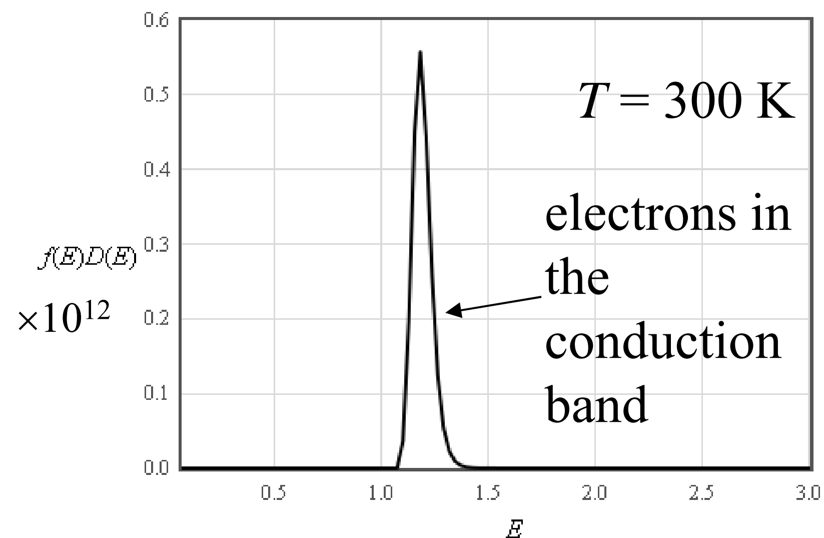


Silicon density of states







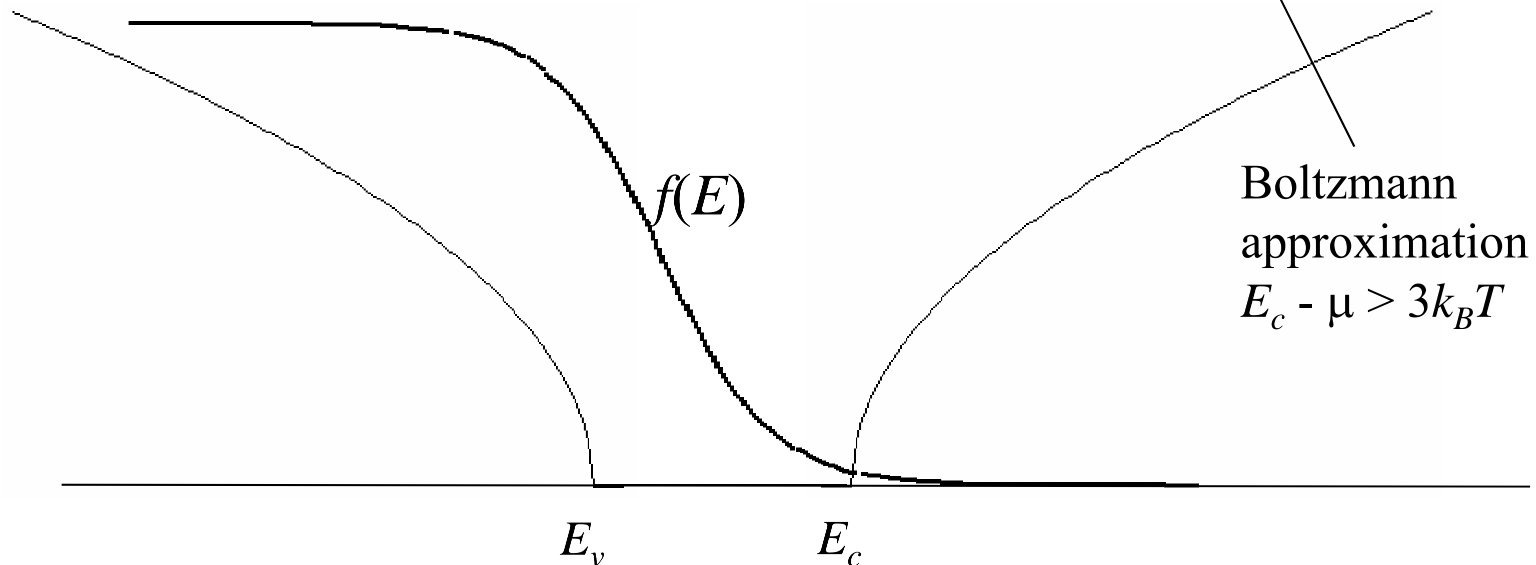


Density of electrons in the conduction band

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

$$D(E) = D_c\sqrt{E - E_c}$$

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



$$n = \int_{E_c}^{\infty} D(E) f(E) dE \approx D_c \int_{E_c}^{\infty} \exp\left(\frac{\mu - E}{k_B T}\right)\sqrt{E - E_c}\, dE$$

Density of electrons in the conduction band

$$n = \int_{E_c}^{\infty} D(E) f(E) dE \approx D_c \int_{E_c}^{\infty} \exp\left(\frac{\mu - E}{k_B T}\right) \sqrt{E - E_c}\, dE$$

$$x = E - E_c \qquad \int_0^{\infty} \sqrt{x} \exp\left(\frac{-x}{k_B T}\right) dx = \frac{2}{\sqrt{\pi}} \left(k_B T\right)^{3/2}$$

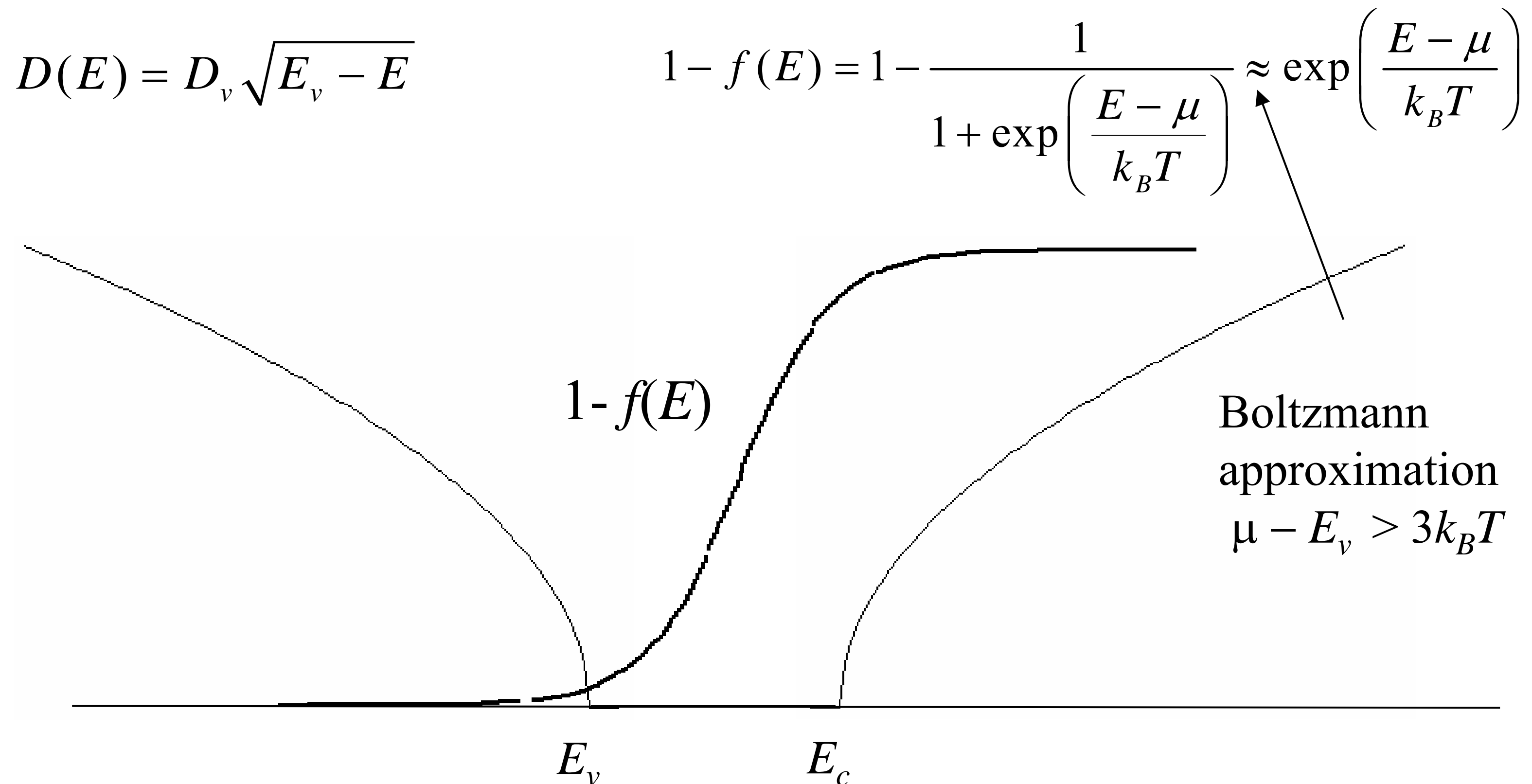
$$\boxed{n = N_c(T) \exp\left(\frac{\mu - E_c}{k_B T}\right)} = \frac{2D_c}{\sqrt{\pi}} \left(k_B T\right)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T}\right)$$

$$N_c = \frac{2D_c}{\sqrt{\pi}} \left(k_B T\right)^{3/2} = 2\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)^{3/2} \quad = \text{effective density of states}$$

Density of holes in the valence band

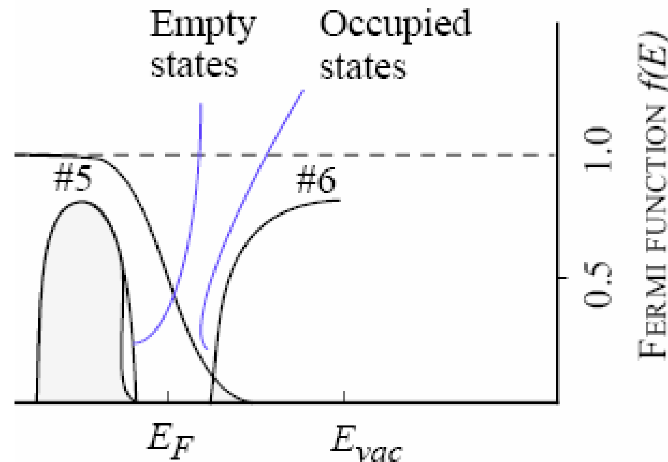
$$D(E) = D_v\sqrt{E_v - E}$$

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



$$p = \int_{-\infty}^{E_v} D(E)\left(1 - f(E)\right)dE \approx D_v \int_{-\infty}^{E_v} \exp\left(\frac{E-\mu}{k_B T}\right)\sqrt{E_v - E}\,dE$$

Density of holes in the valence band



$$p = \int_{-\infty}^{E_v} D(E)\left(1 - f(E)\right) dE \approx D_v \int_{-\infty}^{E_v} \exp\left(\frac{E-\mu}{k_B T}\right)\sqrt{E_v - E}\, dE$$

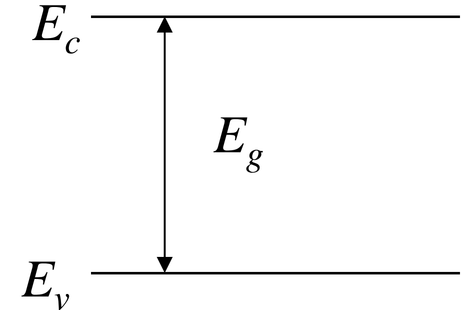
$$\boxed{p = N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)} = \frac{2D_v}{\sqrt{\pi}}\left(k_B T\right)^{3/2} \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

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

= Effective density of states in the valence band

Law of mass action

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



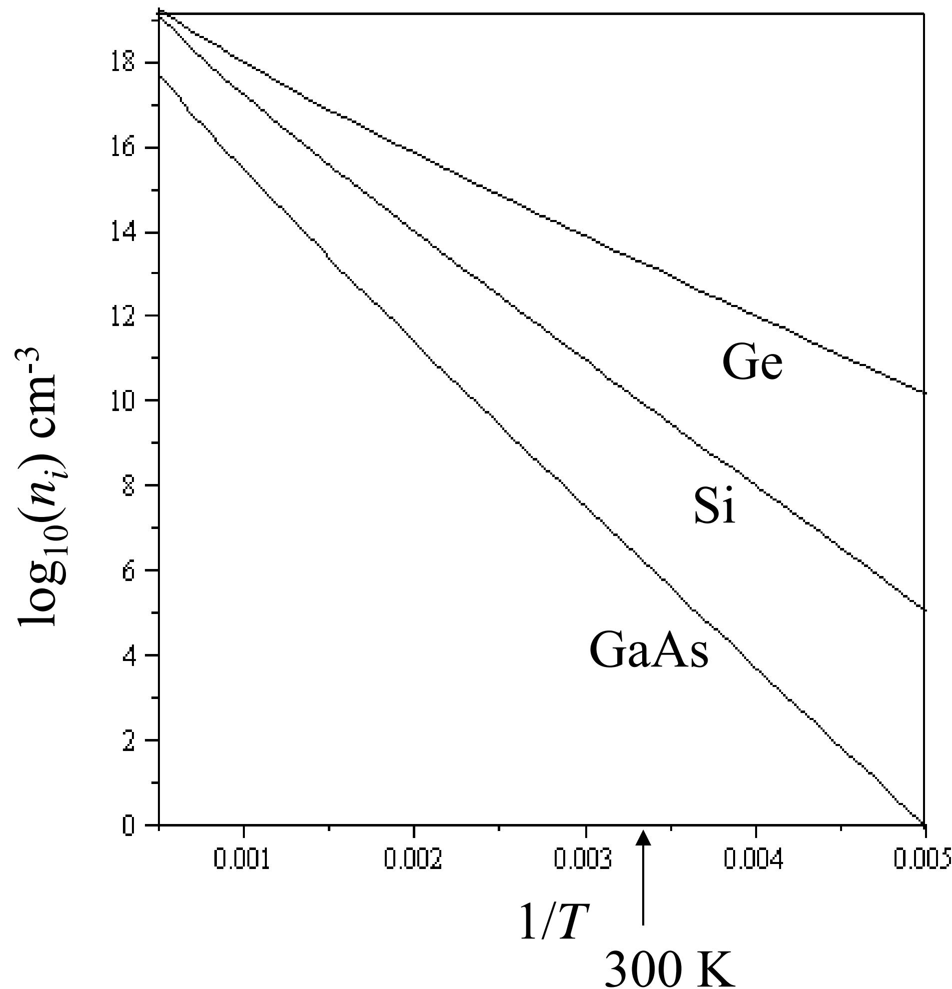
$$np = N_c N_v \exp\left(\frac{-E_g}{k_B T}\right)$$

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

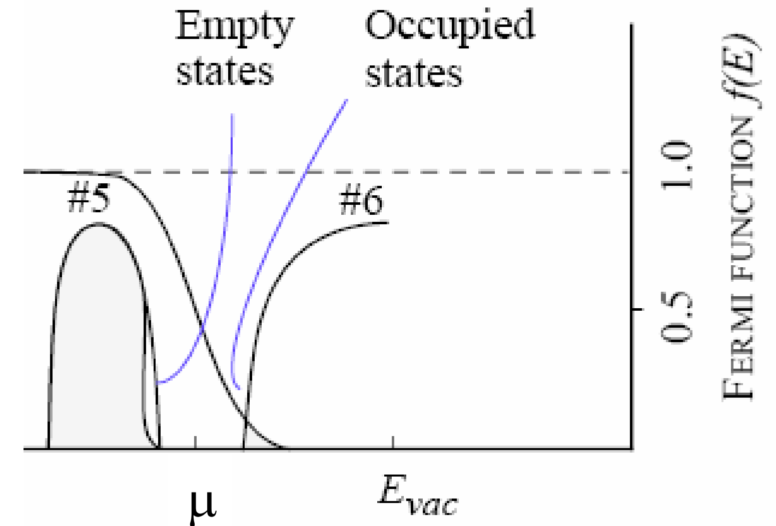


$$n_i = \sqrt{N_v N_c \left(\frac{T}{300}\right)^3} \exp\left(-\frac{E_g}{2k_B T}\right)$$

~ 5 x 10^{22} atoms/cm^3

Chemical potential of an intrinsic semiconductor

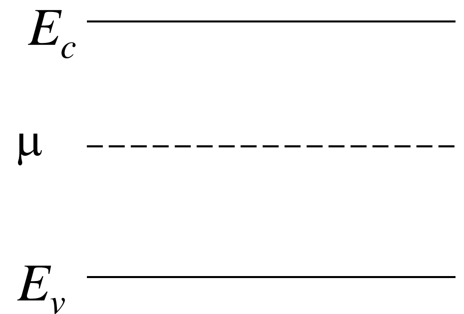
$$n = p = N_c \exp\left(\frac{\mu - E_c}{k_B T}\right) = N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)$$



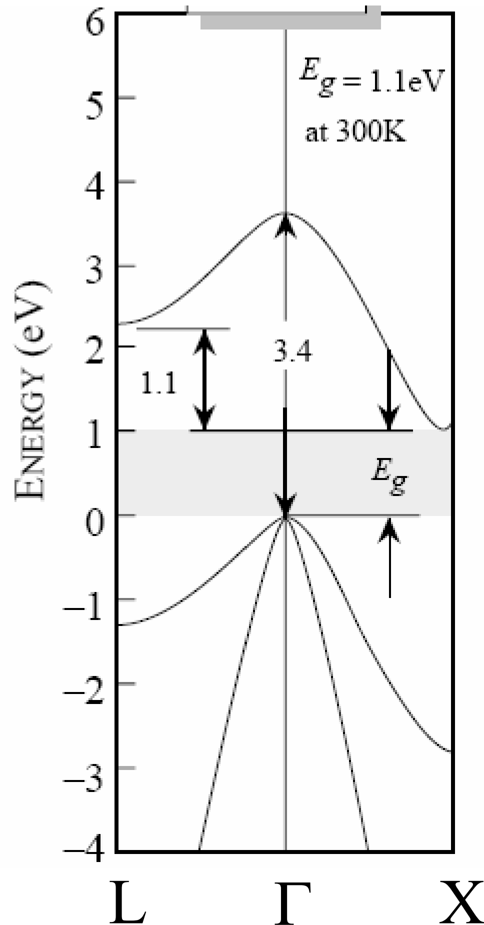
$$\exp\left(\frac{\mu - E_c - E_v + \mu}{k_B T}\right) = \frac{N_v}{N_c}$$

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

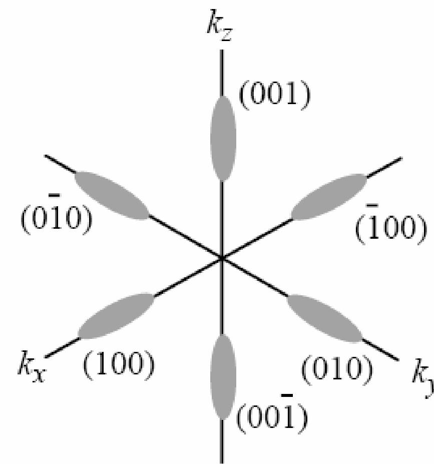
$$\boxed{\mu = \frac{E_c + E_v}{2} + \frac{k_B T}{2} \ln\left(\frac{N_v}{N_c}\right)}$$



Density of electrons in the conduction band



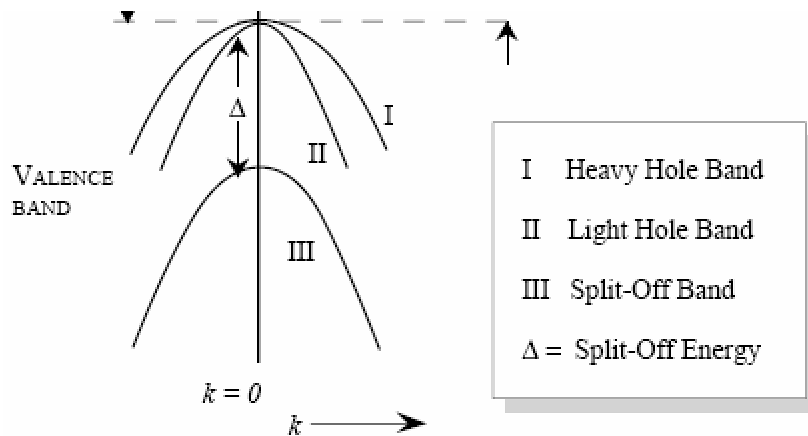
$$n = N_c(T)\exp\left(\frac{\mu - E_c}{k_B T}\right) = \frac{2D_v}{\sqrt{\pi}}(k_B T)^{3/2}\exp\left(\frac{\mu - E_c}{k_B T}\right)$$



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

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}

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}

The electrical contribution to the thermodynamic properties of insulators depend on band edges

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
Density of states m_e^* and m_h^* are 'density of states' effective masses	$D(E)=\begin{cases}\frac{1}{\hbar\pi}\sqrt{\frac{2m_h^*}{(E_v-E)}} & E<E_v\\ 0 & E_v<E<E_c\\ \frac{1}{\hbar\pi}\sqrt{\frac{2m_e^*}{(E-E_c)}} & E>E_c\end{cases}$ 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 $x>0$
Density of states N_v and N_c are the effective densities of states	$D(E)=\begin{cases}N_v(300)\sqrt{\frac{2}{300\pi k_B(E_v-E)}} & E<E_v\\ 0 & E_v<E<E_c\\ N_c(300)\sqrt{\frac{2}{300\pi k_B(E-E_c)}} & E>E_c\end{cases}$ J^{-1} m^{-1}	$D(E)=\begin{cases}\frac{N_v(300)}{300k_B}H(E_v-E) & E<E_v\\ 0 & E_v<E<E_c\\ \frac{N_c(300)}{300k_B}H(E-E_c) & E>E_c\end{cases}$ J^{-1} m^{-2}
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} $=N_c\exp\left(\frac{\mu-E_c}{k_BT}\right)$	$n=\frac{m_e^*k_BT}{\hbar^2\pi}\exp\left(\frac{\mu-E_c}{k_BT}\right)$ m^{-2} $=N_c\exp\left(\frac{\mu-E_c}{k_BT}\right)$
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} $=N_v\exp\left(\frac{\mu-E_c}{k_BT}\right)$	$p=\frac{m_h^*k_BT}{\hbar^2\pi}\exp\left(\frac{E_v-\mu}{k_BT}\right)$ m^{-2} $=N_v\exp\left(\frac{\mu-E_c}{k_BT}\right)$

Intrinsic semiconductors

Near the top of the valence band and the bottom of the conduction band the density of states of a semiconductor can be approximated as,

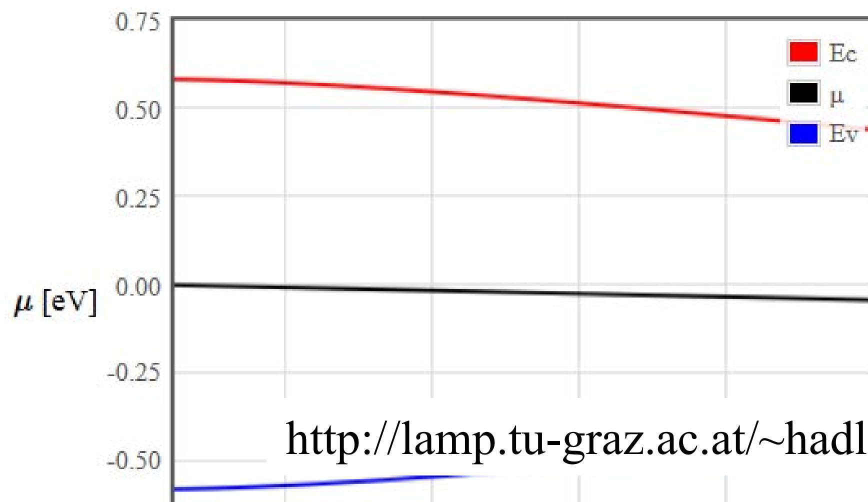
$$D(E) = \begin{cases} D_v\sqrt{E_v - E}, & \text{for } E < E_v \\ 0, & \text{for } E_v < E < E_c \\ D_c\sqrt{E - E_c}, & \text{for } E_c < E \end{cases}$$

Where D_v and D_c are constants that describe the form of the density of states near the band edges. Often in the literature, these constants are given in terms of the 'density of states effective masses' m_h^* and m_e^* or the 'effective density of states at 300 K' $N_v(300)$ and $N_c(300)$. To calculate m_h^* and m_e^* you determine D_v and D_c from a band structure calculation and then calculate the effect mass that would be needed to produce the same density of states from a dispersion relation consisting of a single isotropic parabola $E = \frac{\hbar^2 k^2}{2m^*}$.

$$D_v = \frac{(2m_h^*)^{3/2}}{2\pi^2\hbar^3} \qquad D_c = \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3}$$

In the Boltzmann approximation, the concentration of holes in the valence band p and electrons in the conduction band n are given by,

$$p = \frac{2D_v}{\sqrt{\pi}}\left(k_BT\right)^{3/2}\exp\left(\frac{E_v-\mu}{k_BT}\right), \qquad n = \frac{2D_c}{\sqrt{\pi}}\left(k_BT\right)^{3/2}\exp\left(\frac{\mu-E_c}{k_BT}\right).$$



$N_c(300\text{ K}) =$ 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

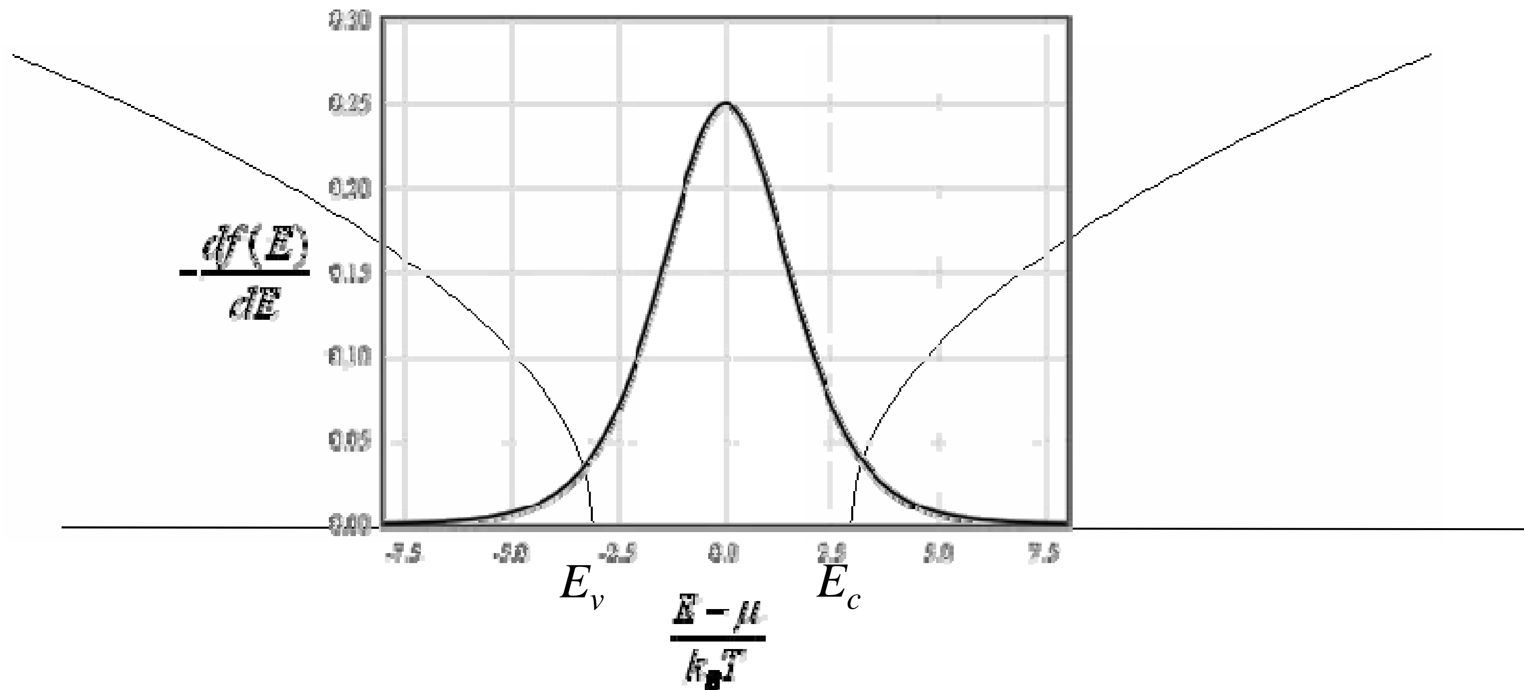
Semiconductor

Si | Ge | GaAs | GaP

InAs | InP | InSb

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

Narrow bandgap semiconductors



Use the programs for metals for small bandgap semiconductors.

www.ioffe.rssi.ru/SVA/NSM/Semicond/index.html

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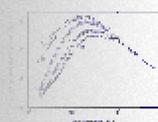
Semiconductors on NSM



Semiconductors | n, k database | InGaAsP | Equivalents

Si	- Silicon	Ge	- Germanium
GaP	- Gallium Phosphide	GaAs	- Gallium Arsenide
InAs	- Indium Arsenide	C	- Diamond
GaSb	- Gallium Antimonide	InSb	- Indium Antimonide
InP	- Indium Phosphide	$GaAs_{1-x}Sb_x$	- Gallium Arsenide Antimonide
$Al_xGa_{1-x}As$	- Aluminium Gallium Arsenide		
AlN	- Aluminium Nitride	InN	- Indium Nitride
BN	- Boron Nitride	GaN	- Gallium Nitride

We are going to add new data for:

$Ga_xIn_{1-x}As_ySb_{1-y}$	- Gallium Indium Arsenide Antimonide	$Ga_xIn_{1-x}P$	- Gallium Indium Phosphide
$Ga_xIn_{1-x}As$	- Gallium Indium Arsenide	$Ga_xIn_{1-x}Sb$	- Gallium Indium Antimonide
$InAs_{1-x}Sb_x$	- Indium Arsenide Antimonide	$Ga_xIn_{1-x}As_yP_{1-y}$	- Gallium Indium Arsenide Phosphide
$Si_{1-x}Ge_x$	- Silicon Germanium	SiC	- Silicon Carbide

Effective Masses

Electrons:

The surfaces of equal energy are ellipsoids.

$m_l = 0.98m_o$

$m_t = 0.19m_o$

Effective mass of density of states $m_c = 0.36m_o$

There are 6 equivalent valleys in the conduction band.

$m_{cc} = 0.26m_o$

Holes:

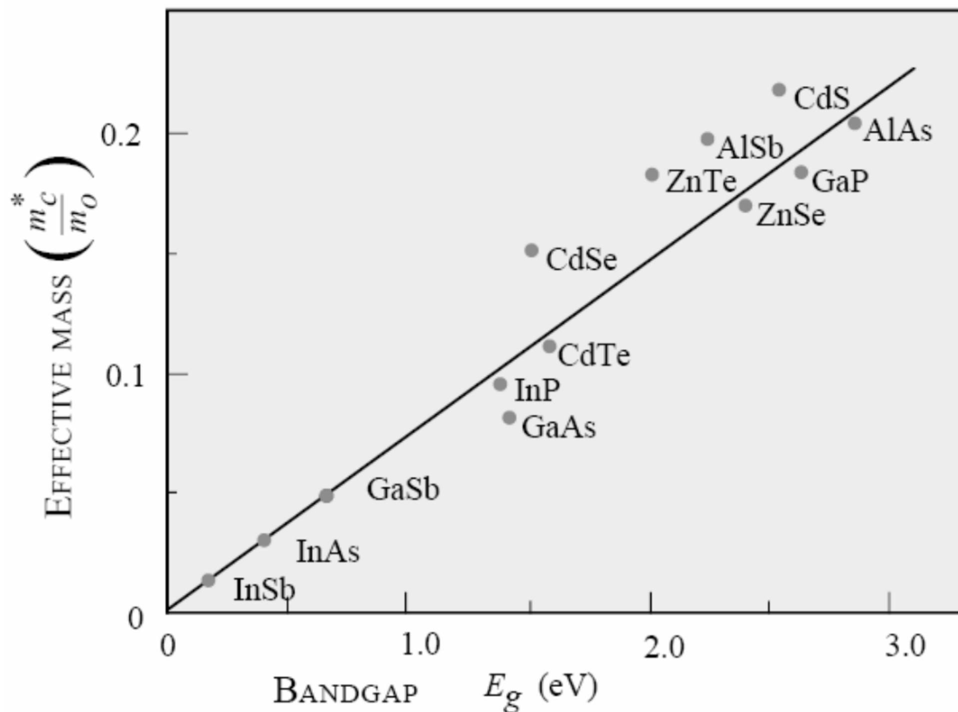
Heavy $m_h = 0.49m_o$

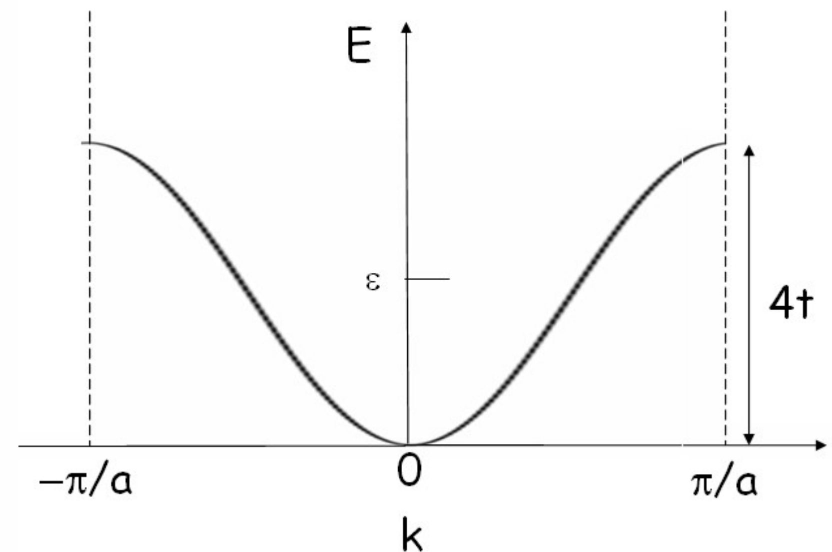
Light $m_{lp} = 0.16m_o$

Split-off band $m_{so} = 0.24m_o$

Effective mass of density of states $m_v = 0.81m_o$

Large gap -> large effective mass





$$E_k = \varepsilon - 2t\cos(ka)$$

$$m^* = \frac{\hbar^2}{\frac{d^2E}{dk^2}}$$

$$\frac{d^2E}{dk^2} = 2ta^2$$

$$m^* \sim \frac{1}{t}$$

narrow bands -> large effective mass