7. Semiconductors

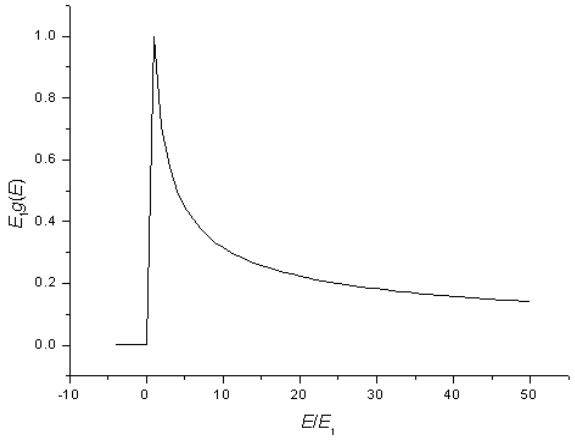
Oct 24, 2019

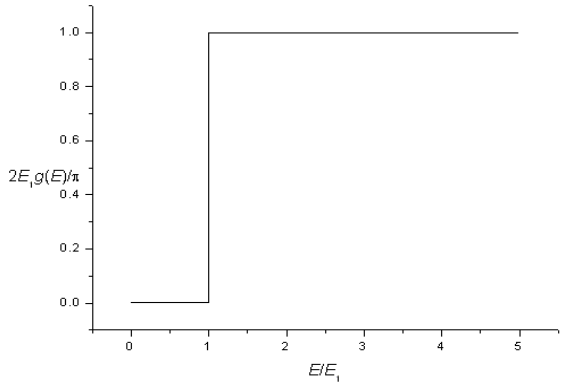
Free electron Fermi gas

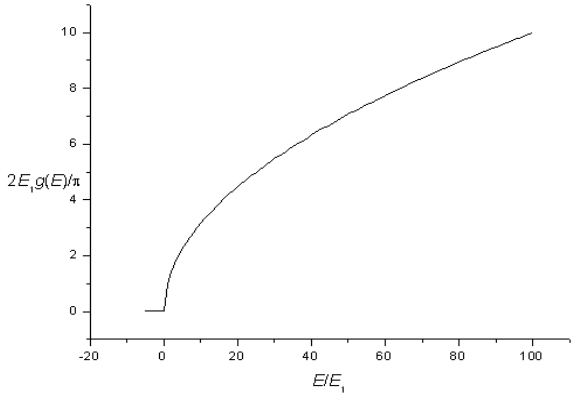
1 - d $$D(E) = \sqrt{\frac{2m}{\hbar^2 \pi^2 E}} = \frac{n}{2\sqrt{E_F E}} \qquad \mathrm{J^{-1}m^{-1}}$$

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

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



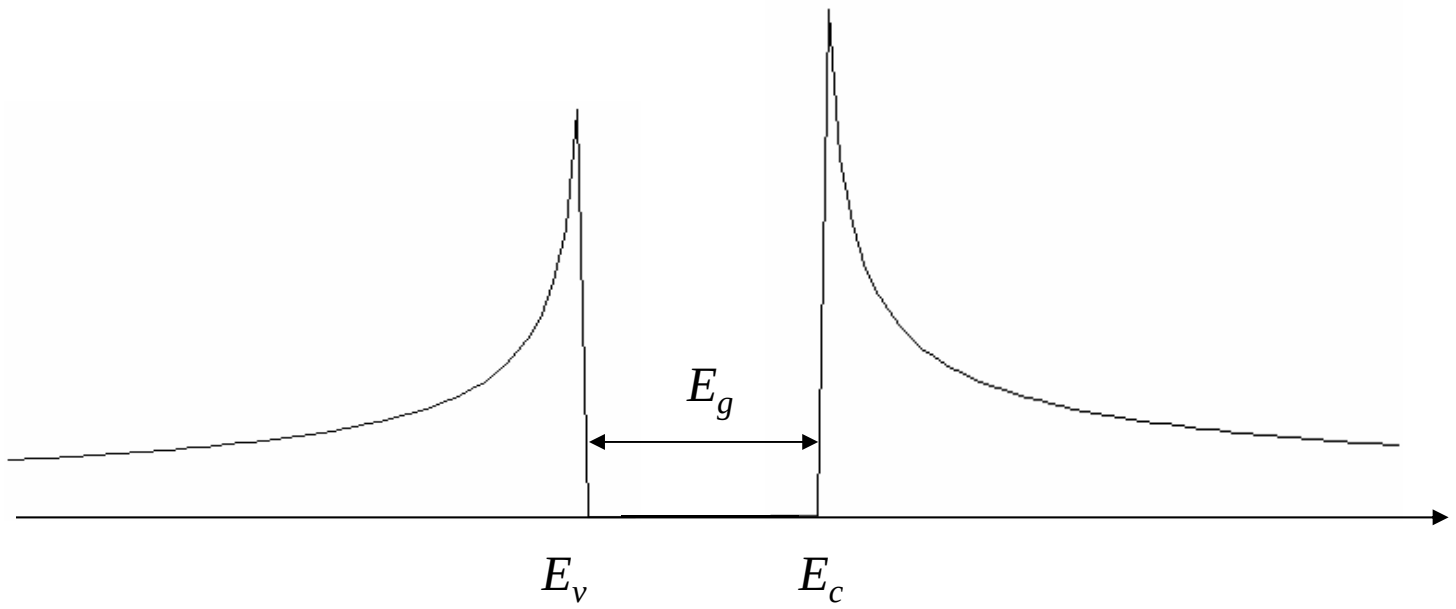




Semiconductors and insulators - 1d

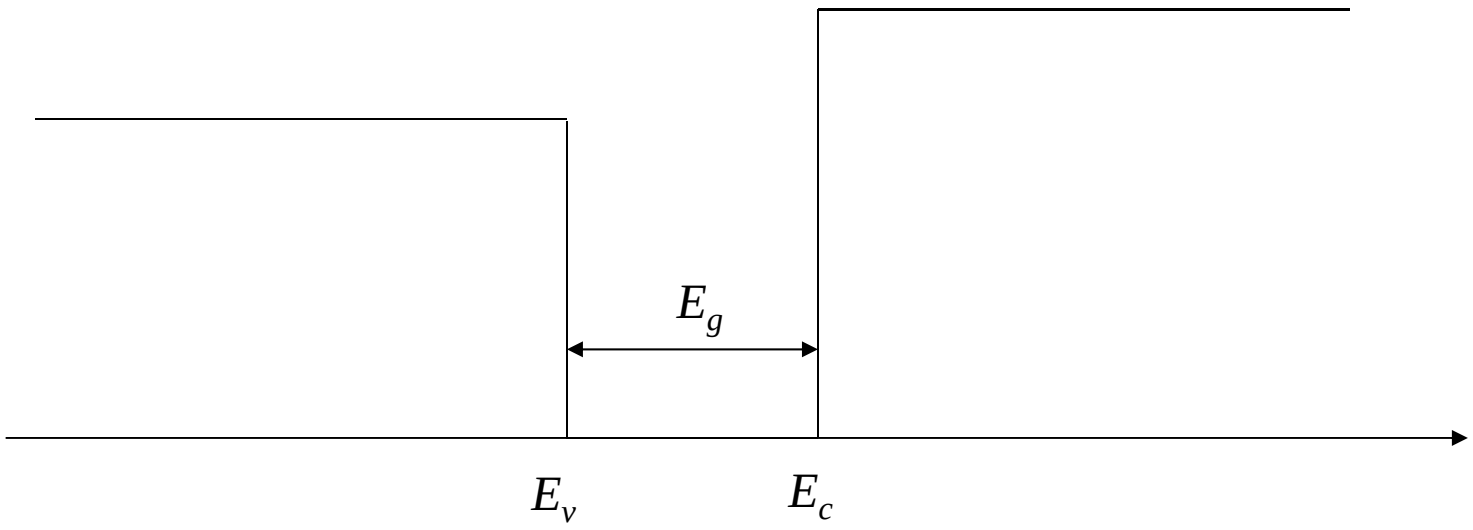
$$E = \frac{\hbar^2 (\vec{k} - \vec{k}_0)^2}{2m^*}$$

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



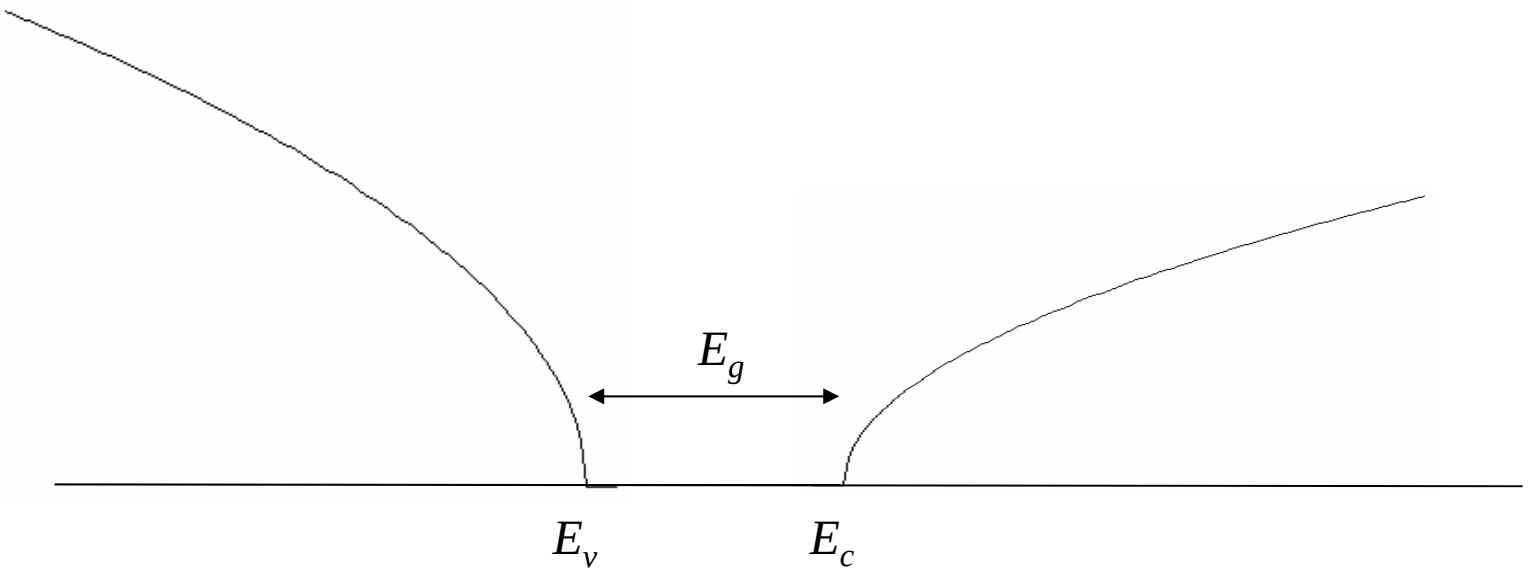
Semiconductors and insulators - 2d

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



Semiconductors and insulators - 3d

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



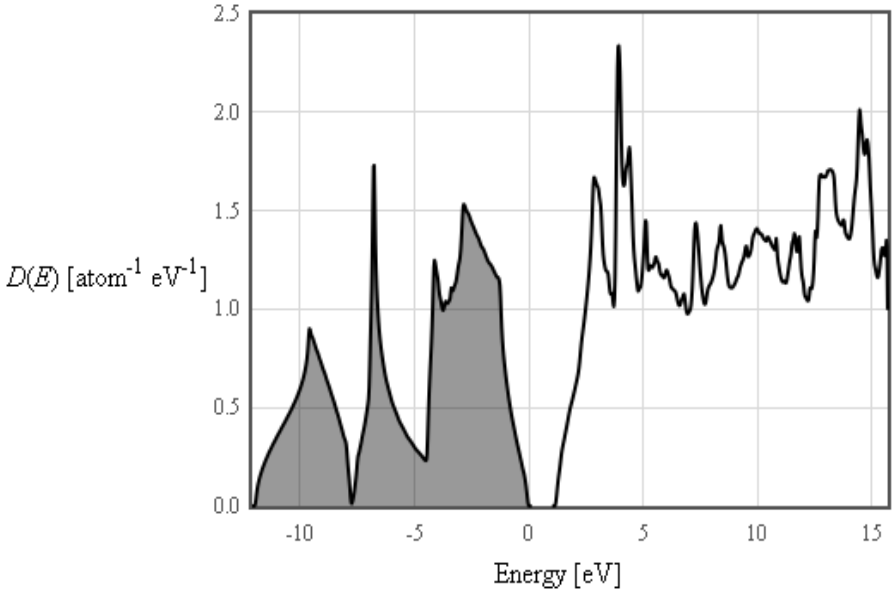
The electrical contribution to the thermodynamic properties of insulators depend on band edges

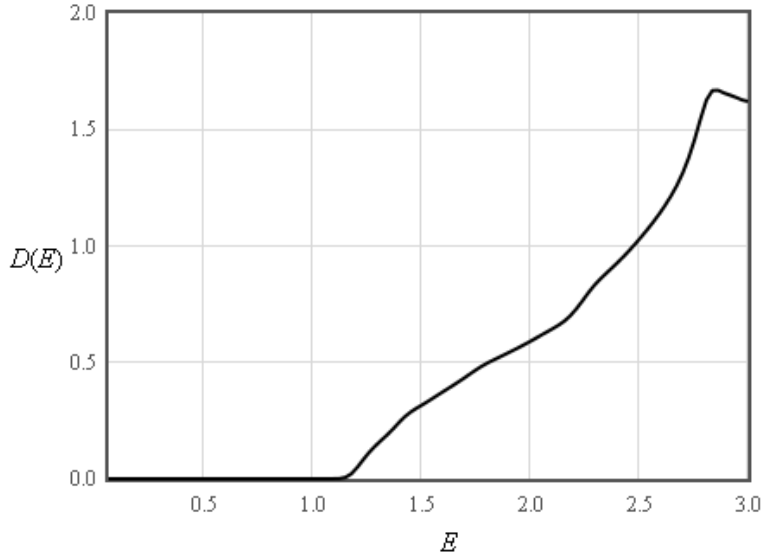
Boltzmann approximation

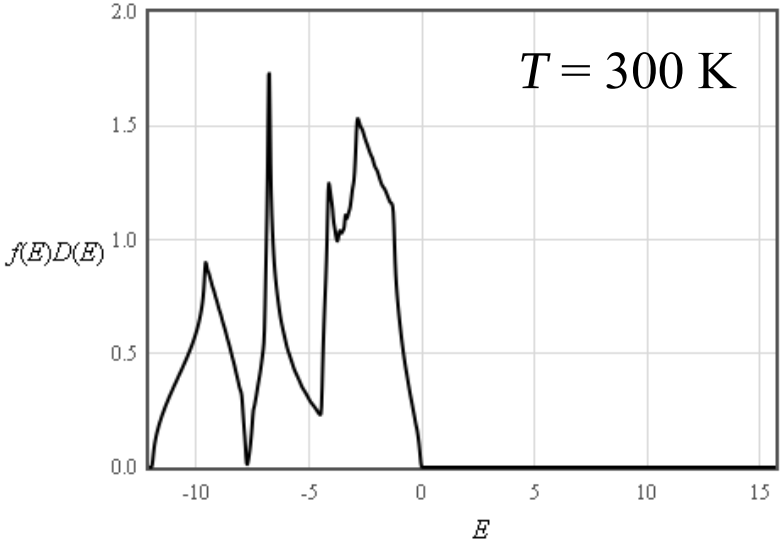
The table below gives the contribution of electrons in intrinsic semiconductors and insulators to some thermodynamic quantities. These results where calculated in the Boltzmann approximation where it is assumed that the chemical potential lies in the band gap more than $3k_BT$ from the band edge. The 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.

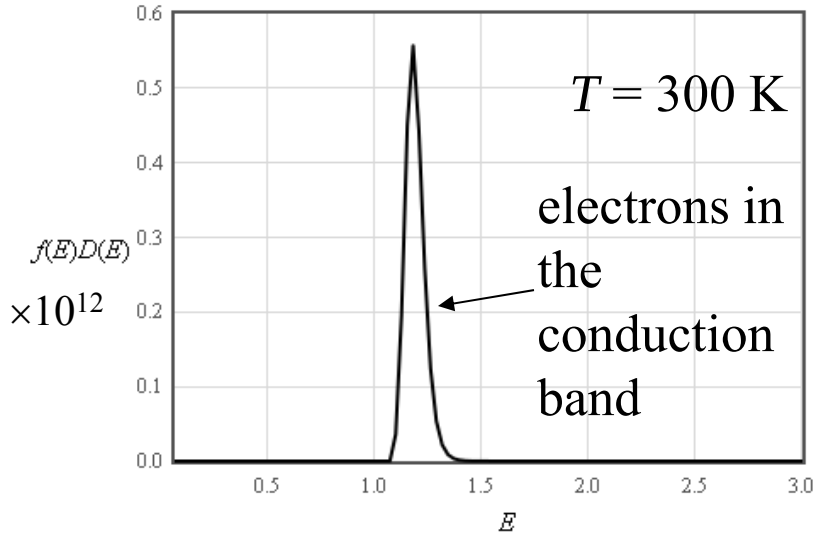
	1-d	2-d
Density of states m_e^* and m_h^* are 'density of states' effective masses	$D(E) = \begin{cases} \frac{1}{\hbar\pi}\sqrt{\frac{2m_h^*}{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \frac{1}{\hbar\pi}\sqrt{\frac{2m_e^*}{(E - E_c)}} & E > E_c \end{cases}$ J^{-1} m^{-1}	$D(E) = \begin{cases} \frac{m_h^*}{\hbar^2\pi} H(E_v - E) & E < E_v \\ 0 & E_v < E < E_c \\ \frac{m_e^*}{\hbar^2\pi} H(E - E_c) & E > E_c \end{cases}$ 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 $n = \int_{E_c}^{\infty} D(E) f(E) dE$	$n = \sqrt{\frac{m_e^* k_B T}{\hbar^2\pi}} \exp\left(\frac{\mu - E_c}{k_B T}\right)$ m^{-1} $= N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$	$n = \frac{m_e^* k_B T}{\hbar^2\pi} \exp\left(\frac{\mu - E_c}{k_B T}\right)$ m^{-2} $= N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$
Density of holes in the valence band $p = \int_{-\infty}^{E_v} D(E)(1 - f(E)) dE$	$p = \sqrt{\frac{m_h^* k_B T}{\hbar^2\pi}} \exp\left(\frac{E_v - \mu}{k_B T}\right)$ m^{-1} $= N_v \exp\left(\frac{\mu - E_c}{k_B T}\right)$	$p = \frac{m_h^* k_B T}{\hbar^2\pi} \exp\left(\frac{E_v - \mu}{k_B T}\right)$ m^{-2} $= N_v \exp\left(\frac{\mu - E_c}{k_B T}\right)$

Silicon density of states

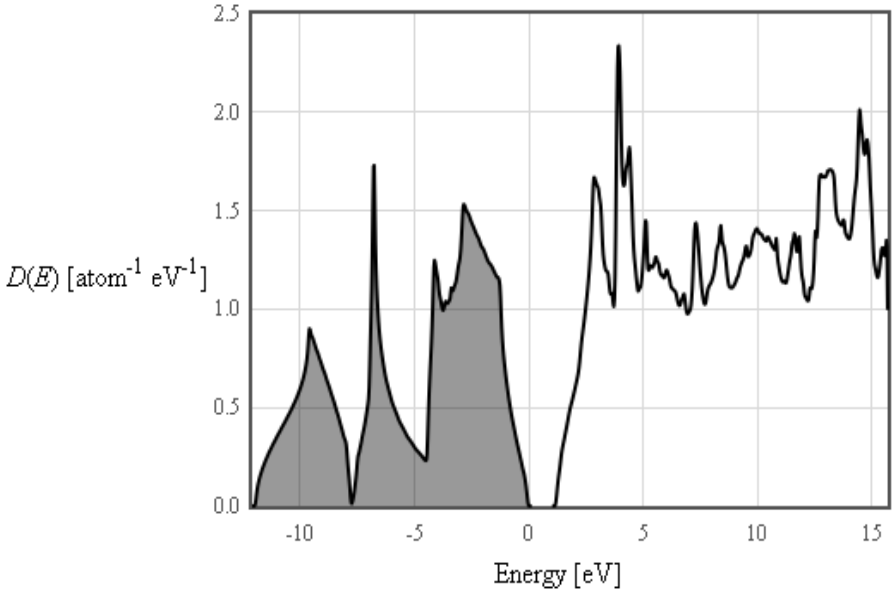


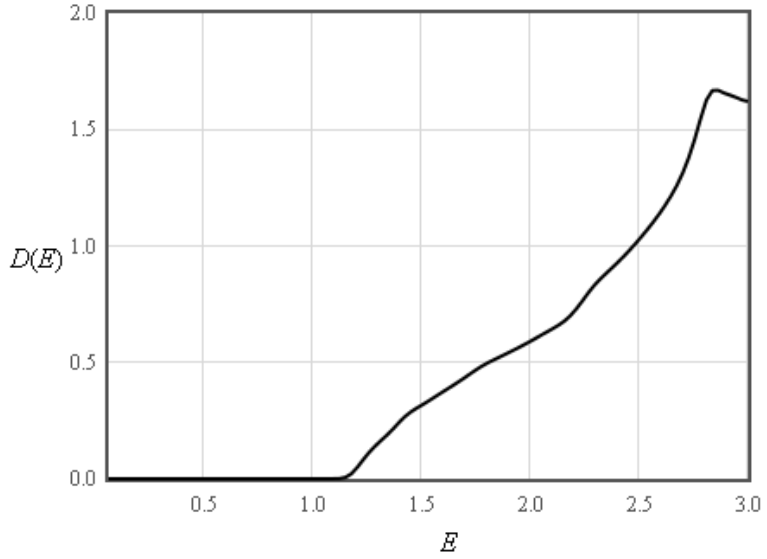


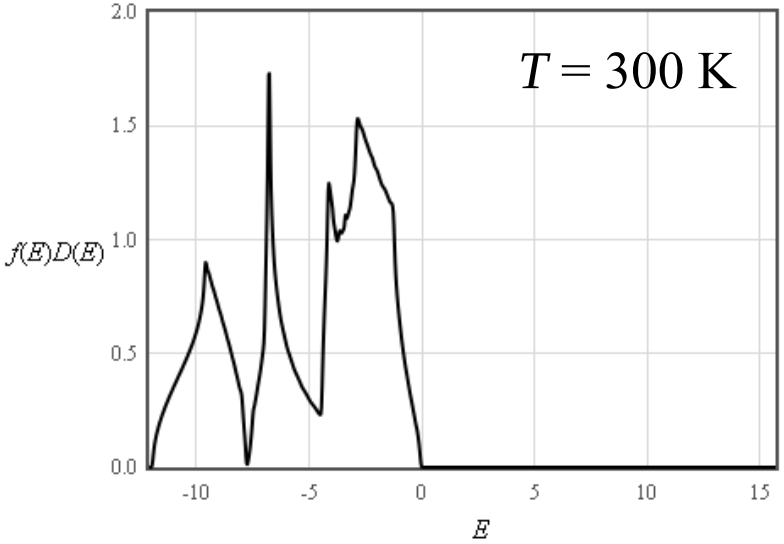


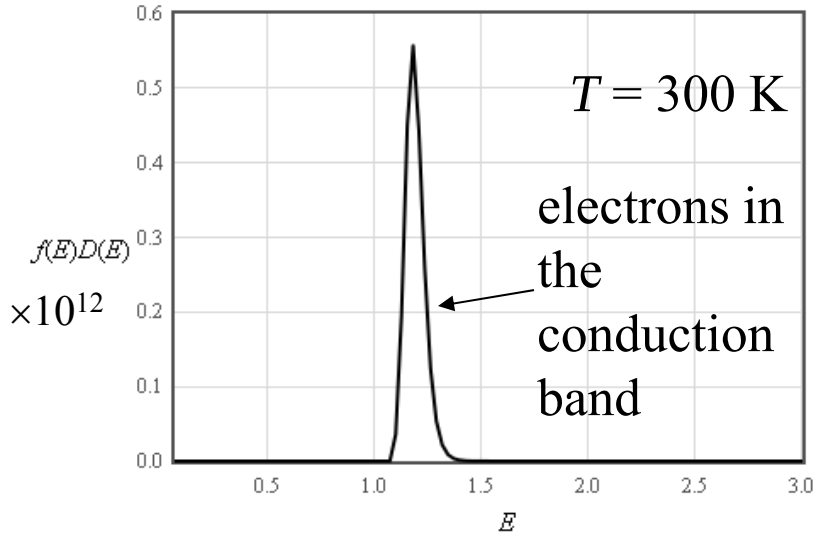


Silicon density of states







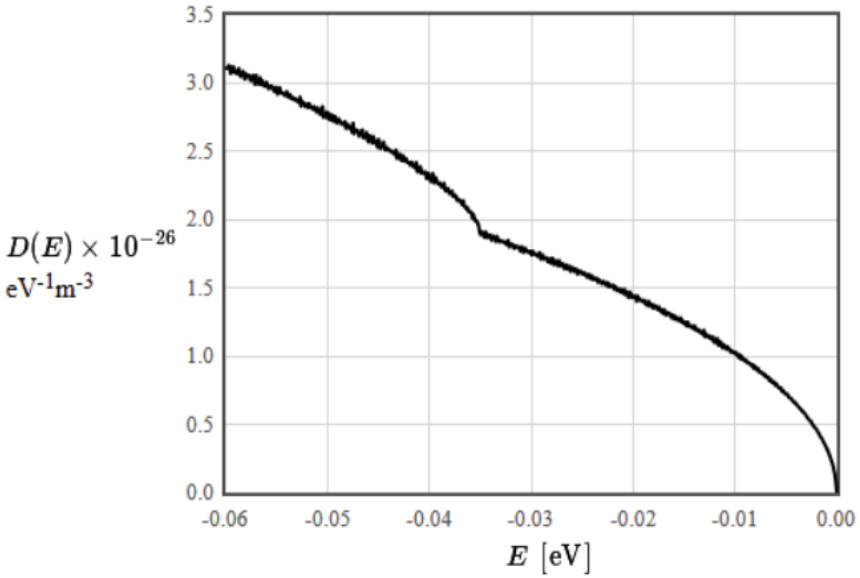


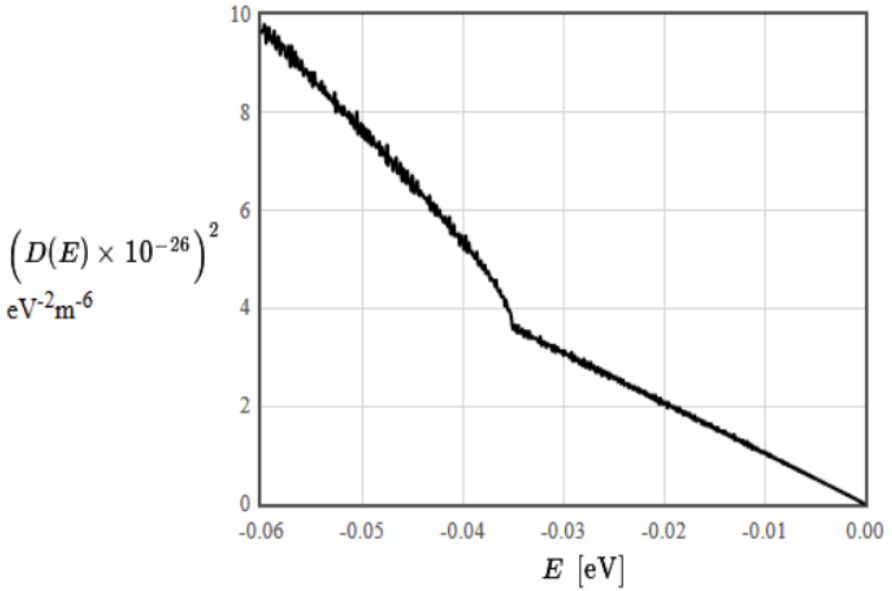
Silicon valence bands

$$E_{v,lh} = -\frac{\hbar^2}{2m_e}\left(4.1k^2 - \sqrt{1.21k^4 + 4.1(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)}\right),$$

$$E_{v,hh} = -\frac{\hbar^2}{2m_e}\left(4.1k^2 + \sqrt{1.21k^4 + 4.1(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)}\right),$$

$$E_{v,so} = -E_{so} - \frac{\hbar^2k^2}{2m_{so}}.$$



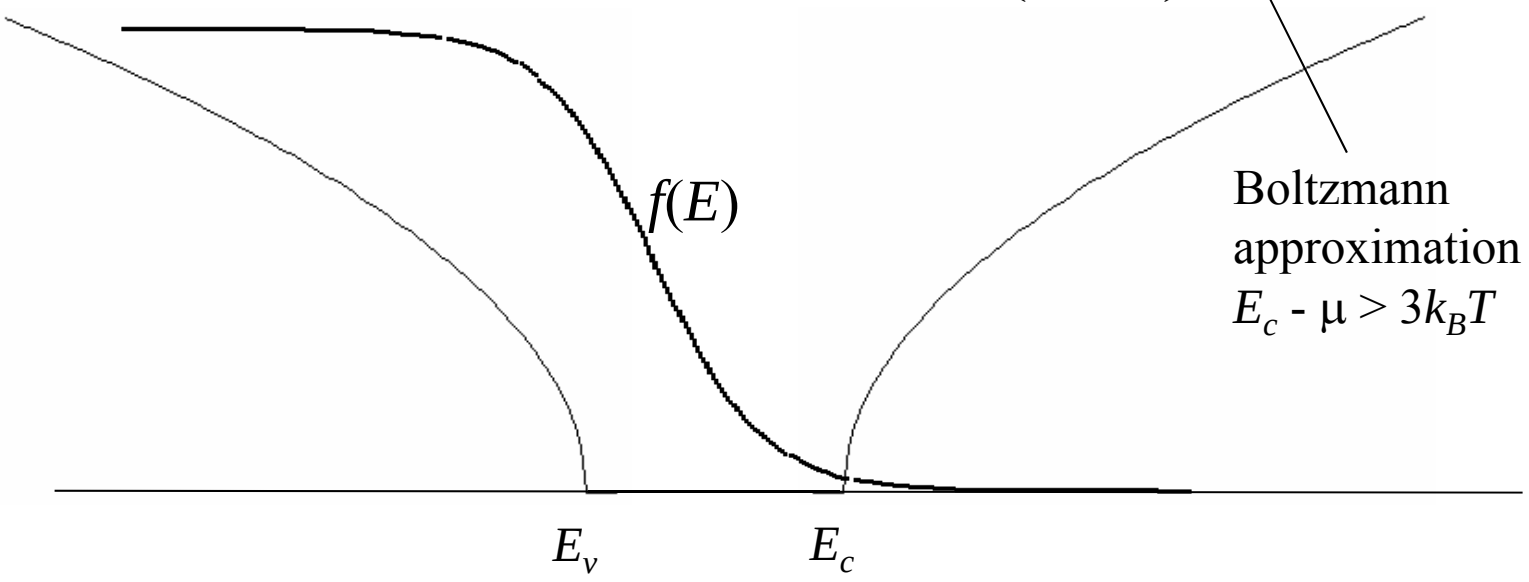


Density of electrons in the conduction band

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

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

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

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

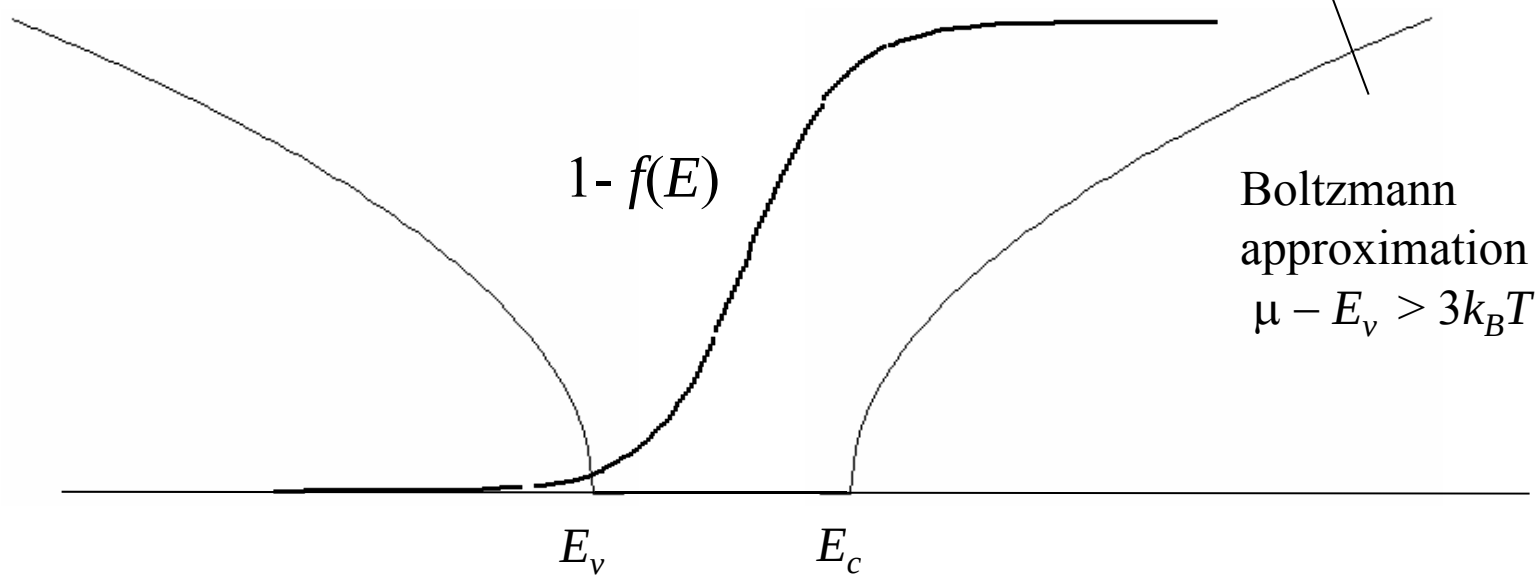
$$\boxed{n = N_c(T) \exp\left(\frac{\mu - E_c}{k_B T}\right)} = \frac{2D_c}{\sqrt{\pi}} \left(k_B T\right)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T}\right)$$

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

Density of holes in the valence band

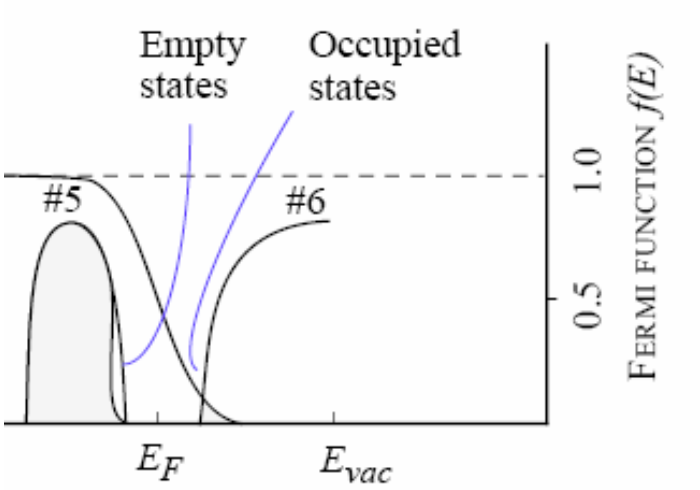
$$D(E) = D_v\sqrt{E_v - E}$$

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



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

Density of holes in the valence band



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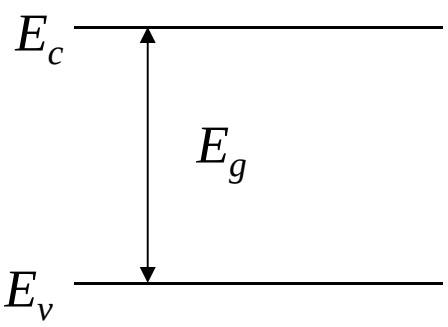
$$\boxed{p = N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)} = \frac{2D_v}{\sqrt{\pi}}\left(k_B T\right)^{3/2} \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

$$N_v = 2\left(\frac{m_h^* k_B T}{2\pi\hbar^2}\right)^{3/2}$$ = Effective density of states in the valence band

Law of mass action

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

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

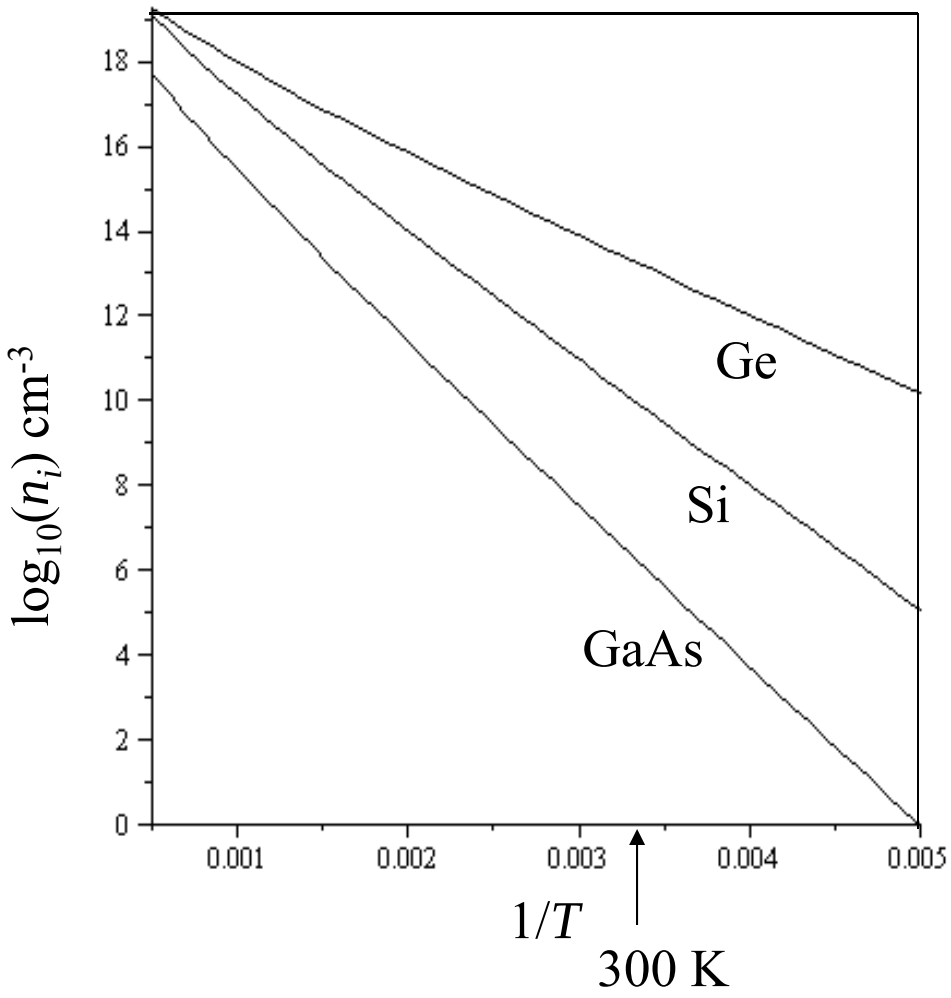


For intrinsic semiconductors (no impurities)

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

intrinsic carrier density

Intrinsic carrier concentration



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

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

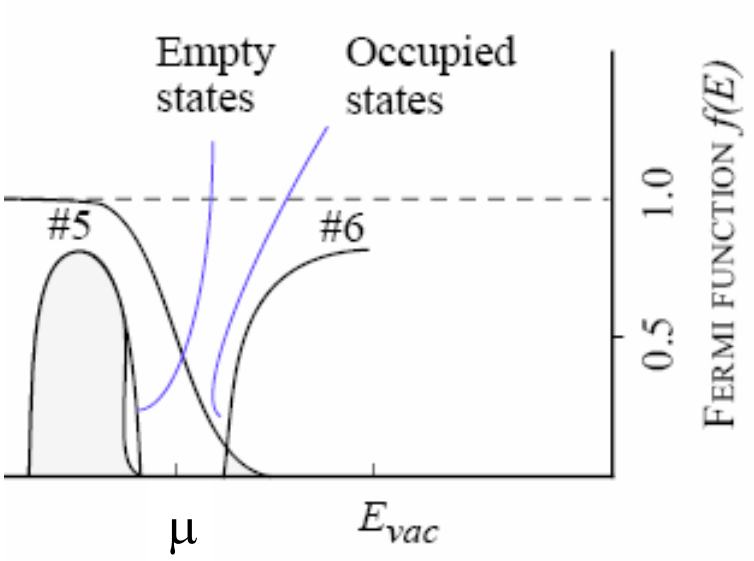
Chemical potential of an intrinsic semiconductor

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

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

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

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

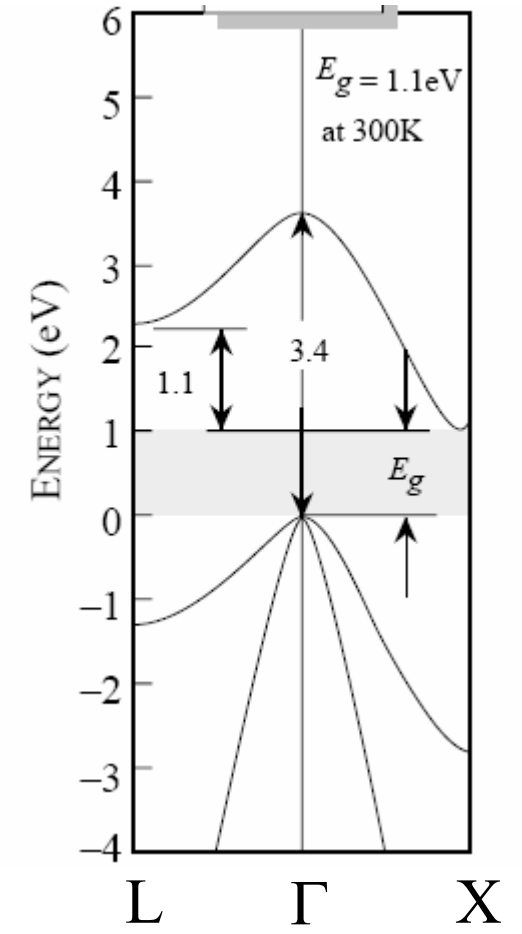


E_c ——————————

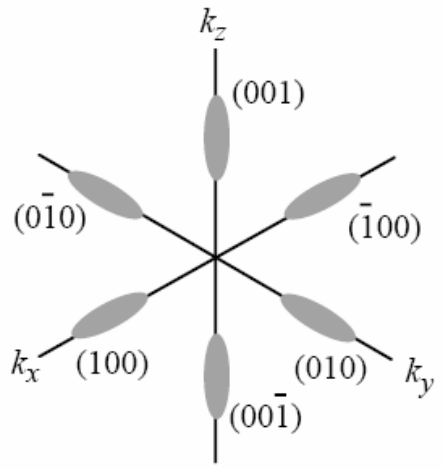
μ ----------

E_v ——————————

Density of electrons in the conduction band



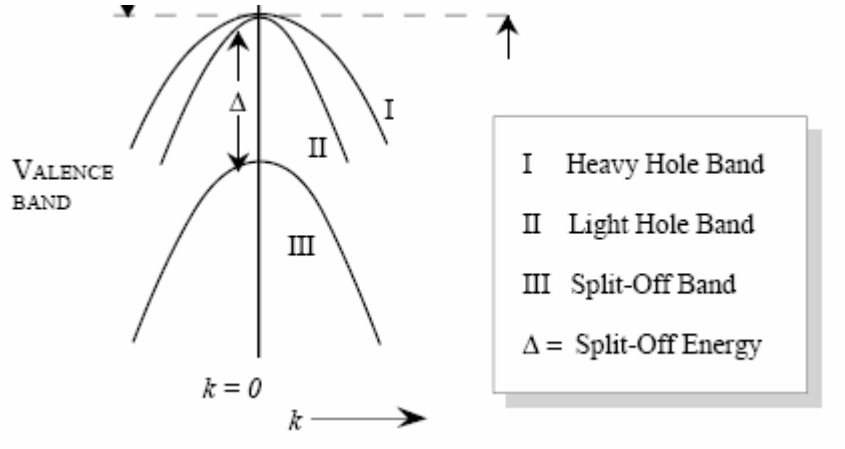
$$n = N_c(T)\exp\left(\frac{\mu - E_c}{k_B T}\right) = \frac{2D_v}{\sqrt{\pi}}\left(k_B T\right)^{3/2}\exp\left(\frac{\mu - E_c}{k_B T}\right)$$



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

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**
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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}

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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 $n = \int_{E_c}^{\infty} D(E) f(E) dE$	$n = \sqrt{\frac{m_e^* k_B T}{\hbar^2\pi}} \exp\left(\frac{\mu - E_c}{k_B T}\right)$ m^{-1} $= N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$	$n = \frac{m_e^* k_B T}{\hbar^2\pi} \exp\left(\frac{\mu - E_c}{k_B T}\right)$ m^{-2} $= N_c \exp\left(\frac{\mu - E_c}{k_B T}\right)$
Density of holes in the valence band $p = \int_{-\infty}^{E_v} D(E)(1 - f(E)) dE$	$p = \sqrt{\frac{m_h^* k_B T}{\hbar^2\pi}} \exp\left(\frac{E_v - \mu}{k_B T}\right)$ m^{-1} $= N_v \exp\left(\frac{\mu - E_c}{k_B T}\right)$	$p = \frac{m_h^* k_B T}{\hbar^2\pi} \exp\left(\frac{E_v - \mu}{k_B T}\right)$ m^{-2} $= N_v \exp\left(\frac{\mu - E_c}{k_B T}\right)$

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,

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

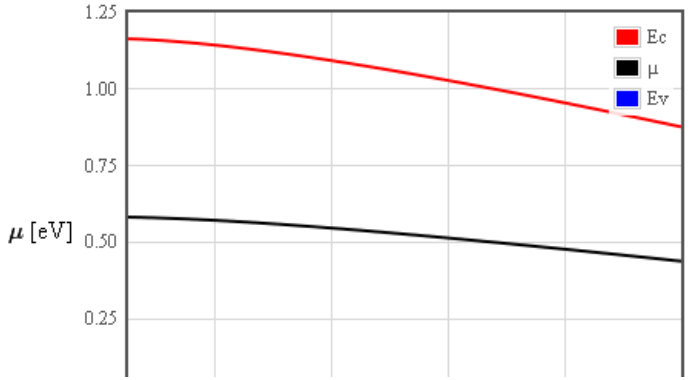
$$m_e^* = \frac{\pi\hbar^2}{300k_B}\left(\sqrt{2}N_c(300)\right)^{2/3}$$

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