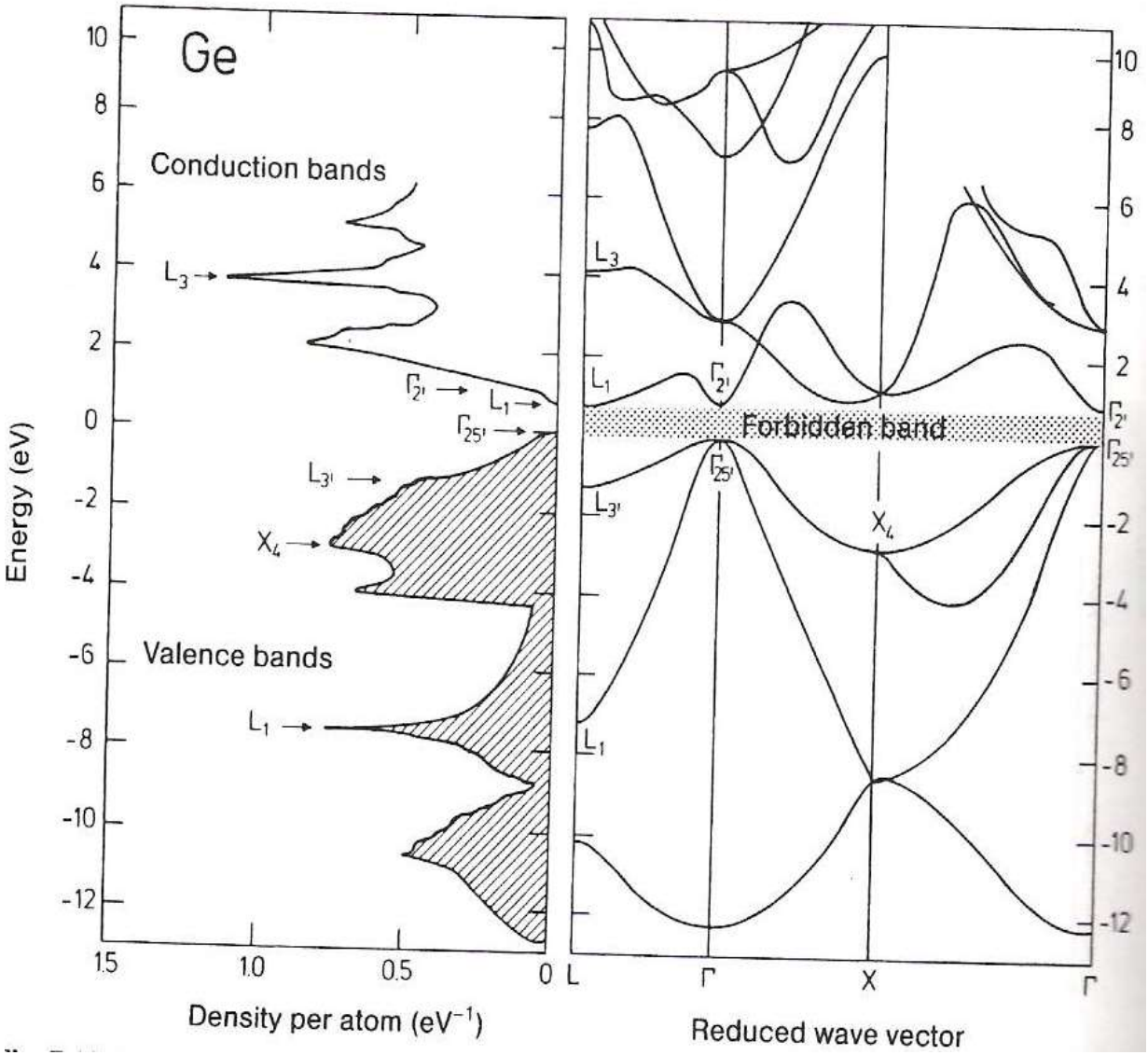
Intrinsic semiconductors

Germanium

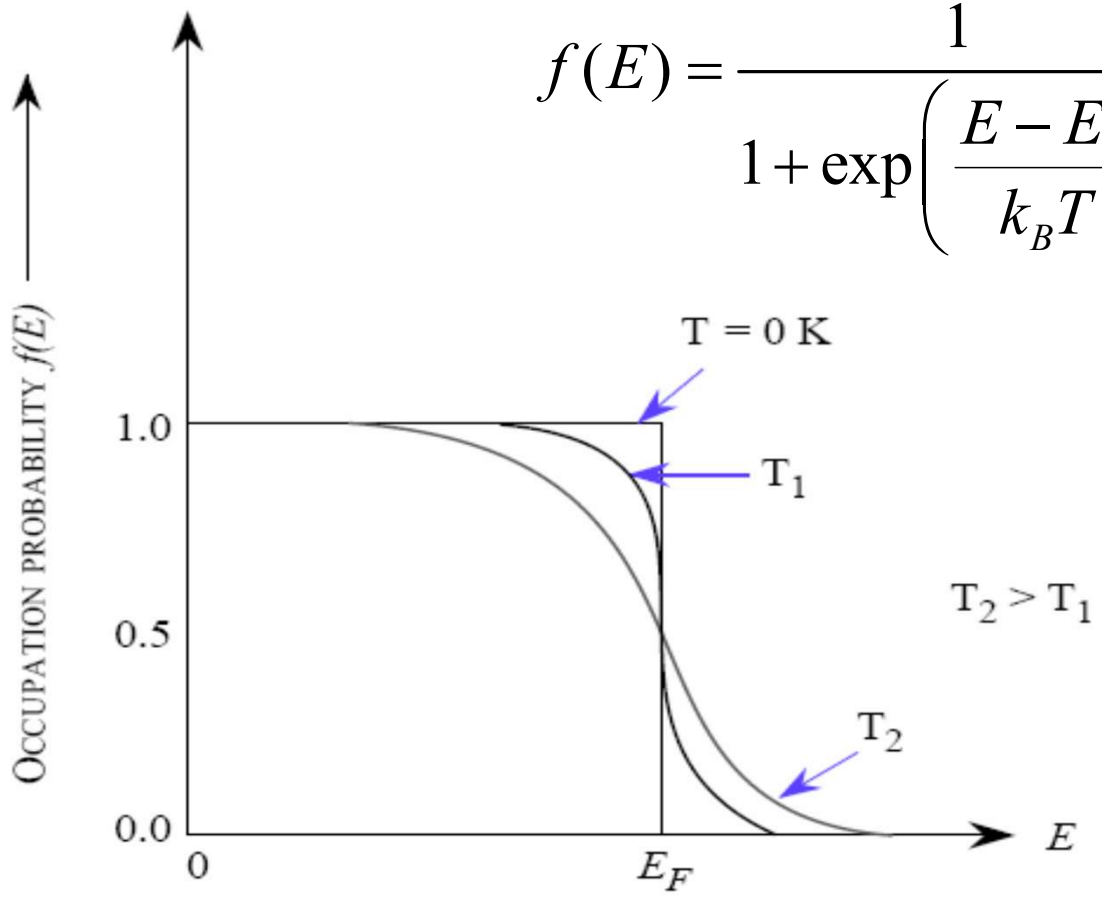


from Ibach & Lueth

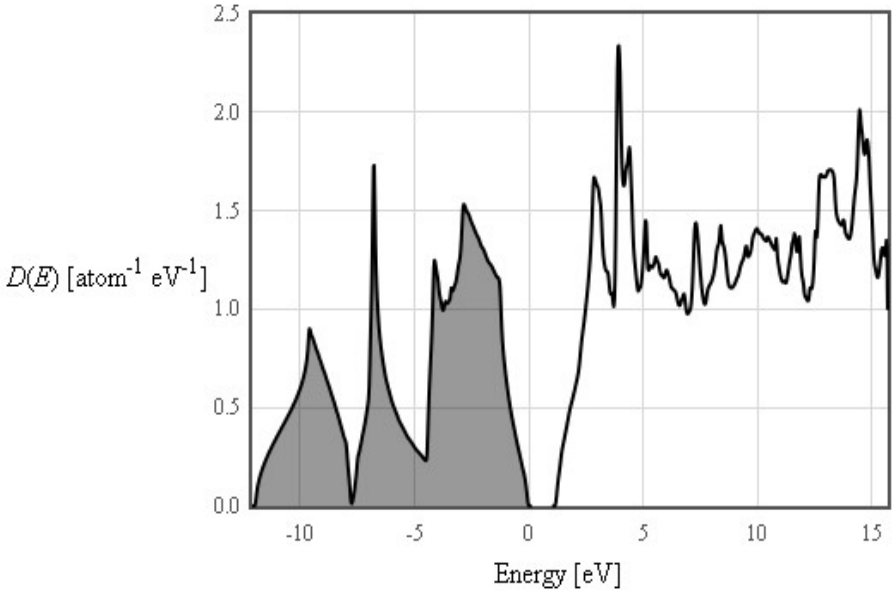
Fermi function

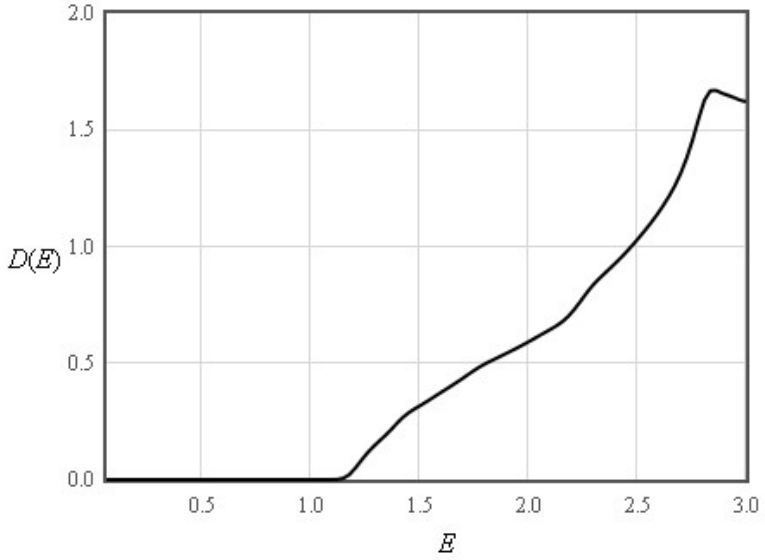
$f(E)$ is the probability that a state at energy E is occupied.

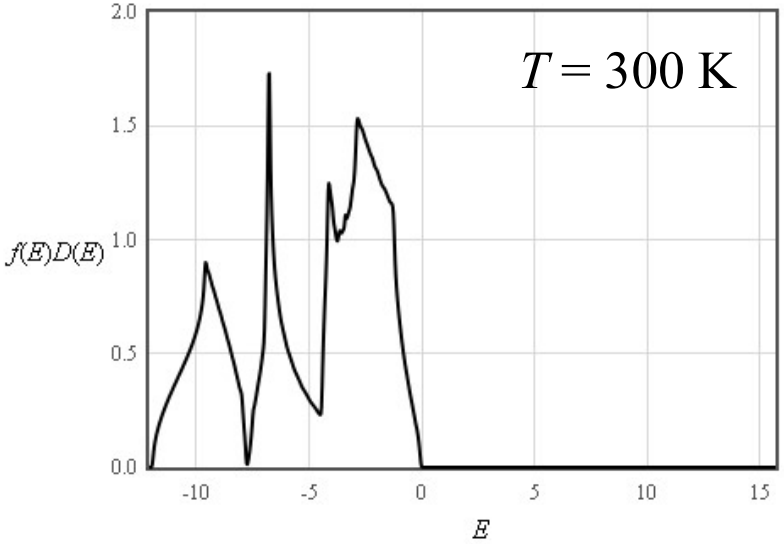
$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)}$$

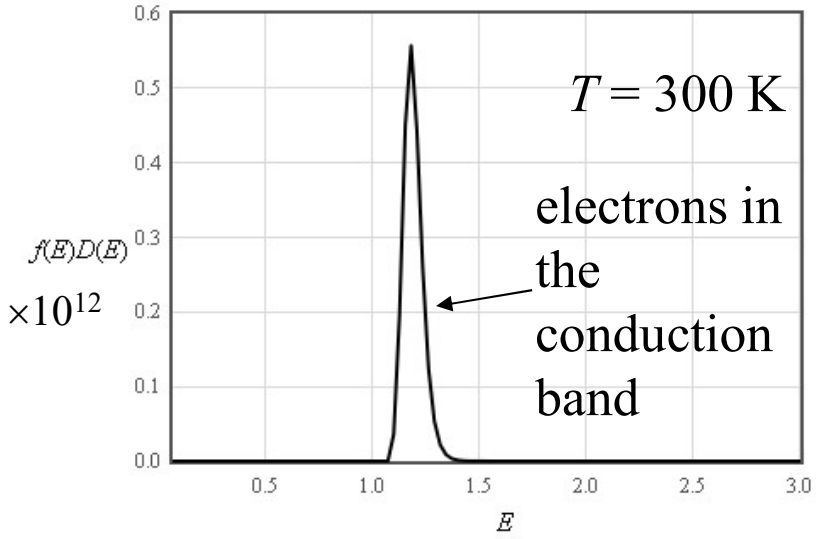


Silicon density of states









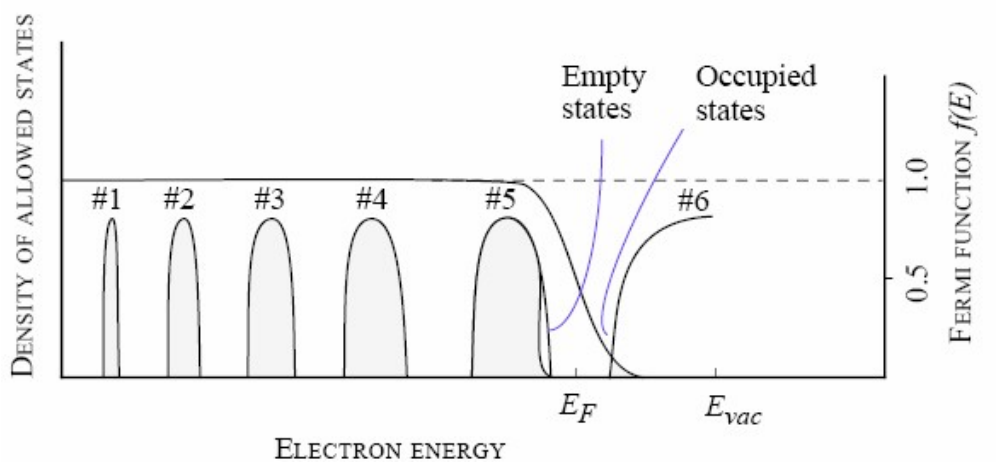
Fermi energy

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

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

Here n is the electron density.

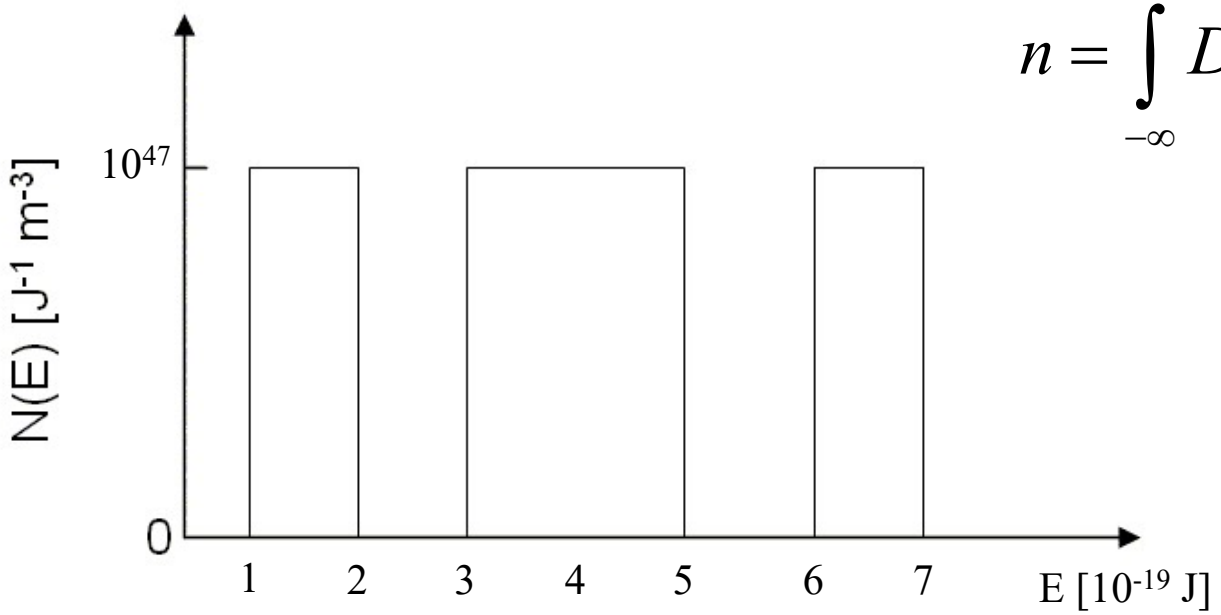
The density of states, the total number of electrons and the temperature are given. To find the Fermi energy, guess one and evaluate the integral. If n turns out too low, guess a higher E_F and if n turns out too high, guess a lower E_F.



Calculate the Fermi energy

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

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



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

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

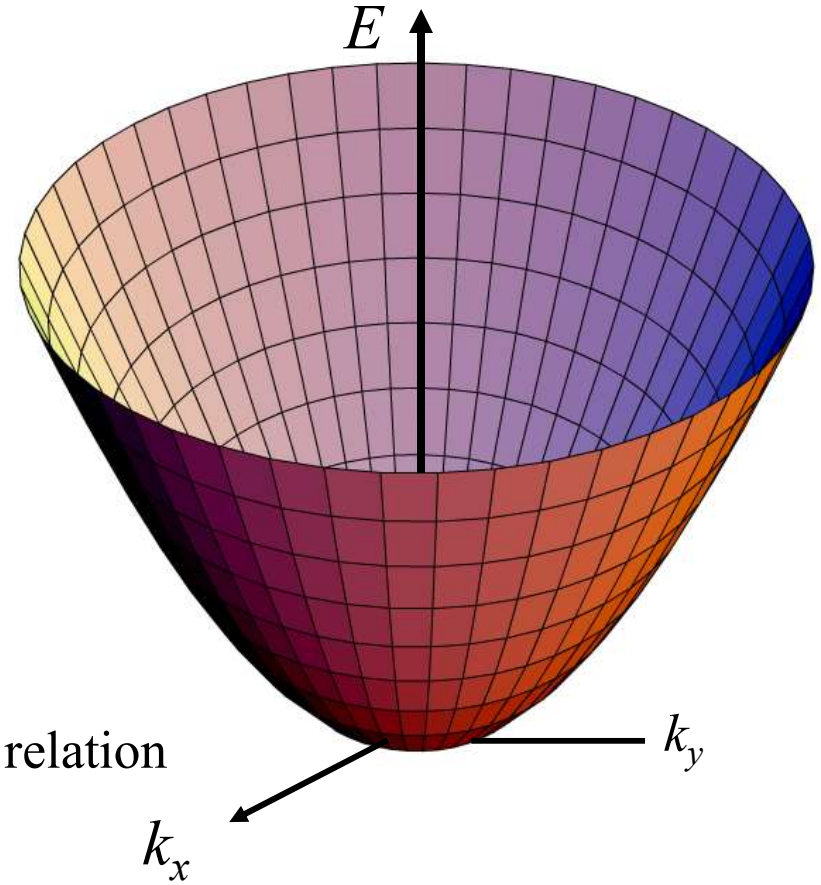
What kind of material is this?

Metal

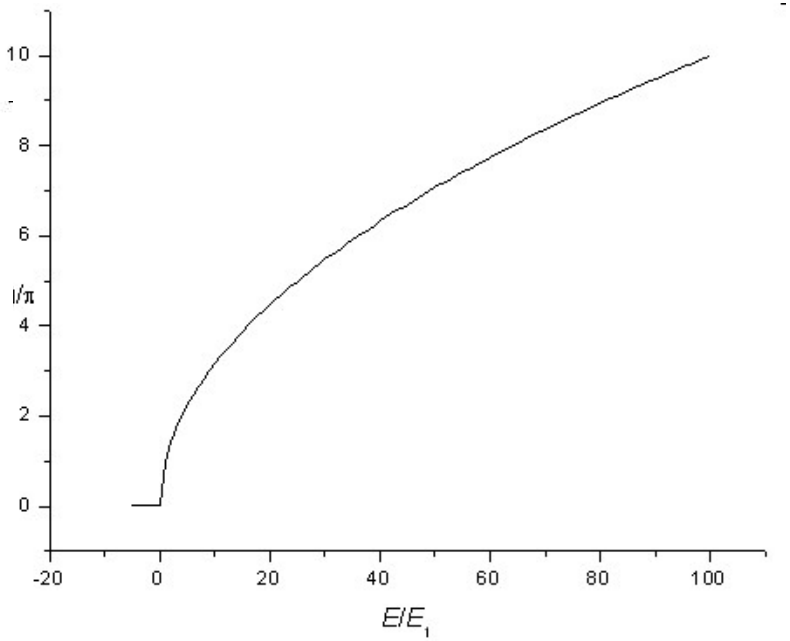
free electrons (simple model for a metal)

$$E(\vec{k}) = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) = \frac{p^2}{2m} = \tfrac{1}{2}mv^2$$

dispersion relation



3-d density of states



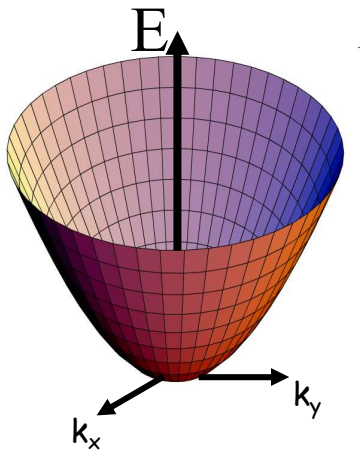
$$D(E) = \begin{cases} 0 & \text{for} \quad E < 0 \\ \dfrac{(2m)^{3/2}}{2\pi^2\hbar^3}\sqrt{E} & \text{for} \quad E > 0 \end{cases}$$

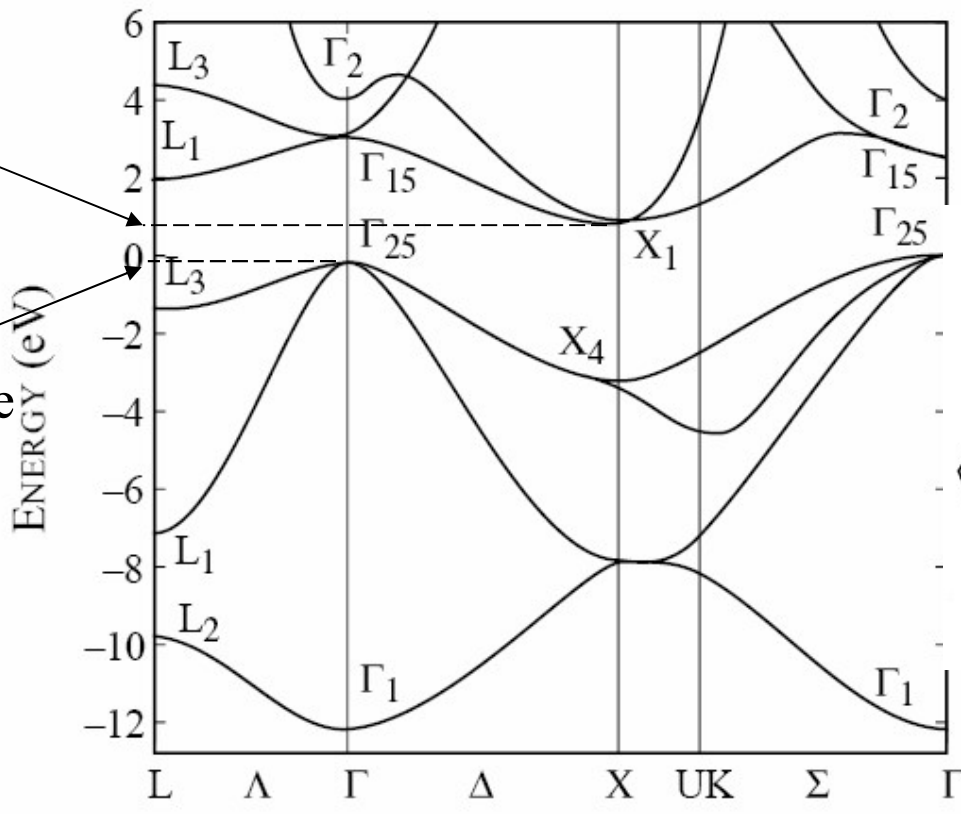
Silicon band structure

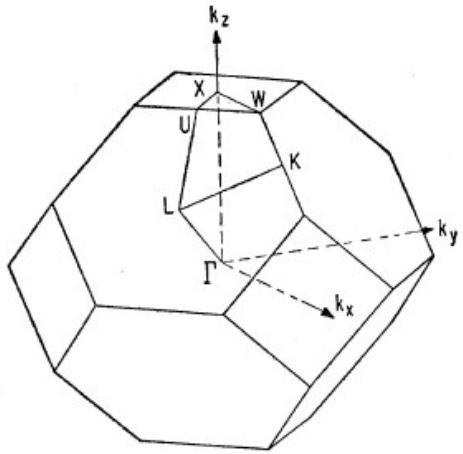
E_c = bottom of the conduction band

$E_g = E_c - E_v$

E_v = top of the valence band







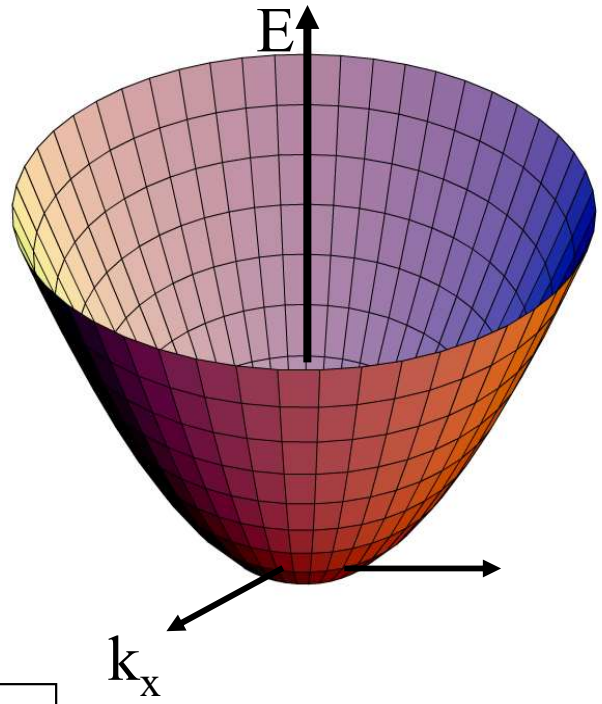
Near the bottom of the conduction band, the band structure looks like a parabola.

Effective mass

$$E(\vec{k}) = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) = \frac{p^2}{2m} = \tfrac{1}{2}mv^2$$

$$\frac{dE(\vec{k})}{dk_x} = \frac{\hbar^2 k_x}{m}$$

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



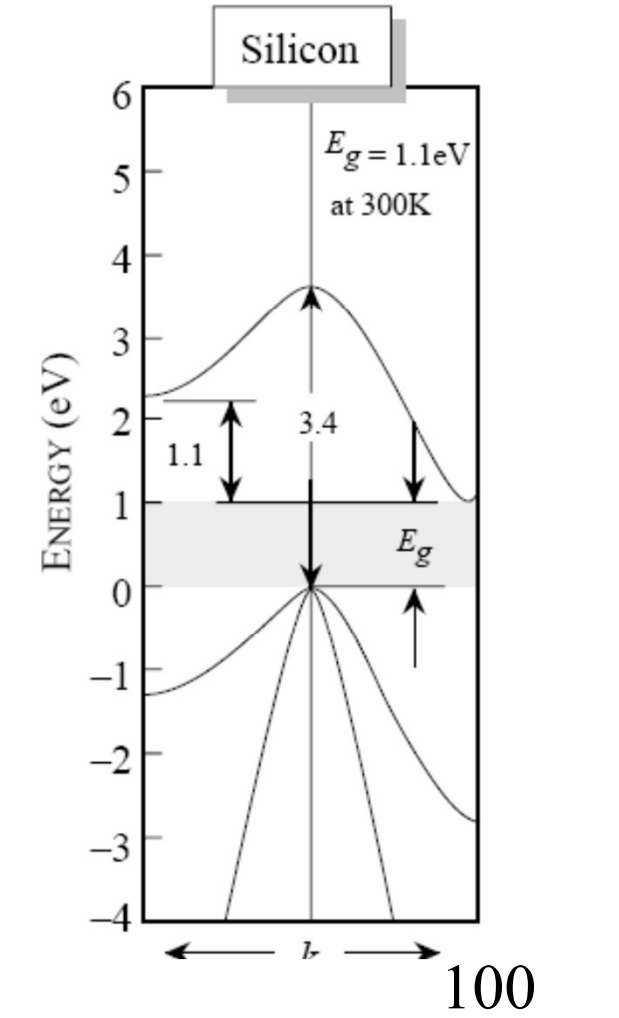
Effective mass

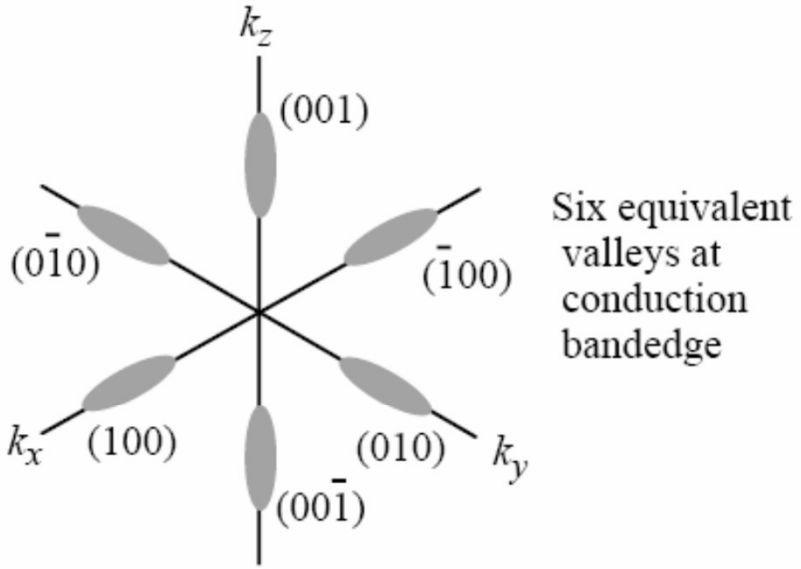
$$m_x^* = \frac{\hbar^2}{\dfrac{d^2E(\vec{k})}{dk_x^2}}$$

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

$$\vec{F} = -e\vec{E} = m^*\vec{a}$$

Anisotropic effective mass in silicon





The electrons seem to have different masses when the electric field is applied in different directions.

valence band, holes

When all states in a band are occupied, the band does not contribute to the current. There are as many left-moving electrons as right-moving electrons.

$$I \propto \sum_{\text{occupied } \vec{k}} \left(-e\vec{v}_{\vec{k}}\right)$$

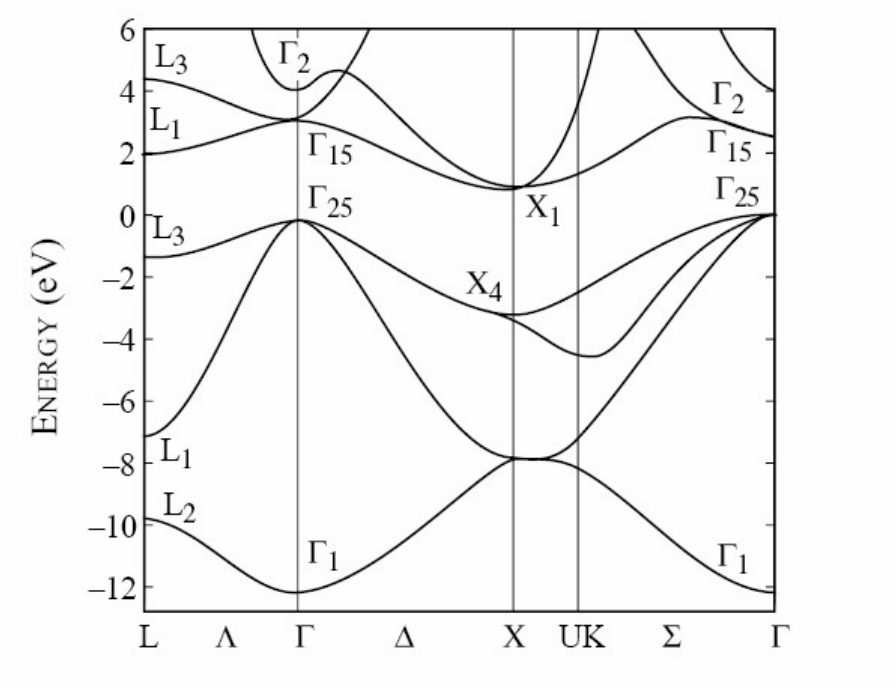
$$I \propto \sum_{\text{all } \vec{k}} \left(-e\vec{v}_{\vec{k}}\right) - \sum_{\text{empty } \vec{k}} \left(-e\vec{v}_{\vec{k}}\right)$$

$$I \propto \sum_{\text{empty } \vec{k}} e\vec{v}_{\vec{k}}$$

valence band, holes

In the valence band, the effective mass is negative.

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



Holes

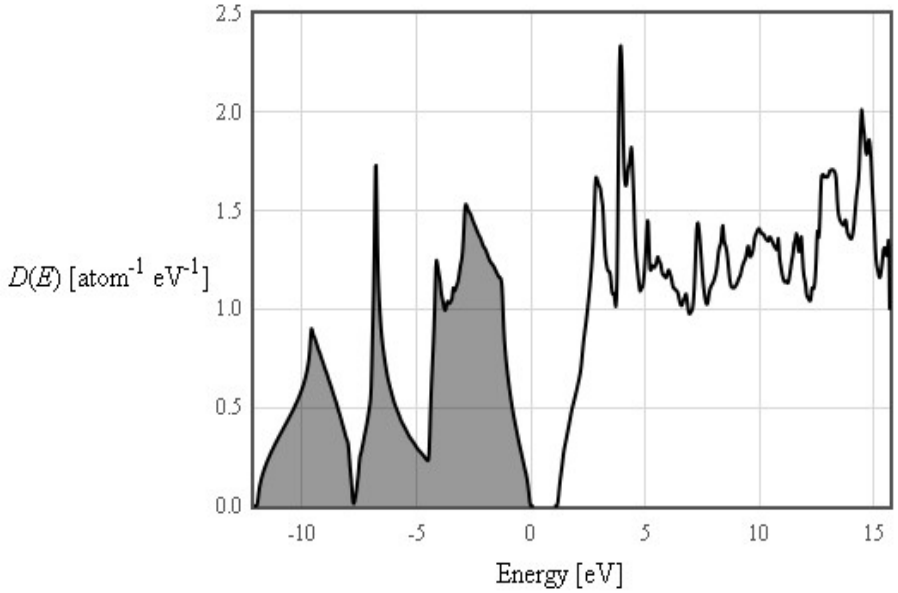
Charge carriers in the valence band can be considered to be positively charged holes. The number of holes in the valence band is the number of missing electrons.

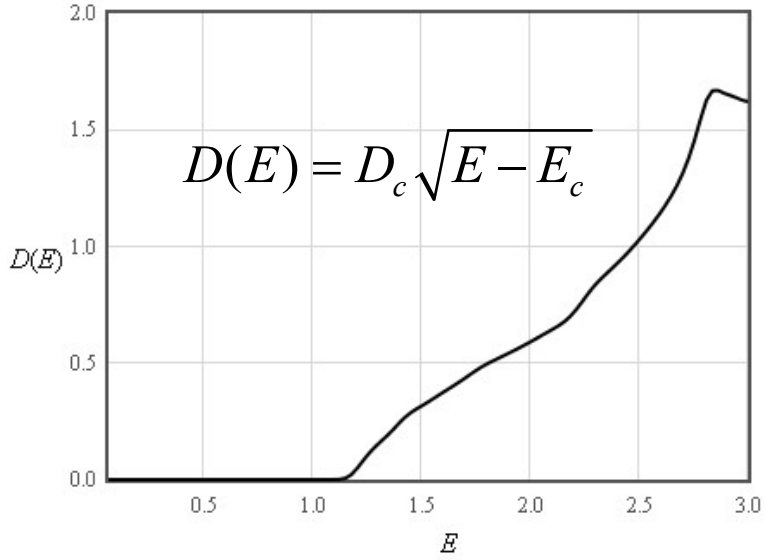
m^*_h = effective mass of holes

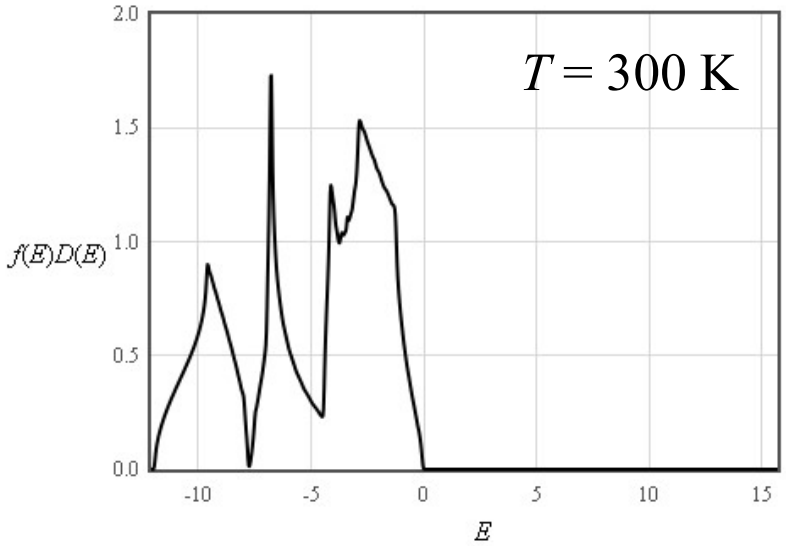
$$m_h^* = -\frac{\hbar^2}{\frac{d^2 E(\vec{k})}{dk_x^2}}$$

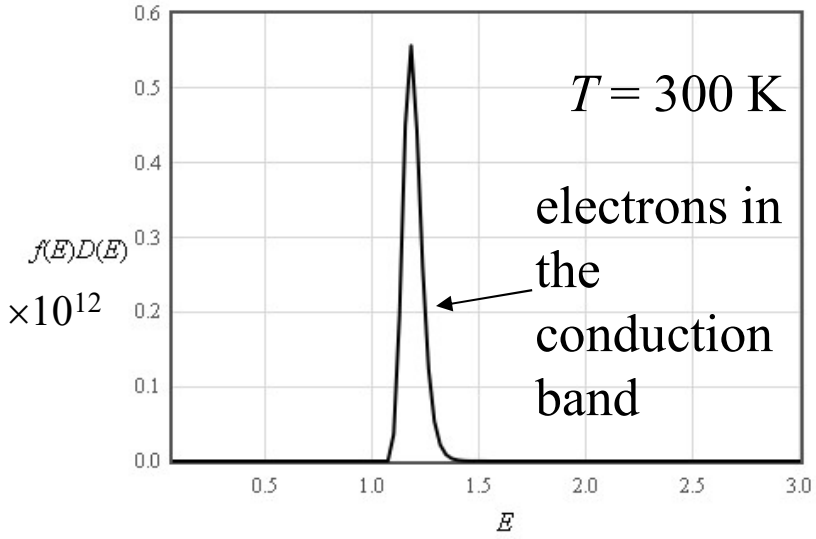
$$\vec{F} = e\vec{E} = m_h^* \vec{a}$$

Silicon density of states



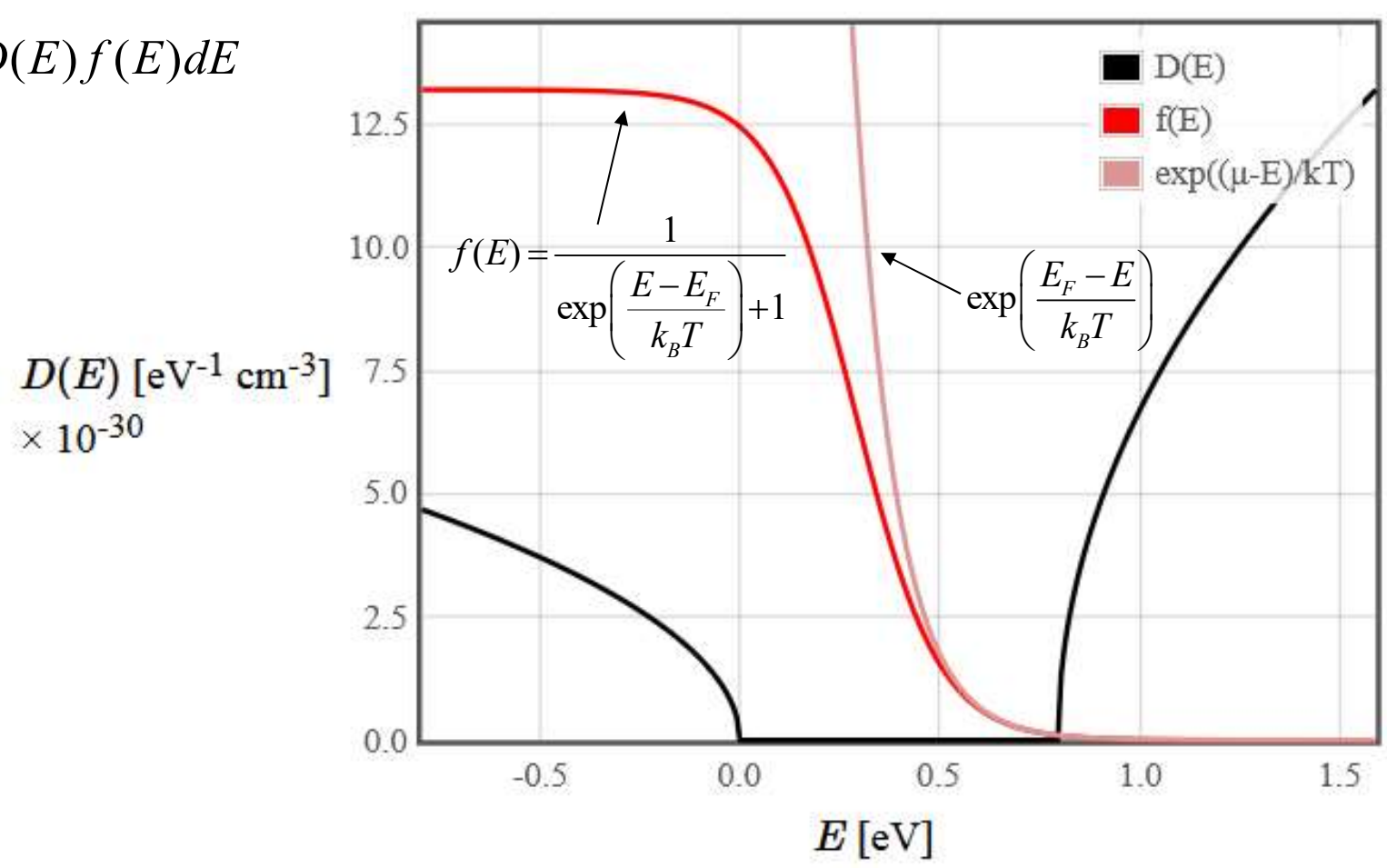






Boltzmann approximation

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



Density of electrons in the conduction band

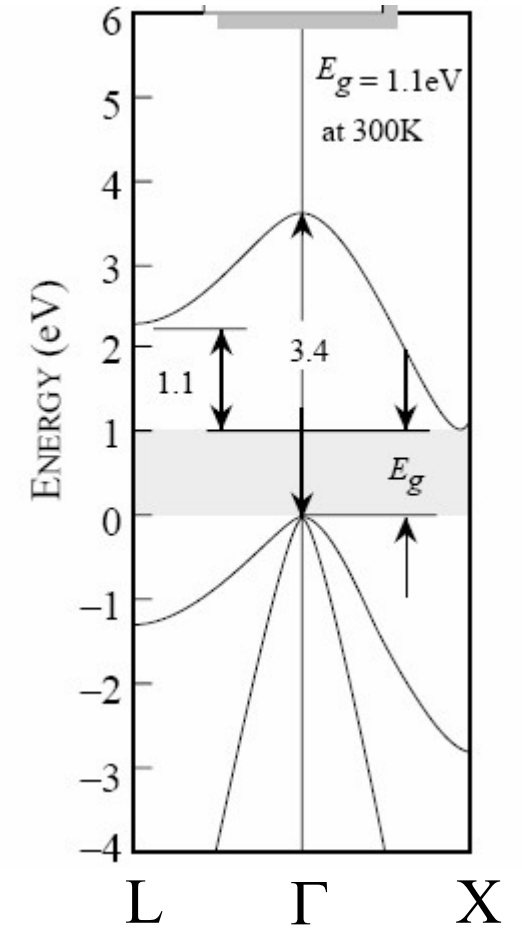
$$n = \int_{E_c}^{\infty} D(E) f(E) dE \approx D_c \int_{E_c}^{\infty} \exp\left(\frac{E_F - E}{k_B T}\right) \sqrt{E - E_c}\, dE$$

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

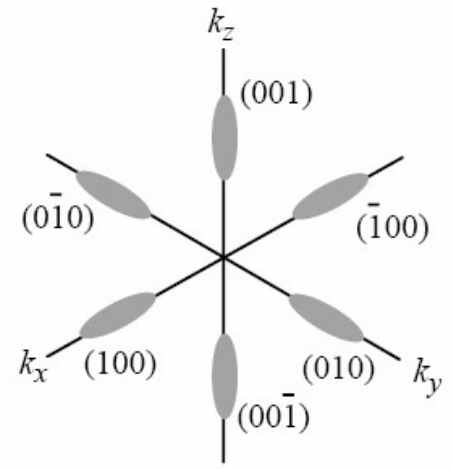
$$\boxed{n = N_c(T) \exp\left(\frac{E_F - E_c}{k_B T}\right)} = \frac{2D_c}{\sqrt{\pi}} \left(k_B T\right)^{3/2} \exp\left(\frac{E_F - E_c}{k_B T}\right)$$

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

Density of electrons in the conduction band



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



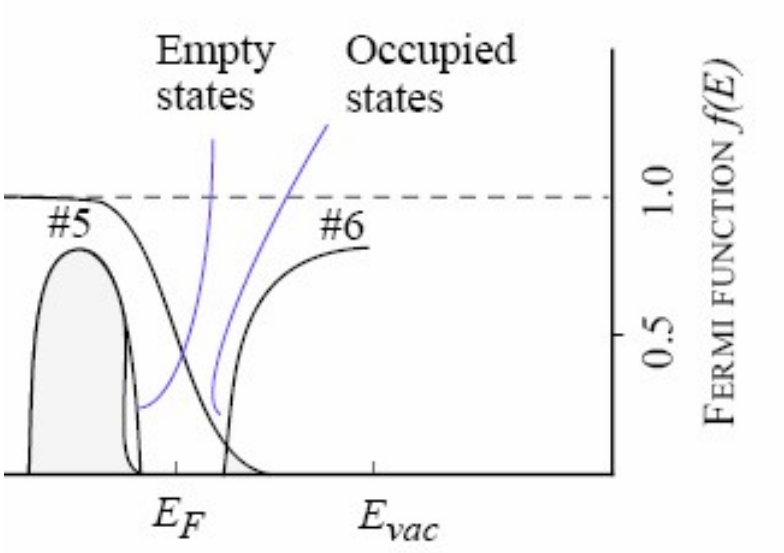
$$n = N_c\left(\frac{T}{300}\right)^{3/2} \exp\left(\frac{E_F - E_c}{k_B T}\right)$$

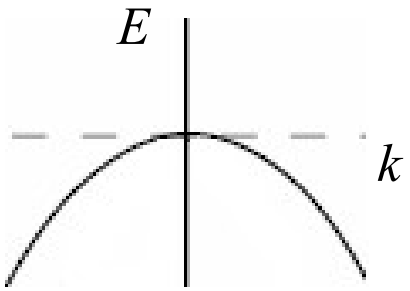
Properties	Si	Ge	GaAs
Bandgap E_g	1.12 eV	0.66 eV	1.424 eV
Effective density of states in conduction band (300 K) N_c	2.78×10^{25} m^{-3}	1.04×10^{25} m^{-3}	4.45×10^{23} m^{-3}

Density of holes in the valence band

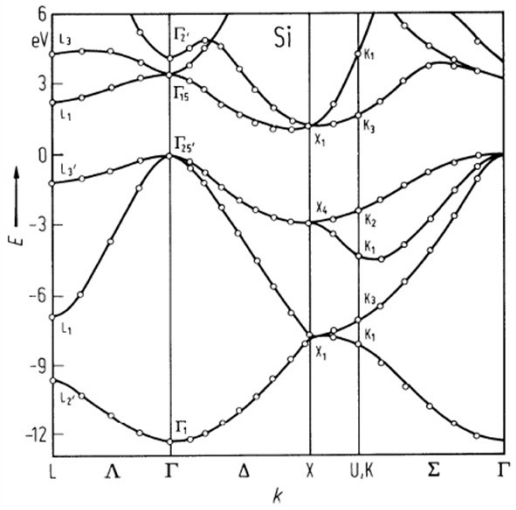
$$D(E) = D_v \sqrt{E_v - E}$$

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





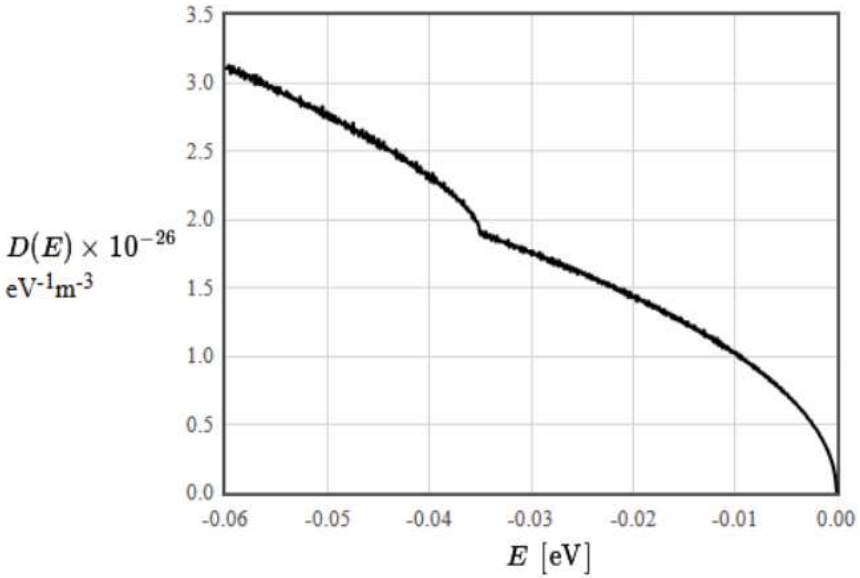
Silicon valence bands

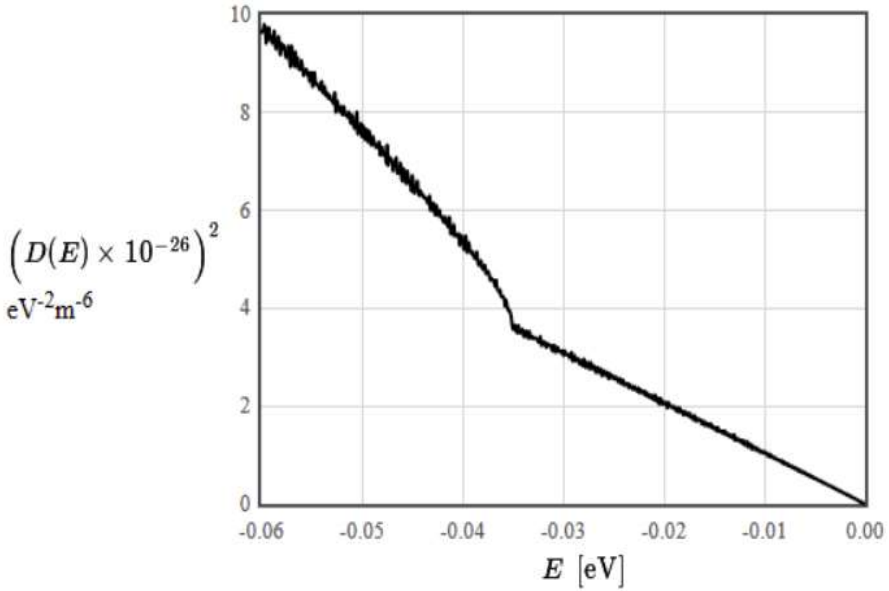


$$E_{v,lh} = -\frac{\hbar^2}{2m_e}\left(4.1k^2 - \sqrt{1.21k^4 + 4.1(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)}\right),$$

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

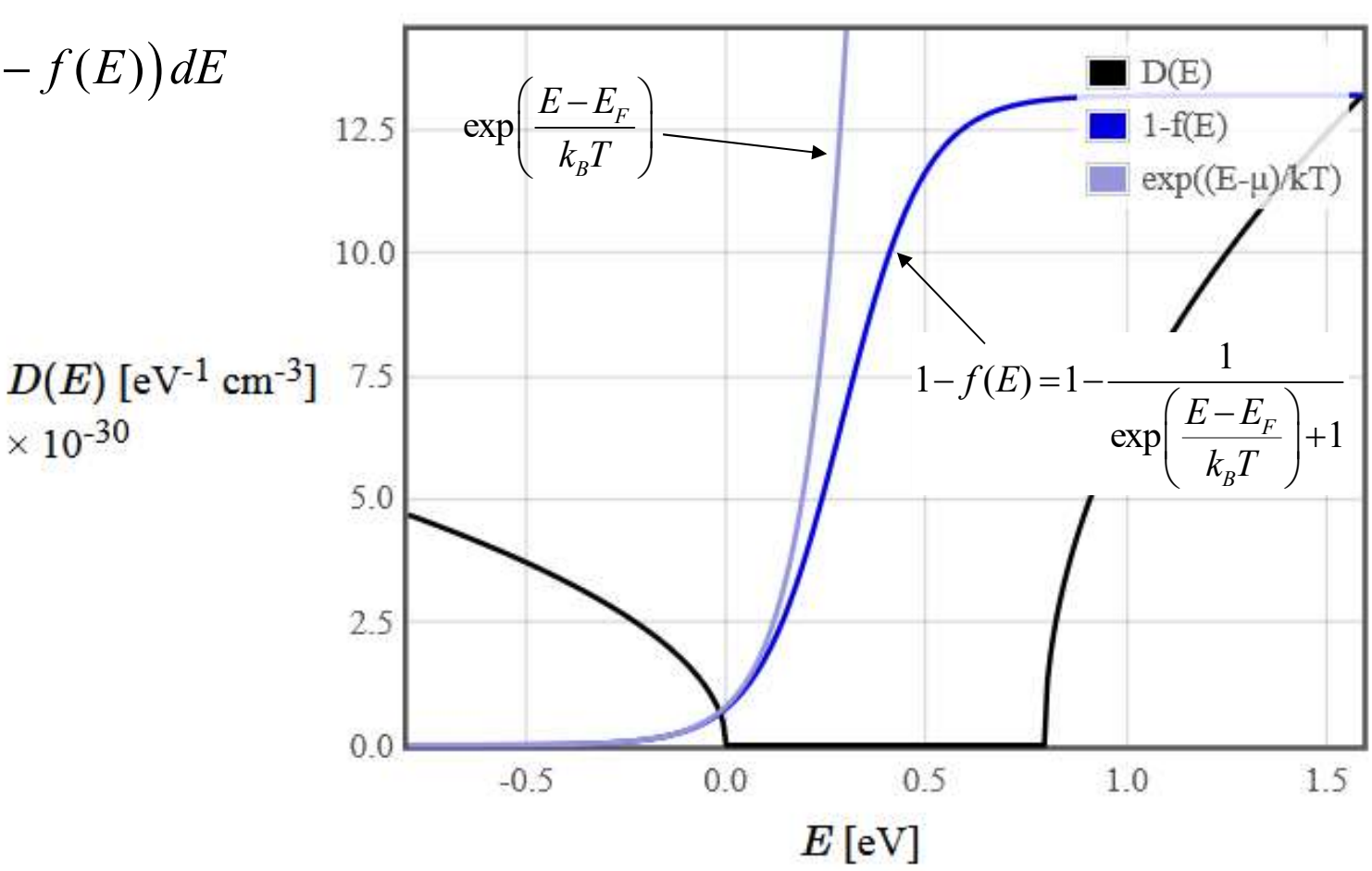
$$E_{v,so} = -E_{so} - \frac{\hbar^2k^2}{2m_{so}}.$$



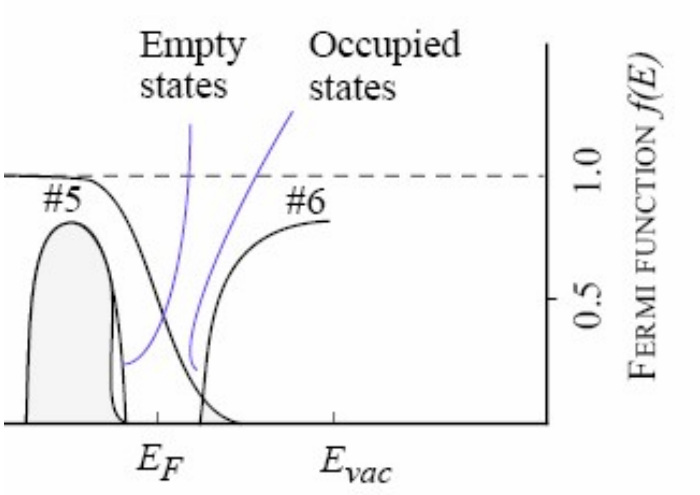


Boltzmann approximation

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



Density of holes in the valence band



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

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

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

Boltzmann approximation

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,

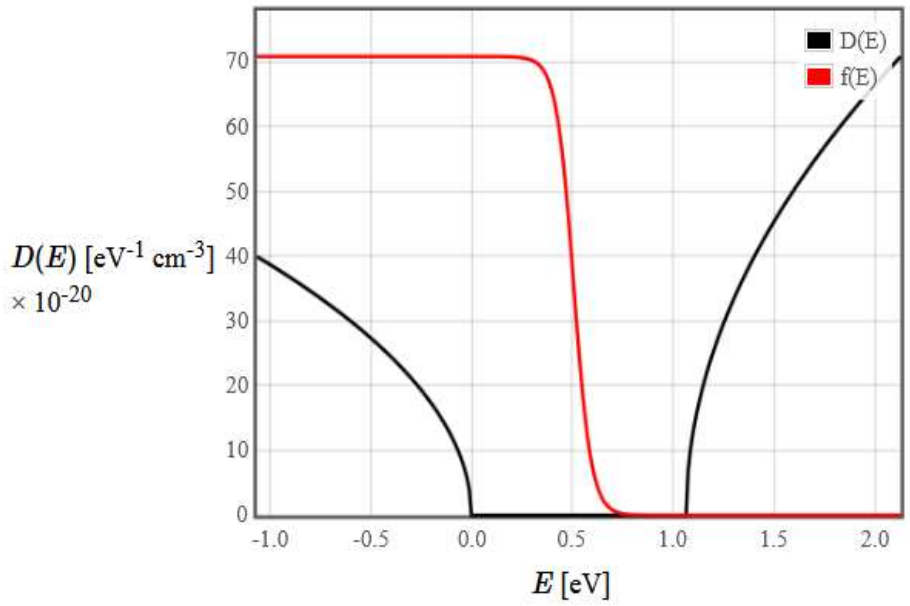
$$D(E) = \begin{cases} D_v\sqrt{E_v - E}, & \text{for } E < E_v \\ 0, & \text{for } E_v < E < E_c \\ D_c\sqrt{E - E_c}, & \text{for } E_c < E \end{cases}$$

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 'densit states effective masses' m_h^* and m_e^* or the 'effective density of states at 300 K' $N_v(300)$ and $N_c(300)$. The relations to D_v and D_c are,

$$D_v = \frac{(2m_h^*)^{3/2}}{2\pi^2\hbar^3} = \frac{\sqrt{\pi}N_v(300)}{2(k_BT)^{3/2}}, \qquad D_c = \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3} = \frac{\sqrt{\pi}N_c(300)}{2(k_B300)^{3/2}}.$$

Data for different semiconducting materials can be found in the NSM Archive.

The plot below shows the density of states of various semiconductors in this approximation. The Fermi function is plotted as well. At low energies the value of the Fermi function is 1 and those states are occupied. At high energies the Fermi function goes to zero and those states are unoccupied. In the limit of low temperture, the Fermi en the middle of the band gap, $E_F = E_g/2$. As the temperature increases, the Fermi energy moves towards the band with the lower density of states.



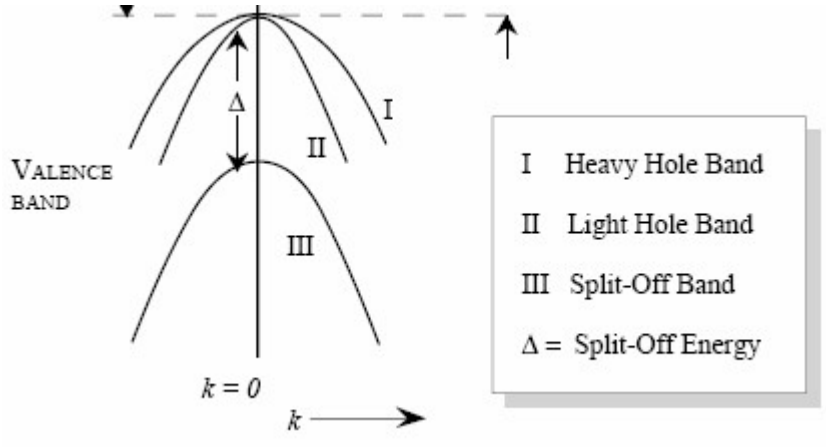
D_c =	6.874E21	$eV^{-3/2}$ cm^{-3}	Semiconductor
D_v =	3.8775E21	$eV^{-3/2}$ cm^{-3}	Si Ge GaAs GaP
E_g =	1.166-4.73E-4*T*T/(T+636)	eV	InAs InP InSb
T =	500	K	

Replot

$E_v = 0$, $E_c = E_g = 1.062$ eV, $\mu = 0.5063$ eV

$N_c(300) = 3.224\text{e+}19$ cm^{-3}, $N_v(300) = 1.819\text{e+}19$ cm^{-3}

Density of holes in the valence band



$$p = 2\left(\frac{m_h^* k_B T}{2\pi\hbar^2}\right)^{3/2} \exp\left(\frac{E_v - E_F}{k_B T}\right)$$

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

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}

New Semiconductor Materials. Biology systems.
Characteristics and Properties

Semiconductors n,k

database InGaAsP Levels Equivalents Bibliografic database

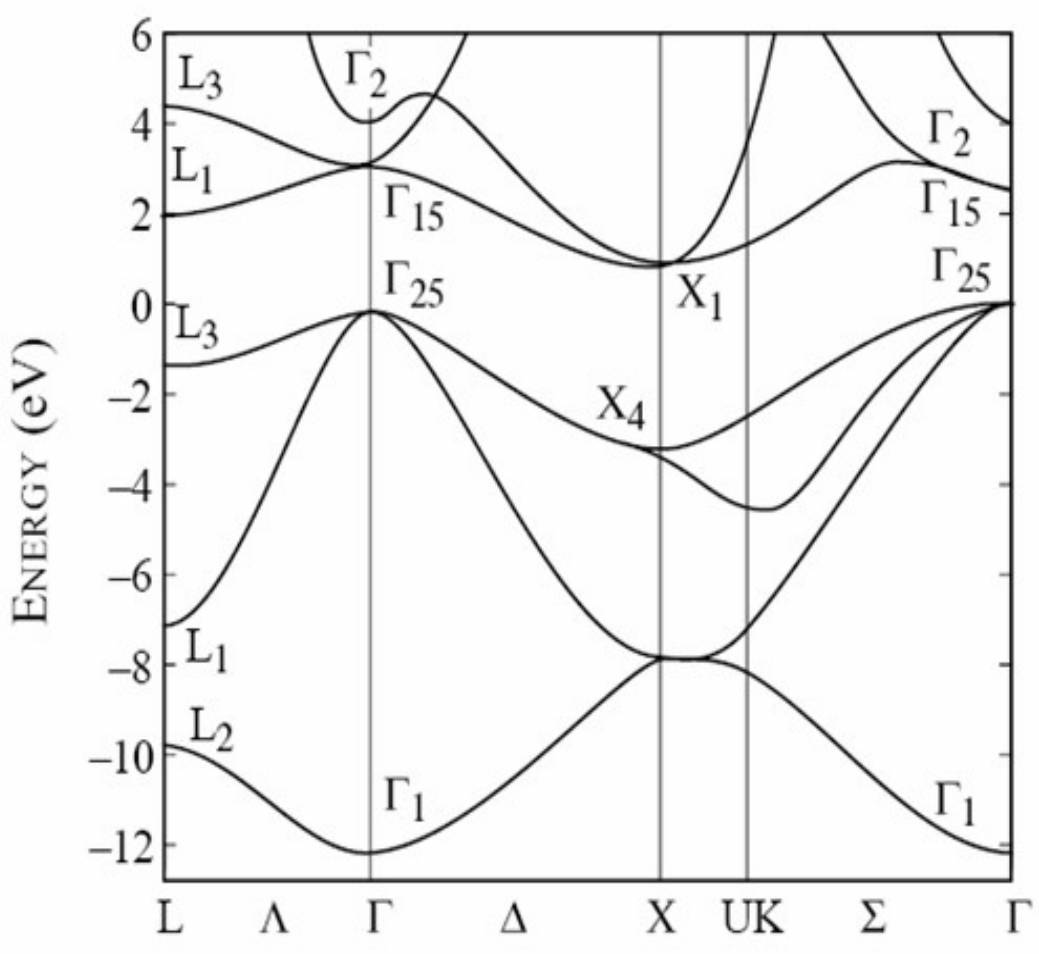
NSM Archive - Physical Properties of Semiconductors

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

http://www.matprop.ru/semicond

Exam March 2007 Problem 1

The band structure of a semiconductor is shown below. The zero of energy is chosen to be the top of the valence band.



(a) Is this a direct or an indirect semiconductor? Why?

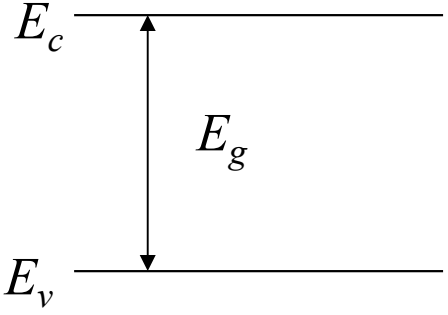
(b) What is the band gap?

(c) What are light holes and heavy holes? Explain how you can determine the effective mass of the holes from this diagram.

Law of mass action

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

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

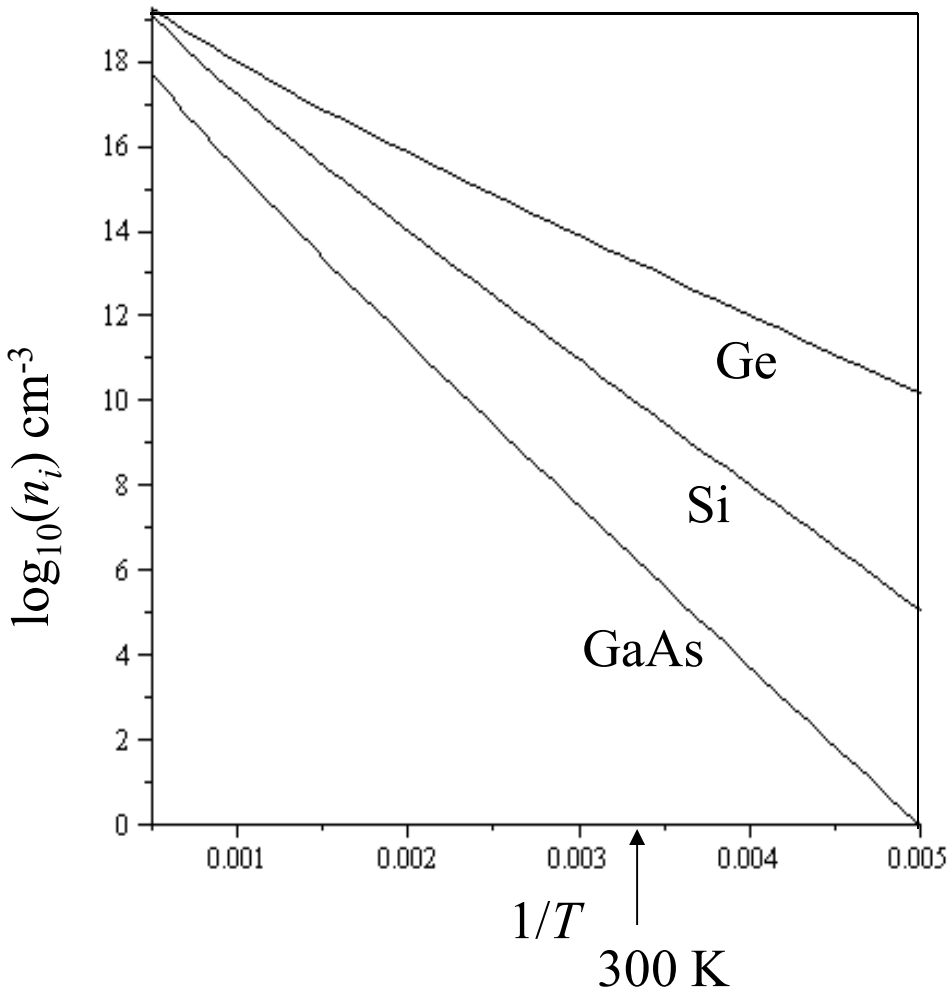


For intrinsic semiconductors (no impurities)

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

intrinsic carrier density

Intrinsic carrier concentration



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

Silicon has ~ 5×10^{22} atoms/cm^3

Good for thermometer, bad for designing circuits.

Fermi energy of an intrinsic semiconductor

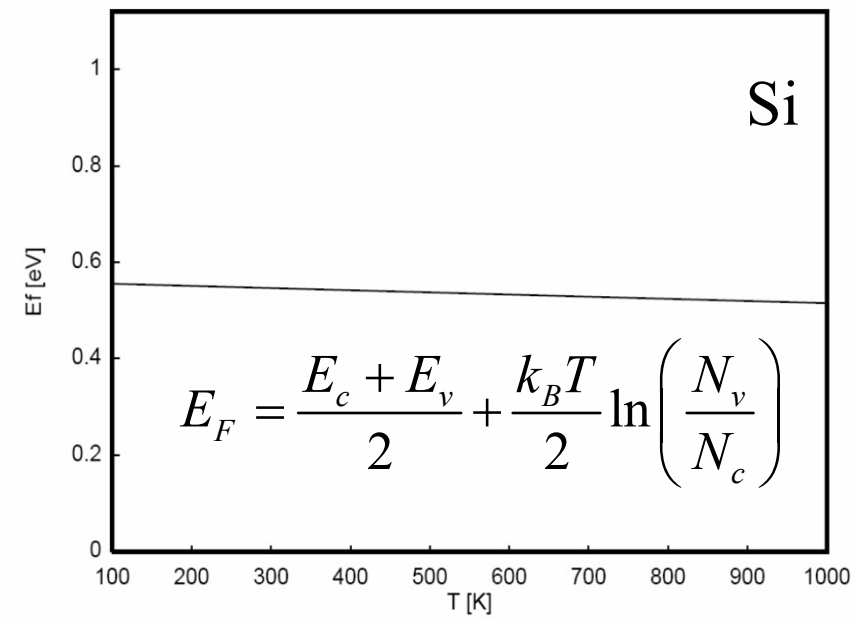
$$n = p = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right) = N_v \exp\left(\frac{E_v - E_F}{k_B T}\right)$$

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

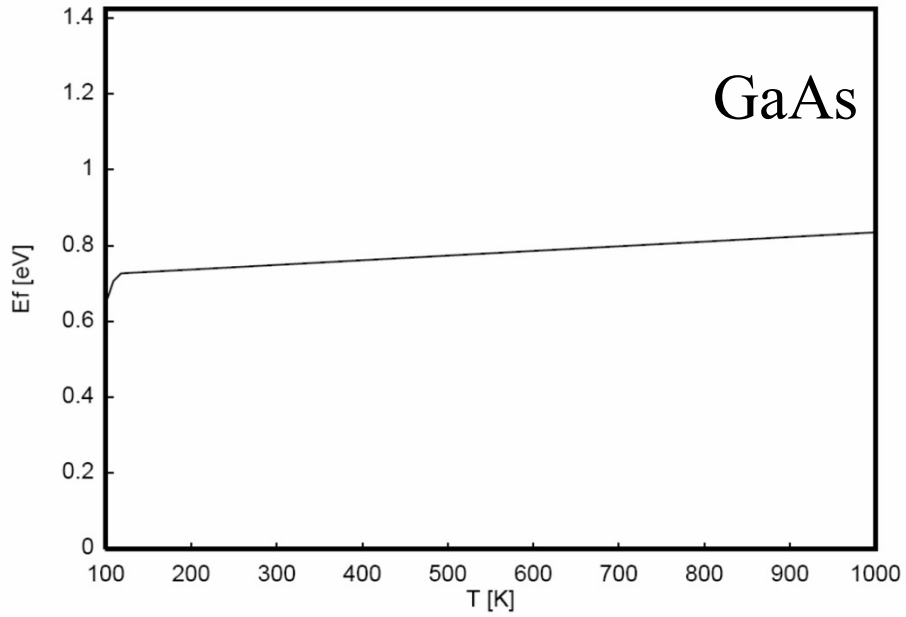
$$\frac{2E_F}{k_B T} = \frac{E_c + E_v}{k_B T} + \ln\left(\frac{N_v}{N_c}\right)$$

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

Temperature dependence of E_F

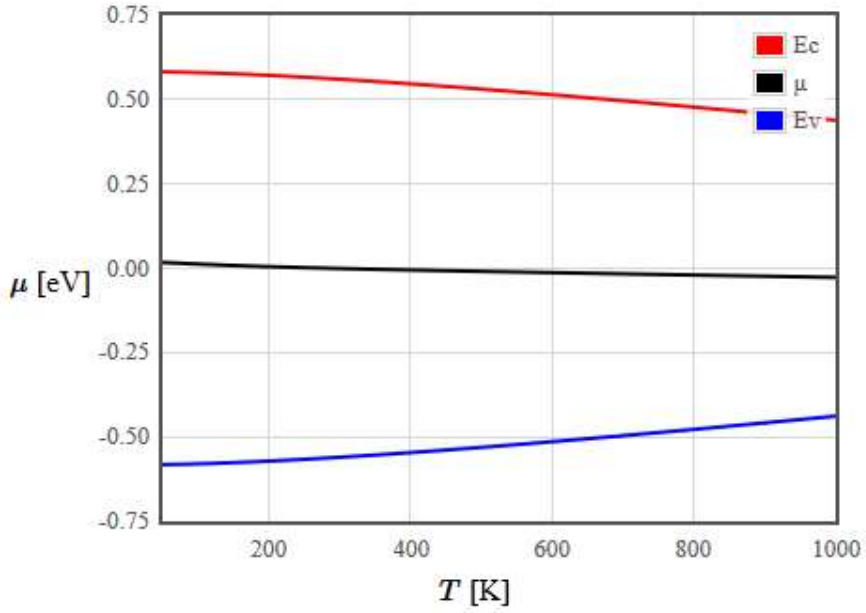


$$E_F = \frac{E_c + E_v}{2} + \frac{k_B T}{2} \ln\left(\frac{N_v}{N_c}\right)$$



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	$m_{lh}^* = 0.16$ $m_{hh}^* = 0.49$	$m_{lh}^* = 0.044$ $m_{hh}^* = 0.28$	$m_{lh}^* = 0.082$ $m_{hh}^* = 0.45$

Intrinsic semiconductors



$N_c(300\ \mathrm{K})$ = 2.78E19 1/cm³

$N_v(300\ \mathrm{K})$ = 9.84E18 1/cm³

$N_{so}(300\ \mathrm{K})$ = 2.98E18 1/cm³

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

E_v-E_{so} = 0.044 eV

T_1 = 50 K

T_2 = 1000 K

Replot

Semiconductor

Si | Ge | GaAs

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

Extrinsic semiconductors

The introduction of impurity atoms that can add electrons or holes is called doping.

n-type : donor atoms contribute electrons to the conduction band.
Examples: P, As in Si.

p-type : acceptor atoms contribute holes to the valence band.
Examples: B, Ga, Al in Si.