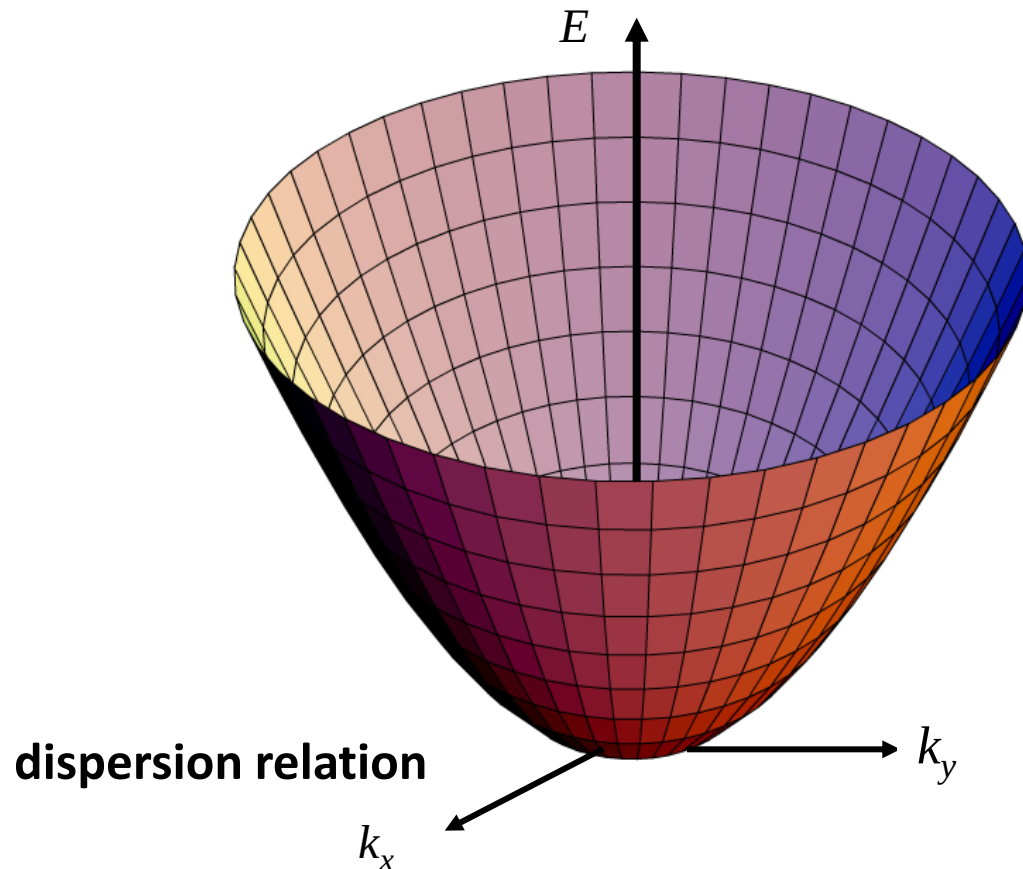


4

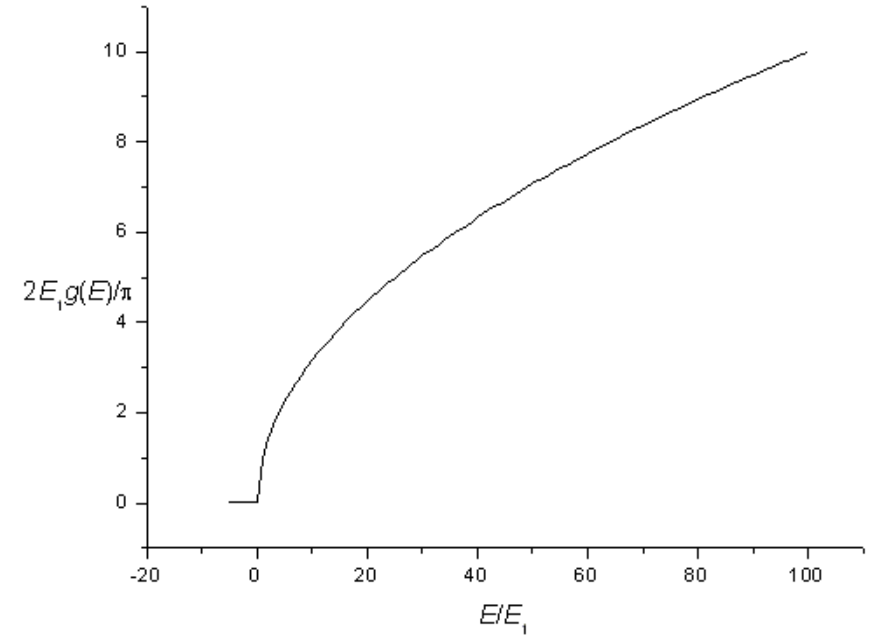
Intrinsic semiconductors

free electrons (simple model for a metal)

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



3-d density of states



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

Effective mass

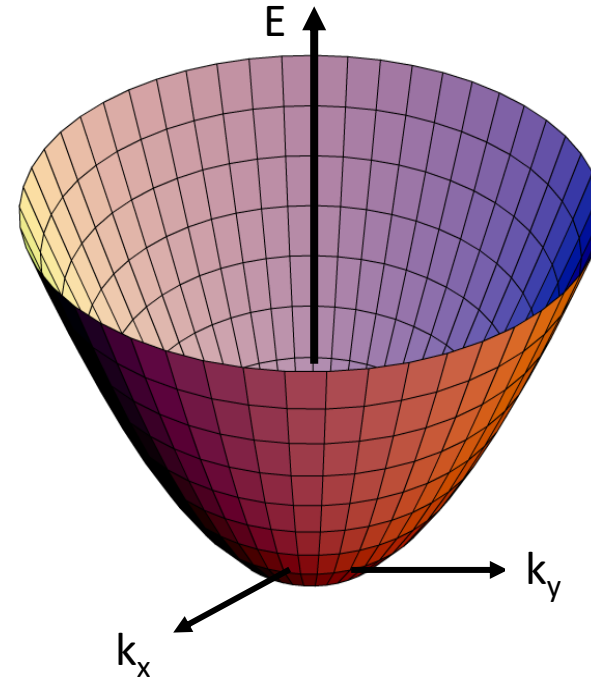
$$E(\vec{k}) = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2) = \frac{p^2}{2m} = \frac{1}{2} m v^2$$

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

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

Effective mass

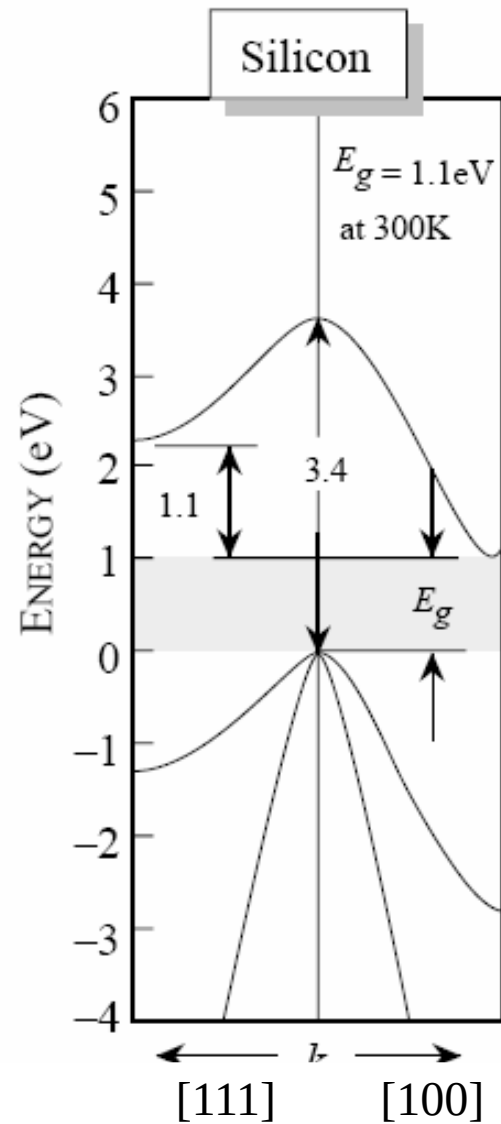
$$m_{x^*} = \frac{\hbar^2}{\frac{d^2 E(\vec{k})}{dk_x^2}}$$



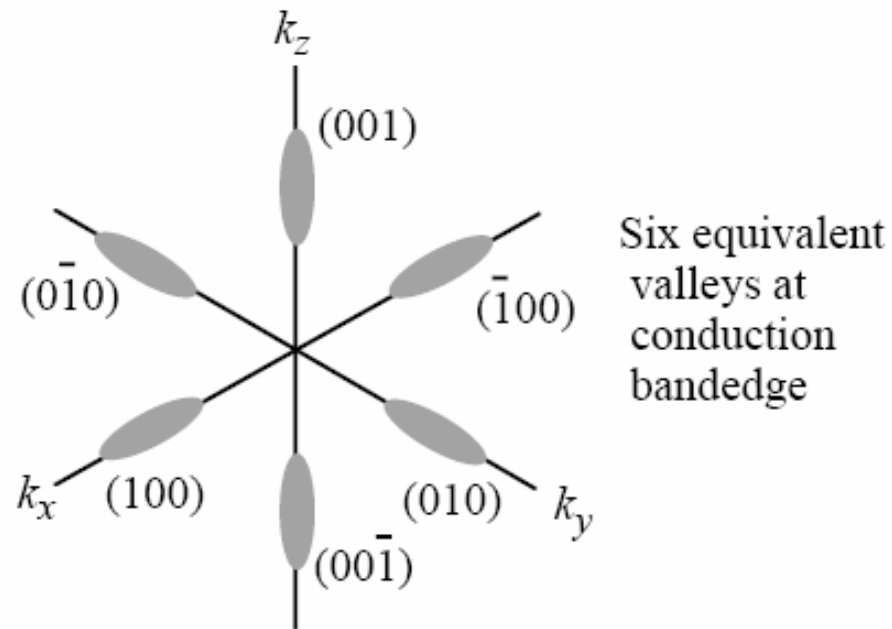
This effective mass is used to describe the response of electrons to external forces in the particle picture.

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

Anisotropic effective mass in silicon



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



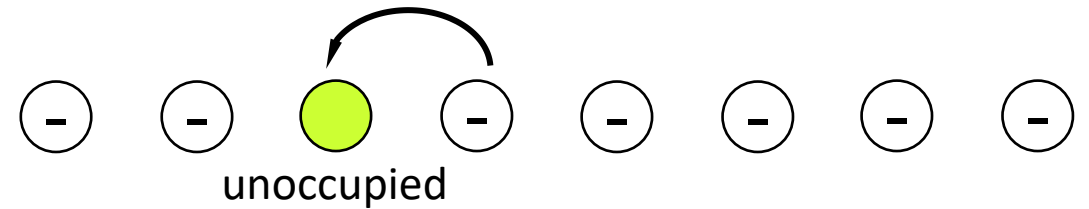
valence band, holes

- 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.

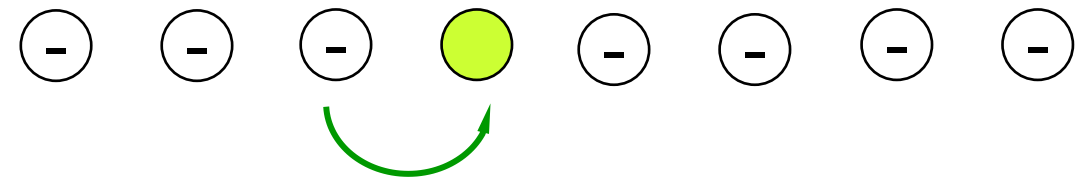
$$I \propto \sum_{\text{occupied } \vec{k}} (-e\vec{v}_{\vec{k}})$$

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

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



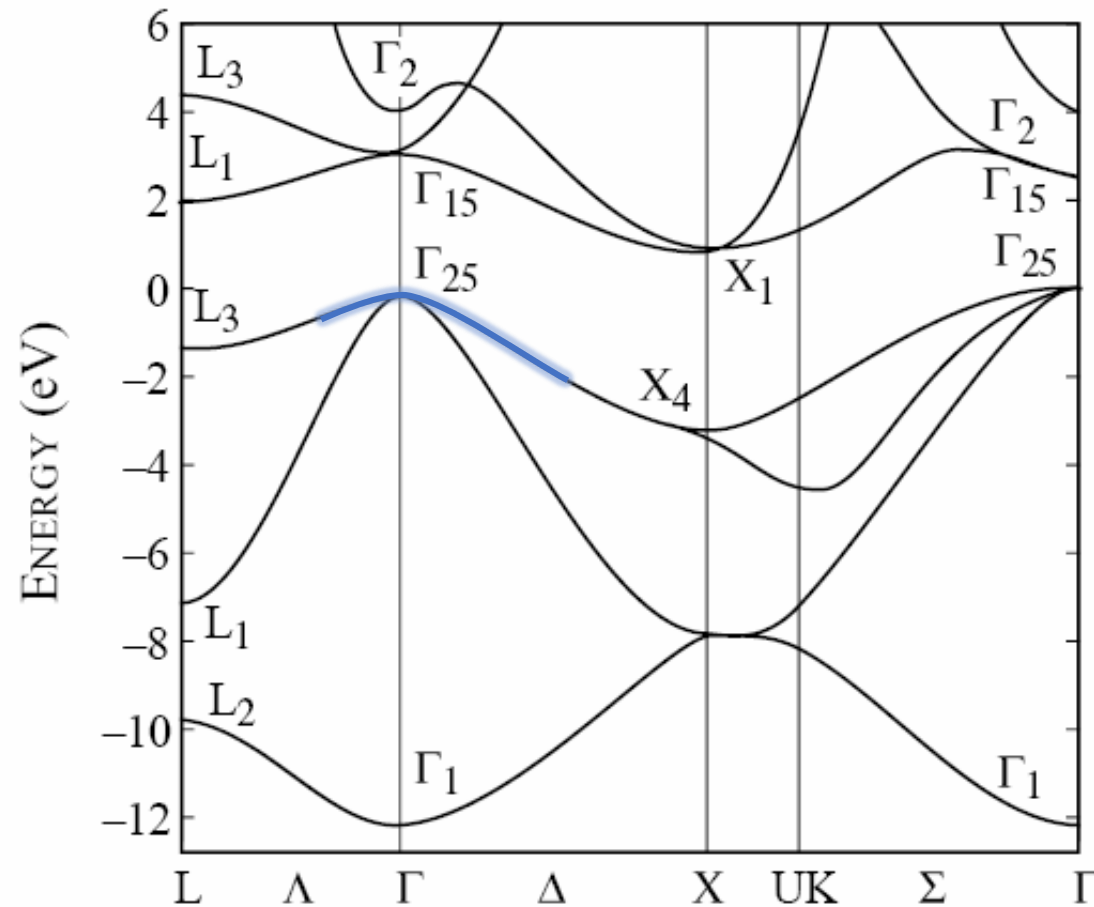
holes move like gaps in a densely packed garage



valence band, holes

In the valence band, the effective mass is negative.

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



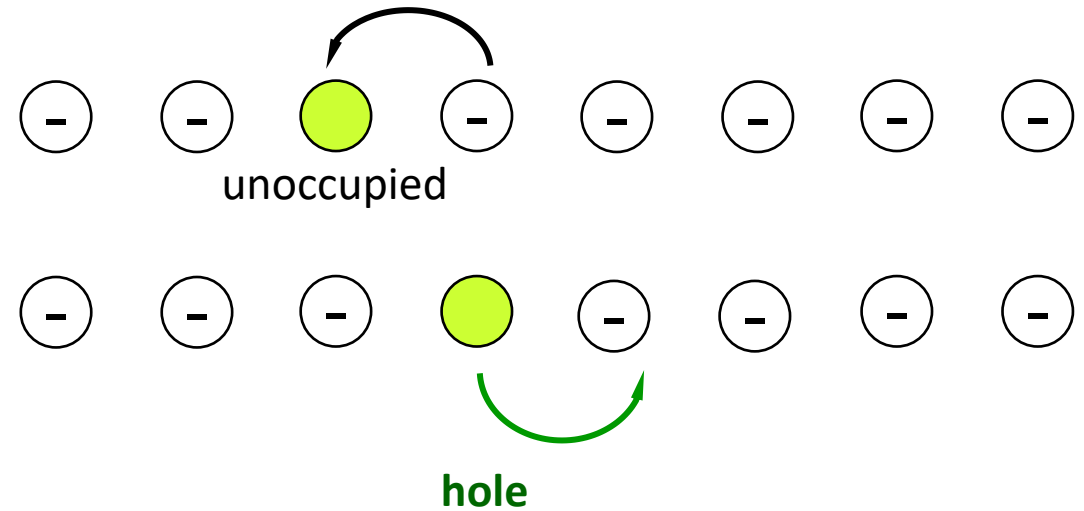
Holes

- 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.

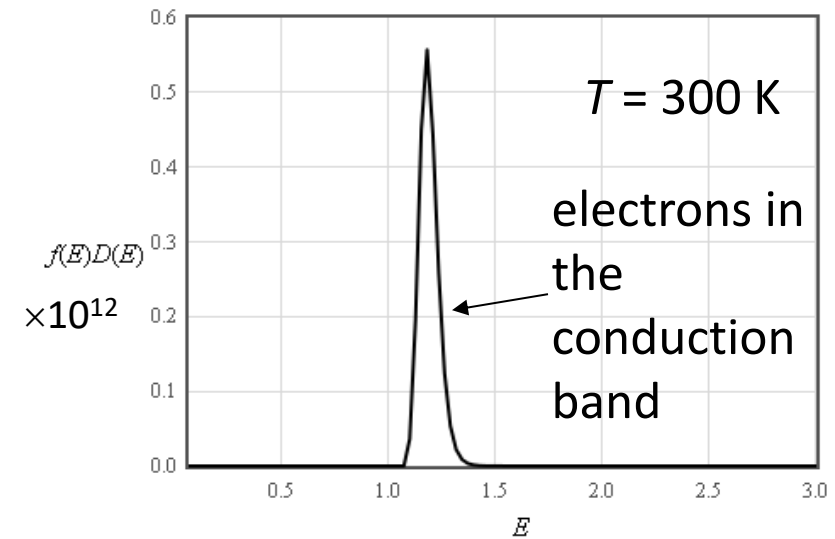
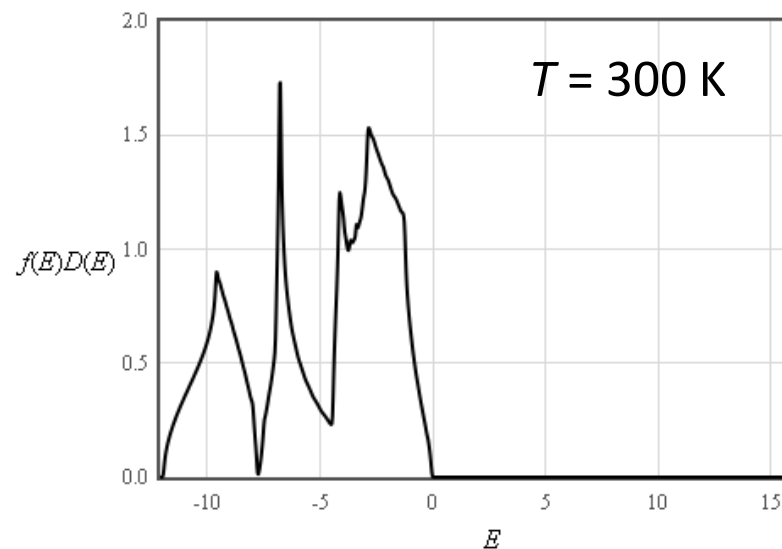
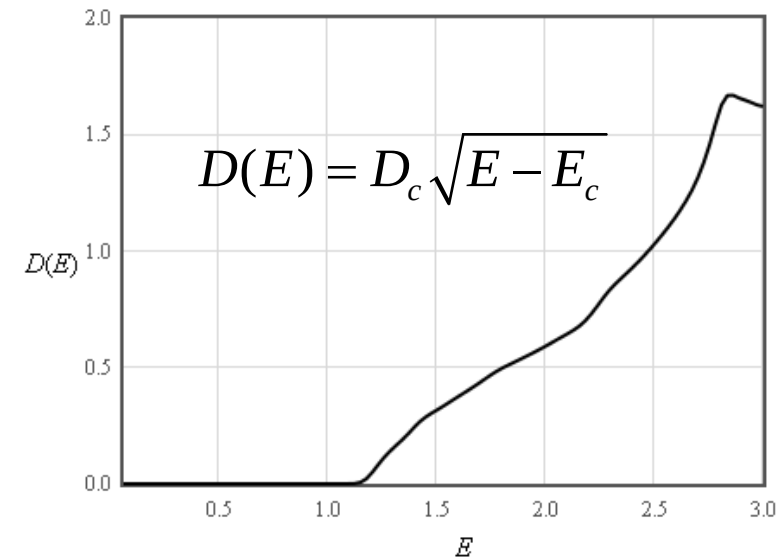
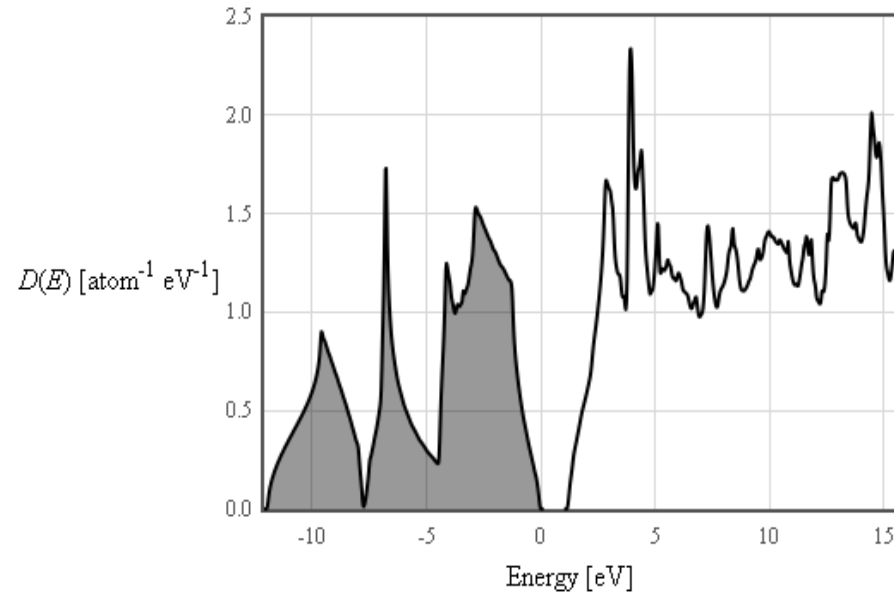
effective mass of holes m_h^*

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

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



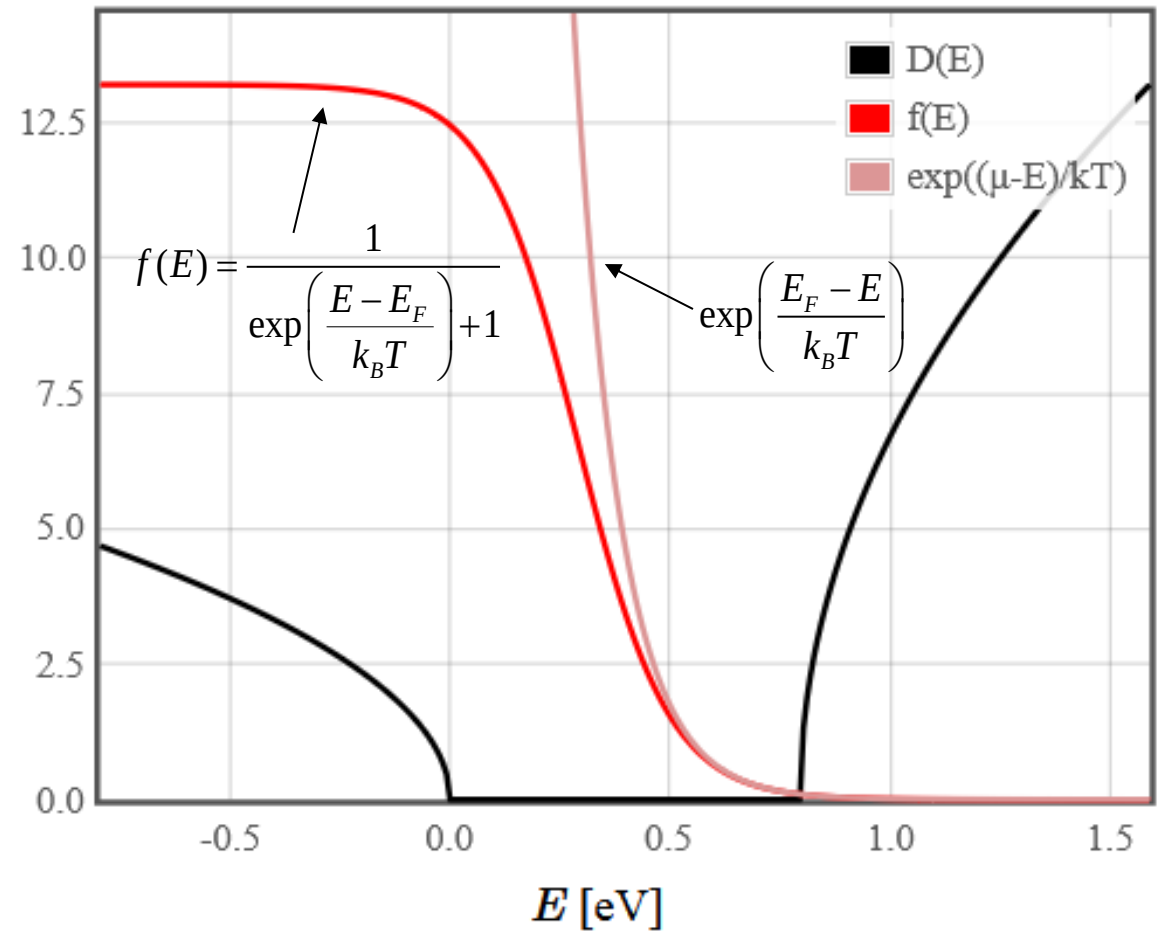
Silicon density of states



Boltzmann approximation

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

$D(E)$ [eV⁻¹ cm⁻³]
× 10⁻³⁰



Density of electrons in the conduction band

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

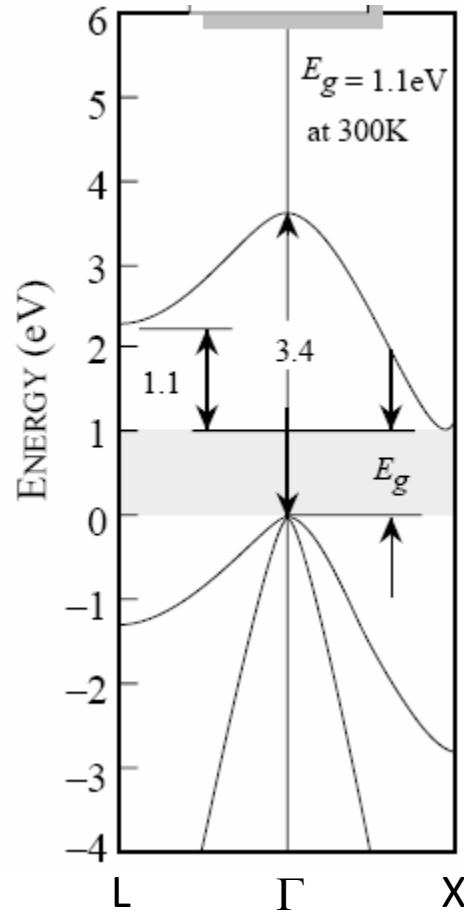
$$x = E - E_c$$

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

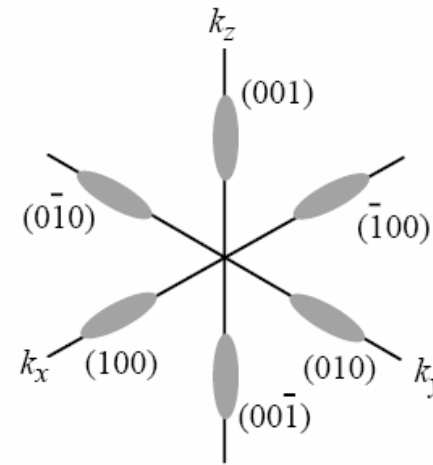
$$n = N_c(T) \exp\left(\frac{E_F - E_c}{k_B T}\right) = \frac{2D_c}{\sqrt{\pi}} (k_B T)^{3/2} \exp\left(\frac{E_F - E_c}{k_B T}\right)$$

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

Density of electrons in the conduction band



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

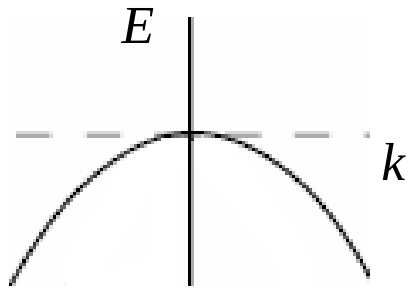


$$n = N_c \left(\frac{T}{300} \right)^{3/2} \exp \left(\frac{E_F - E_c}{k_B T} \right)$$

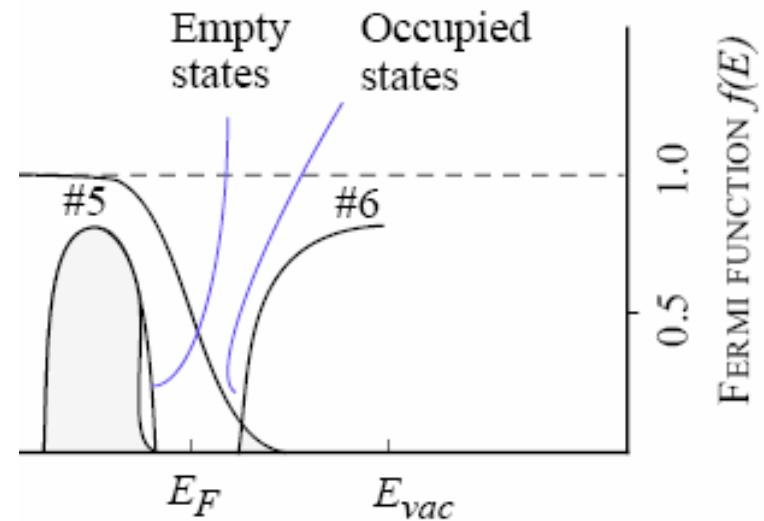
Properties	Si	Ge	GaAs
Bandgap E_g	1.12 eV	0.66 eV	1.424 eV
Effective density of states in conduction band (300 K) N_c	$2.78 \times 10^{25} \text{ m}^{-3}$	$1.04 \times 10^{25} \text{ m}^{-3}$	$4.45 \times 10^{23} \text{ m}^{-3}$

Density of holes in the valence band

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

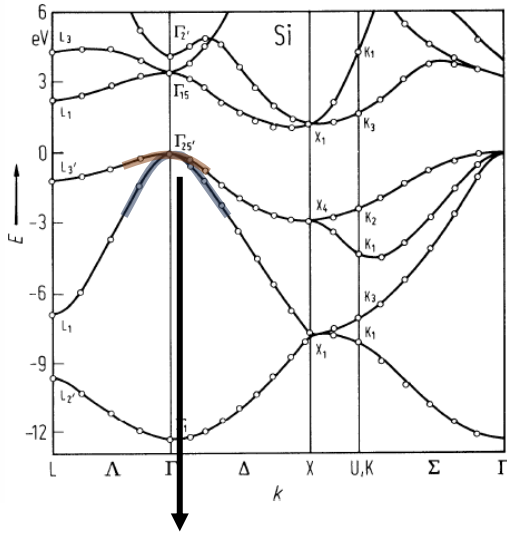


$$1 - f(E) = 1 - \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} \approx \exp\left(\frac{E - E_F}{k_B T}\right)$$



Silicon valence bands

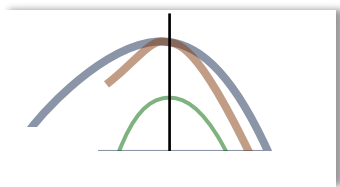
<https://journals.aps.org/rmp/pdf/10.1103/RevModPhys.30.122>



$$E_{v, lh} = -\frac{\hbar^2}{2m_e} \left(4.1k^2 + \sqrt{1.21k^4 + 16.81(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)} \right)$$

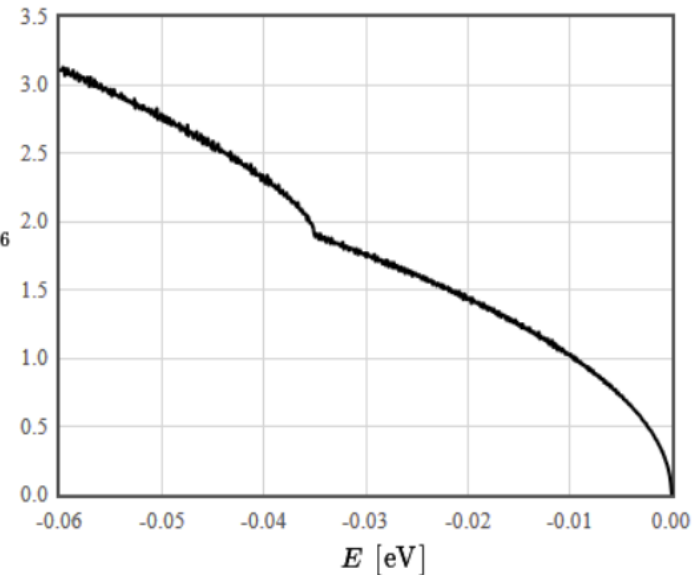
$$E_{v, hh} = -\frac{\hbar^2}{2m_e} \left(4.1k^2 - \sqrt{1.21k^4 + 16.81(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)} \right)$$

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

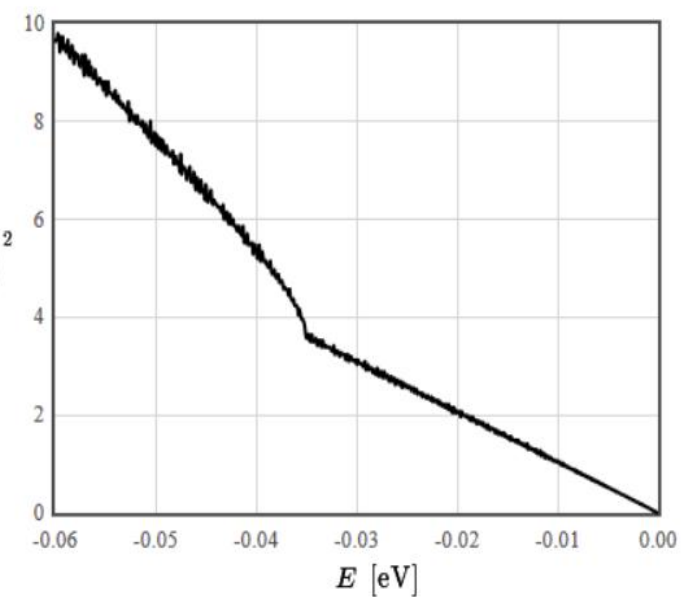


close up

$D(E) \times 10^{-26}$
 $\text{eV}^{-1}\text{m}^{-3}$



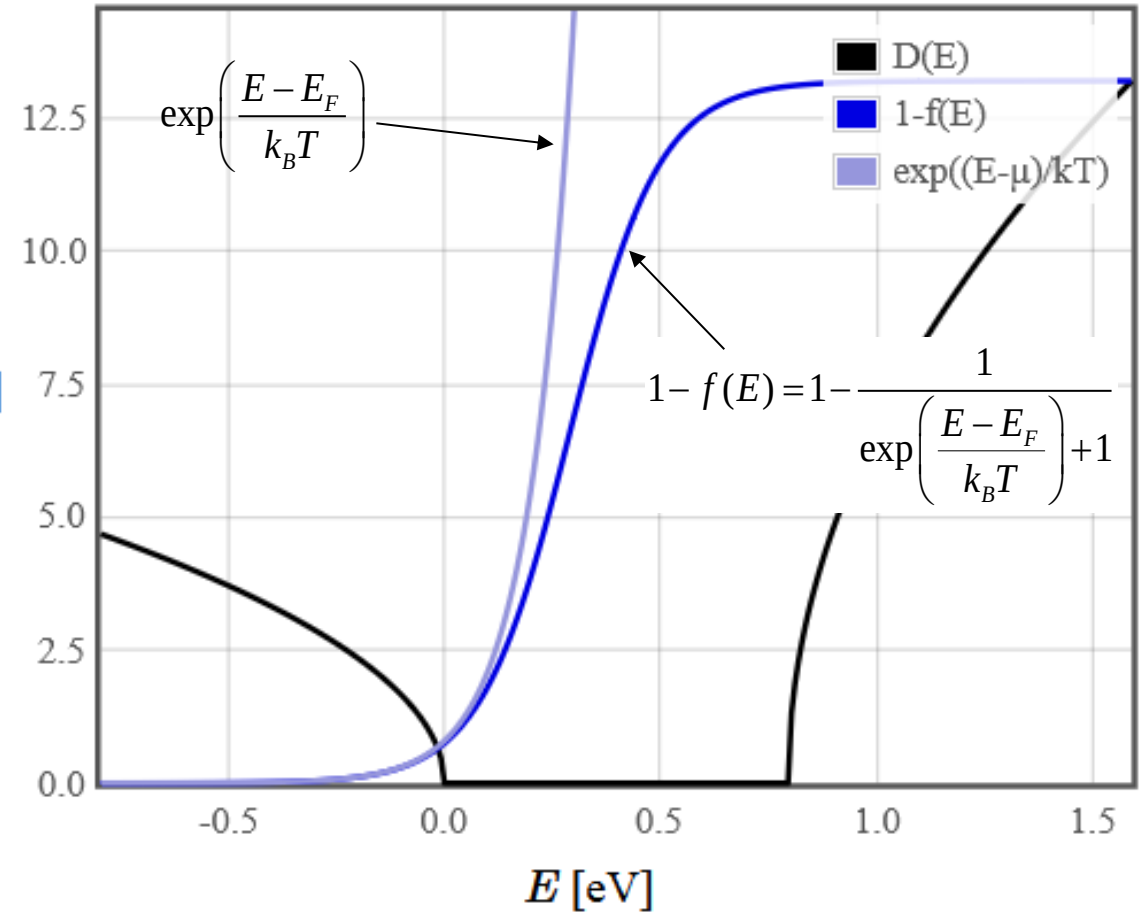
$(D(E) \times 10^{-26})^2$
 $\text{eV}^{-2}\text{m}^{-6}$



Boltzmann approximation

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

$D(E) [\text{eV}^{-1} \text{cm}^{-3}]$
 $\times 10^{-30}$



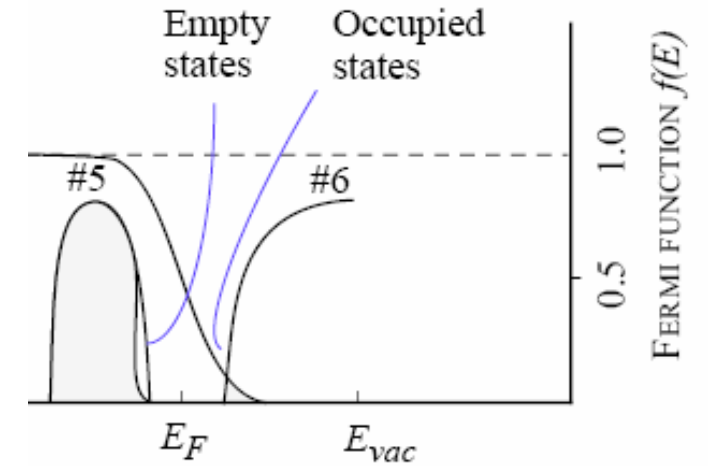
Density of holes in the valence band

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

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

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

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,

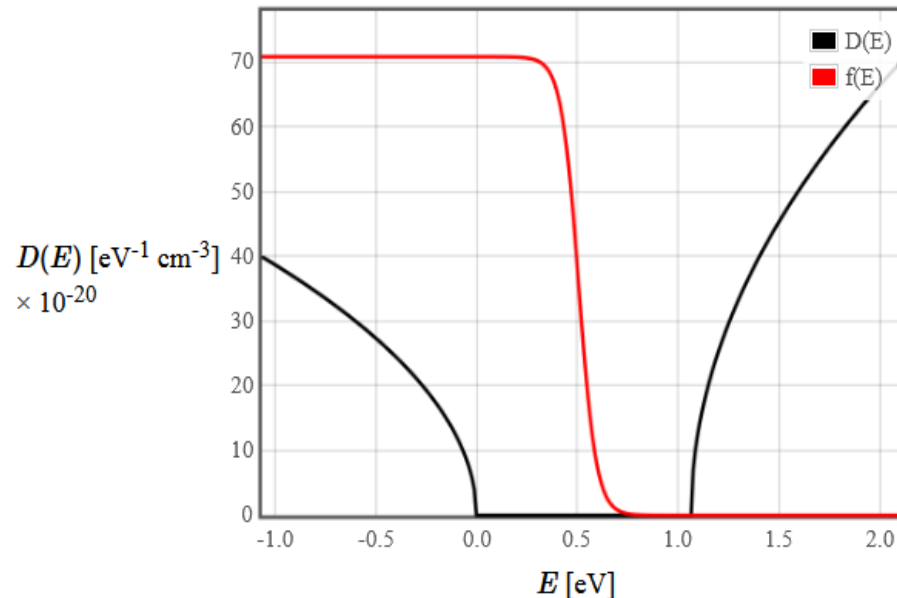
$$D(E) = \begin{cases} D_v \sqrt{E_v - E}, & \text{for } E < E_v \\ 0, & \text{for } E_v < E < E_c \\ D_c \sqrt{E - E_c}, & \text{for } E_c < E \end{cases}$$

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 'density 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,

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

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 temperature, the Fermi energy is 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.

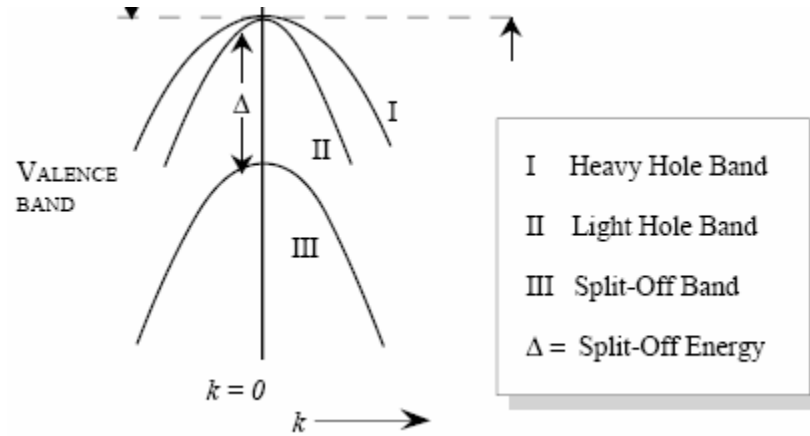


$D_c =$	6.874E21	$\text{eV}^{-3/2} \text{ cm}^{-3}$	Semiconductor Si Ge GaAs GaP InAs InP InSb
$D_v =$	3.8775E21	$\text{eV}^{-3/2} \text{ cm}^{-3}$	
$E_g =$	1.166-4.73E-4*T/(T+636)	eV	
$T =$	500	K	
Replot			

$$E_v = 0, \quad E_c = E_g = 1.062 \text{ eV}, \quad \mu = 0.5063 \text{ eV}$$

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

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	$2.78 \times 10^{25} \text{ m}^{-3}$	$1.04 \times 10^{25} \text{ m}^{-3}$	$4.45 \times 10^{23} \text{ m}^{-3}$
Effective density of states in valence band (300 K) N_v	$9.84 \times 10^{24} \text{ m}^{-3}$	$6.0 \times 10^{24} \text{ m}^{-3}$	$7.72 \times 10^{24} \text{ m}^{-3}$
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/cm ³	5.3267 g/cm ³	5.32 g/cm ³
Atoms/m ³	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

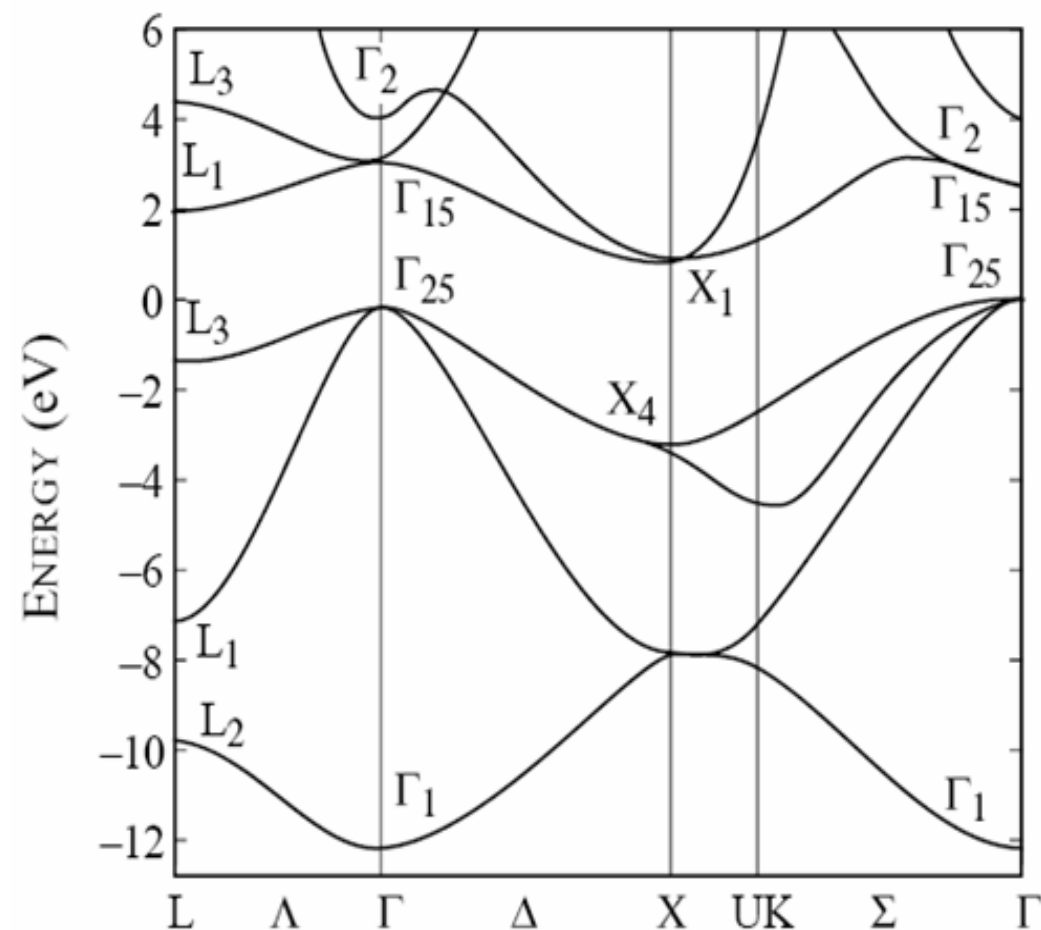
NSM Archive - Physical Properties of Semiconductors

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 _x Ga _{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.

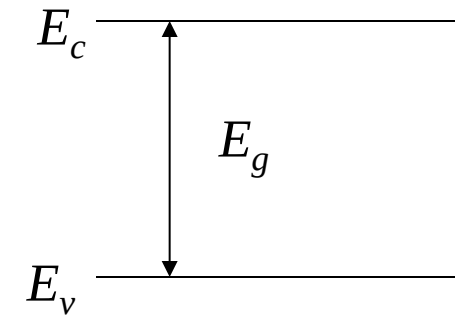


- (a) Is this a direct or an indirect semiconductor? Why?
- (b) What is the band gap?
- (c) What are light holes and heavy holes? Explain how you can determine the effective mass of the holes from this diagram.

Law of mass action

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

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

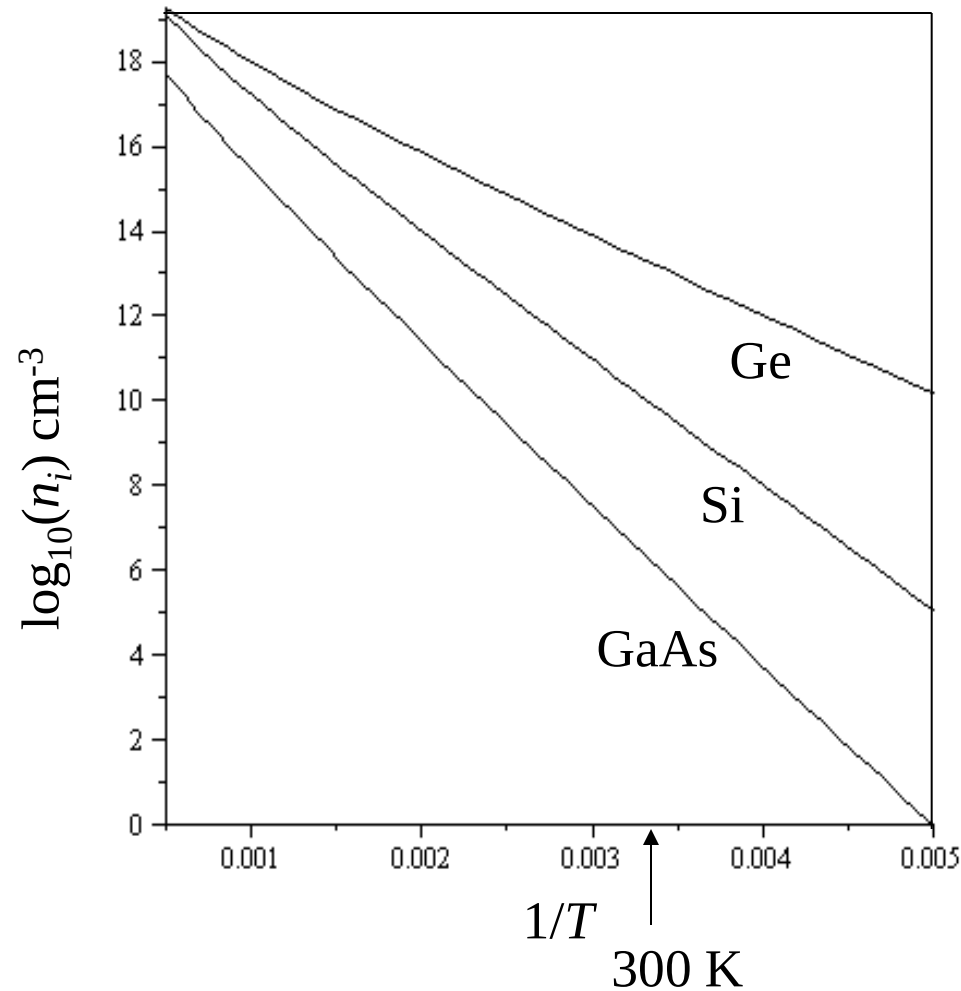


For intrinsic semiconductors (no impurities)

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

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 $\sim 5 \times 10^{22}$ atoms/cm³

Good for thermometer, bad for designing circuits.

Fermi energy of an intrinsic semiconductor

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

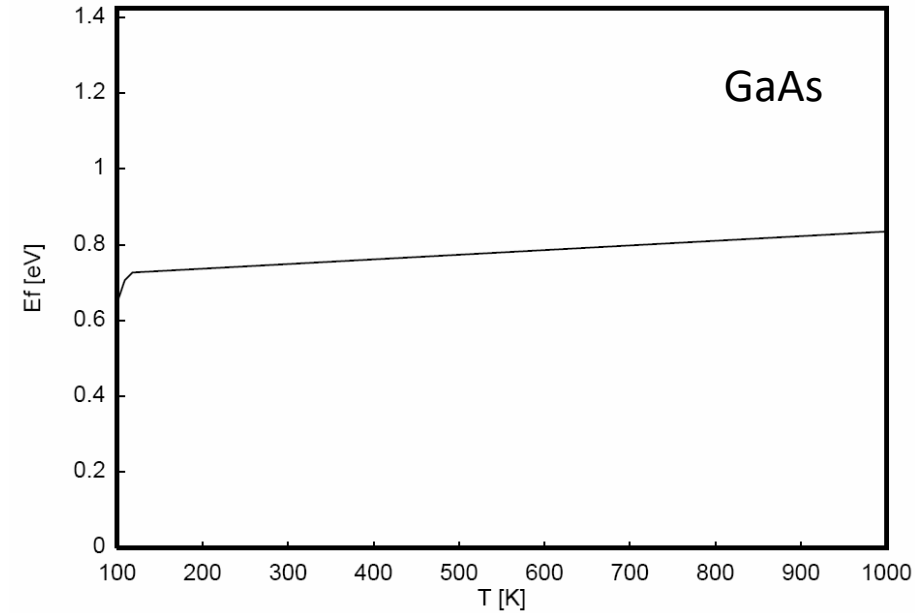
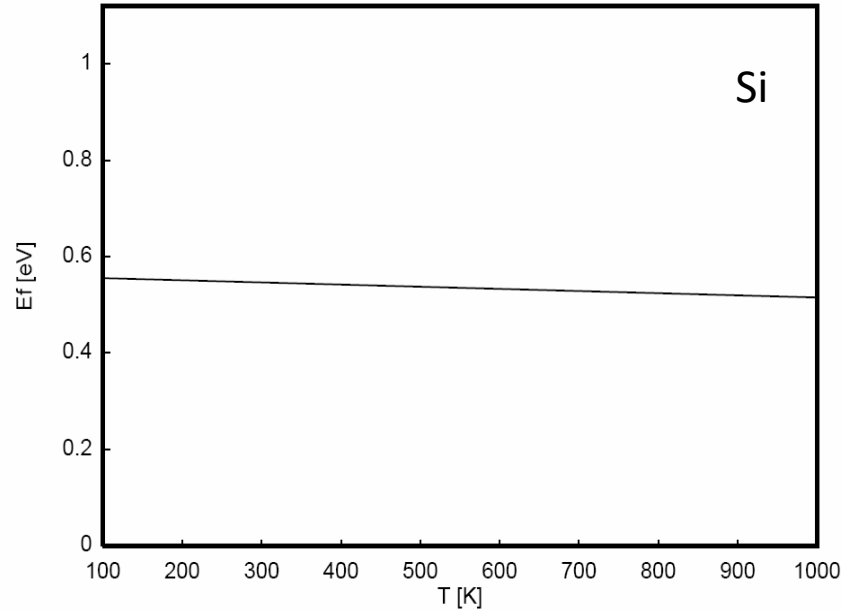
$$n = p \Rightarrow \underset{\blacktriangle}{N_c} \exp \left(\frac{E_F - E_c}{k_B T} \right) \overset{\blacktriangledown}{=} \underset{\blacktriangle}{N_v} \exp \left(\frac{E_v - E_F}{k_B T} \right)$$

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

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

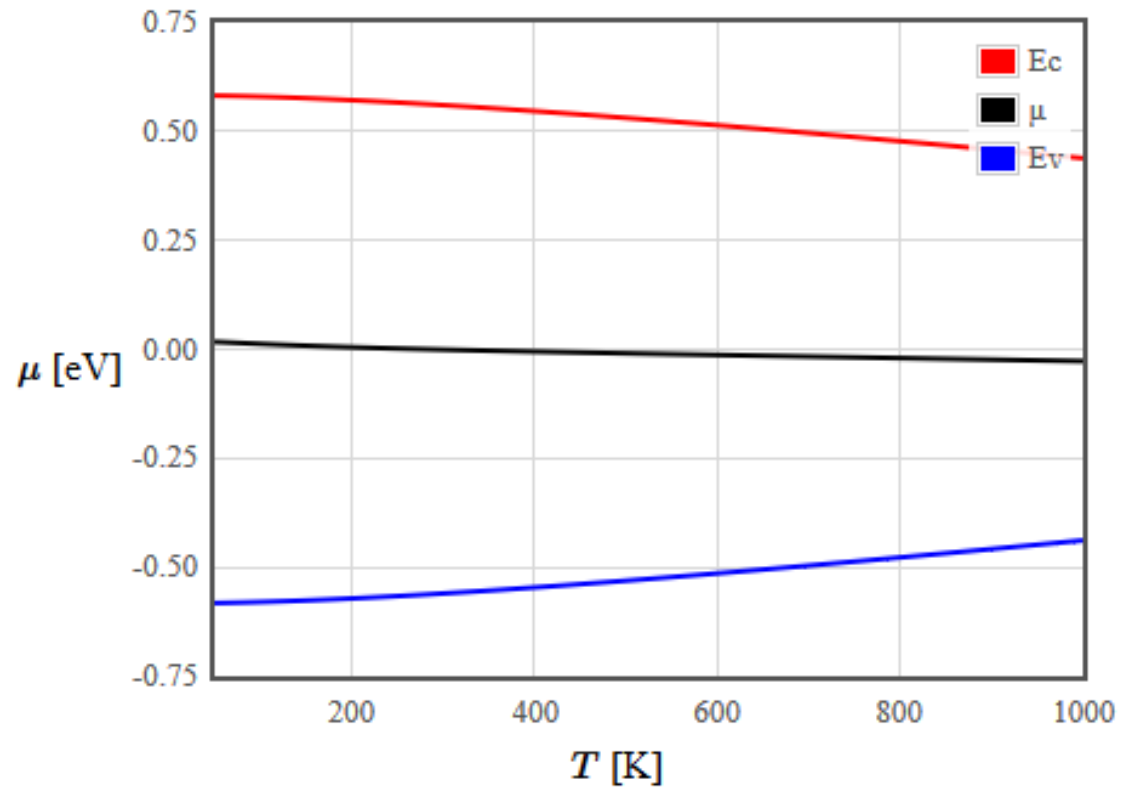
Temperature dependence of E_F

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



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	$2.78 \times 10^{25} \text{ m}^{-3}$	$1.04 \times 10^{25} \text{ m}^{-3}$	$4.45 \times 10^{23} \text{ m}^{-3}$
Effective density of states in valence band (300 K) N_v	$9.84 \times 10^{24} \text{ m}^{-3}$	$6.0 \times 10^{24} \text{ m}^{-3}$	$7.72 \times 10^{24} \text{ m}^{-3}$
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



$N_c(300\text{ K}) =$	2.78E19	$1/\text{cm}^3$	Semiconductor Si Ge GaAs
$N_v(300\text{ K}) =$	9.84E18	$1/\text{cm}^3$	
$N_{so}(300\text{ K}) =$	2.98E18	$1/\text{cm}^3$	
$E_g =$	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			

http://lampz.tugraz.at/~hadley/ss1/semiconductors/intrinsic_so.php