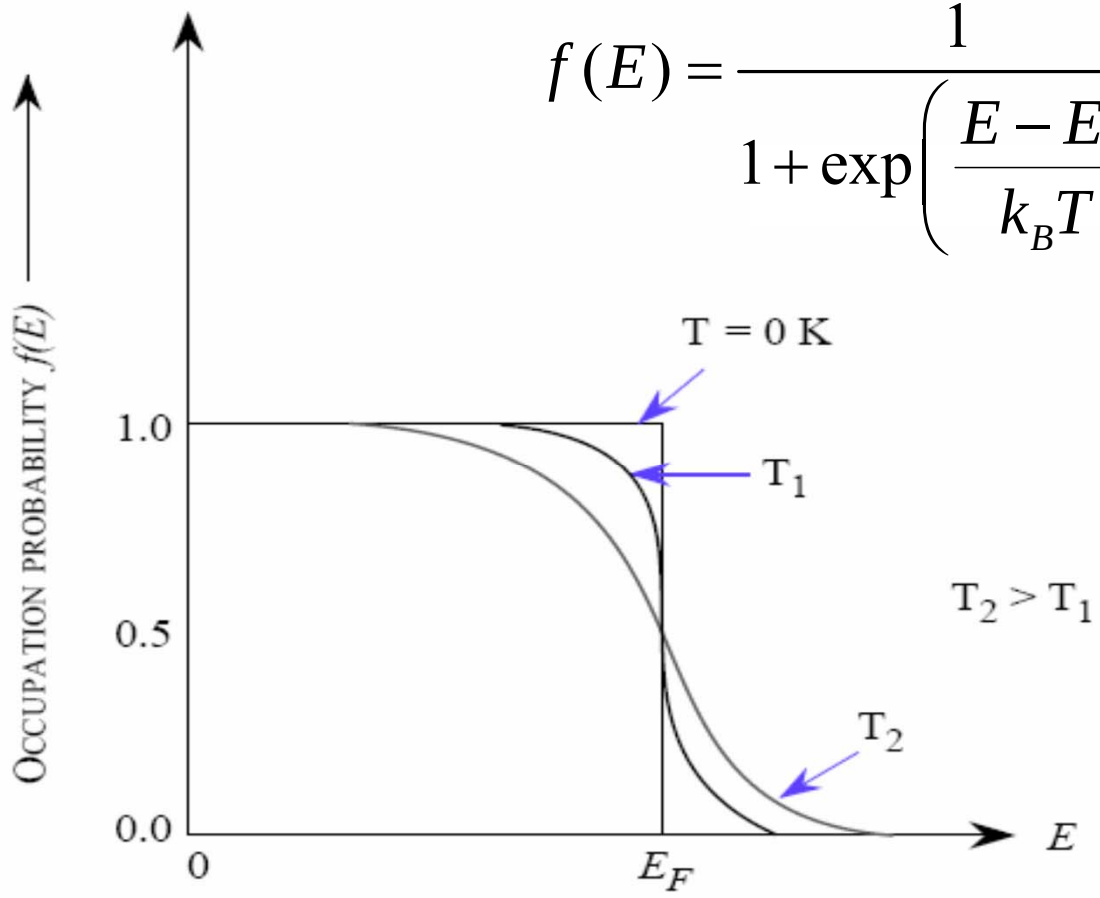
3. Intrinsic and Extrinsic semiconductors

Oct. 17, 2018

Fermi function

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

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



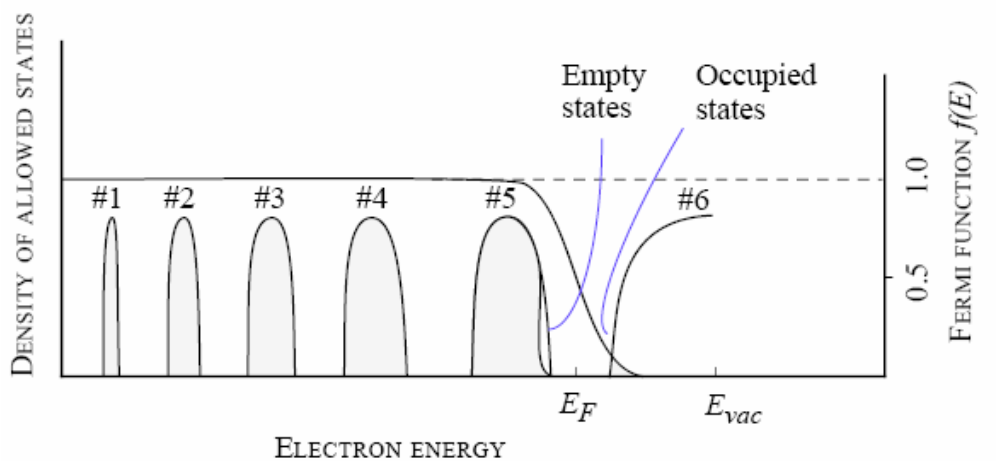
Fermi energy

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.

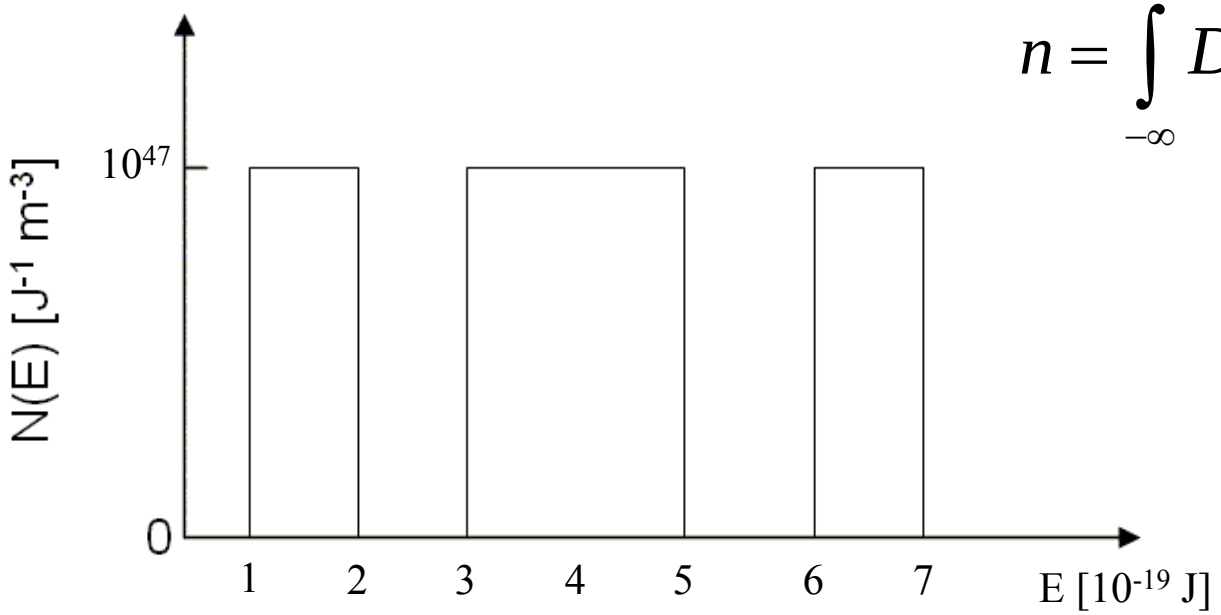
The density of states, the total number of electrons and the temperature are given. To find the Fermi energy, guess one and evaluate the integral. If n turns out too low, guess a higher E_F and if n turns out too high, guess a lower E_F.



Calculate the Fermi energy

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

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



$$n = 3\times10^{28}\ \mathrm{m}^{-3}$$

What is the Fermi energy at zero temperature? For a semiconductor, find the limiting value of the Fermi energy as the temperature approaches zero.

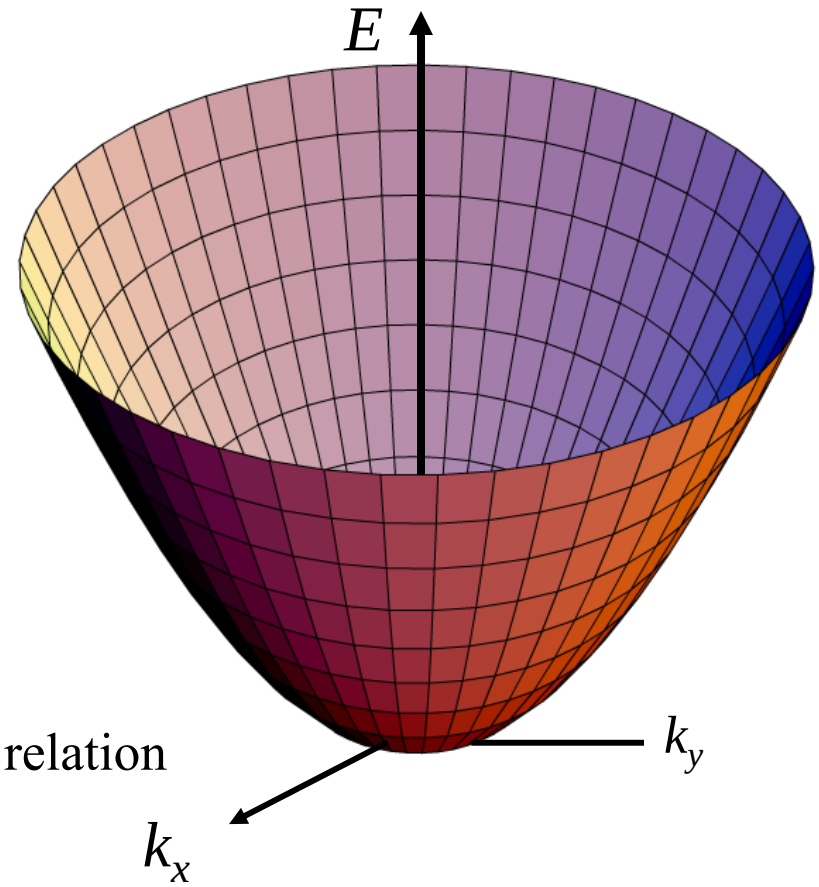
$E_f =$ _____ eV

What kind of material is this?

Metal

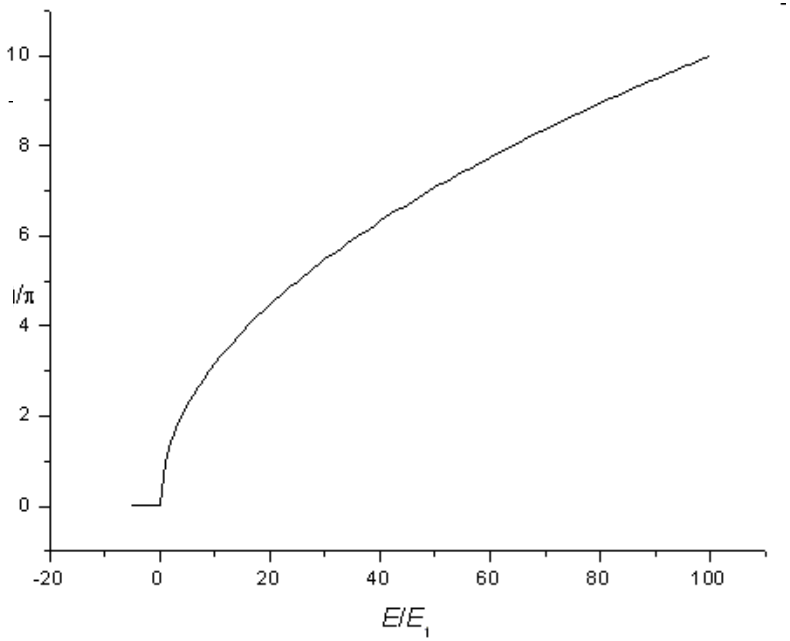
free electrons (simple model for a metal)

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



dispersion relation

3-d density of states



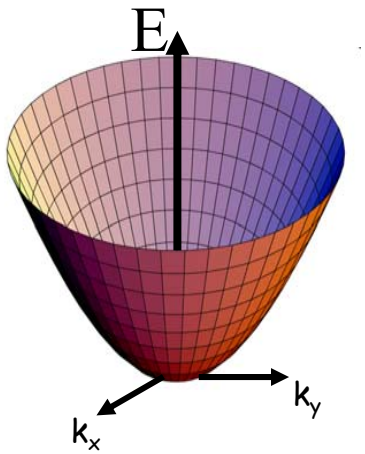
$$D(E) = \begin{cases} 0 & \text{for} \quad E < 0 \\ \dfrac{(2m)^{3/2}}{2\pi^2\hbar^3}\sqrt{E} & \text{for} \quad E > 0 \end{cases}$$

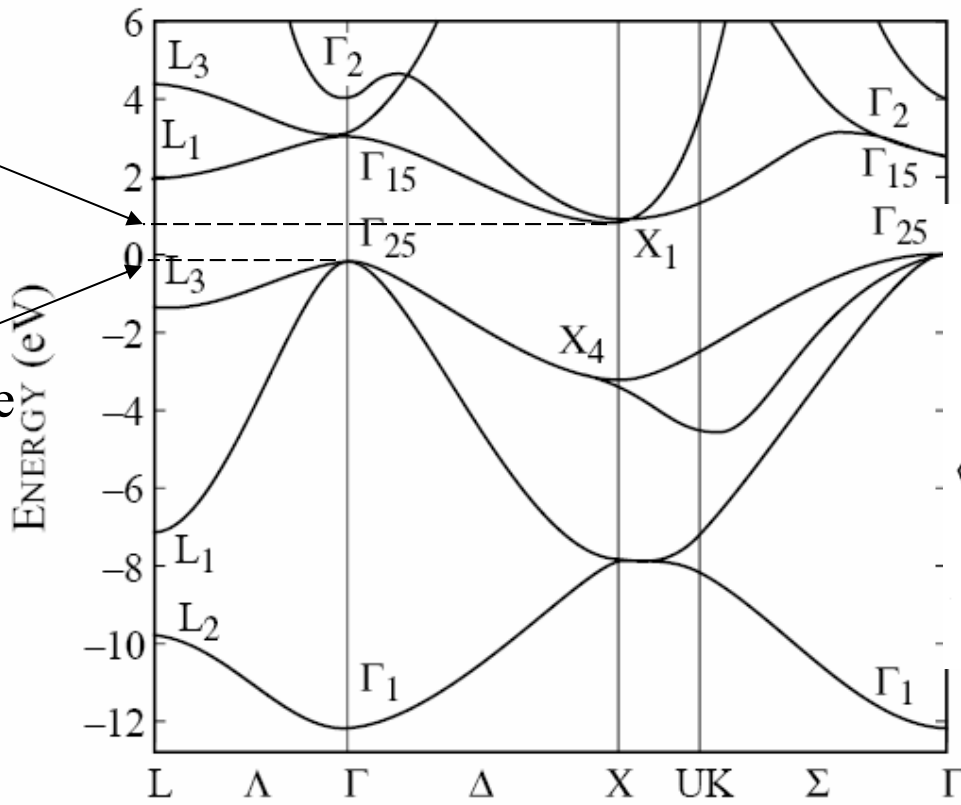
Silicon band structure

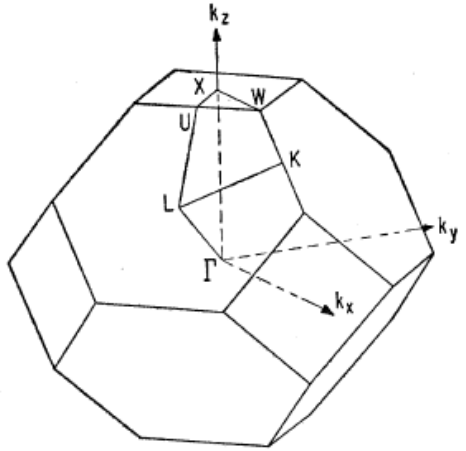
E_c = bottom of the conduction band

$E_g = E_c - E_v$

E_v = top of the valence band







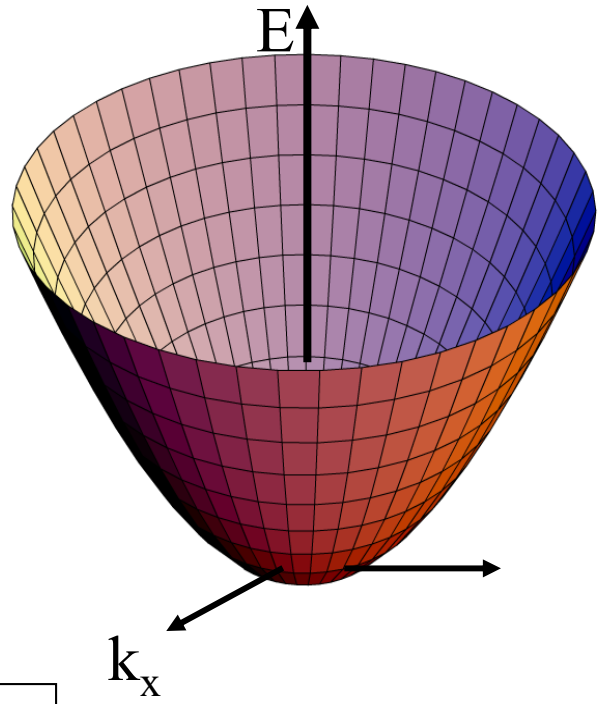
Near the bottom of the conduction band, the band structure looks like a parabola.

Effective mass

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

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

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



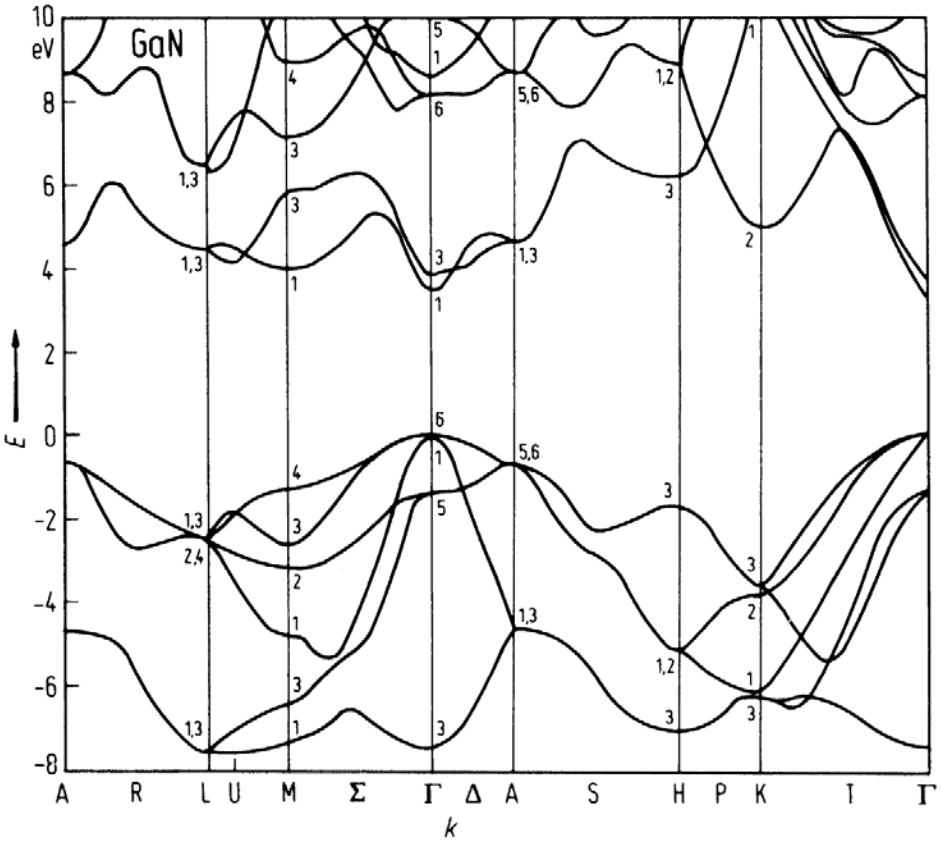
Effective mass

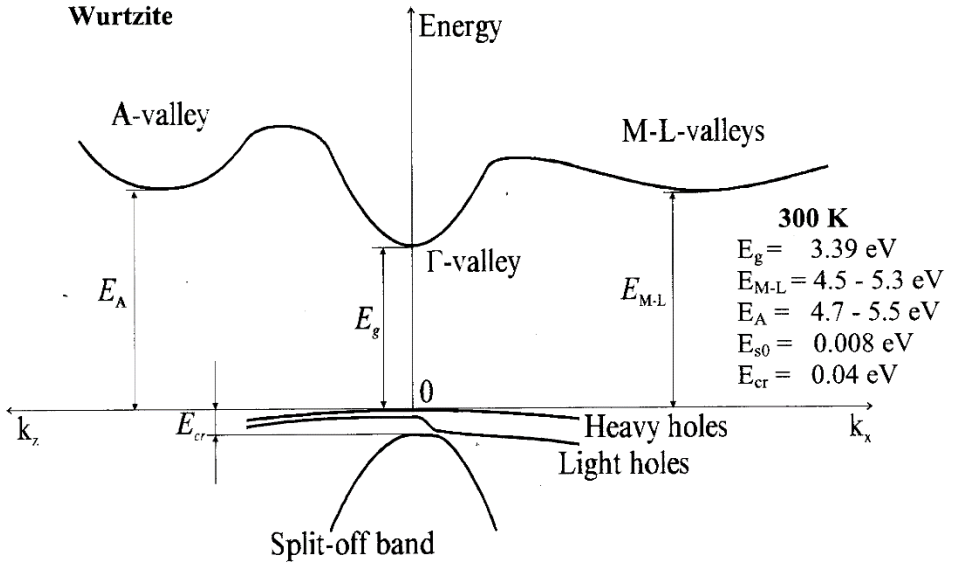
$$m_x^* = \frac{\hbar^2}{\dfrac{d^2E(\vec{k})}{dk_x^2}}$$

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

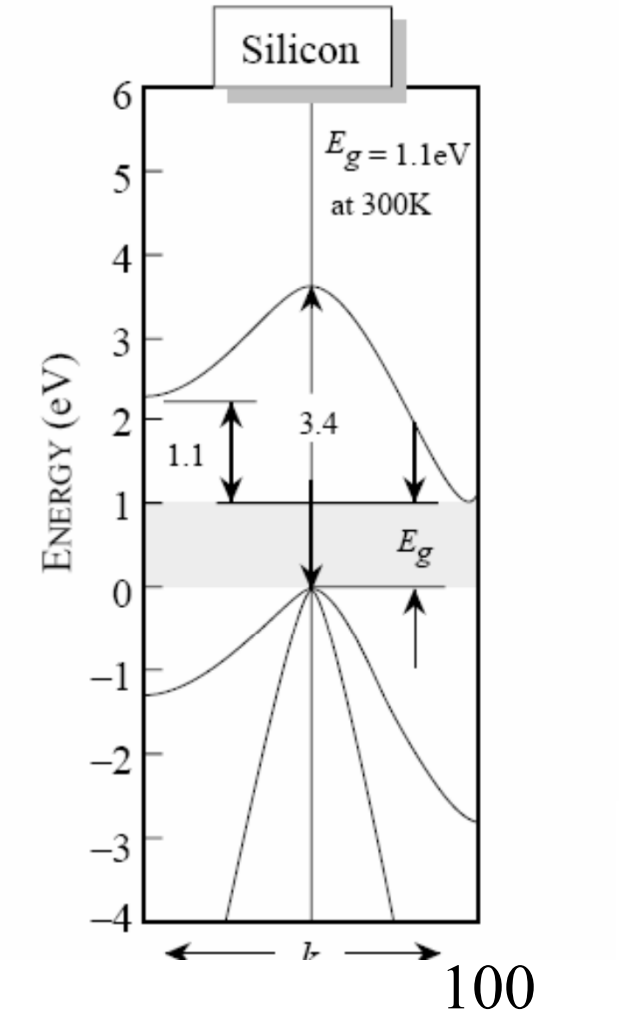
$$\vec{F} = -e\vec{E} = m^*\vec{a}$$

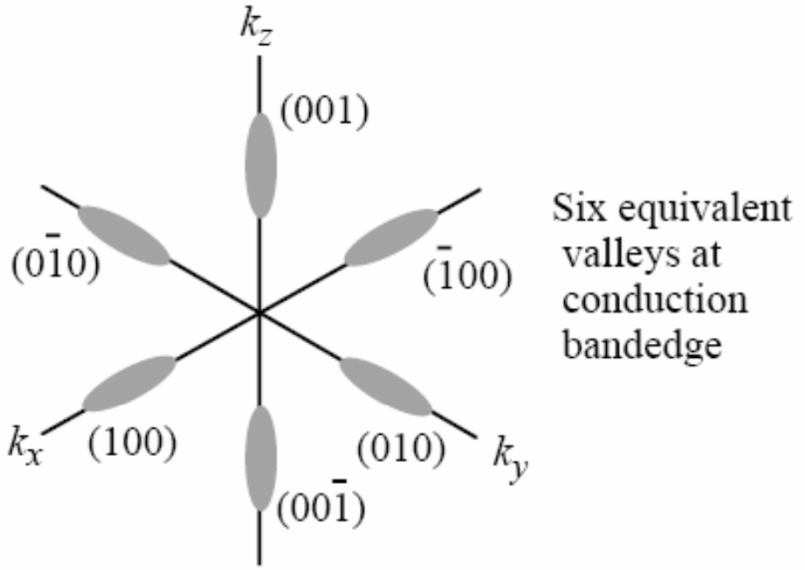
GaN


GaN
10
eV
8
6
4
2
0
-2
-4
-6
-8
E
A R L U M Σ Γ Δ A S H P K T Γ
k


Wurtzite
Energy
A-valley
M-L-valleys
Γ-valley
E_A
E_g
E_{M-L}
E_{cr}
0
k_z
k_x
Heavy holes
Light holes
Split-off band
300 K
E_g = 3.39 eV
E_{M-L} = 4.5 - 5.3 eV
E_A = 4.7 - 5.5 eV
E_{s0} = 0.008 eV
E_{cr} = 0.04 eV

Anisotropic effective mass in silicon





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

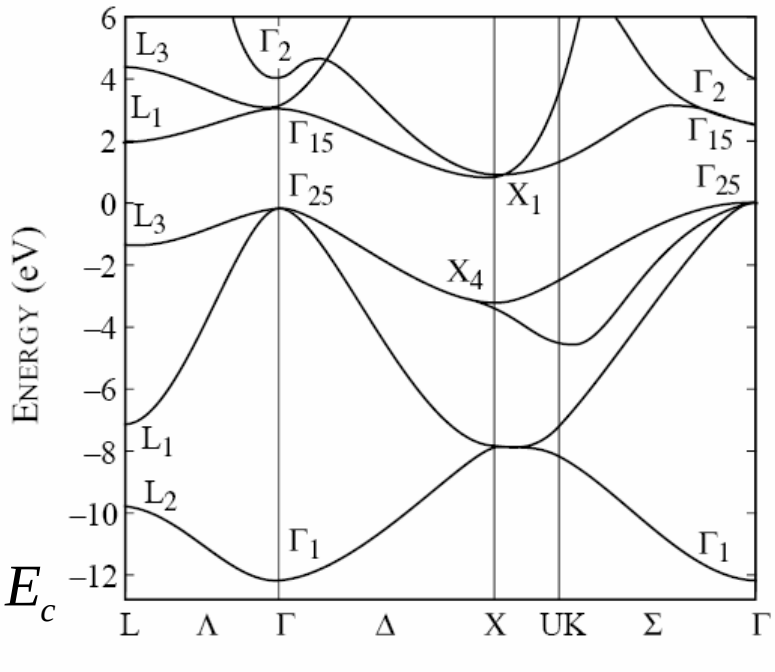
Return to problem list

Conduction band electron energy

In silicon, the bottom of the conduction valley along the (100) direction is at $(2\pi/a)(0.85,0,0)$ where $a = 0.543$ nm. Electrons in this valley have an anisotropic effective mass. The effective mass in the (100) direction is $m_l^* = 0.98m_0$ and the effective mass transverse to the [100] direction is $m_t^* = 0.19m_0$. What is the energy of an electron with a k-vector $(2\pi/a)(0.92,-0.01,0.15)$?

$E =$ _____ eV

Submit answer Clear



$$E = \frac{\hbar^2\left(k_x - 0.85\frac{2\pi}{a}\right)^2}{2m_l} + \frac{\hbar^2 k_y^2}{2m_t} + \frac{\hbar^2 k_z^2}{2m_t} + E_c$$

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.

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

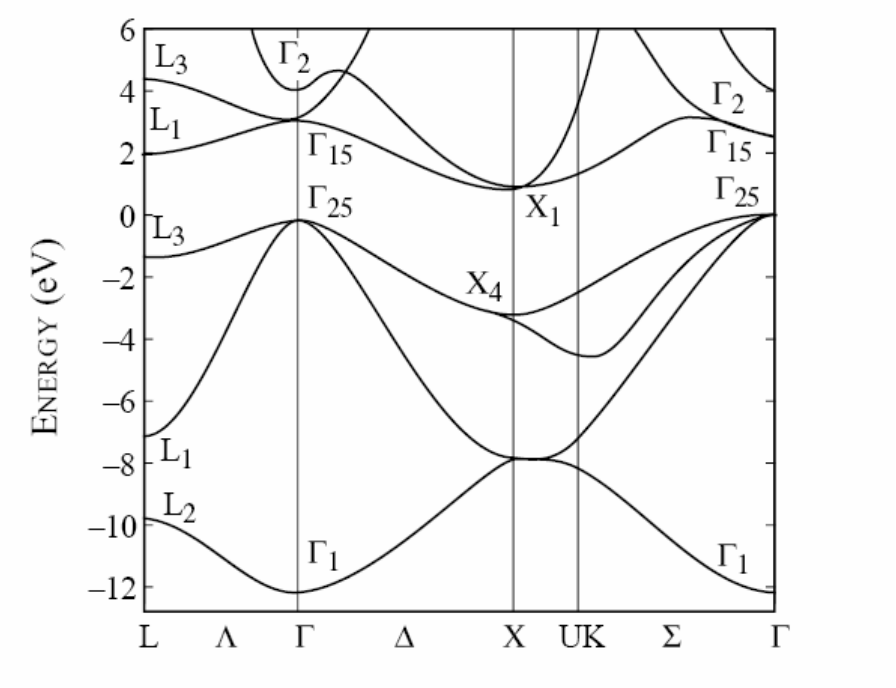
$$I \propto \sum_{\text{all } \vec{k}} \left(-e\vec{v}_{\vec{k}}\right) - \sum_{\text{empty } \vec{k}} \left(-e\vec{v}_{\vec{k}}\right)$$

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

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

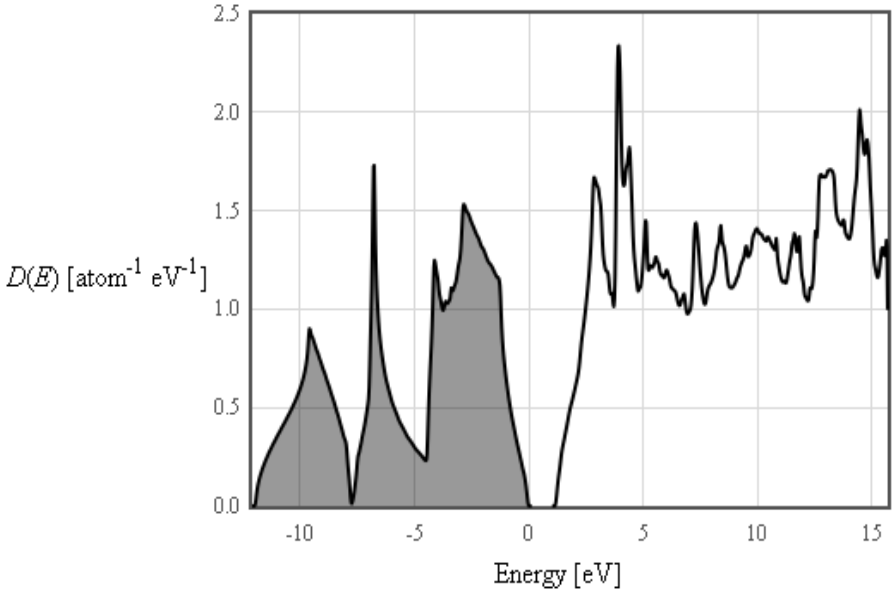
Charge carriers in the valence band can be considered to be positively charged holes. The number of holes in the valence band is the number of missing electrons.

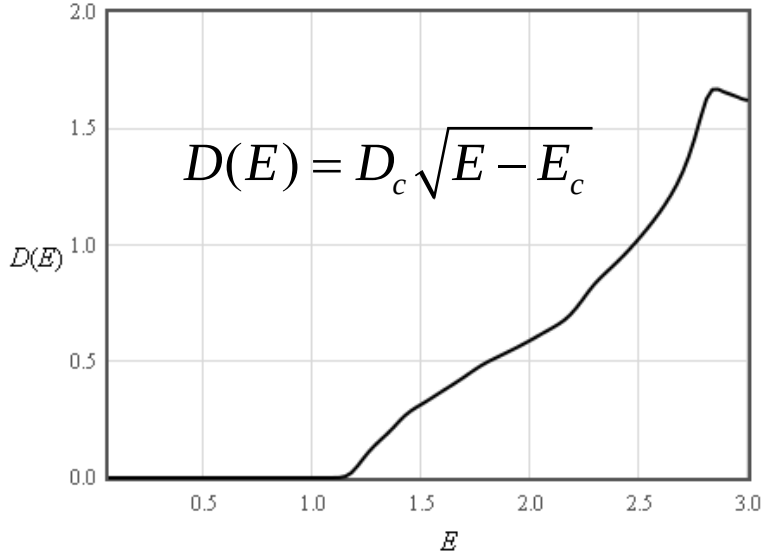
m^*_h = effective mass of holes

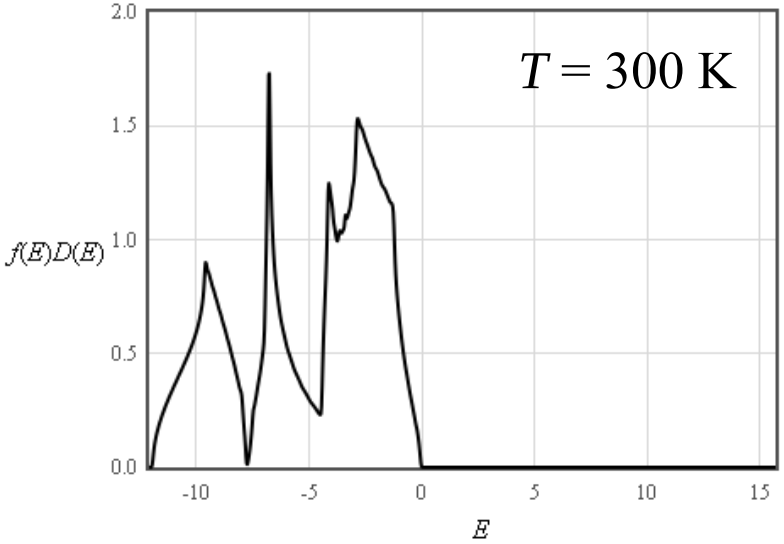
$$m_h^* = -\frac{\hbar^2}{\frac{d^2E(\vec{k})}{dk_x^2}}$$

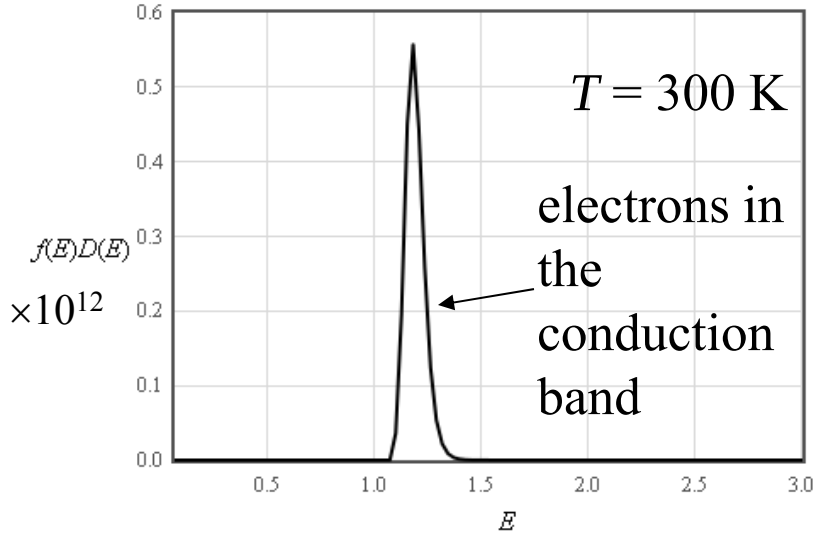
$$\vec{F} = e\vec{E} = m_h^*\vec{a}$$

Silicon density of states

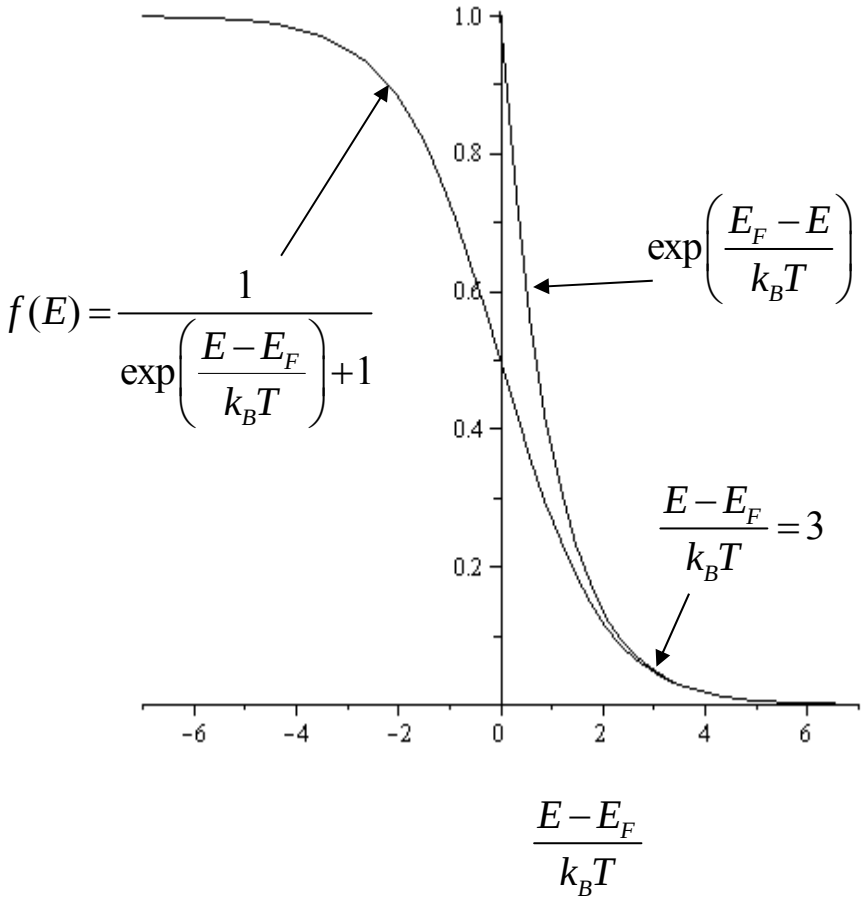








Boltzmann approximation



Density of electrons in the conduction band

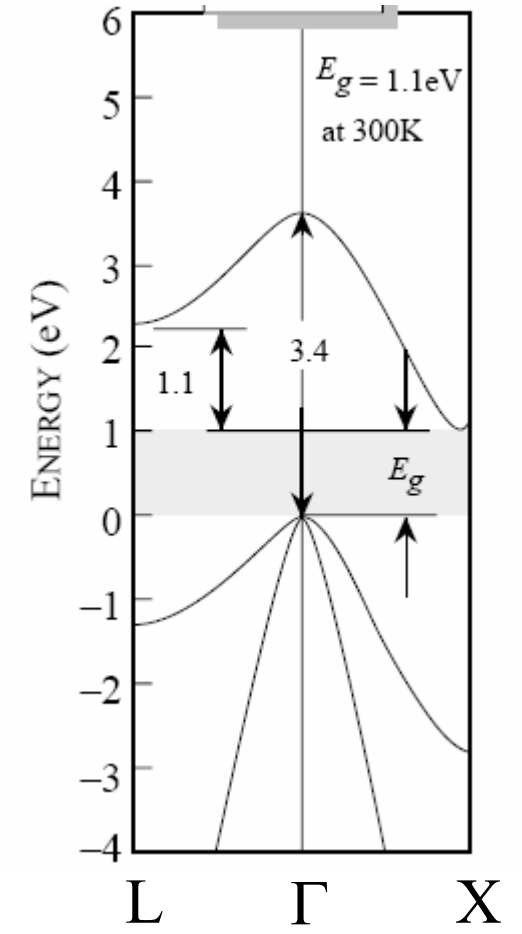
$$n = \int_{E_c}^{\infty} D(E)\, f(E) dE \approx D_c \int_{E_c}^{\infty} \exp\left(\frac{E_F - E}{k_B T}\right) \sqrt{E - E_c}\, dE$$

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

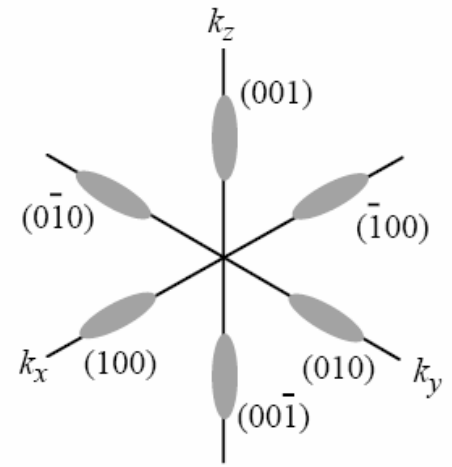
$$\boxed{n = N_c(T) \exp\left(\frac{E_F - E_c}{k_B T}\right)} = \frac{2D_c}{\sqrt{\pi}} \left(k_B T\right)^{3/2} \exp\left(\frac{E_F - E_c}{k_B T}\right)$$

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

Density of electrons in the conduction band



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



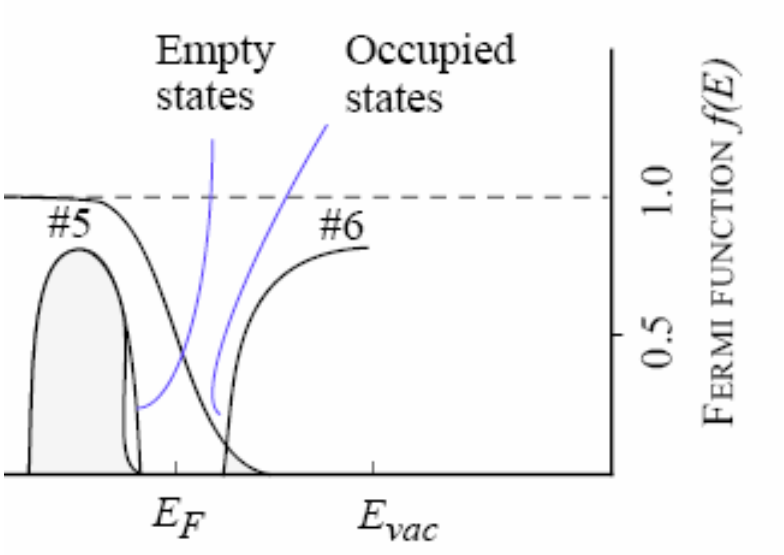
$$n = N_c\left(\frac{T}{300}\right)^{3/2} \exp\left(\frac{E_F - E_c}{k_B T}\right)$$

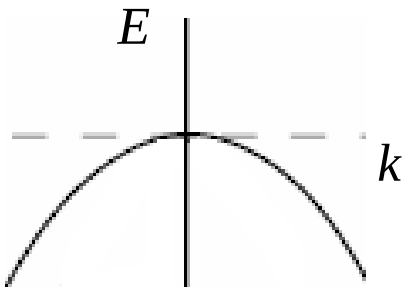
Properties	Si	Ge	GaAs
Bandgap E_g	1.12 eV	0.66 eV	1.424 eV
Effective density of states in conduction band (300 K) N_c	2.78×10^{25} m^{-3}	1.04×10^{25} m^{-3}	4.45×10^{23} m^{-3}

Density of holes in the valence band

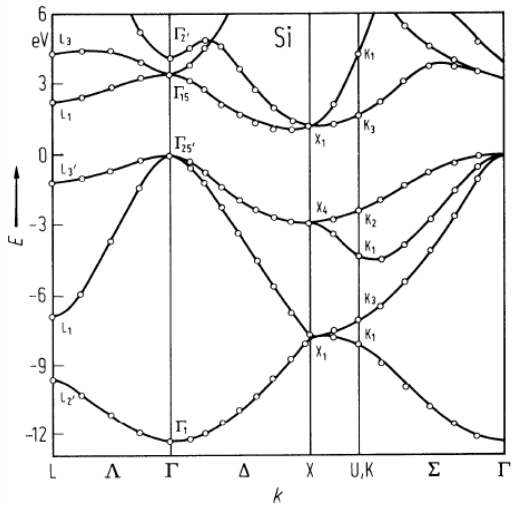
$$D(E) = D_v \sqrt{E_v - E}$$

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





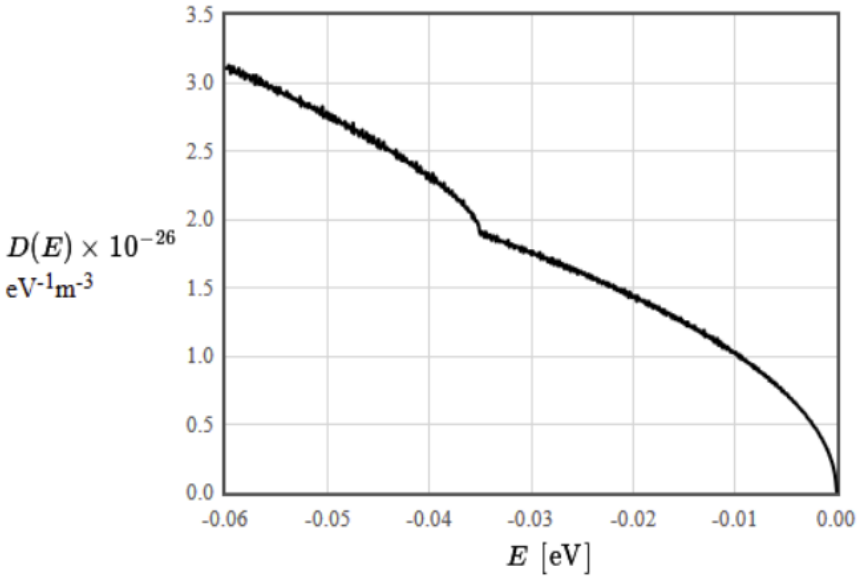
Silicon valence bands

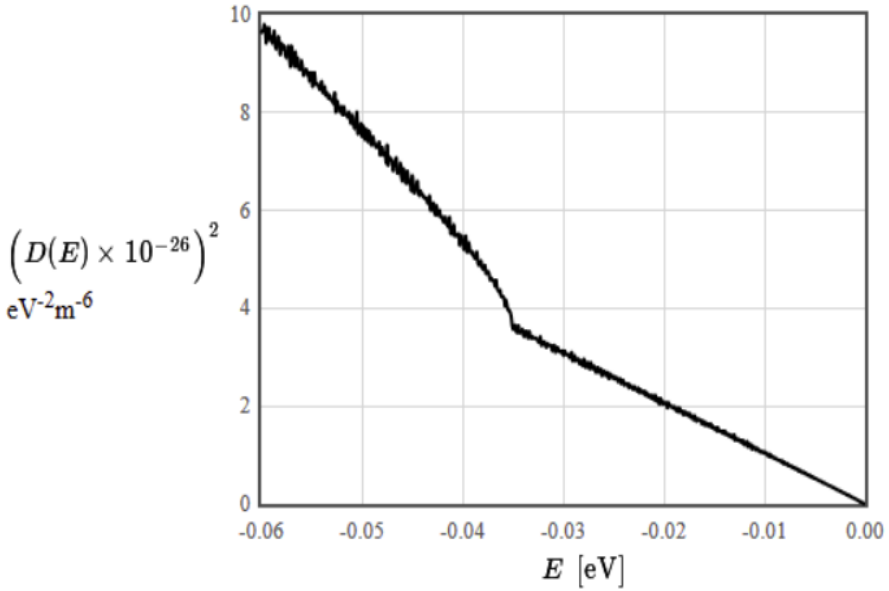


$$E_{v,lh} = -\frac{\hbar^2}{2m_e}\left(4.1k^2 - \sqrt{1.21k^4 + 4.1(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)}\right),$$

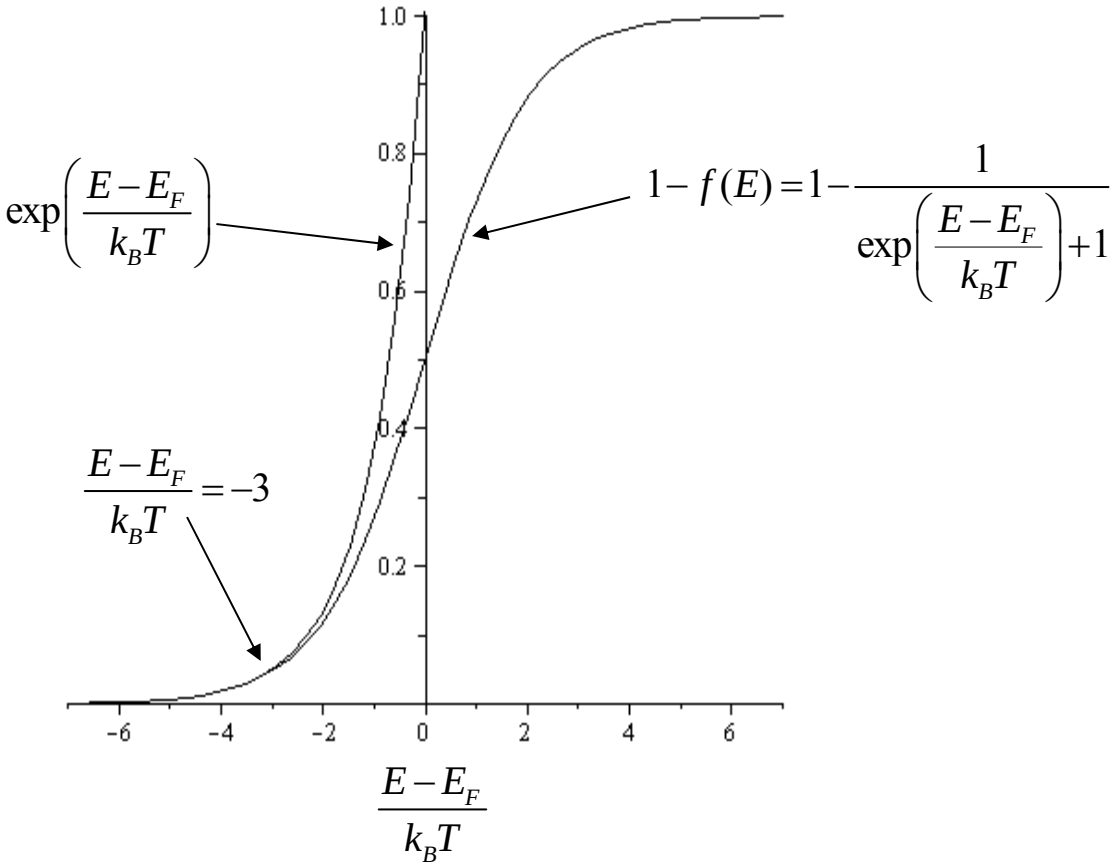
$$E_{v,hh} = -\frac{\hbar^2}{2m_e}\left(4.1k^2 + \sqrt{1.21k^4 + 4.1(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)}\right),$$

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

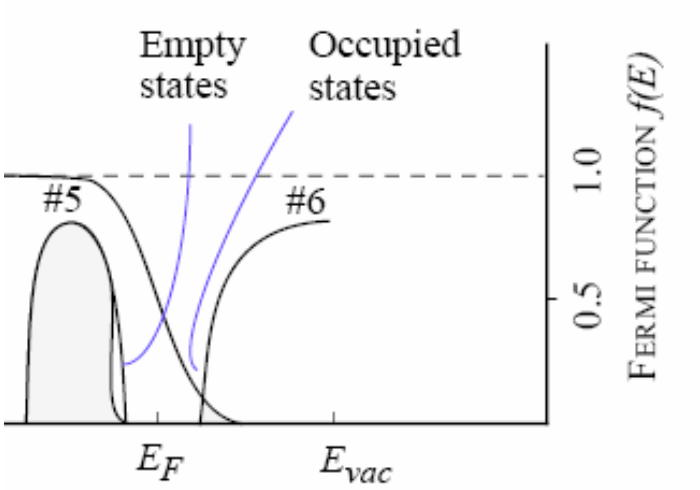




Boltzmann approximation



Density of holes in the valence band

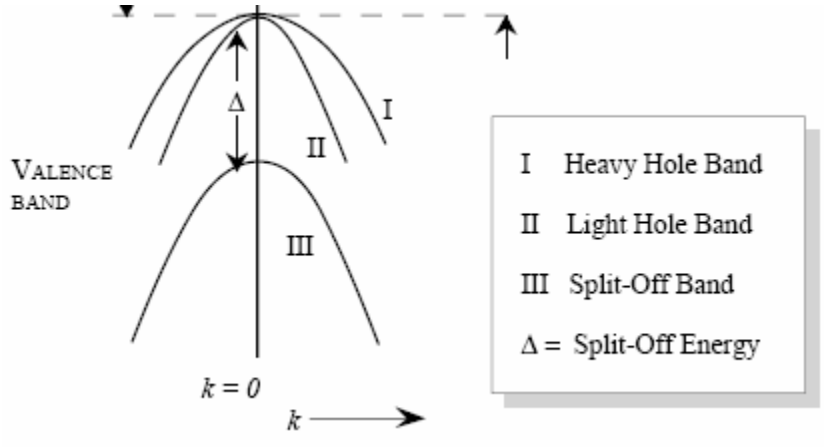


$$p = \int_{-\infty}^{E_v} D(E)\left(1 - f(E)\right)dE \approx D_v \int_{-\infty}^{E_v} \exp\left(\frac{E - E_F}{k_B T}\right)\sqrt{E_v - E}\,dE$$

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

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

Density of holes in the valence band



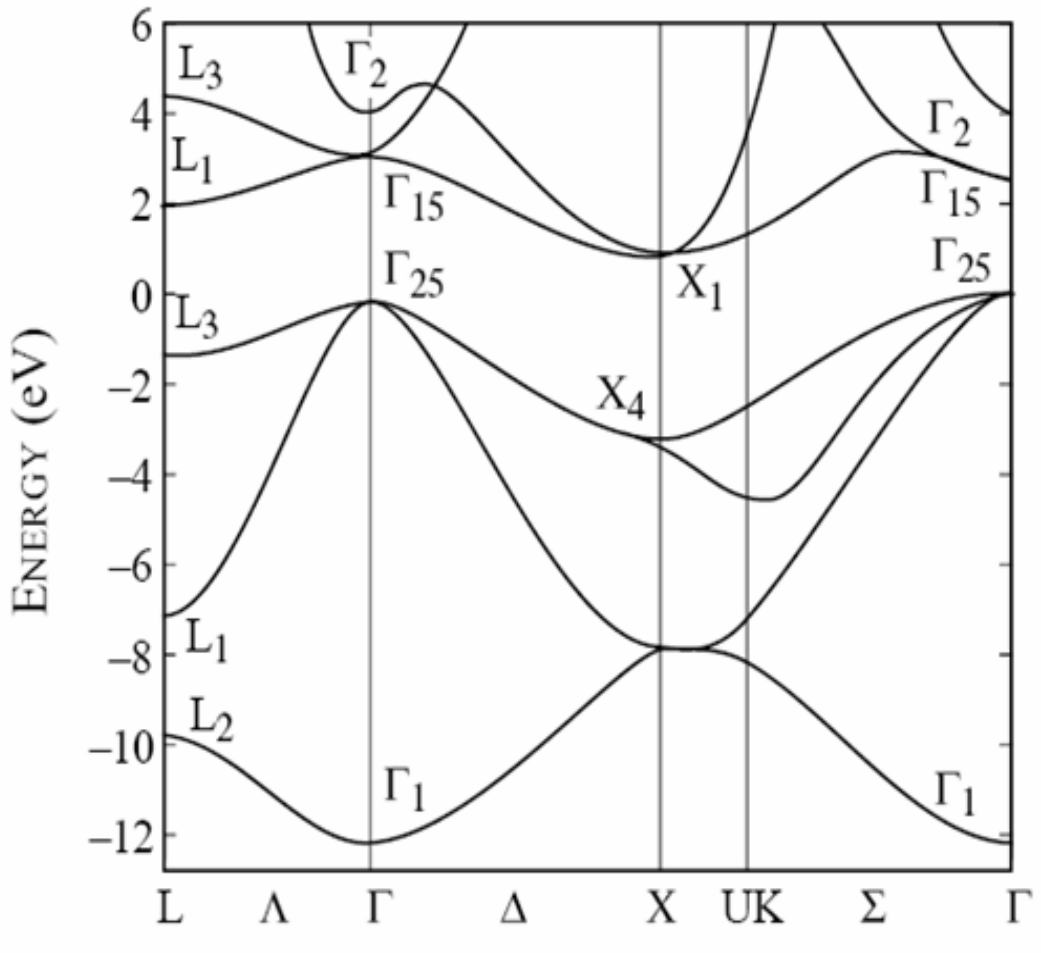
$$p = 2\left(\frac{m_h^* k_B T}{2\pi\hbar^2}\right)^{3/2} \exp\left(\frac{E_v - E_F}{k_B T}\right)$$

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

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}

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?

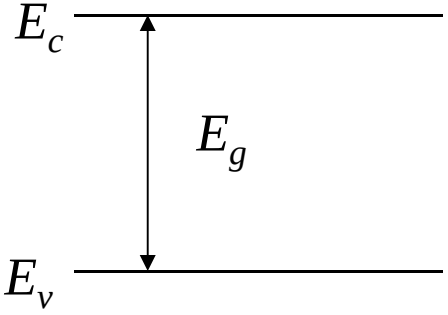
(b) What is the band gap?

(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

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

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

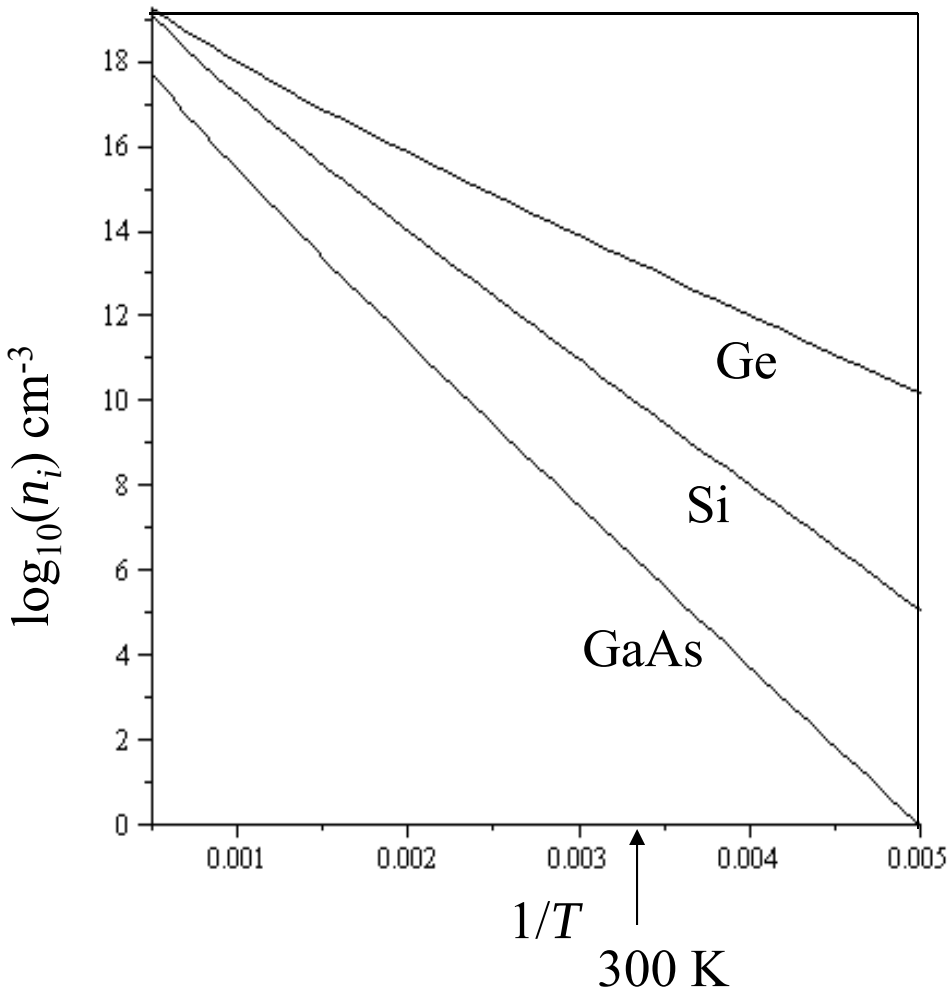


For intrinsic semiconductors (no impurities)

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

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

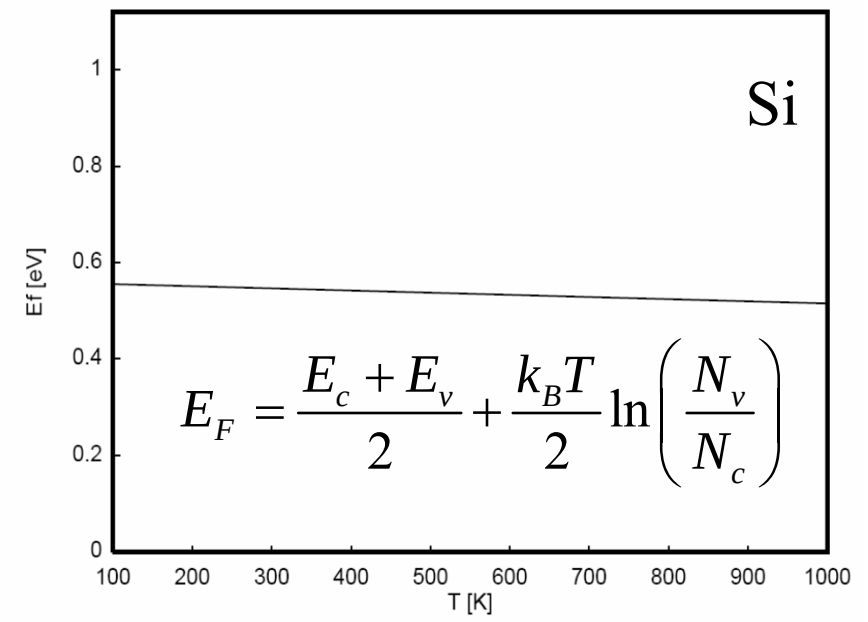
$$n = p = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right) = N_v \exp\left(\frac{E_v - E_F}{k_B T}\right)$$

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

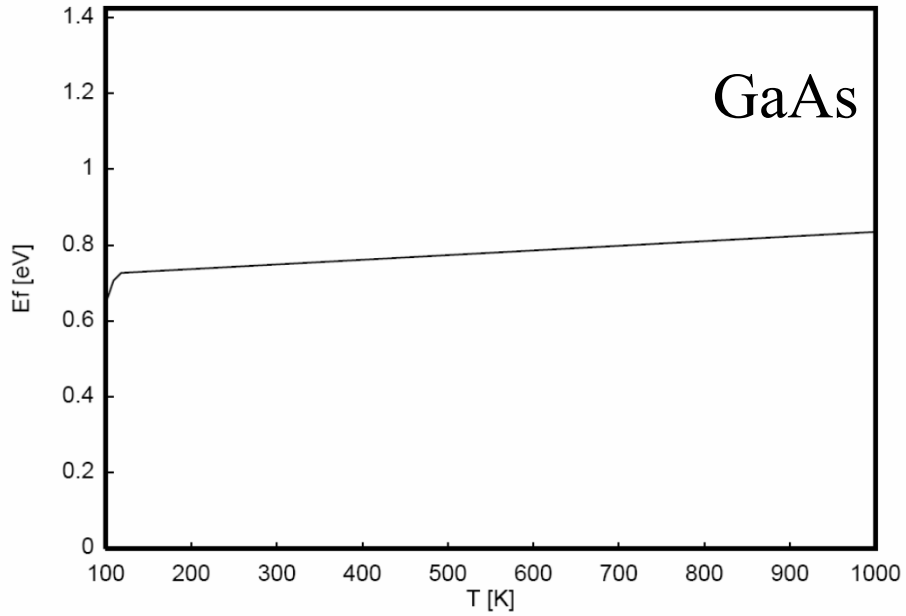
$$\frac{2E_F}{k_B T} = \frac{E_c + E_v}{k_B T} + \ln\left(\frac{N_v}{N_c}\right)$$

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

Temperature dependence of E_F

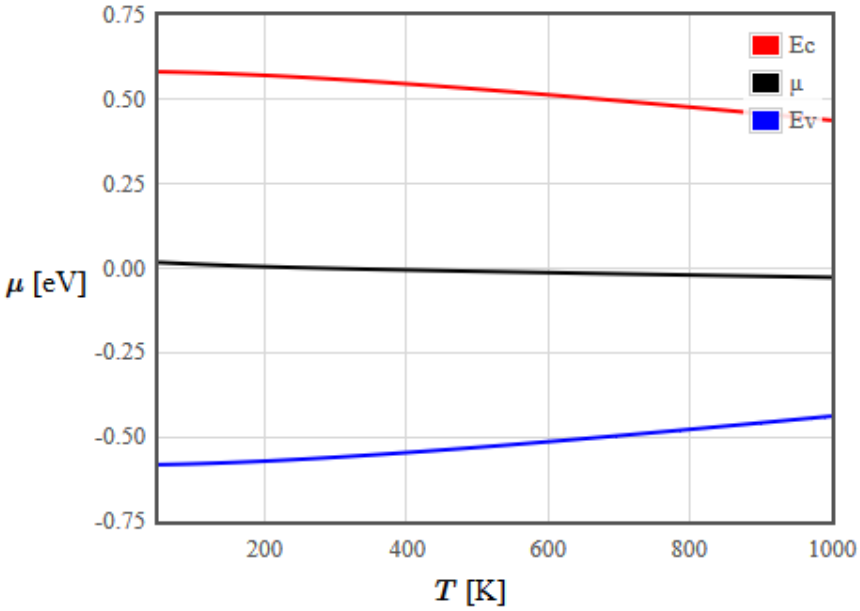


$$E_F = \frac{E_c + E_v}{2} + \frac{k_B T}{2} \ln\left(\frac{N_v}{N_c}\right)$$



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 with a split-off band



$N_c(300\ \mathrm{K}) =$	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.

n and p

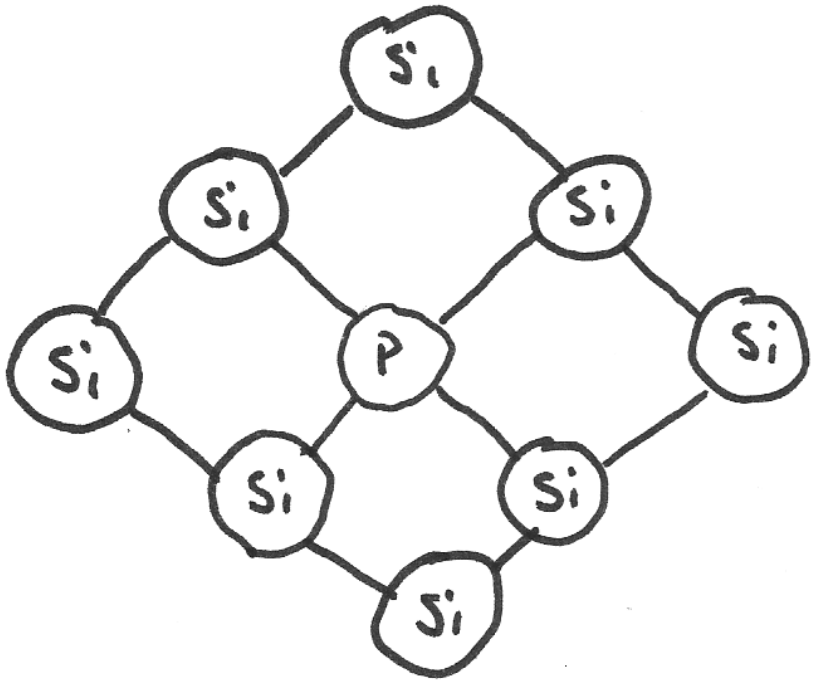
The electron density and hole density are:

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

The law of mass action:

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

Ionization of dopants

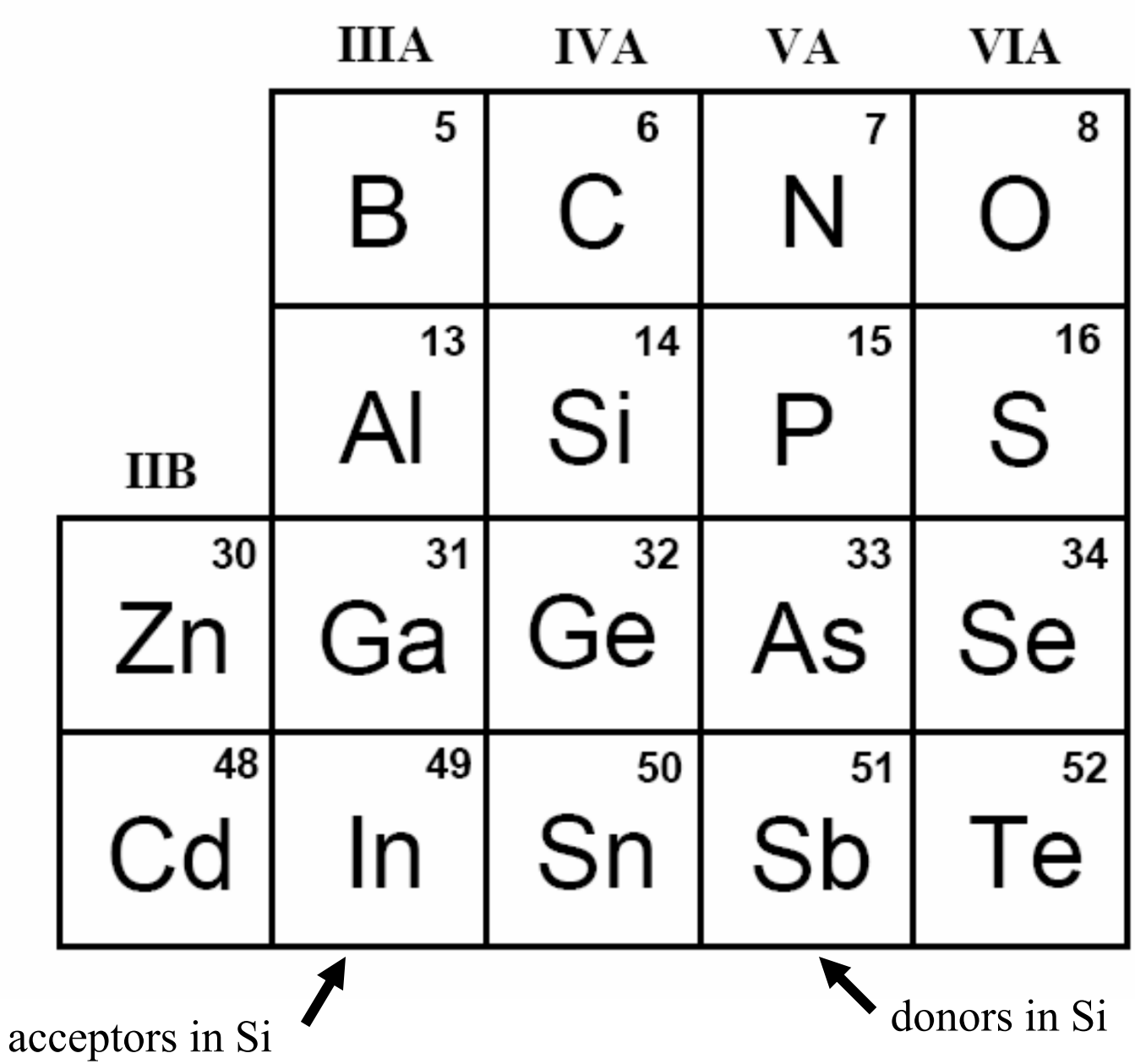


Easier to ionize a P atom in Si than a free P atom

$$E_n = -\frac{me^4}{8\varepsilon_0^2 h^2 n^2}$$

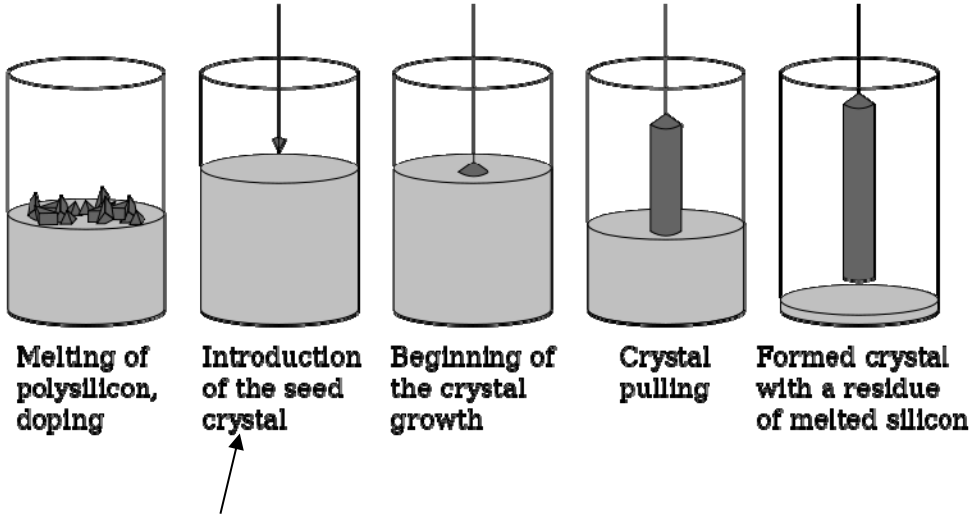
Ionization energy is smaller by a factor: $\frac{m^*}{m}\left(\frac{\varepsilon_0}{\varepsilon_r \varepsilon_0}\right)^2$

Ionization energy ~ 25 meV


IIIA
IVA
VA
VIA
IIB
5
B
6
C
7
N
8
O
13
Al
14
Si
15
P
16
S
30
Zn
31
Ga
32
Ge
33
As
34
Se
48
Cd
49
In
50
Sn
51
Sb
52
Te
acceptors in Si
donors in Si

Crystal growth

Czochralski Process



add dopants to the melt

images from wikipedia

Crystal growth

Float zone Process

Neutron transmutation

$^{30}Si + n \rightarrow {}^{31}Si + \gamma$

$^{31}Si \rightarrow {}^{31}P + \beta$

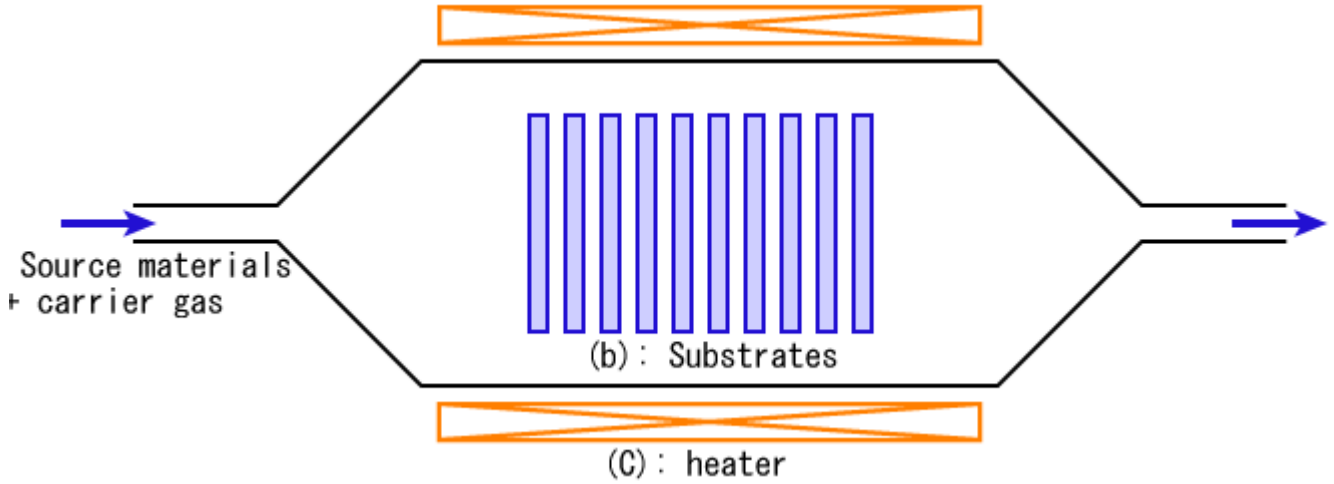
image from wikipedia

Gas phase diffusion

AsH_3 (Arsine) or PH_3 (phosphine) for n-doping
B_2H_6 (diborane) for p-doping.

http://www.microfab.de/foundry/services/diffusion/index.html

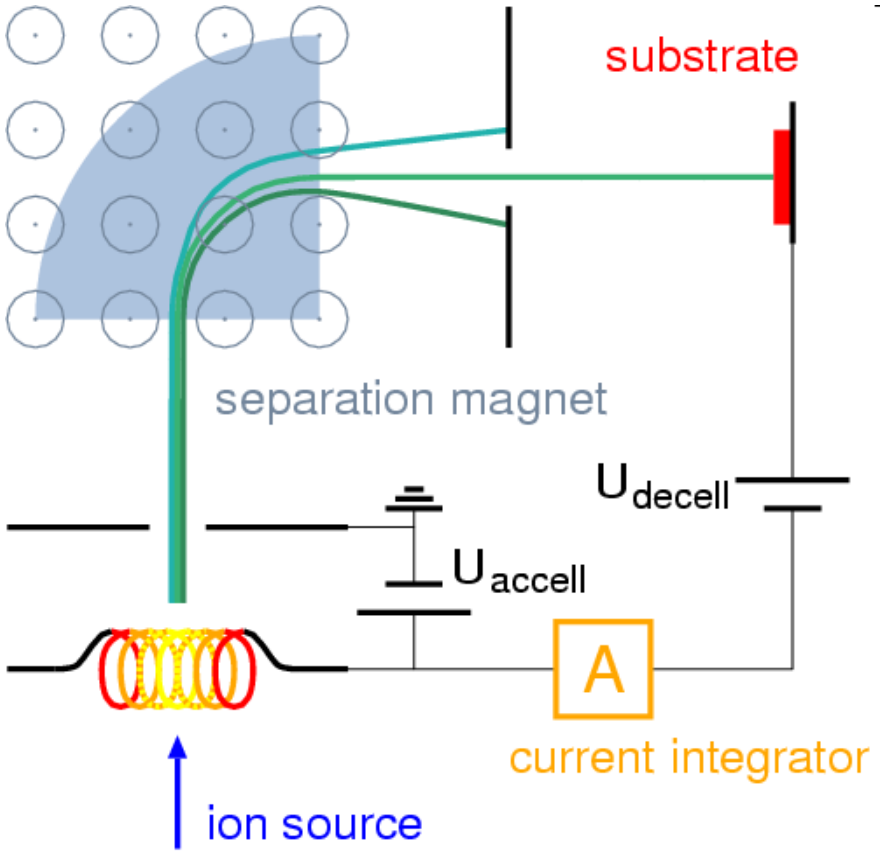
Chemical vapor deposition



Epitaxial silicon CVD SiH_4 (silane) or SiH_2Cl_2 (dichlorosilane)
PH_3 (phosphine) for n-doping or B_2H_6 (diborane) for p-doping.

image from wikipedia

Ion implantation

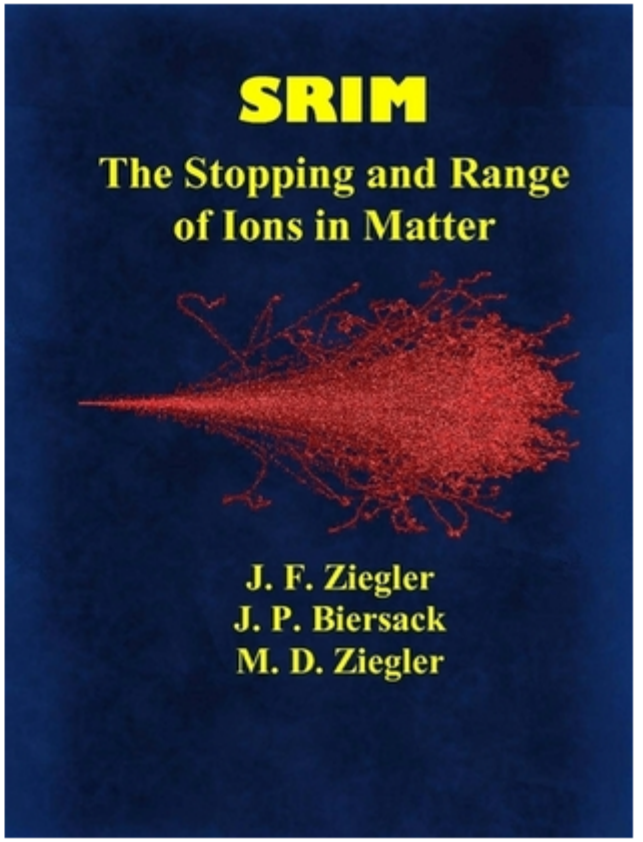


Implant at 7º to avoid channeling

SRIM

The Stopping and Range of Ions in Matter

James F. Ziegler, Jochen P. Biersack, Matthias D. Ziegler



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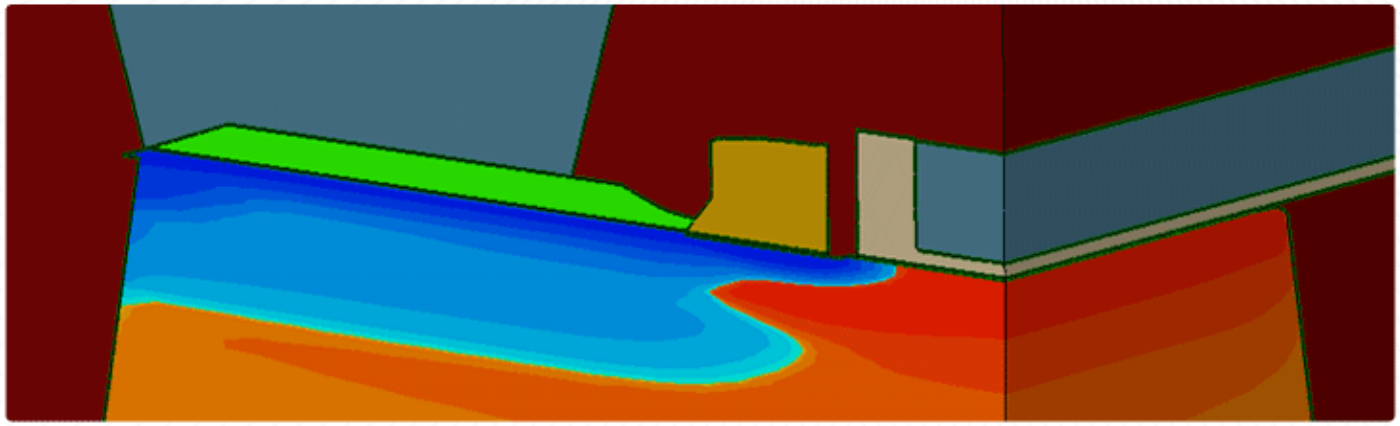
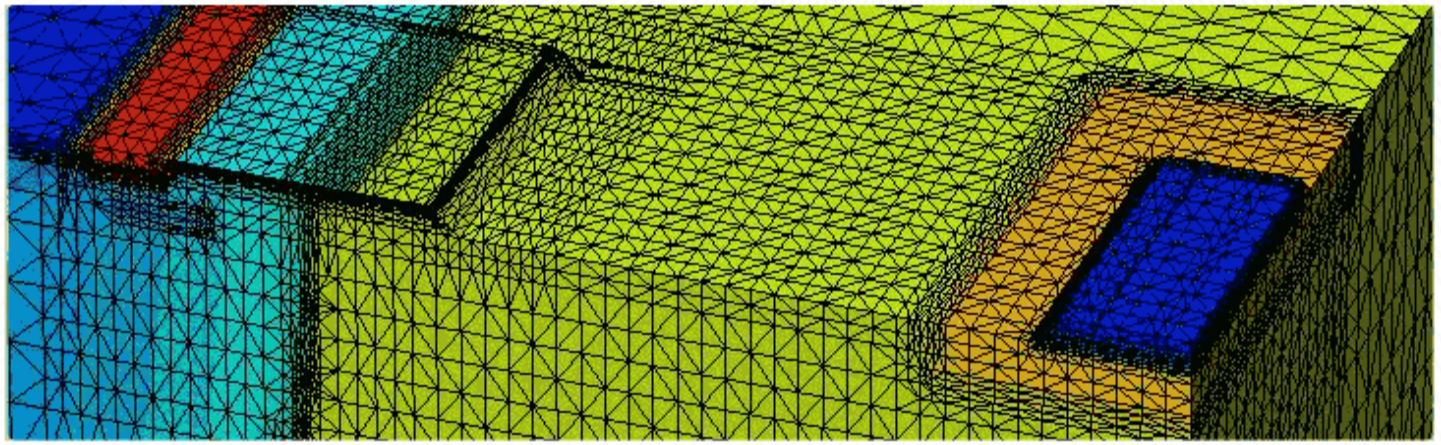
Process Simulation



Device Simulation



http://www.synopsys.com