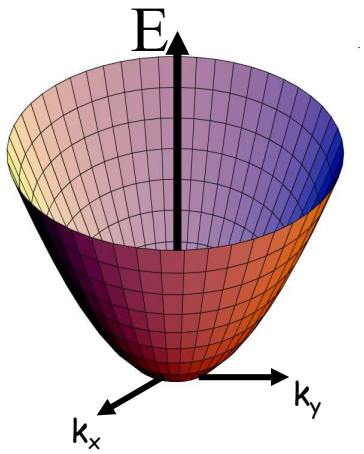
Intrinsic semiconductors

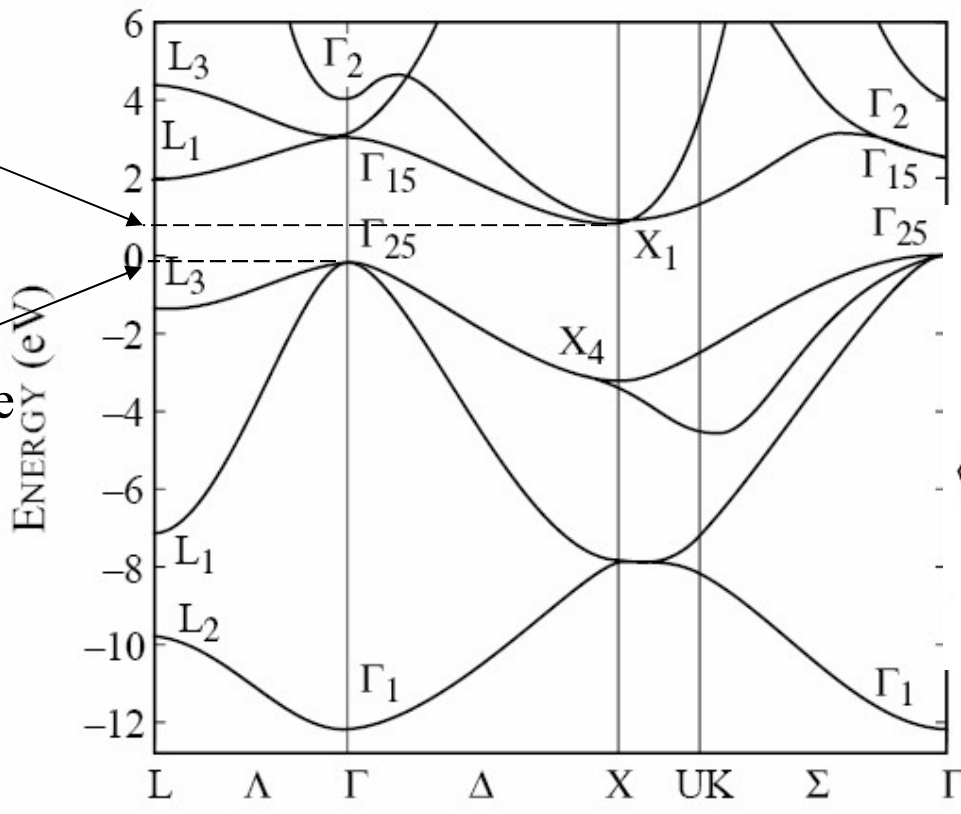
Silicon band structure

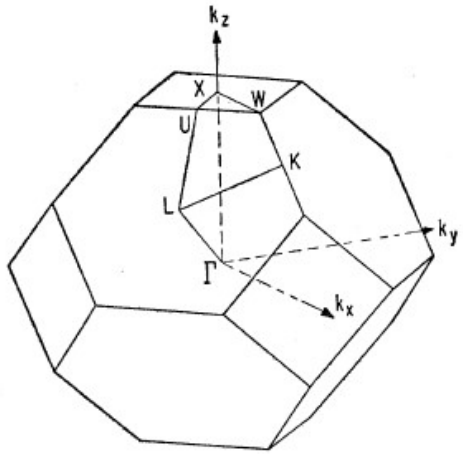
E_c = bottom of the conduction band

$E_g = E_c - E_v$

E_v = top of the valence band







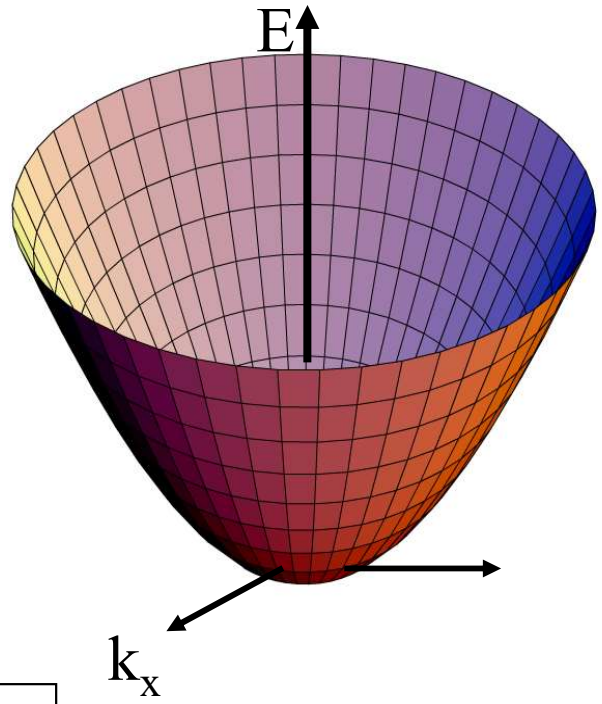
Near the bottom of the conduction band, the band structure looks like a parabola.

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.

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

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.

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

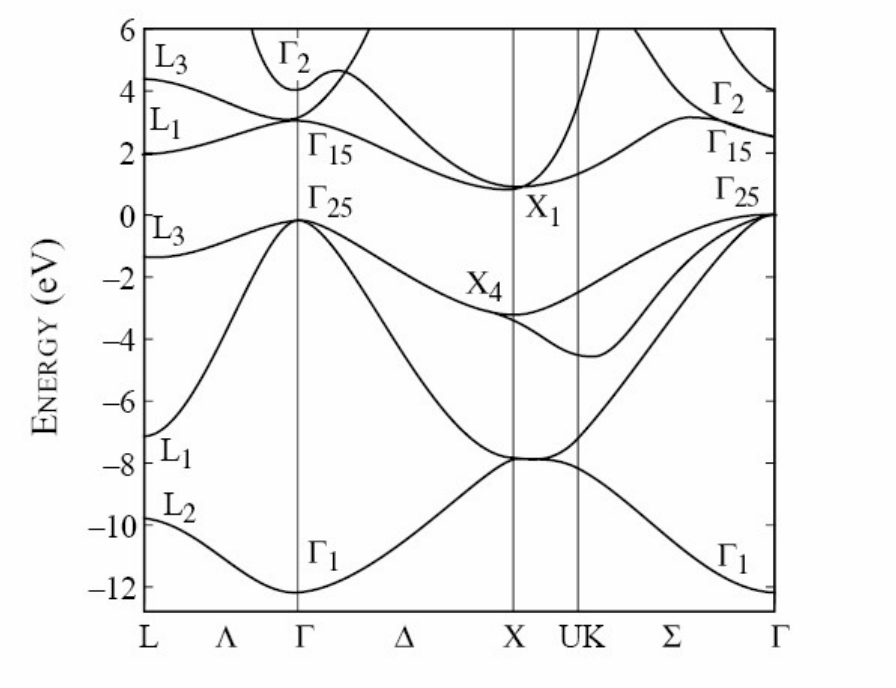
$$I \propto \sum_{\text{all } \vec{k}} \left(-e\vec{v}_{\vec{k}}\right) - \sum_{\text{empty } \vec{k}} \left(-e\vec{v}_{\vec{k}}\right)$$

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

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

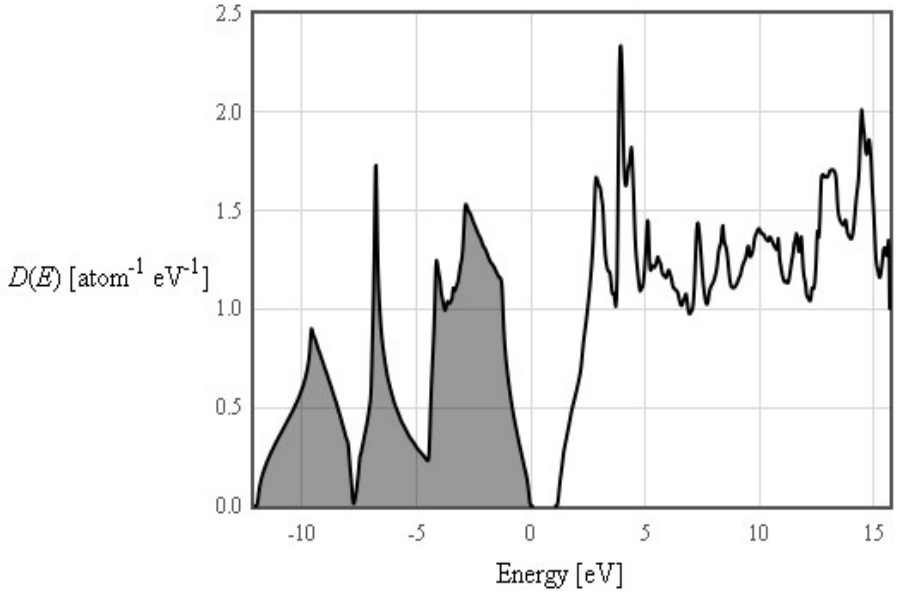
Charge carriers in the valence band can be considered to be positively charged holes. The number of holes in the valence band is the number of missing electrons.

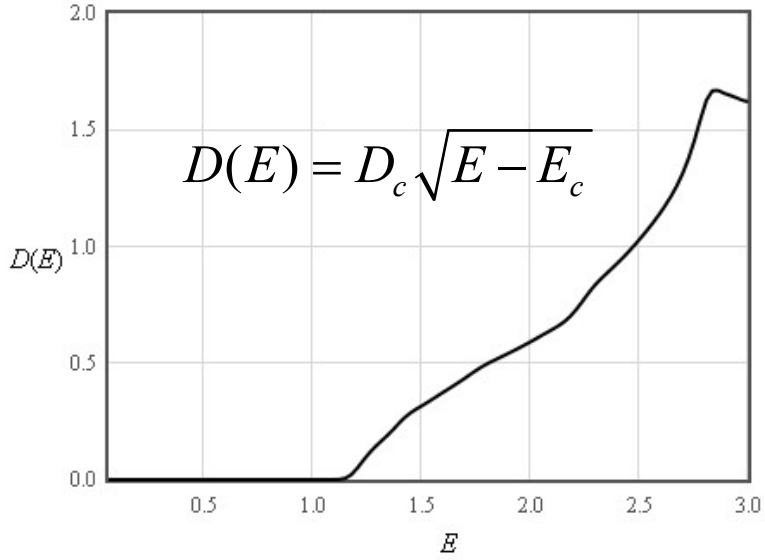
m^*_h = effective mass of holes

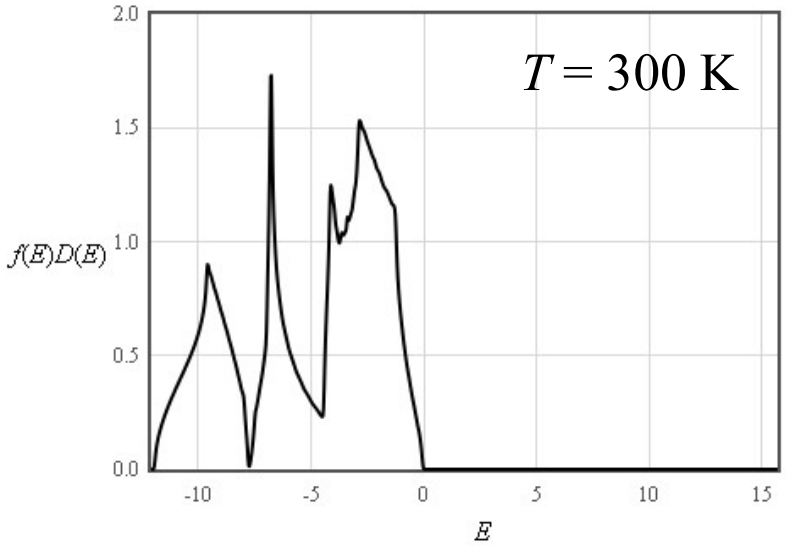
$$m_h^* = -\frac{\hbar^2}{\frac{d^2 E(\vec{k})}{dk_x^2}}$$

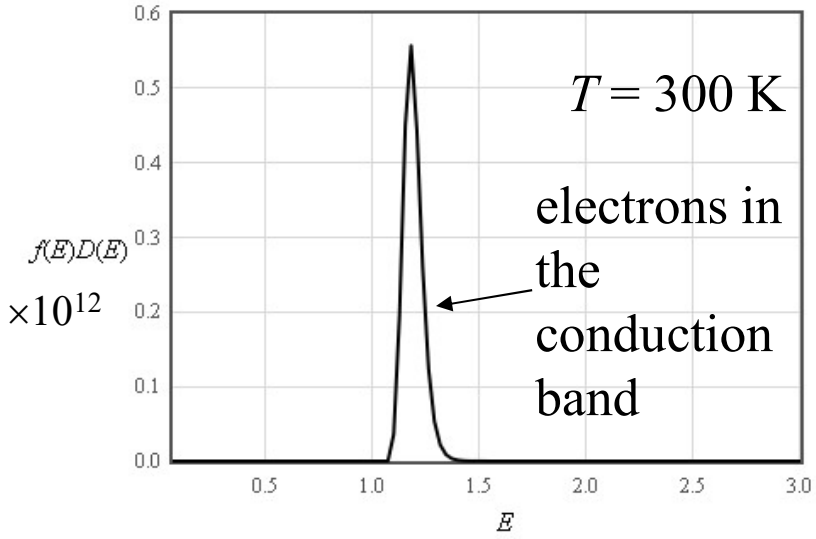
$$\vec{F} = e\vec{E} = m_h^* \vec{a}$$

Silicon density of states



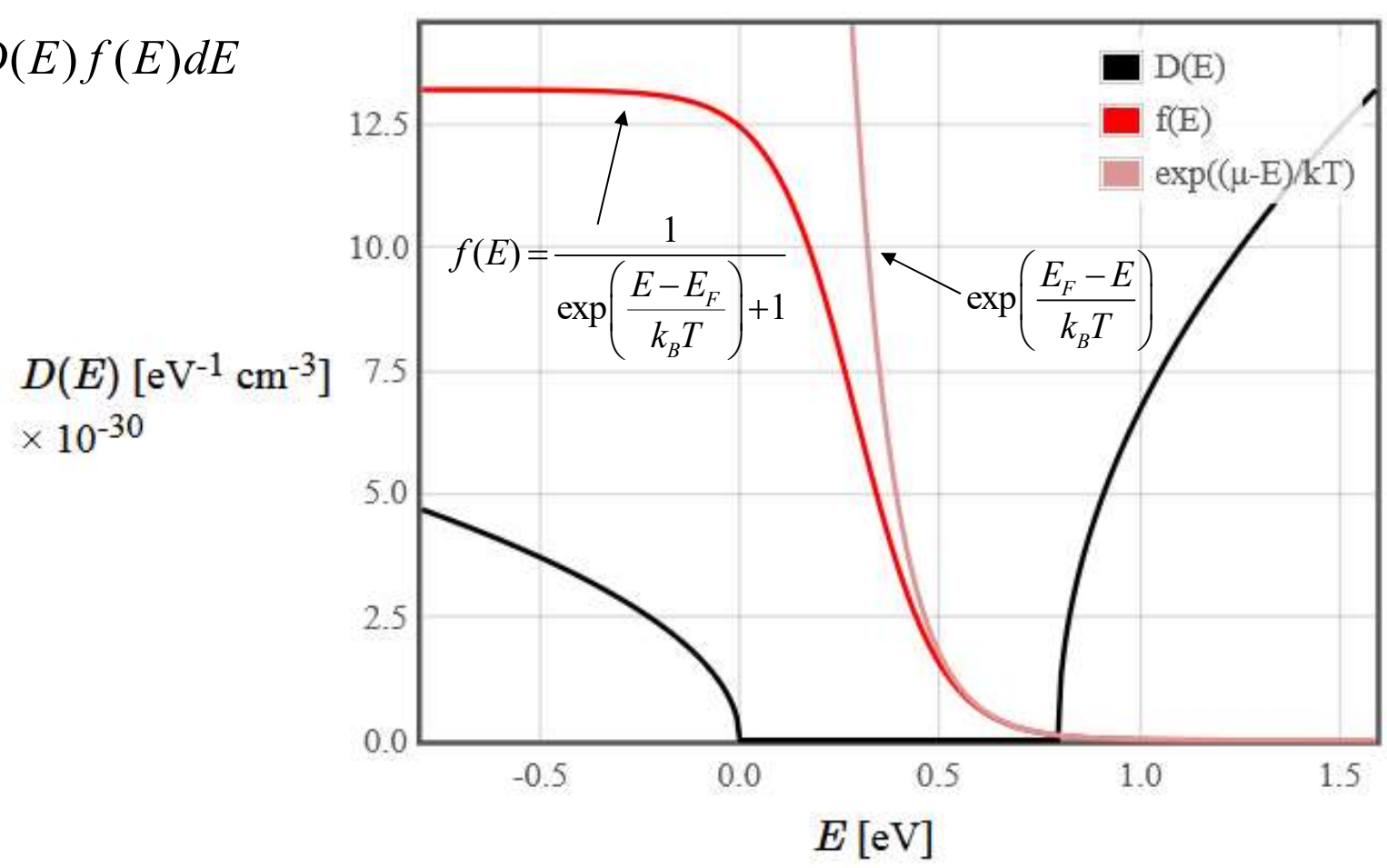






Boltzmann approximation

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



Density of electrons in the conduction band

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

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

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

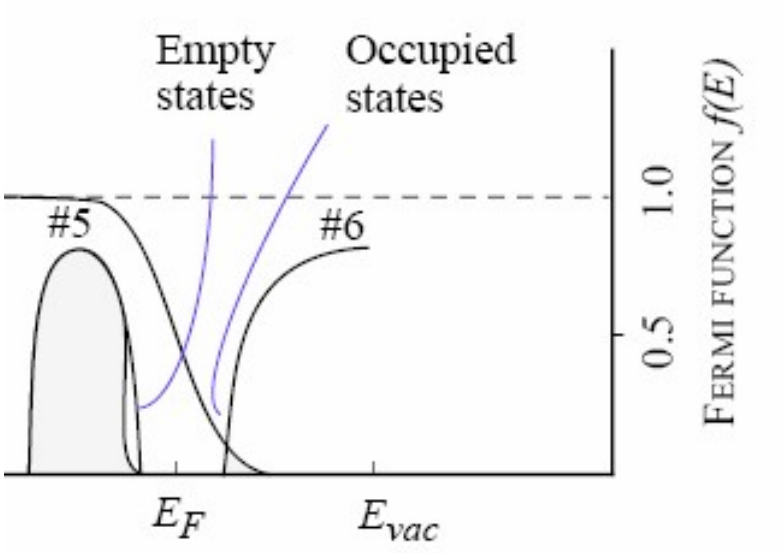
$$N_c = \frac{2D_c}{\sqrt{\pi}} \left(k_B T\right)^{3/2} = 2\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)^{3/2}$$

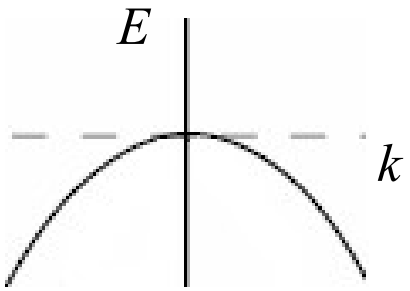
= effective density of states of the conduction band

Density of holes in the valence band

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

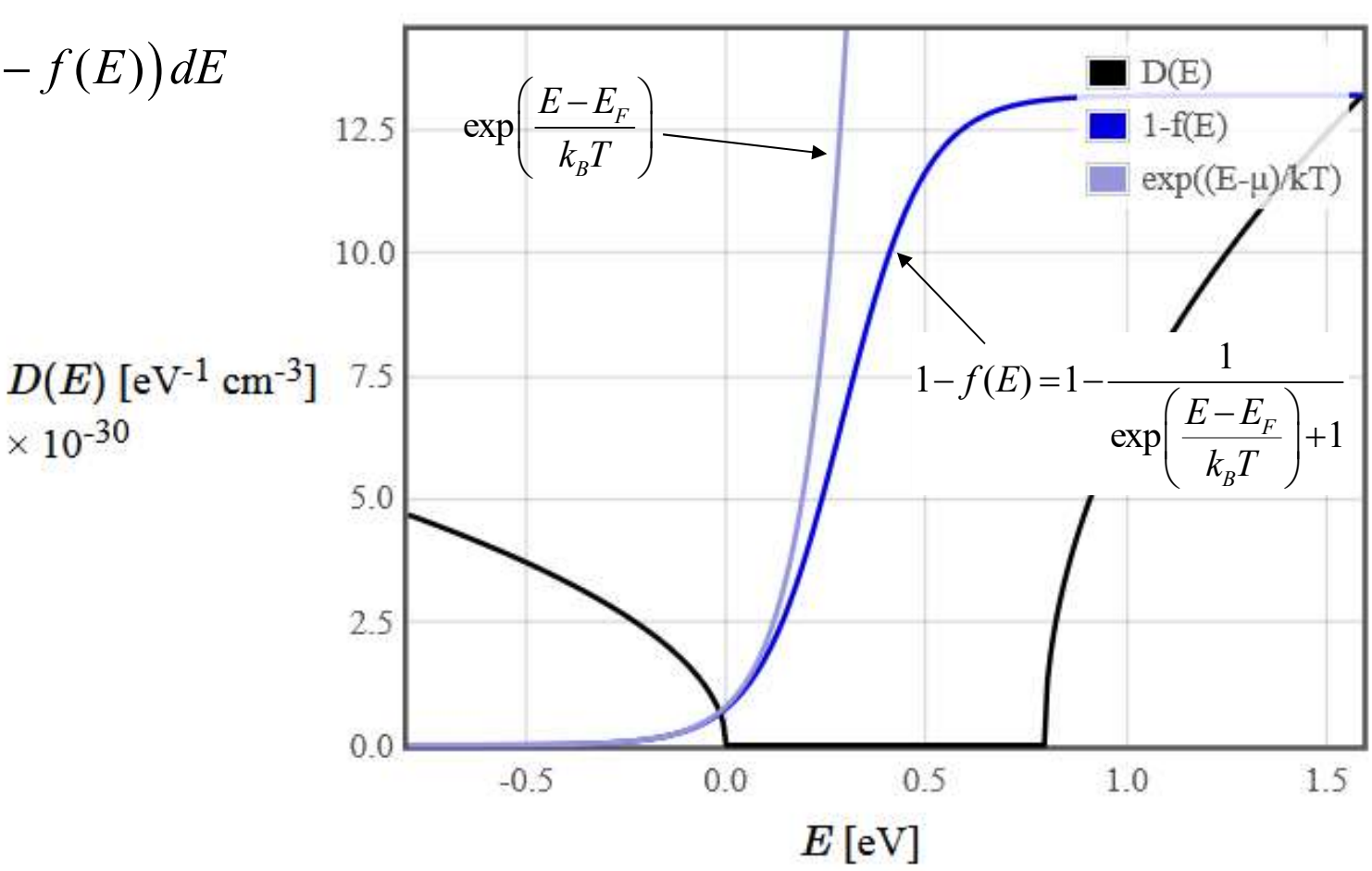
$$1 - f(E) = 1 - \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} \approx \exp\left(\frac{E - E_F}{k_B T}\right)$$



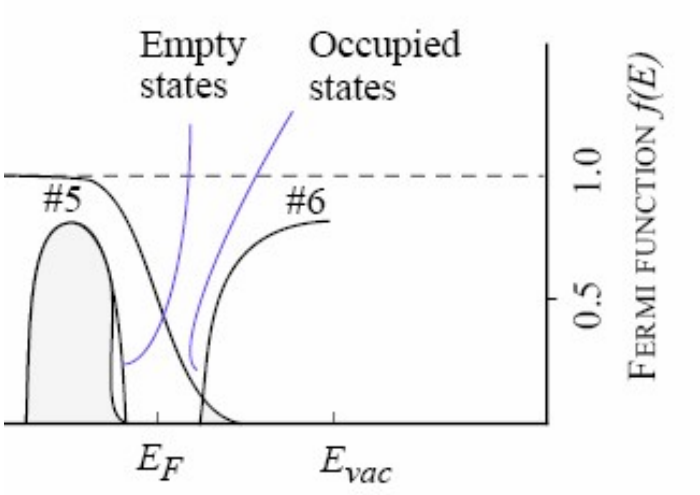


Boltzmann approximation

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



Density of holes in the valence band



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

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

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

= 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,

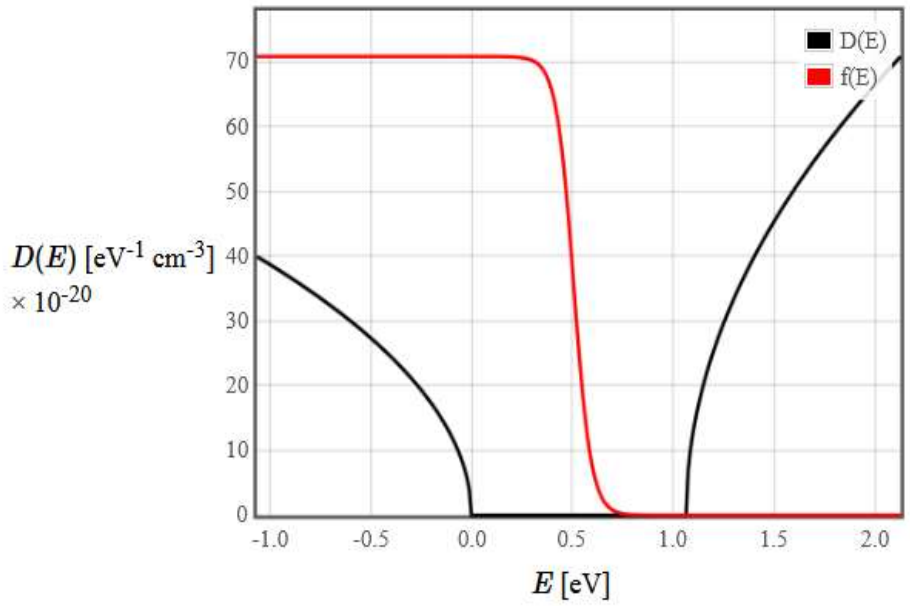
$$D(E) = \begin{cases} D_v\sqrt{E_v - E}, & \text{for } E < E_v \\ 0, & \text{for } E_v < E < E_c \\ D_c\sqrt{E - E_c}, & \text{for } E_c < E \end{cases}$$

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.



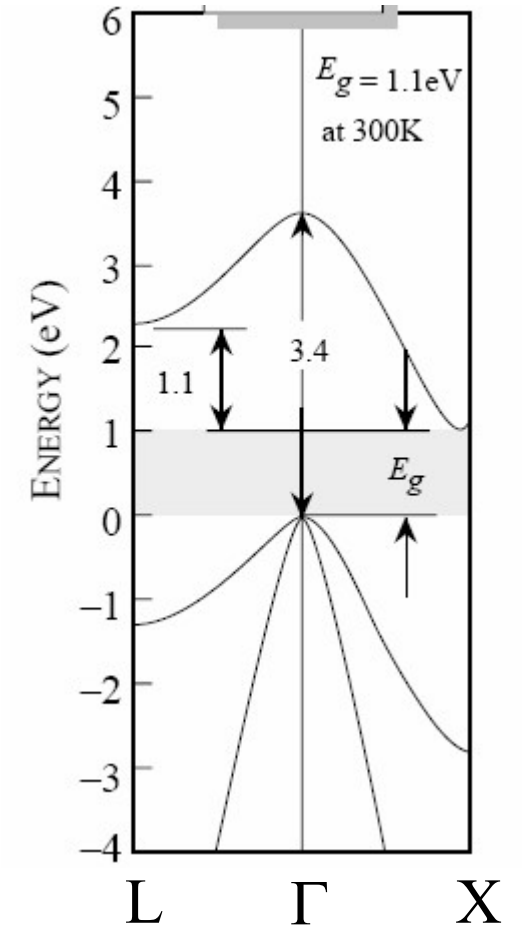
D_c =	6.874E21	$eV^{-3/2}$ cm^{-3}	Semiconductor
D_v =	3.8775E21	$eV^{-3/2}$ cm^{-3}	Si Ge GaAs GaP
E_g =	1.166-4.73E-4*T*T/(T+636)	eV	InAs InP InSb
T =	500	K	

Replot

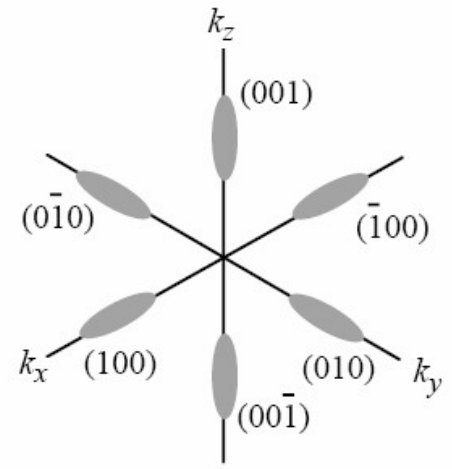
$E_v = 0$, $E_c = E_g = 1.062$ eV, $\mu = 0.5063$ eV

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

Density of electrons in the conduction band



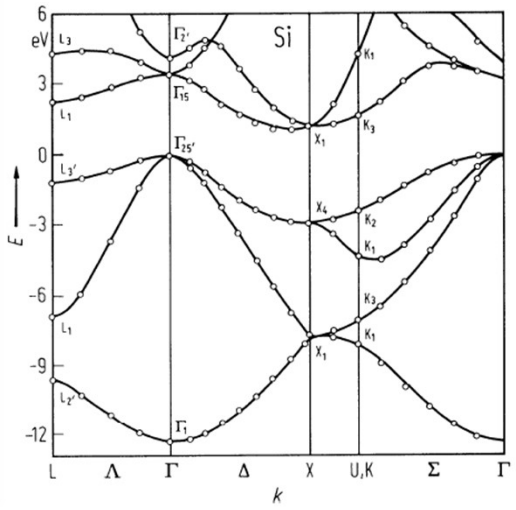
$$n = 2\left(\frac{m^* k_B T}{2\pi\hbar^2}\right)^{3/2} \exp\left(\frac{E_F - E_c}{k_B T}\right)$$



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

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}

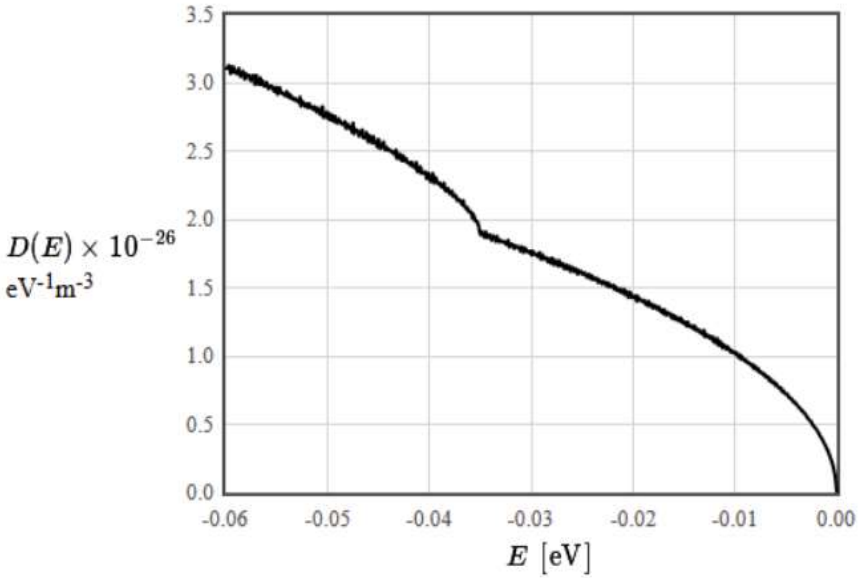
Silicon valence bands

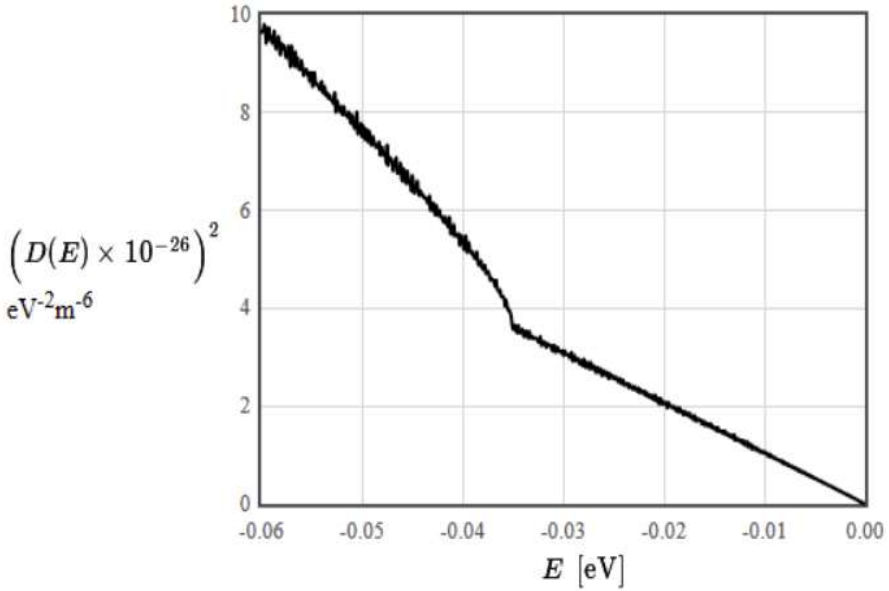


$$E_{v,lh} = -\frac{\hbar^2}{2m_e}\left(4.1k^2 - \sqrt{1.21k^4 + 4.1(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)}\right),$$

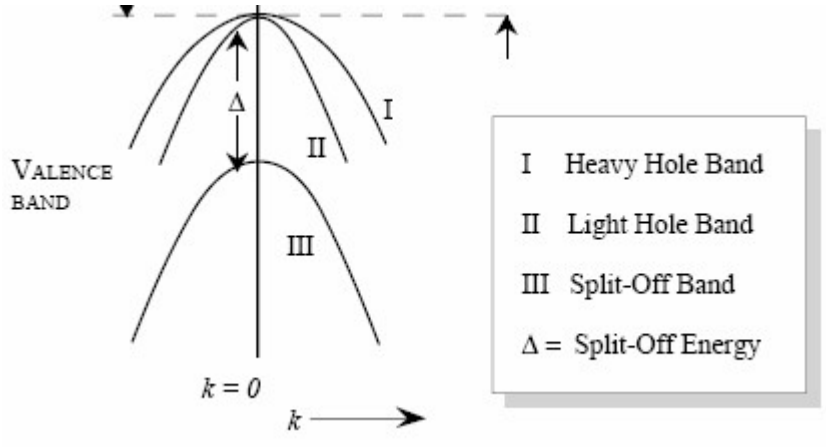
$$E_{v,hh} = -\frac{\hbar^2}{2m_e}\left(4.1k^2 + \sqrt{1.21k^4 + 4.1(k_x^2k_y^2 + k_x^2k_z^2 + k_y^2k_z^2)}\right),$$

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





Density of 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

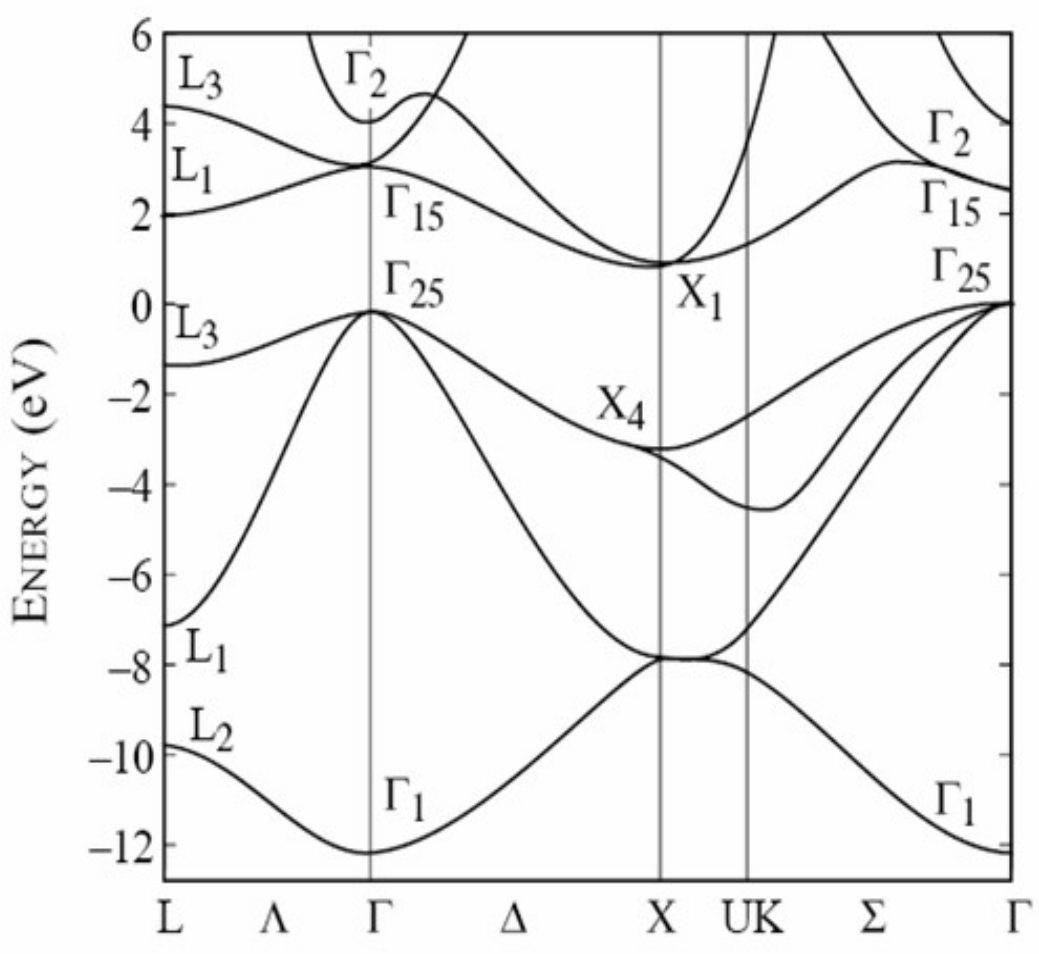
NSM Archive - Physical Properties of Semiconductors

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?

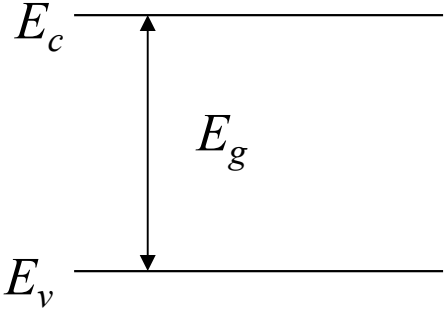
(b) What is the band gap?

(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

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

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

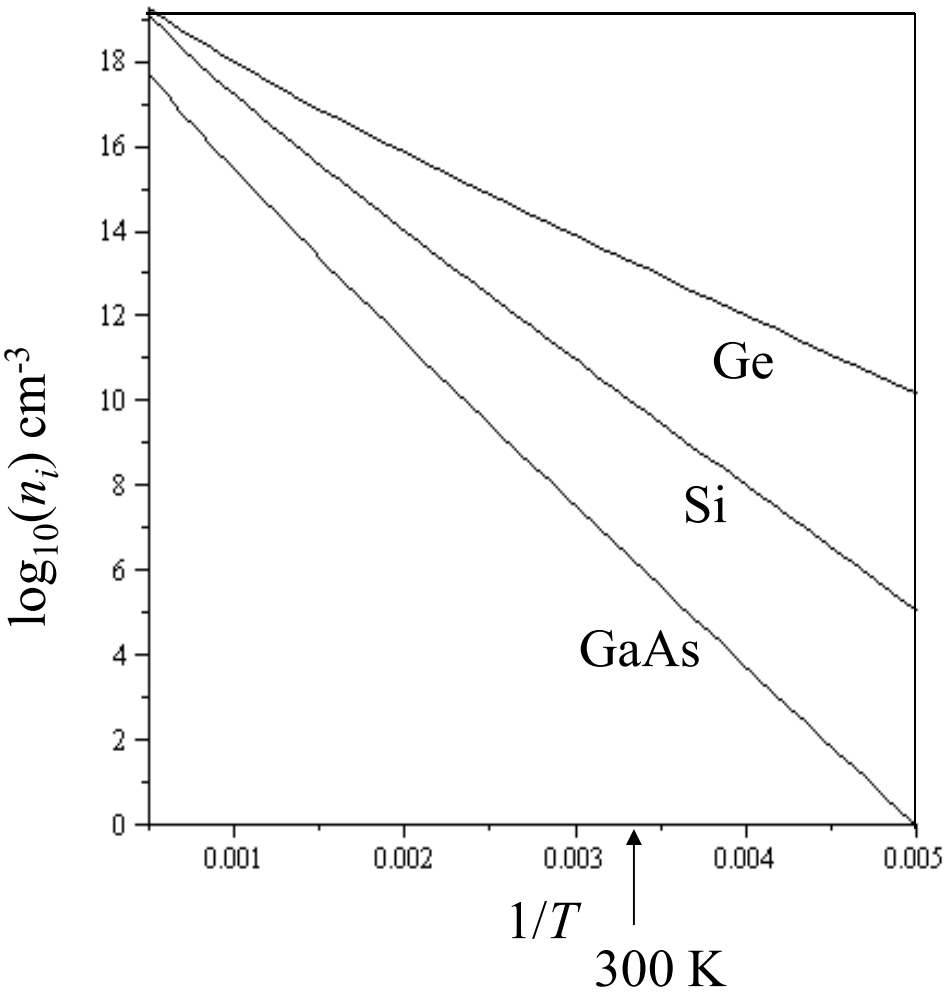


For intrinsic semiconductors (no impurities)

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

intrinsic carrier density

Intrinsic carrier concentration



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

Silicon has ~ 5×10^{22} atoms/cm^3

Good for thermometer, bad for designing circuits.

Fermi energy of an intrinsic semiconductor

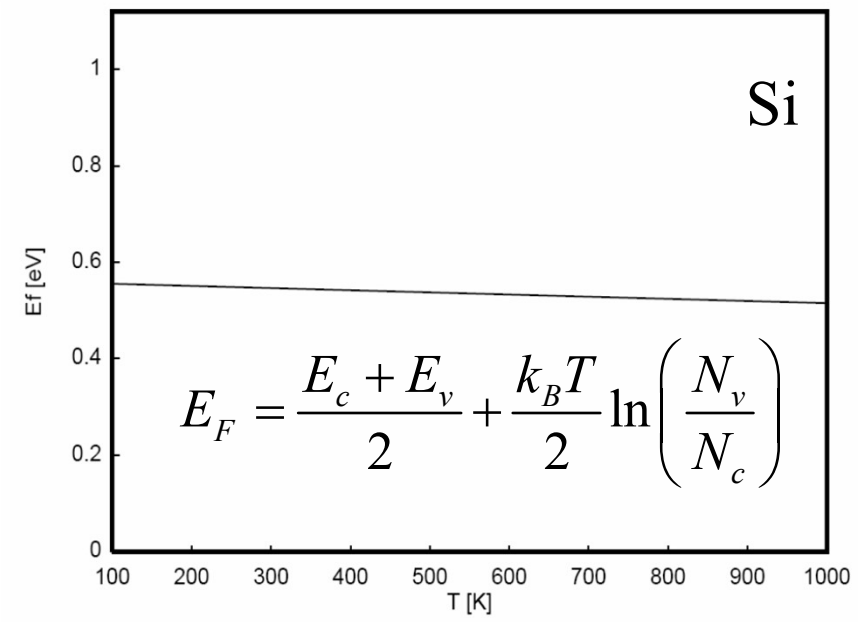
$$n = p = N_c \exp\left(\frac{E_F - E_c}{k_B T}\right) = N_v \exp\left(\frac{E_v - E_F}{k_B T}\right)$$

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

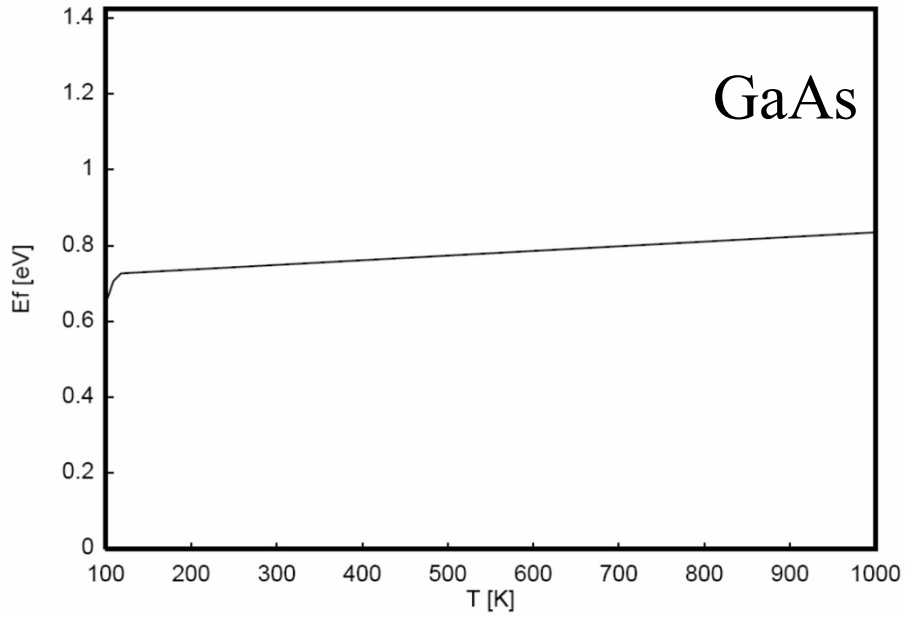
$$\frac{2E_F}{k_B T} = \frac{E_c + E_v}{k_B T} + \ln\left(\frac{N_v}{N_c}\right)$$

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

Temperature dependence of E_F



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



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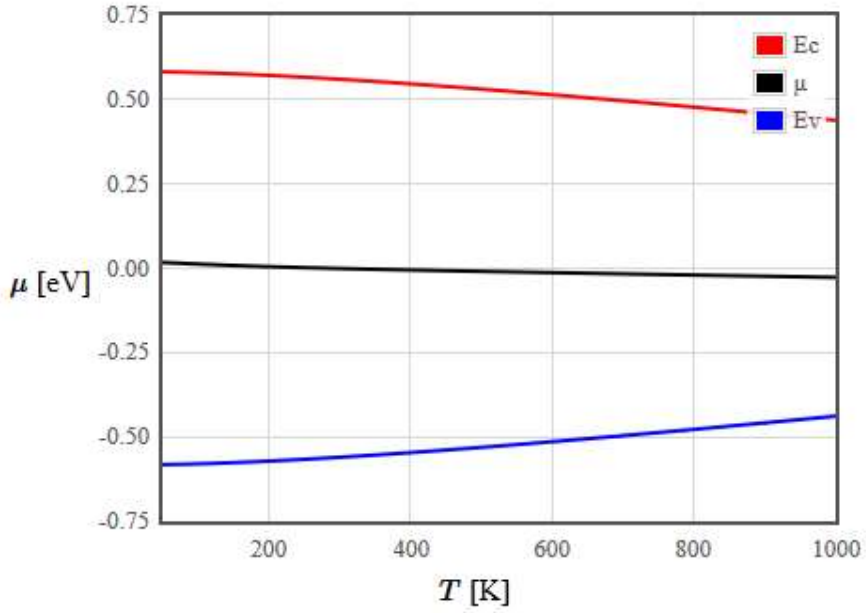
Intrinsic semiconductors



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

n and p

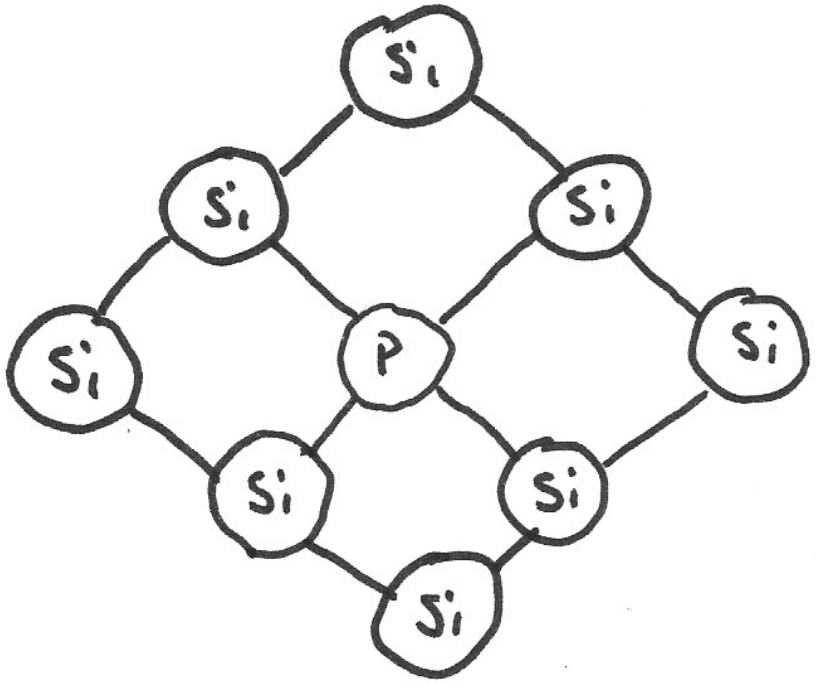
The electron density and hole density are:

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

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

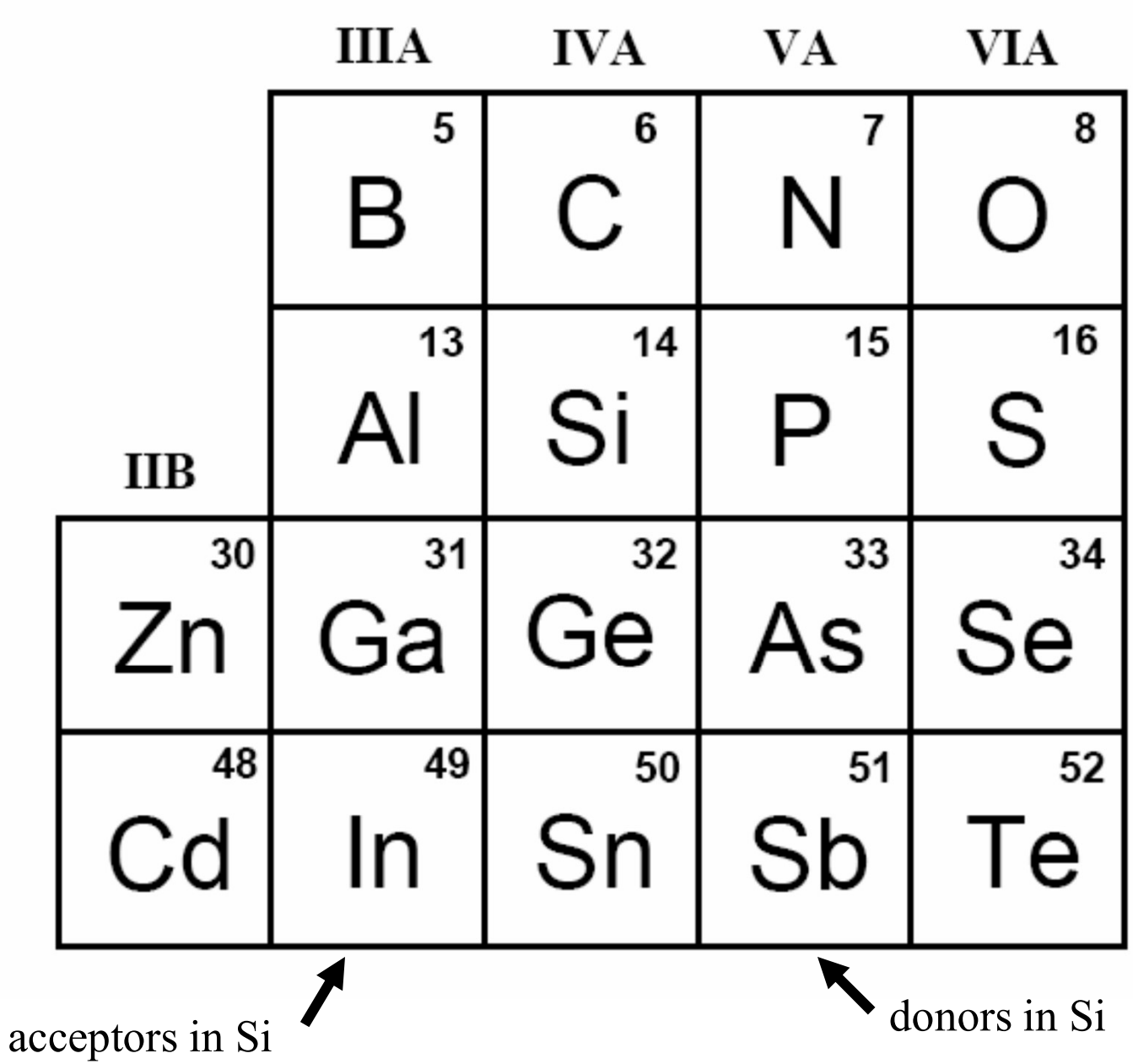


Easier to ionize a P atom in Si than a free P atom

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

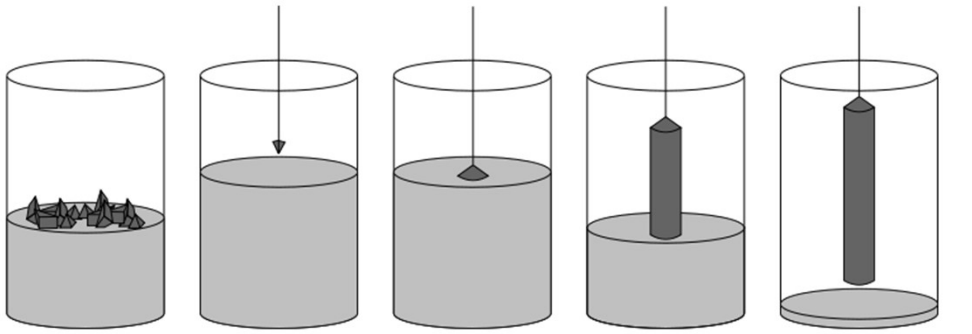
Ionization energy is smaller by a factor: $\frac{m^*}{m}\left(\frac{\varepsilon_0}{\varepsilon_r \varepsilon_0}\right)^2$

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

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

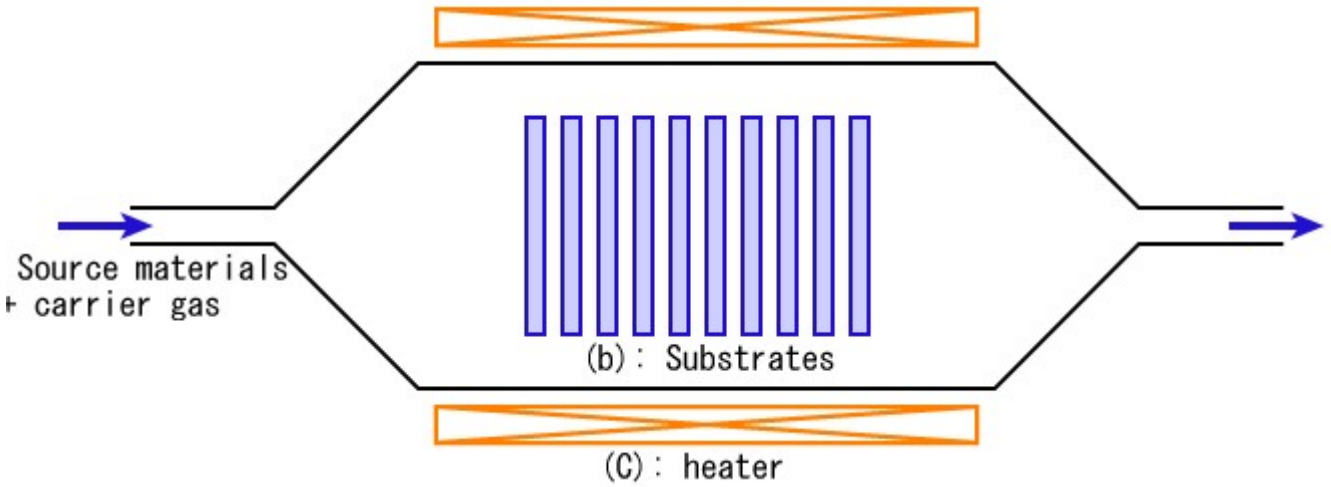
image from wikipedia

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

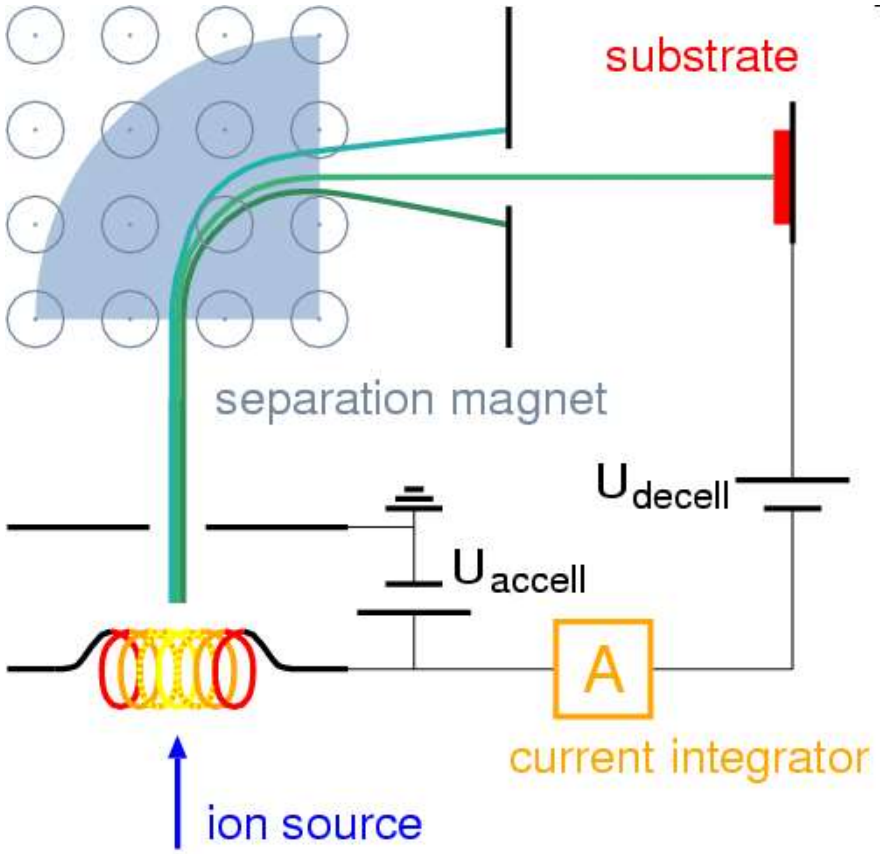
Chemical vapor deposition



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

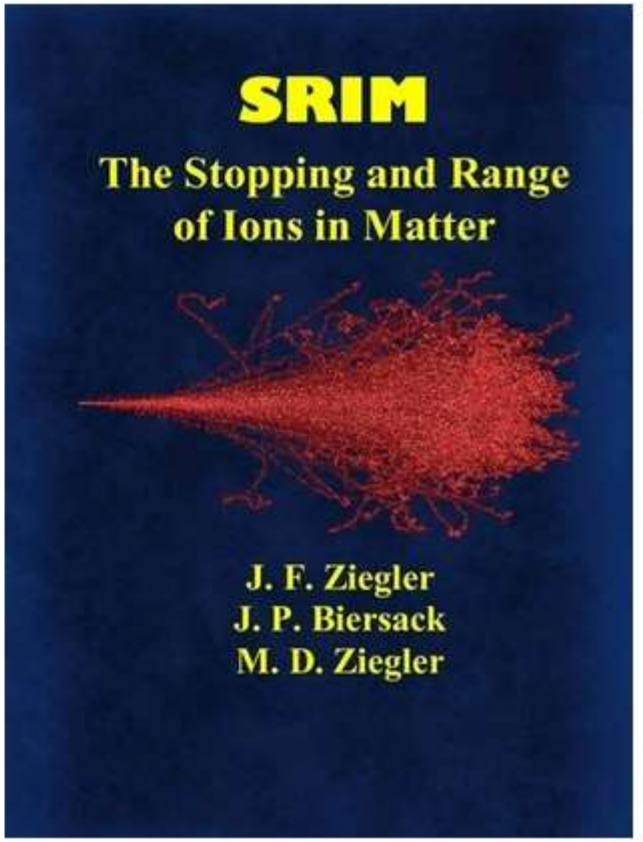


Implant at 7º to avoid channeling

SRIM

The Stopping and Range of Ions in Matter

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

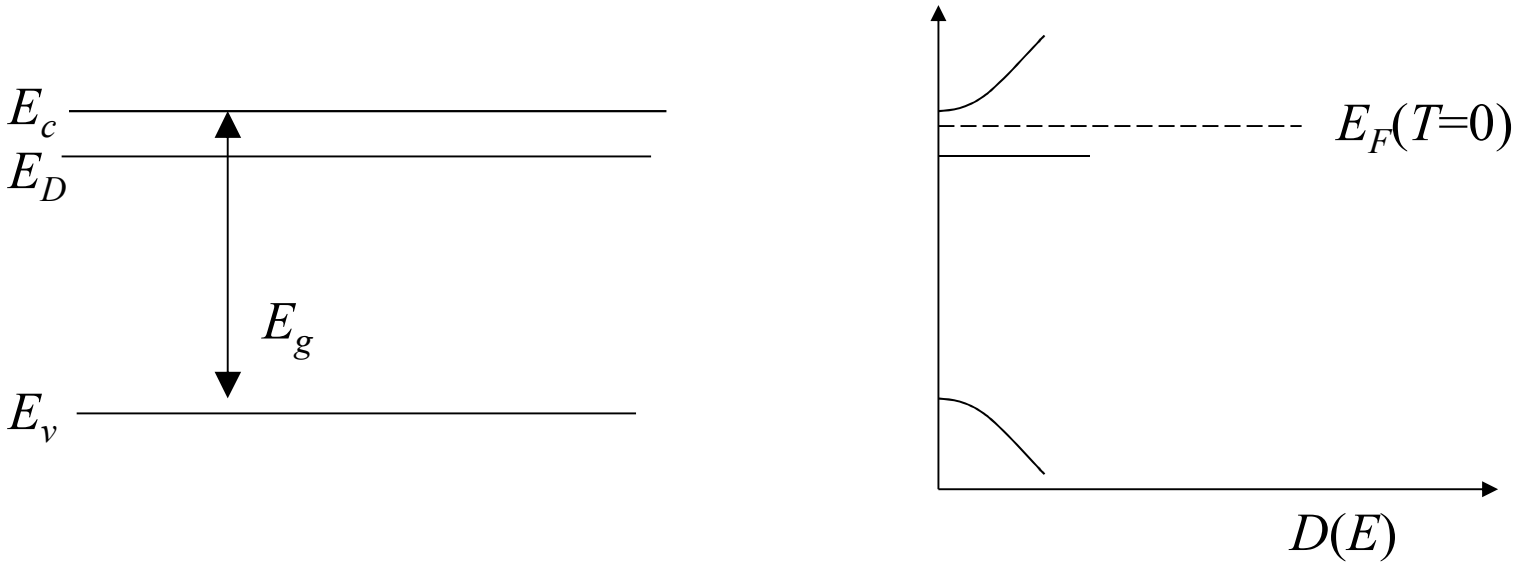


http://www.synopsys.com

Donors

Five valence electrons: P, As

States are added in the band gap just below the conduction band



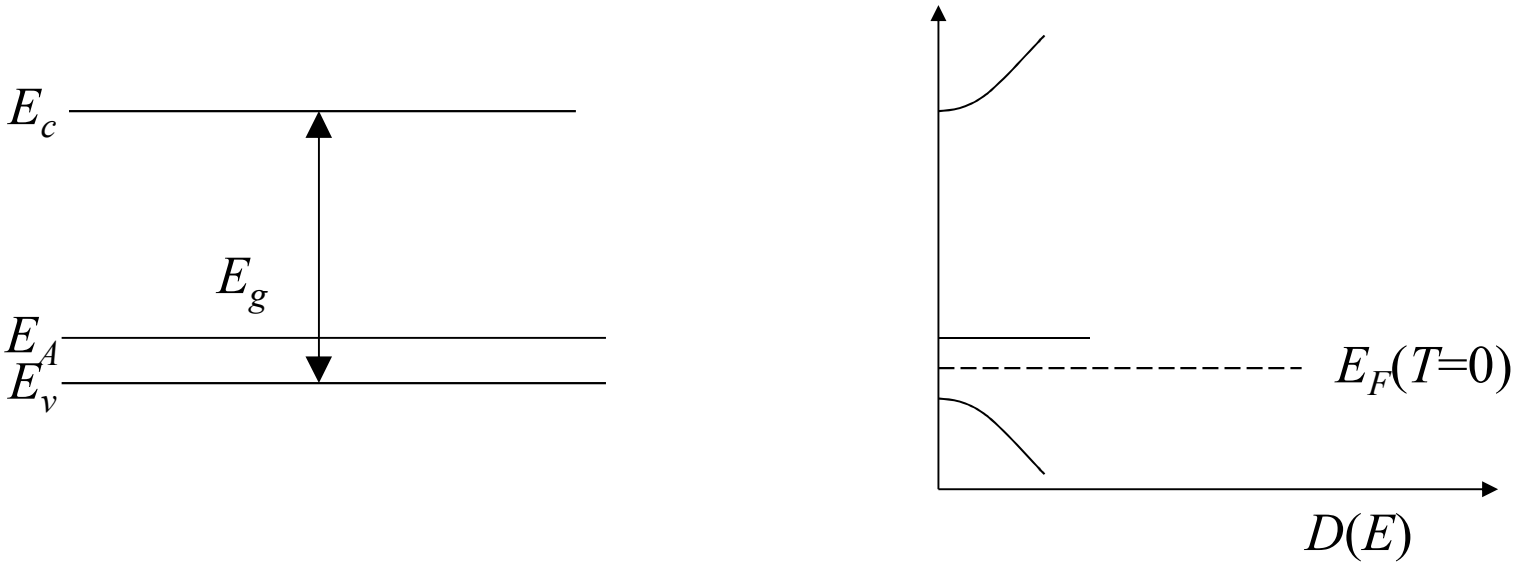
n-type: $n \sim N_D$ Many more electrons in the conduction band than holes in the valence band.

majority carriers: electrons; minority carriers: holes

Acceptors

Three valence electrons: B, Al, Ga

States are added in the band gap just above the valence band



p-type: $p \sim N_A$ Many more holes in the valence band than electrons in the conduction band.

majority carriers: holes; minority carriers: electrons

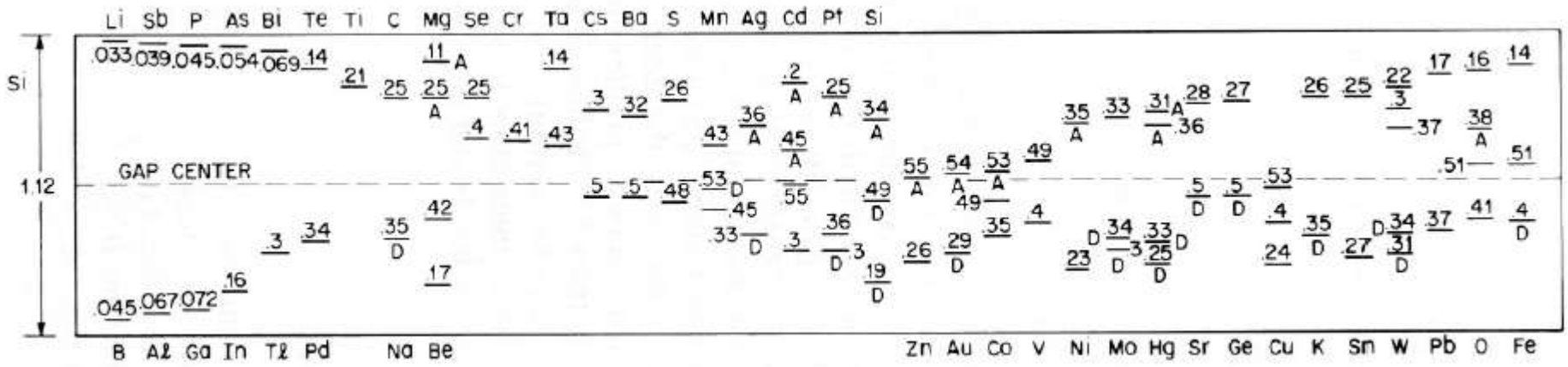
Donor and Acceptor Energies

Semiconductor	Donor	Energy (meV)
Si	Li	33
	Sb	39
	P	45
	As	54
Ge	Li	9.3
	Sb	9.6
	P	12
	As	13
GaAs	Si	5.8
	Ge	6.0
	S	6.0
	Sn	6.0

Energy below the conduction band

Semiconductor	Acceptor	Energy (meV)
Si	B	45
	Al	67
	Ga	72
	In	160
Ge	B	10
	Al	10
	Ga	11
	In	11
GaAs	C	26
	Be	28
	Mg	28
	Si	35

Energy above the valence band



Source: Semiconductor Devices Physics and Technology, S.M. Sze, 1985

Direct Observation of Friedel Oscillations around Incorporated Si_{Ga} Dopants in GaAs by Low-Temperature Scanning Tunneling Microscopy

M. C. M. M. van der Wielen, A. J. A. van Roij, and H. van Kempen
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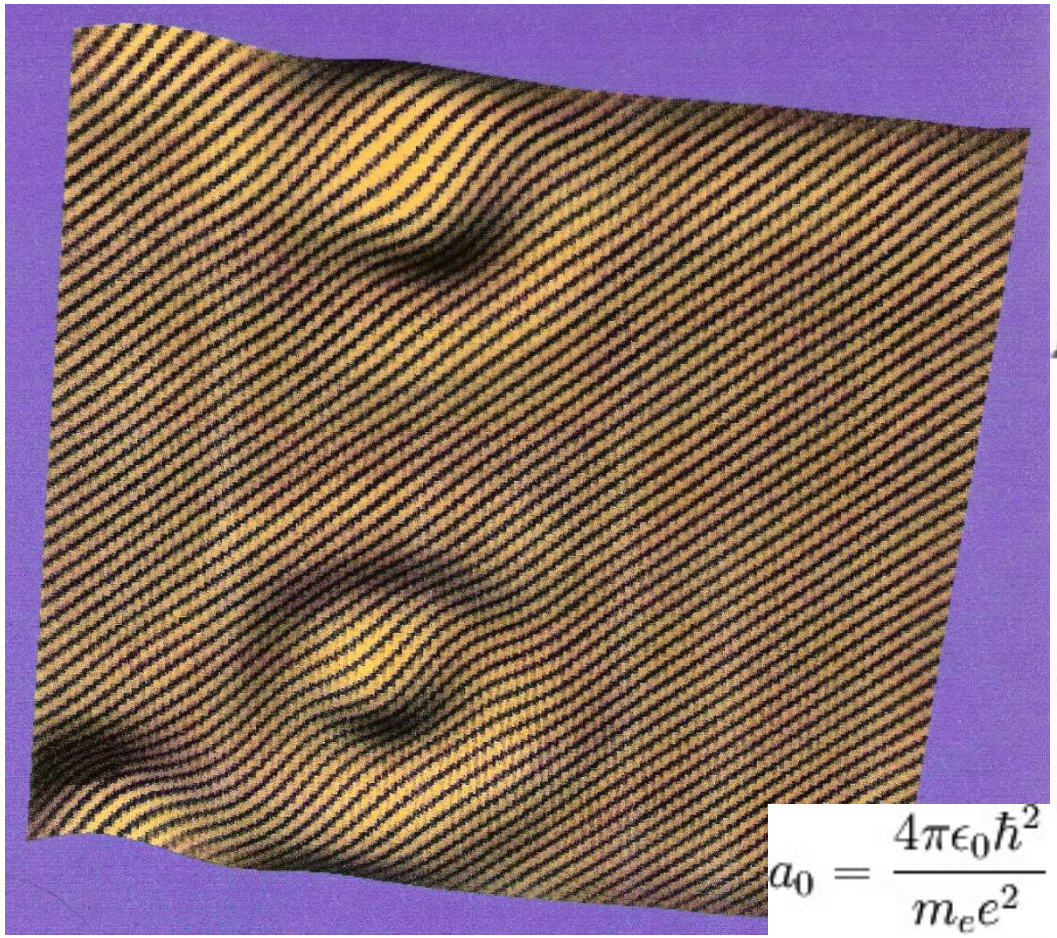
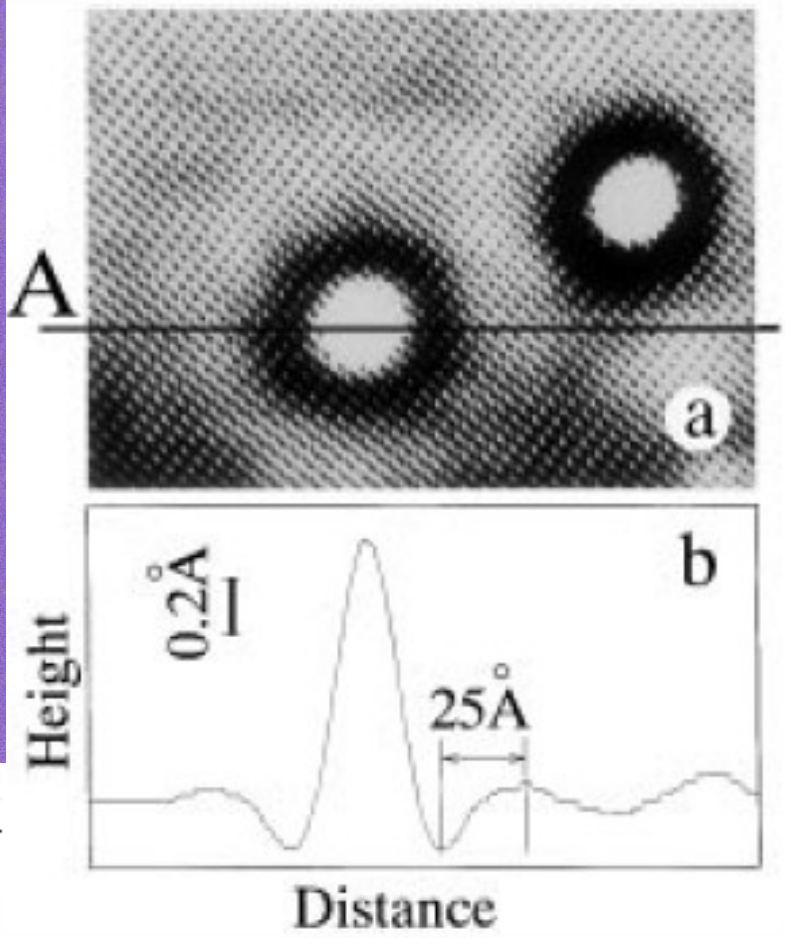
(Received 25 July 1995)



$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2}$$



Temperature dependence