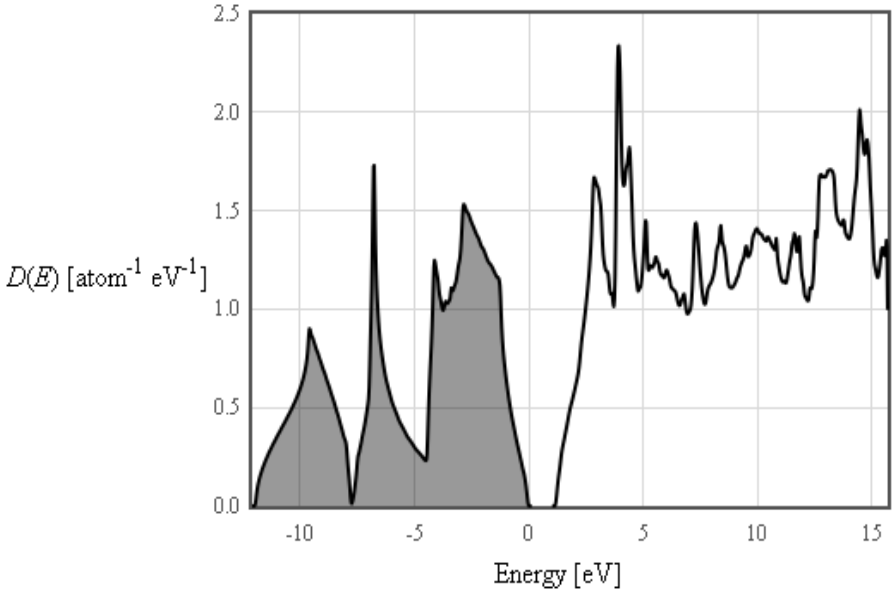
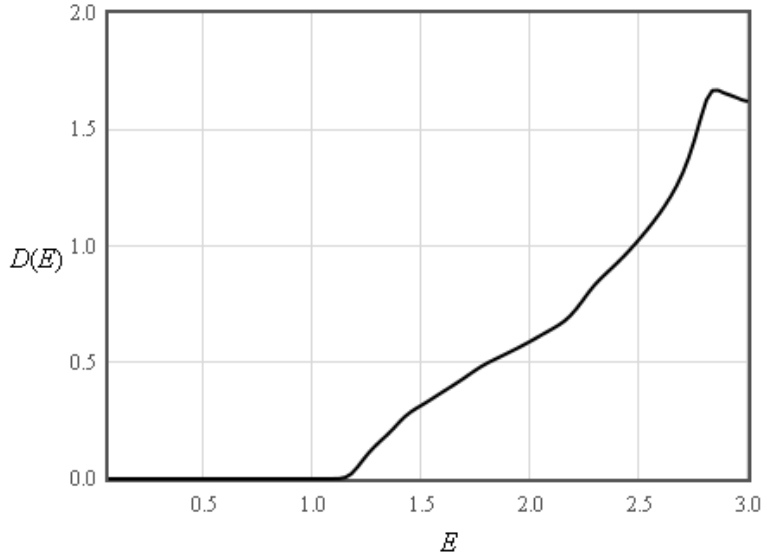
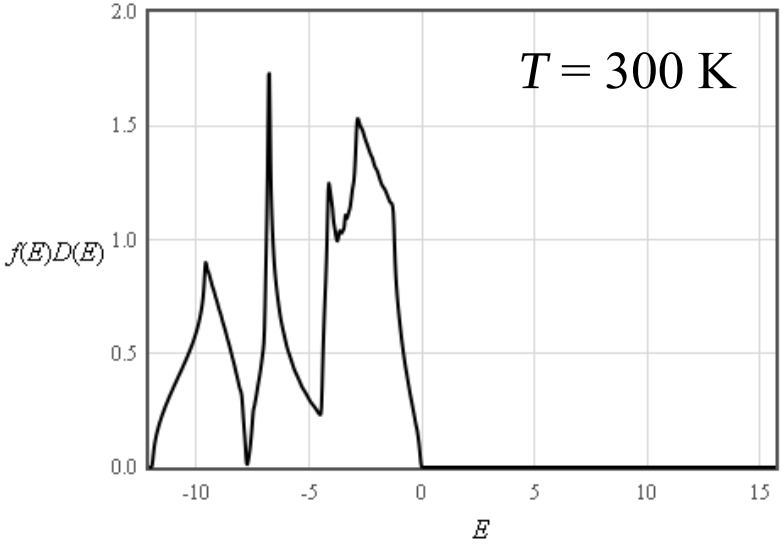
7. Semiconductors

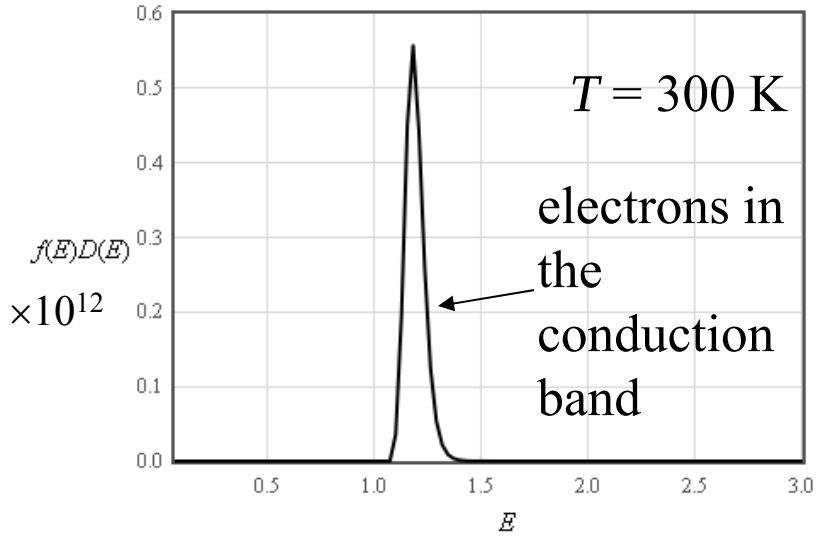
Oct 22, 2018

Silicon density of states







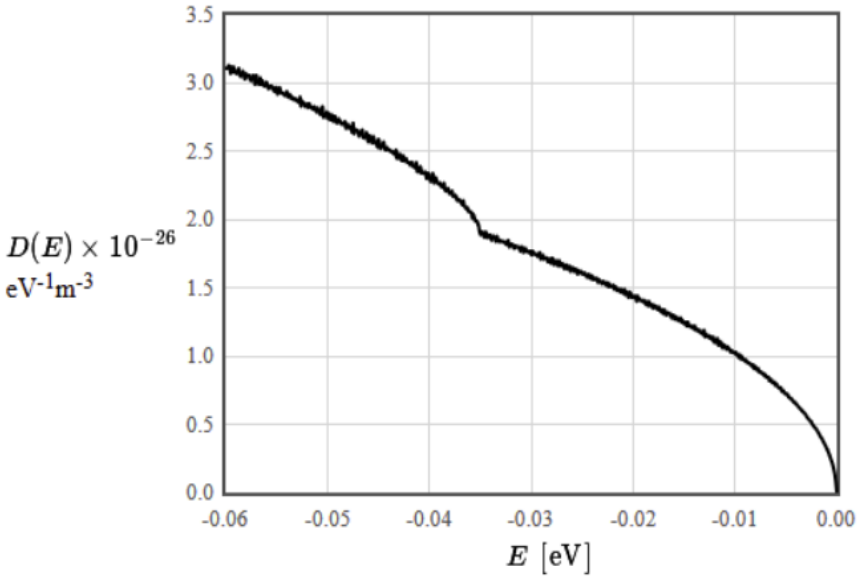


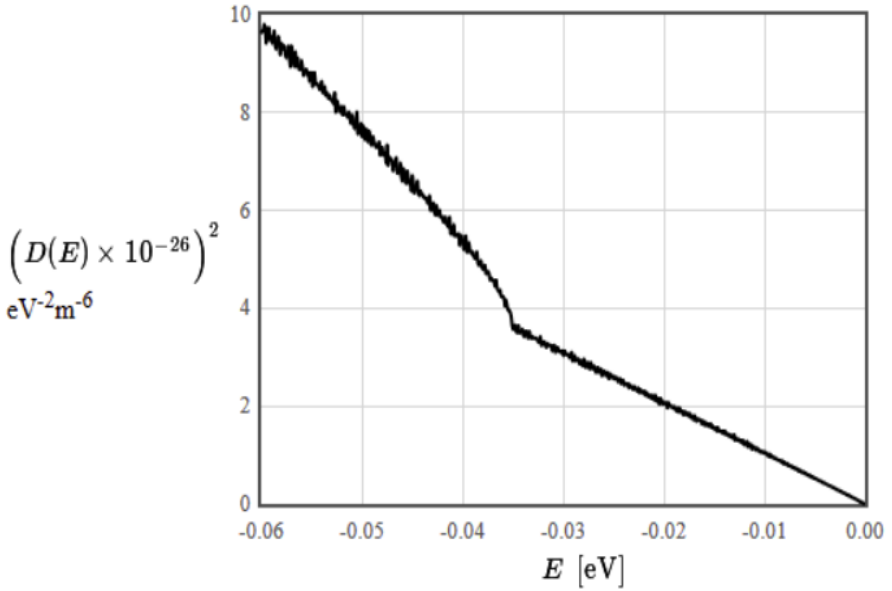
Silicon valence bands

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

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

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



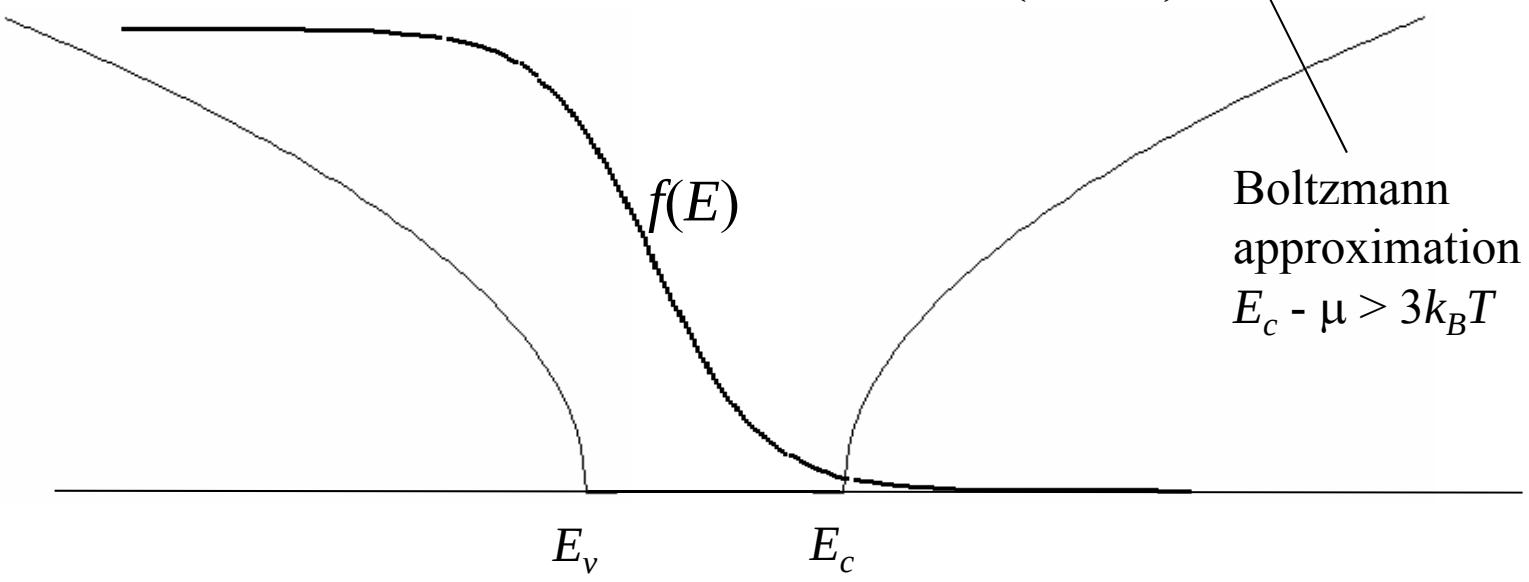


Density of electrons in the conduction band

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

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

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

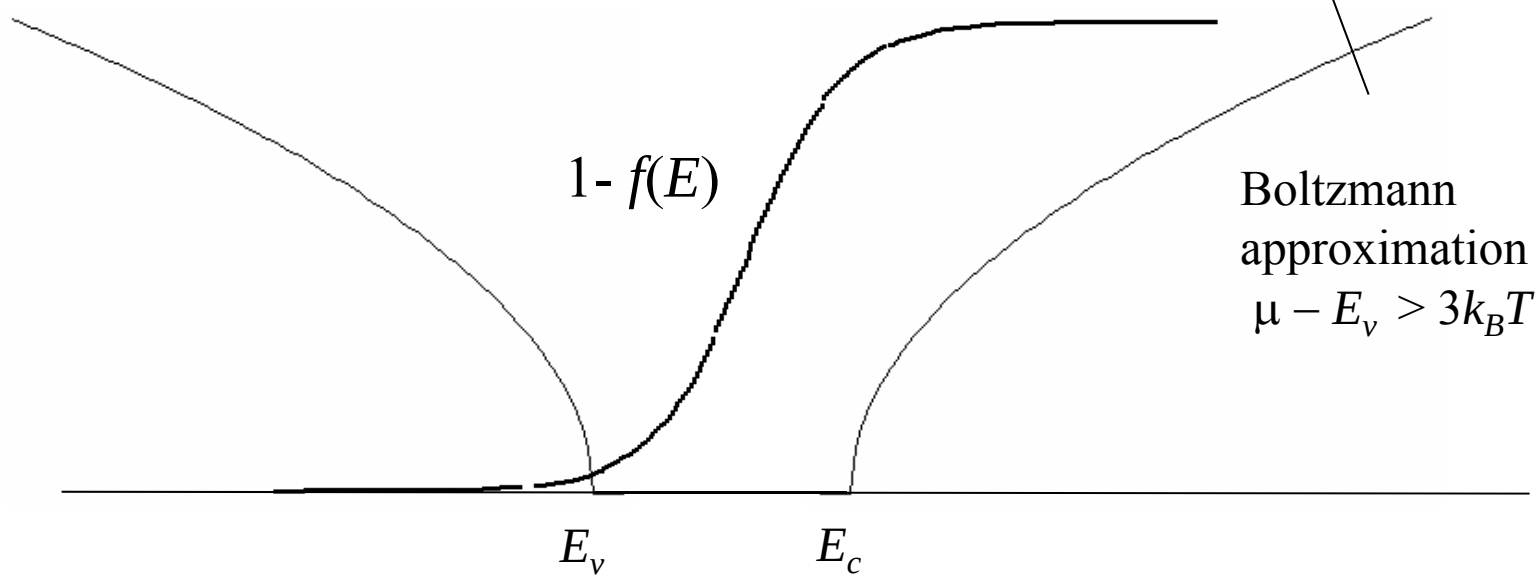
$$\boxed{n = N_c(T) \exp\left(\frac{\mu - E_c}{k_B T}\right)} = \frac{2D_c}{\sqrt{\pi}} \left(k_B T\right)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T}\right)$$

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

Density of holes in the valence band

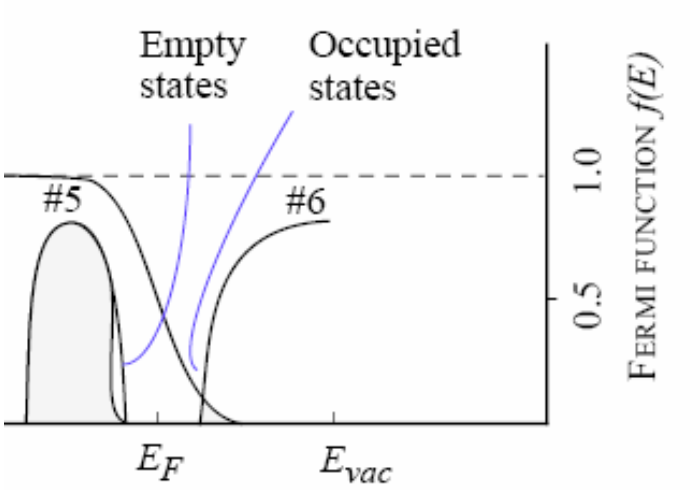
$$D(E) = D_v\sqrt{E_v - E}$$

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



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

Density of holes in the valence band



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

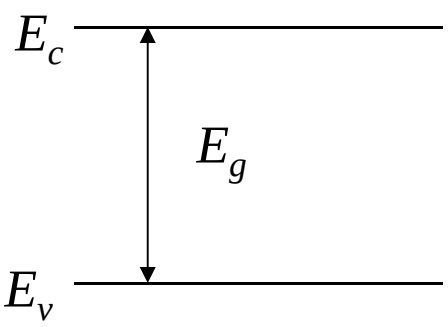
$$\boxed{p = N_v \exp\left(\frac{E_v - \mu}{k_B T}\right)} = \frac{2D_v}{\sqrt{\pi}}\left(k_B T\right)^{3/2} \exp\left(\frac{E_v - \mu}{k_B T}\right)$$

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

Law of mass action

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

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

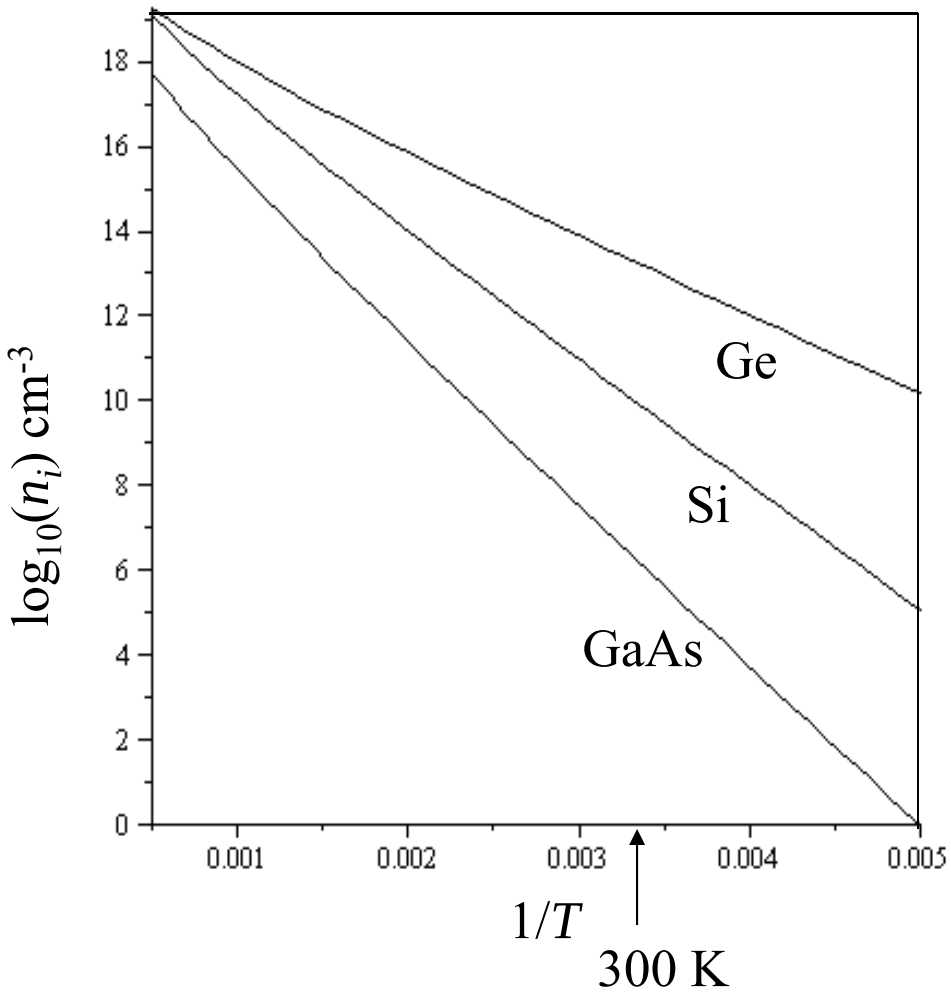


For intrinsic semiconductors (no impurities)

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

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

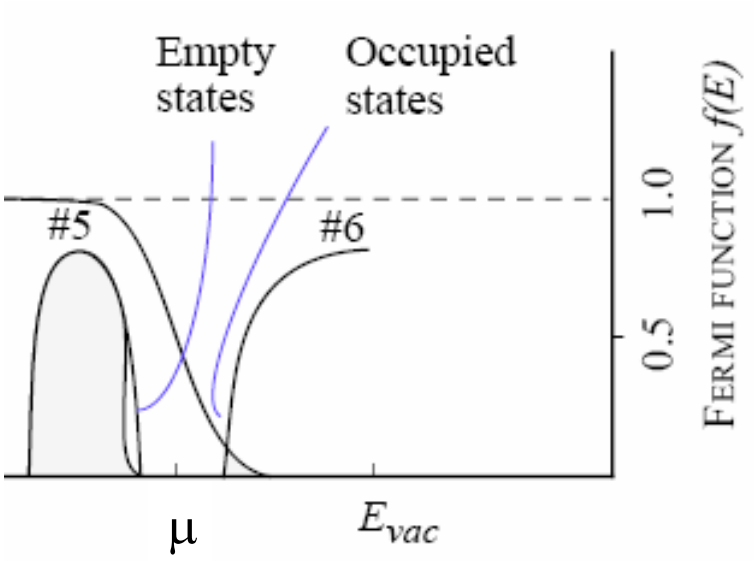
Chemical potential of an intrinsic semiconductor

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

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

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

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

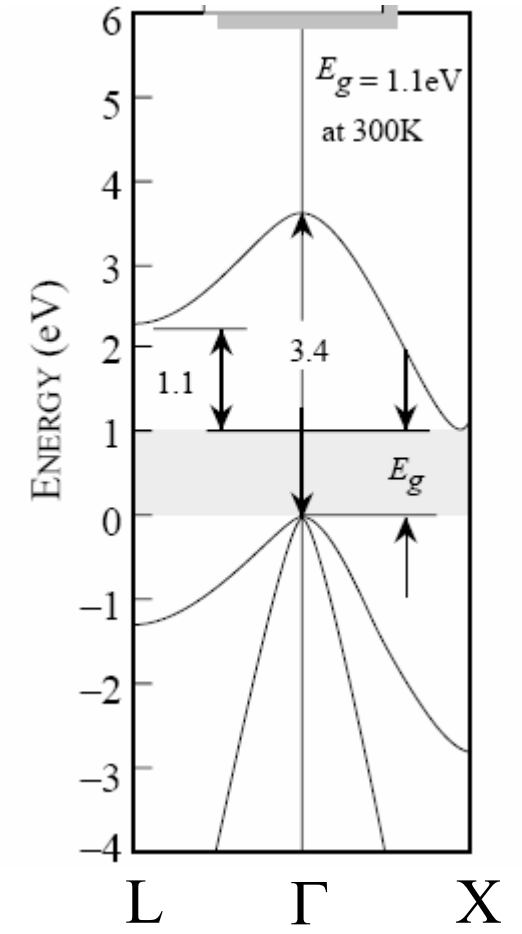


E_c ——————————

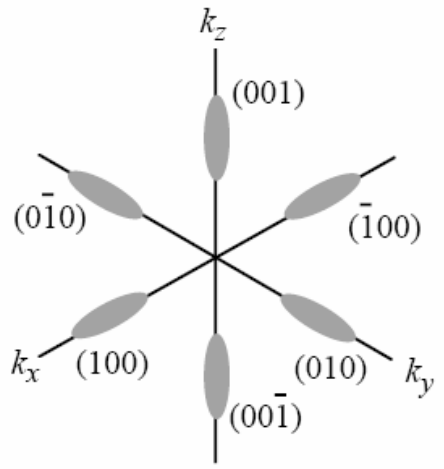
μ ----------

E_v ——————————

Density of electrons in the conduction band



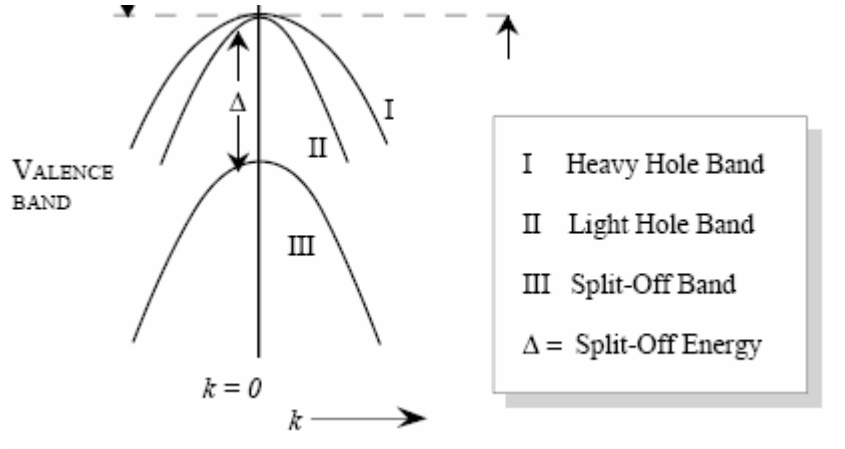
$$n = N_c(T)\exp\left(\frac{\mu - E_c}{k_B T}\right) = \frac{2D_v}{\sqrt{\pi}}\left(k_B T\right)^{3/2}\exp\left(\frac{\mu - E_c}{k_B T}\right)$$



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

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
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}

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

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,

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

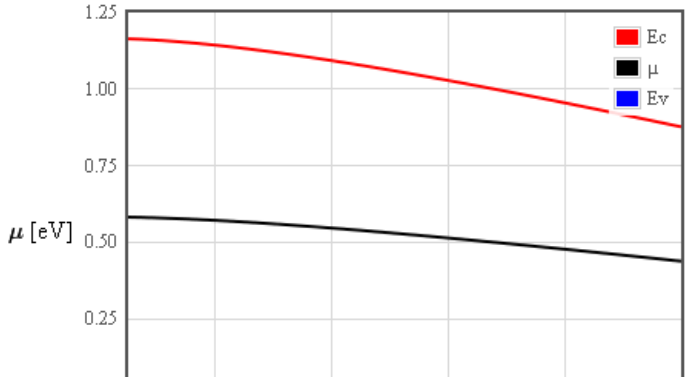
$$m_e^* = \frac{\pi\hbar^2}{300k_B}\left(\sqrt{2}N_c(300)\right)^{2/3}$$

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

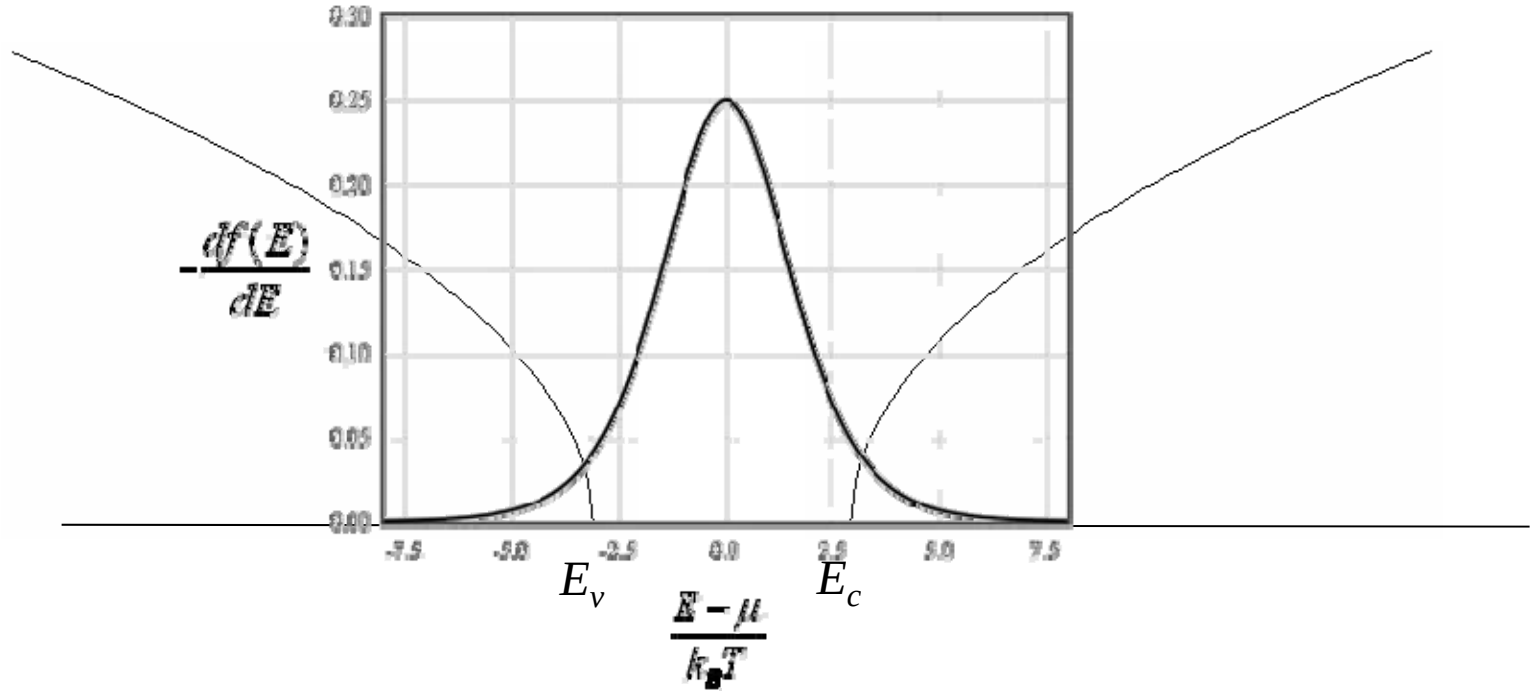
Replot

Semiconductor

Si | Ge | GaAs

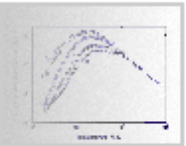
http://lamp.tu-graz.ac.at/~hadley/ss1/semiconductors/intrinsic.php

Narrow bandgap semiconductors



Use the programs for metals for small bandgap semiconductors.

Semiconductors on NSM



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

We are going to add new data for:

$Ga_xIn_{1-x}As_ySb_{1-y}$	- Gallium Indium Arsenide Antimonide	$Ga_xIn_{1-x}P$	- Gallium Indium Phosphide
$Ga_xIn_{1-x}As$	- Gallium Indium Arsenide	$Ga_xIn_{1-x}Sb$	- Gallium Indium Antimonide
$InAs_{1-x}Sb_x$	- Indium Arsenide Antimonide	$Ga_xIn_{1-x}As_yP_{1-y}$	- Gallium Indium Arsenide Phosphide
$Si_{1-x}Ge_x$	- Silicon Germanium	SiC	- Silicon Carbide

Effective Masses

Electrons:

The surfaces of equal energy are ellipsoids.

$m_l = 0.98m_o$

$m_t = 0.19m_o$

Effective mass of density of states $m_c = 0.36m_o$

There are 6 equivalent valleys in the conduction band.

$m_{cc} = 0.26m_o$

Holes:

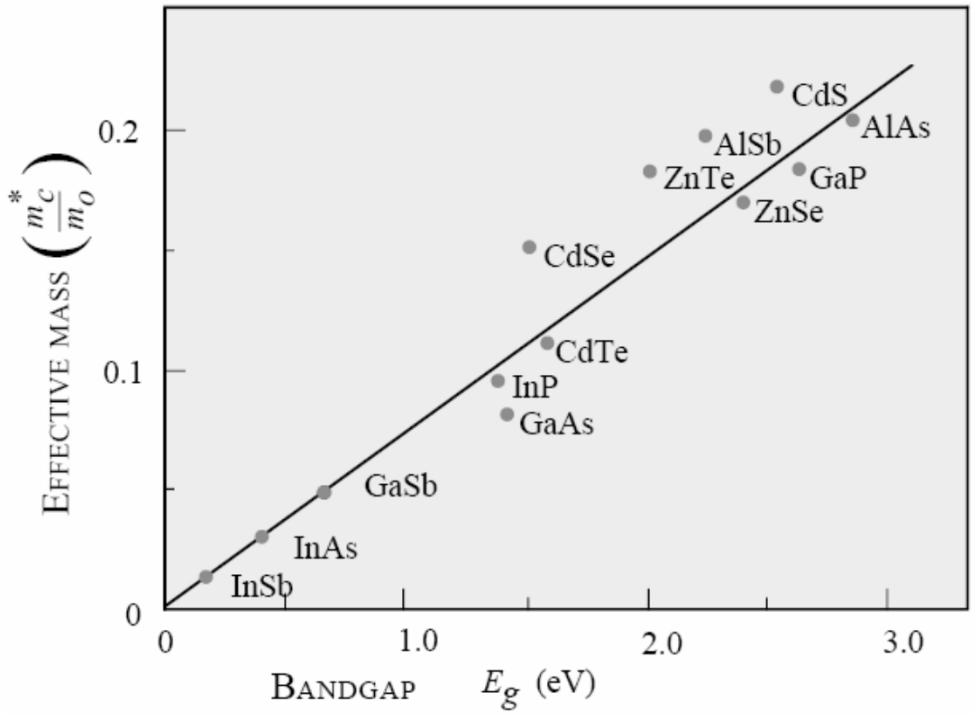
Heavy $m_h = 0.49m_o$

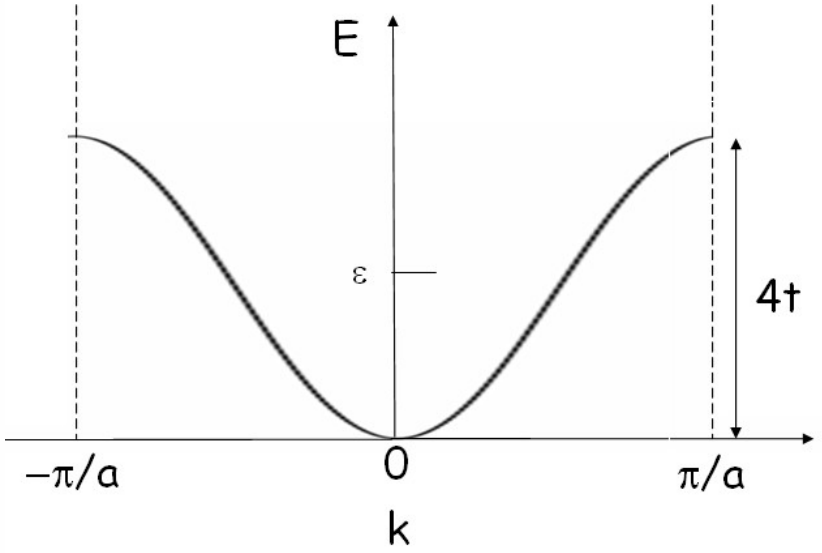
Light $m_{lp} = 0.16m_o$

Split-off band $m_{so} = 0.24m_o$

Effective mass of density of states $m_v = 0.81m_o$

Large gap -> large effective mass





$$E_k = \varepsilon - 2t\cos(ka)$$

$$m^* = \frac{\hbar^2}{\frac{d^2E}{dk^2}}$$

$$\frac{d^2E}{dk^2} = 2ta^2$$

$$m^* \sim \frac{1}{t}$$

narrow bands -> large effective mass

Measuring the effective mass

Cyclotron resonance $\omega_c = \frac{eB}{m^*}$

Resonant absorption occurs when rf waves with the cyclotron resonance frequency are applied. This can be used to experimentally determine the effective mass.

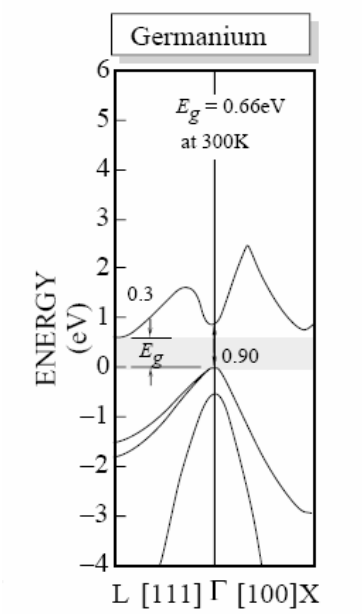
Knowing the effective mass, the scattering time can be calculated from the measured conductivity.

$$\sigma = \frac{ne^2\tau_{sc}}{m^*}$$

Direct and indirect band gaps

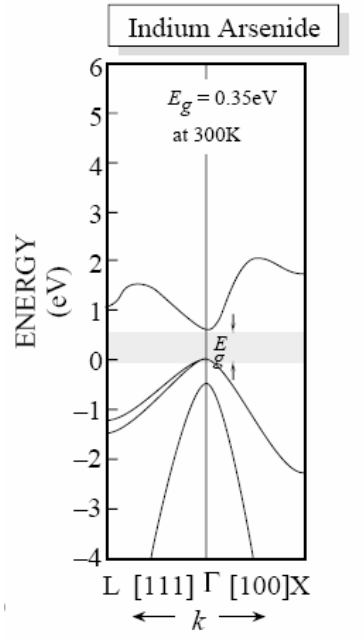
indirect bandgap
$\Delta k \neq 0$

phonons are emitted



direct bandgap:
$\Delta k = 0$

photons can be emitted

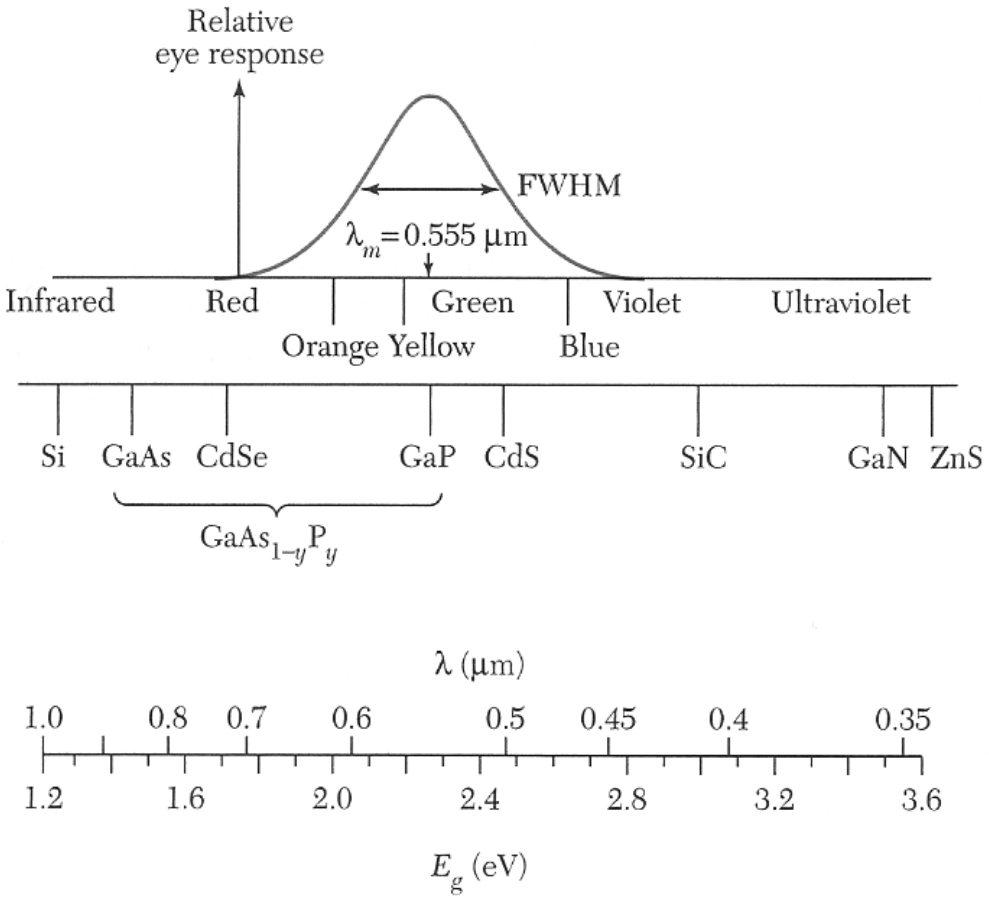


Momentum must be conserved when photons are absorbed or emitted.

Light emitting diodes

TABLE 1 Common III-V materials used to produce LEDs and their emission wavelengths.

Material	Wavelength (nm)
InAsSbP/InAs	4200
InAs	3800
GaInAsP/GaSb	2000
GaSb	1800
$Ga_xIn_{1-x}As_{1-y}P_y$	1100-1600
$Ga_{0.47}In_{0.53}As$	1550
$Ga_{0.27}In_{0.73}As_{0.63}P_{0.37}$	1300
GaAs:Er,InP:Er	1540
Si:C	1300
GaAs:Yb,InP:Yb	1000
$Al_xGa_{1-x}As$:Si	650-940
GaAs:Si	940
$Al_{0.11}Ga_{0.89}As$:Si	830
$Al_{0.4}Ga_{0.6}As$:Si	650
$GaAs_{0.6}P_{0.4}$	660
$GaAs_{0.4}P_{0.6}$	620
$GaAs_{0.15}P_{0.85}$	590
$(Al_xGa_{1-x})_{0.5}In_{0.5}P$	655
GaP	690
GaP:N	550-570
$Ga_xIn_{1-x}N$	340,430,590
SiC	400-460
BN	260,310,490

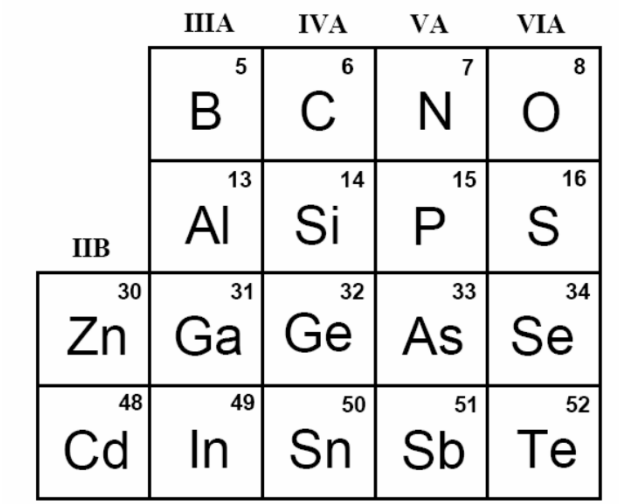


Extrinsic semiconductors

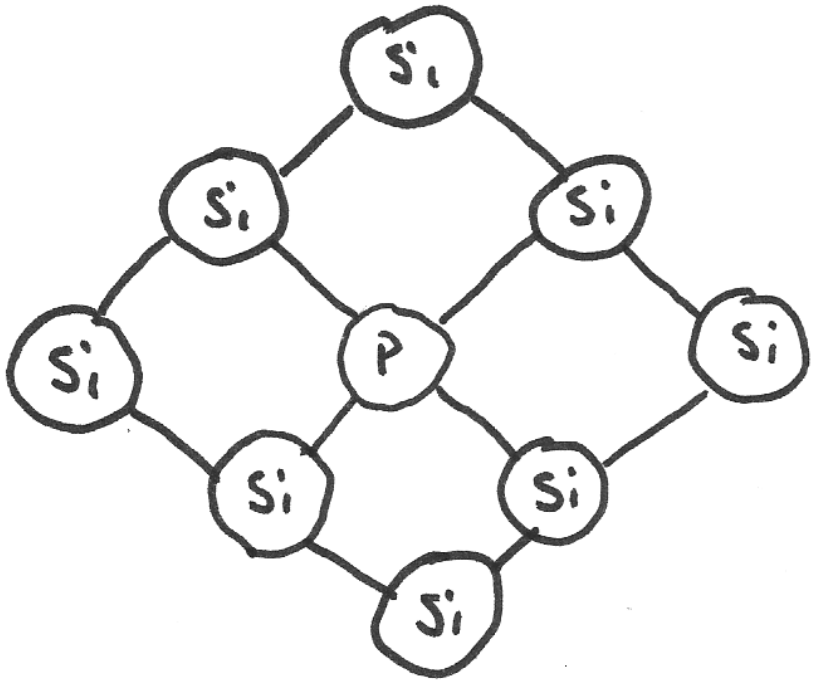
The introduction of impurity atoms that can and electrons or holes is called doping.

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.



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

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

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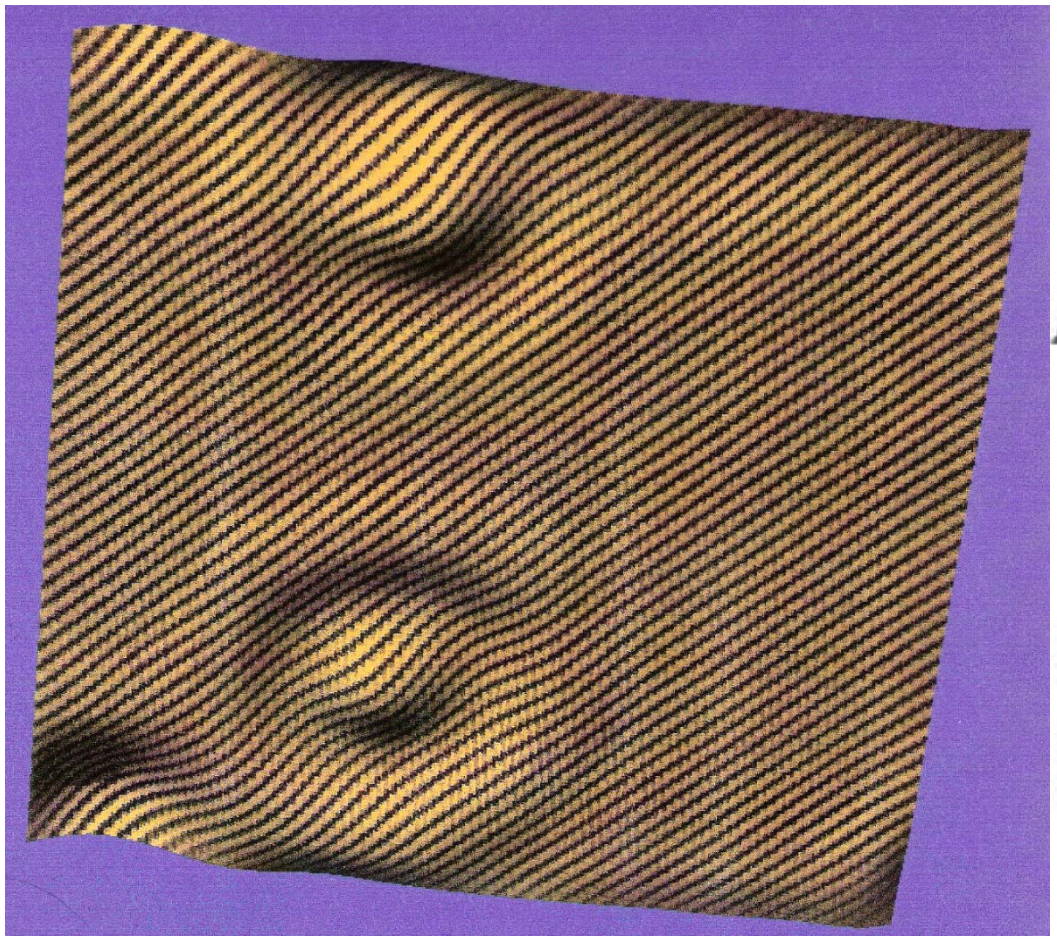
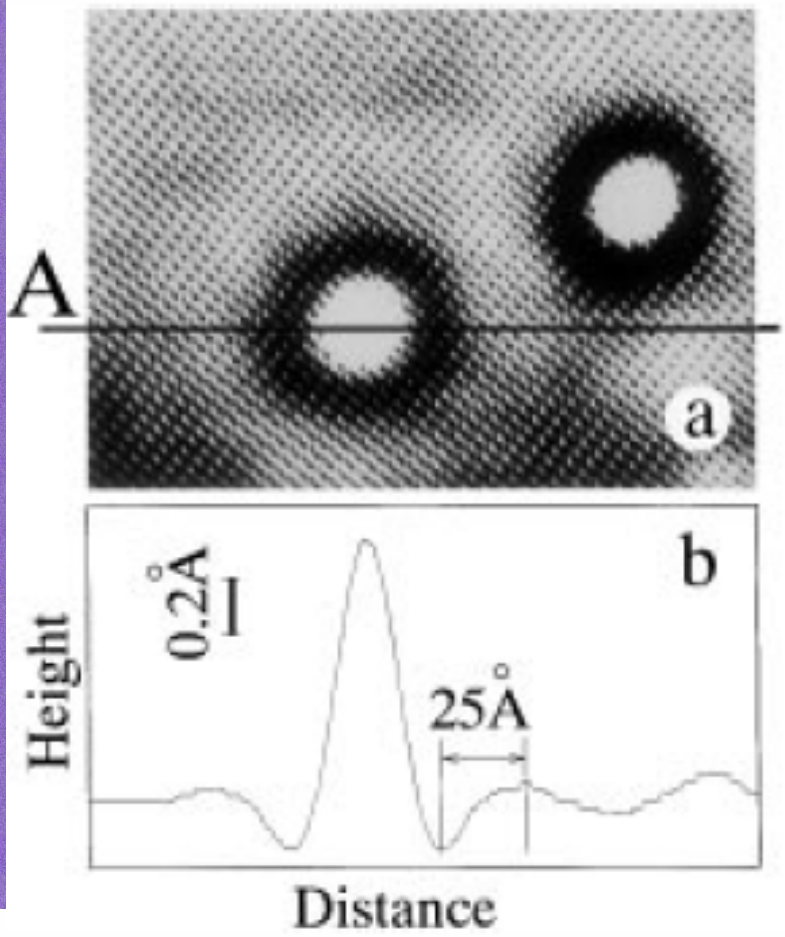
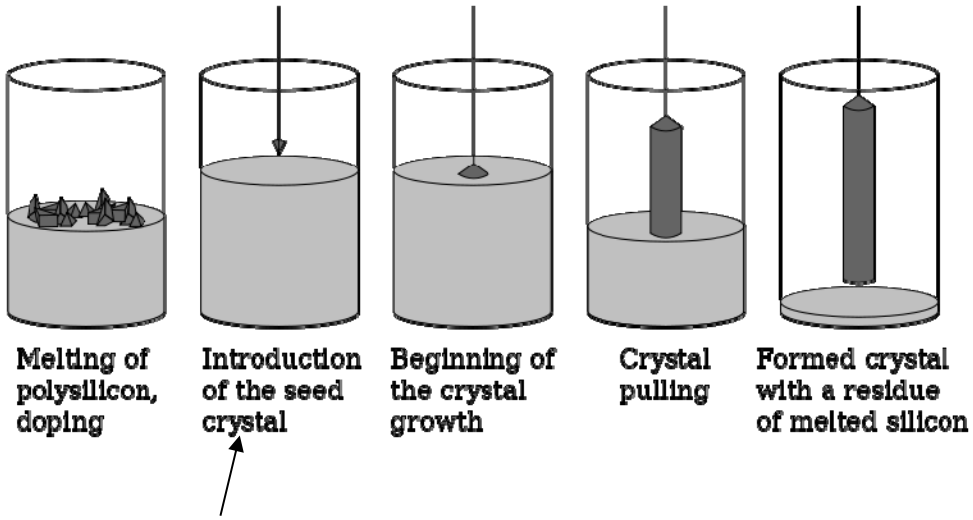
Research Institute for Materials, University of Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands
(Received 25 July 1995)





Crystal growth

Czochralski Process



add dopants to the melt

images from wikipedia

Crystal growth

Float zone Process

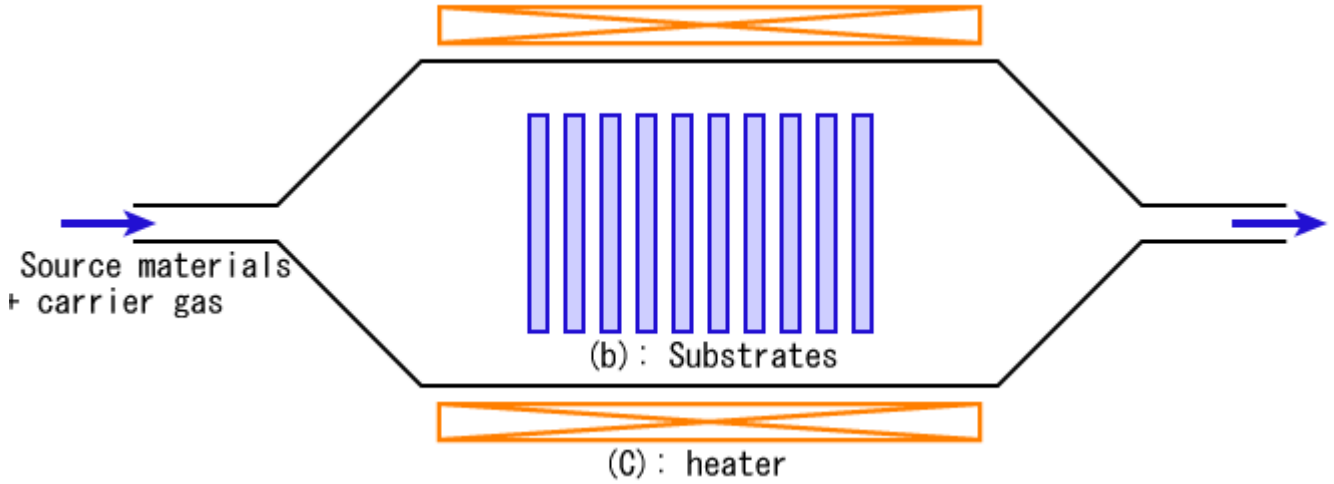
Neutron transmutation

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

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

image from wikipedia

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.

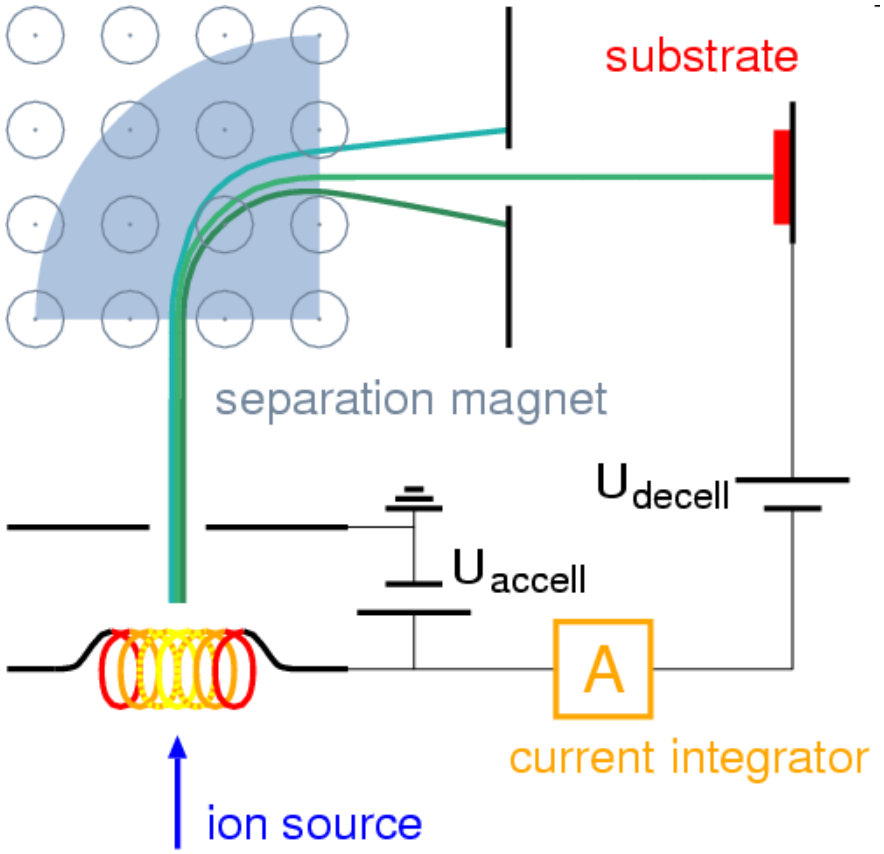
image from wikipedia

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

Ion implantation

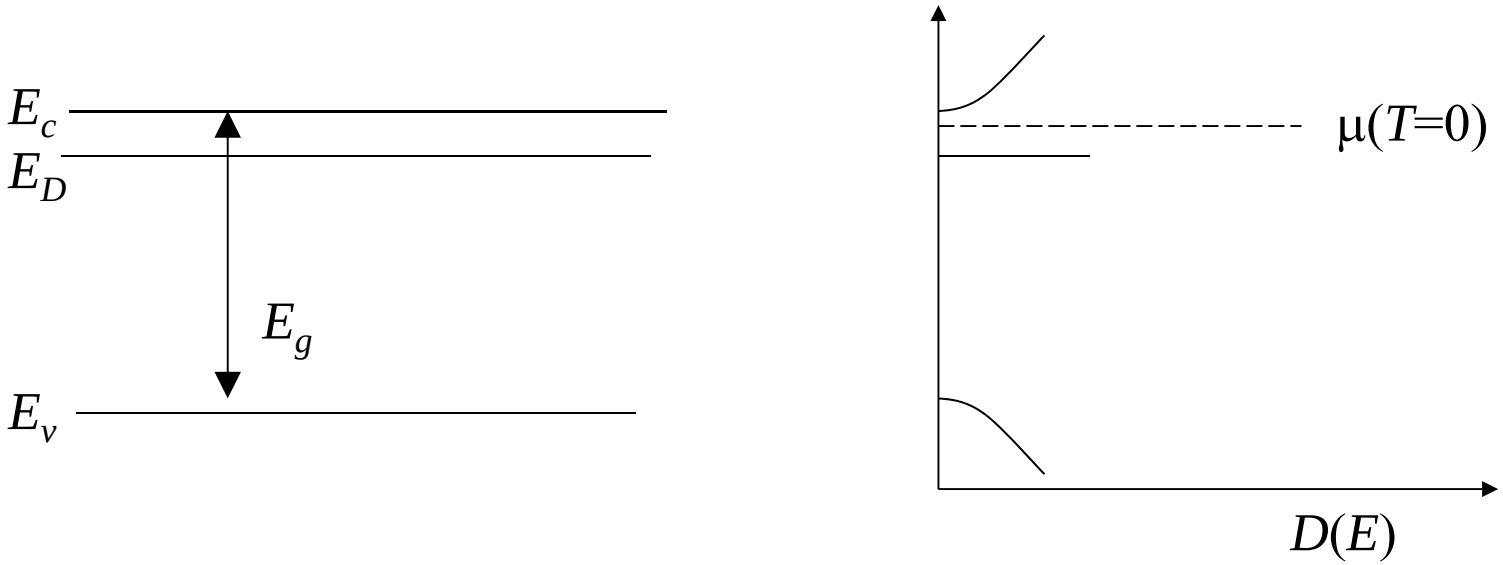


Implant at 7º to avoid channeling

Donors

Five valence electrons: P, As

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



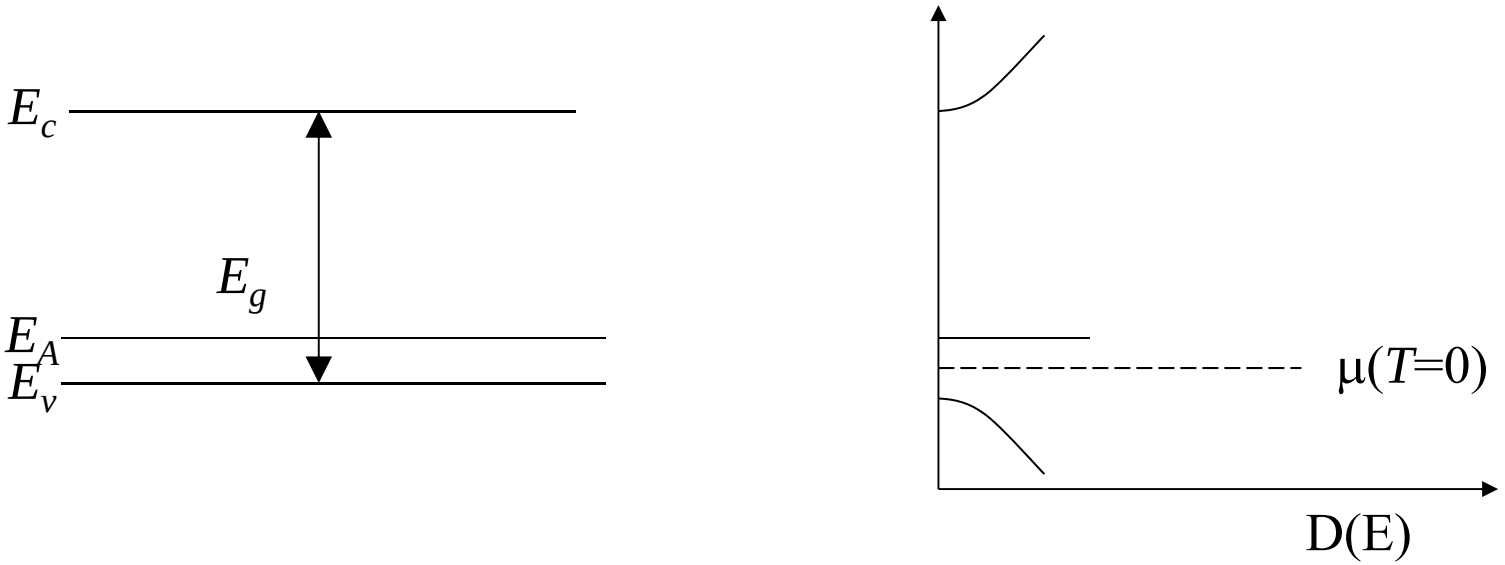
n-type: $n \sim N_D$ Many more electrons in the conduction band than holes in the valence band.

majority carriers: electrons; minority carriers: holes

Acceptors

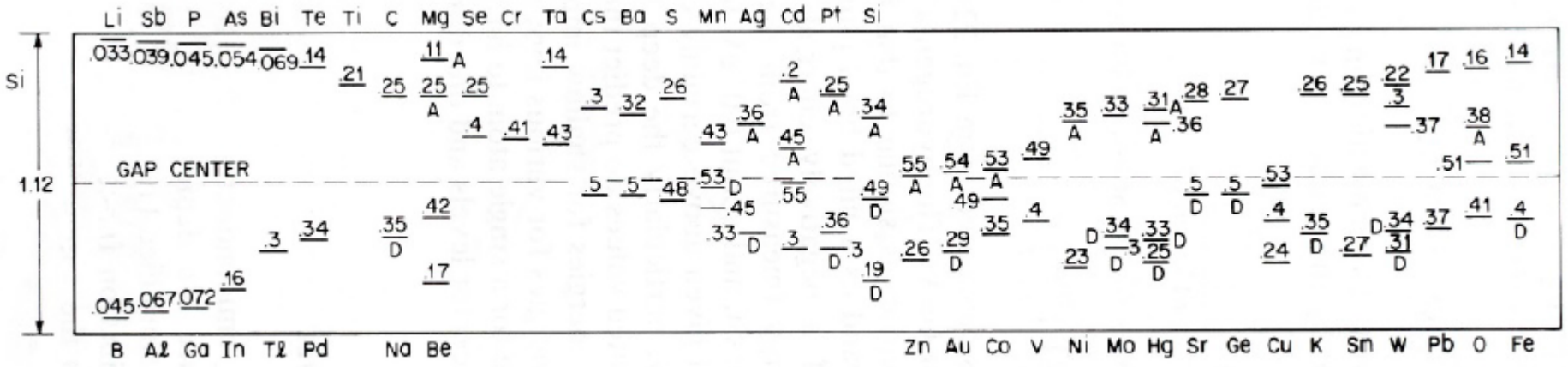
Three valence electrons: B, Al, Ga

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



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

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