Semiconductors

Semiconductors

density of electrons in the conduction band

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

effective density of states in the conduction band at 300 K

density of holes in the valence band

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

effective density of states in the valence band at 300 K

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

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,

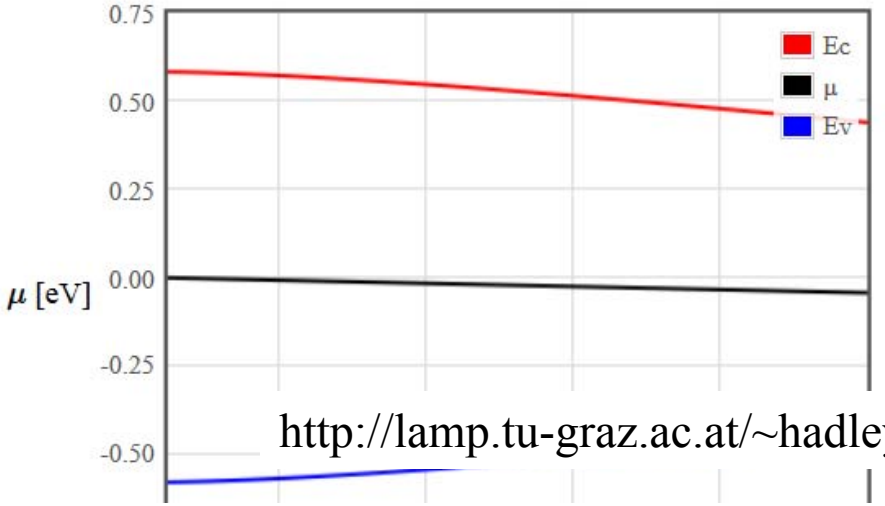
$$D(E) = \begin{cases} D_v\sqrt{E_v - E}, & \text{for } E < E_v \\ 0, & \text{for } E_v < E < E_c \\ D_c\sqrt{E - E_c}, & \text{for } E_c < E \end{cases}$$

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 of states effective masses' m_h^* and m_e^* or the 'effective density of states at 300 K' $N_v(300)$ and $N_c(300)$. To calculate m_h^* and m_e^* you determine D_v and D_c from a band structure calculation and then calculate the effect mass that would be needed to produce the same density of states from a dispersion relation consisting of a single isotropic parabola $E = \frac{\hbar^2 k^2}{2m^*}$.

$$D_v = \frac{(2m_h^*)^{3/2}}{2\pi^2\hbar^3} \qquad D_c = \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3}$$

In the Boltzmann approximation, the concentration of holes in the valence band p and electrons in the conduction band n are given by,

$$p = \frac{2D_v}{\sqrt{\pi}}(k_B T)^{3/2}\exp\left(\frac{E_v - \mu}{k_B T}\right), \qquad n = \frac{2D_c}{\sqrt{\pi}}(k_B T)^{3/2}\exp\left(\frac{\mu - E_c}{k_B T}\right).$$



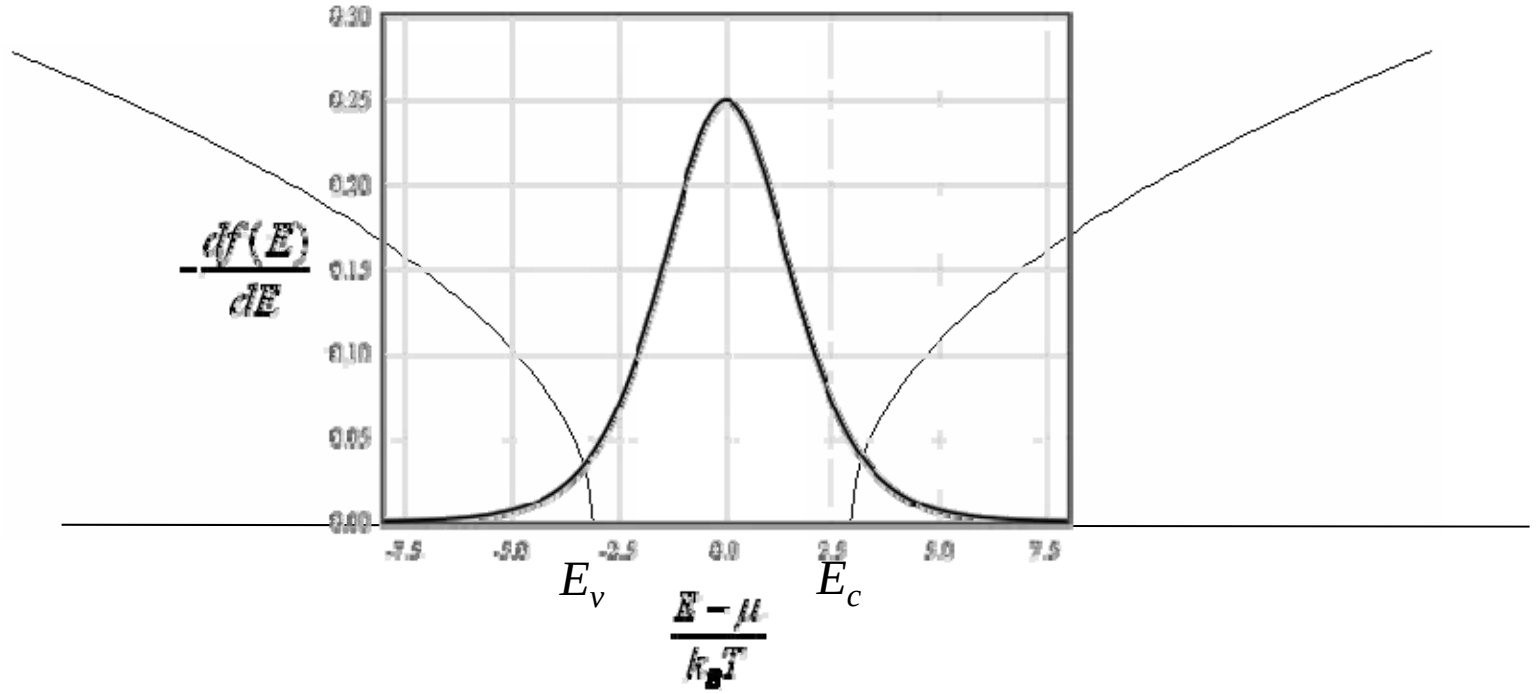
$N_c(300\ \text{K}) =$	2.78E19	1/cm³
$N_v(300\ \text{K}) =$	9.84E18	1/cm³
$E_g =$	1.166-4.73E-4*T*T/(T+636)	eV
$T_1 =$	50	K

Semiconductor

Si | Ge | GaAs | GaP | InAs | InP | InSb

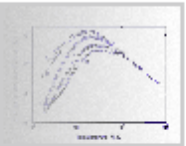
http://lamp.tu-graz.ac.at/~hadley/ss1/semiconductors/intrinsic.php

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:

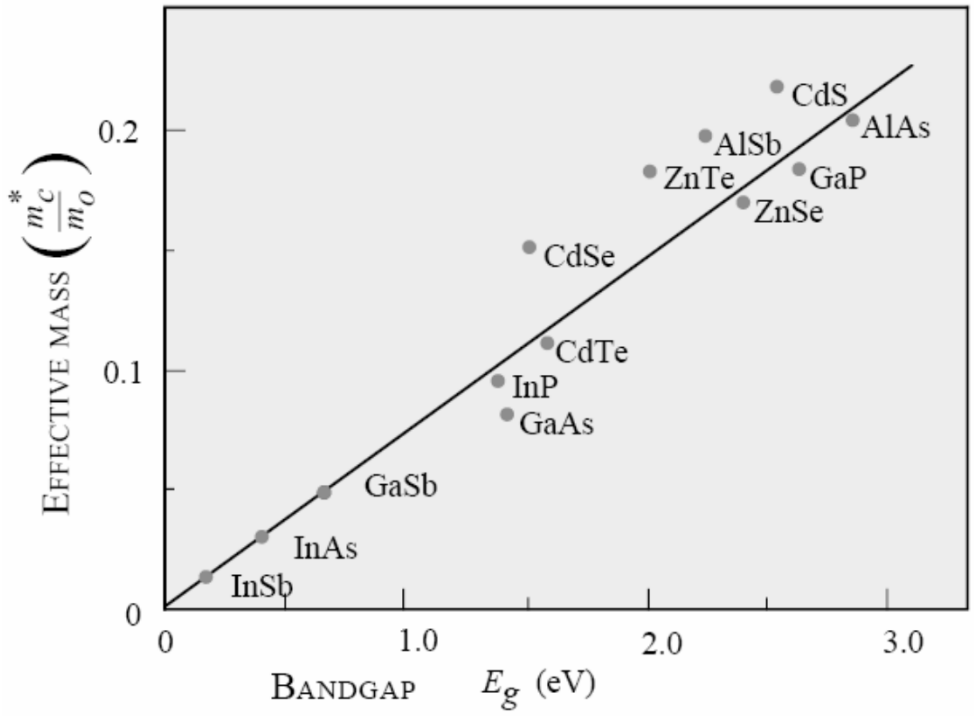
Heavy $m_h = 0.49m_o$

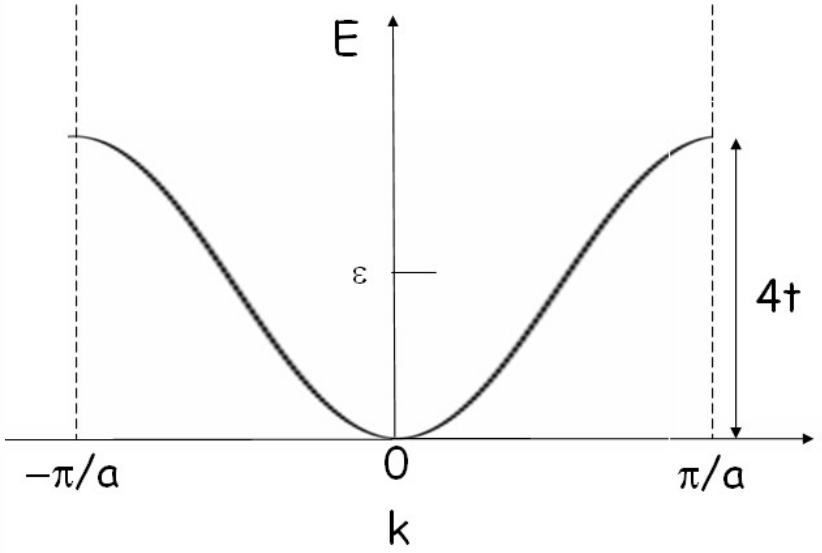
Light $m_{lp} = 0.16m_o$

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.

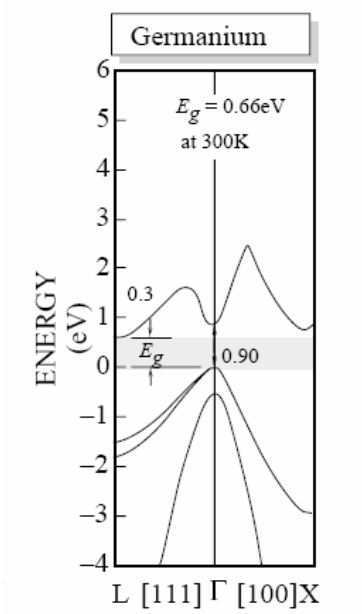
Knowing the effective mass, the scattering time can be calculated from the measured conductivity.

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

Direct and indirect band gaps

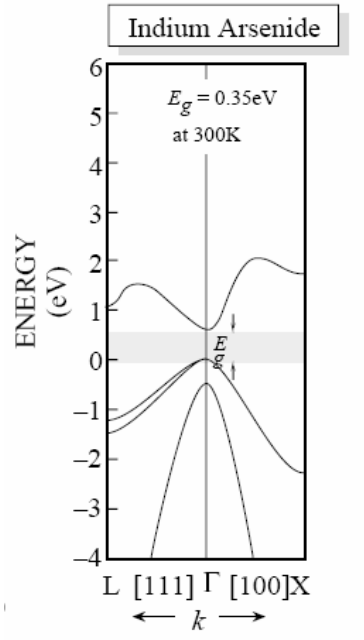
indirect bandgap
$\Delta k \neq 0$

phonons are emitted



direct bandgap:
$\Delta k = 0$

photons can be emitted

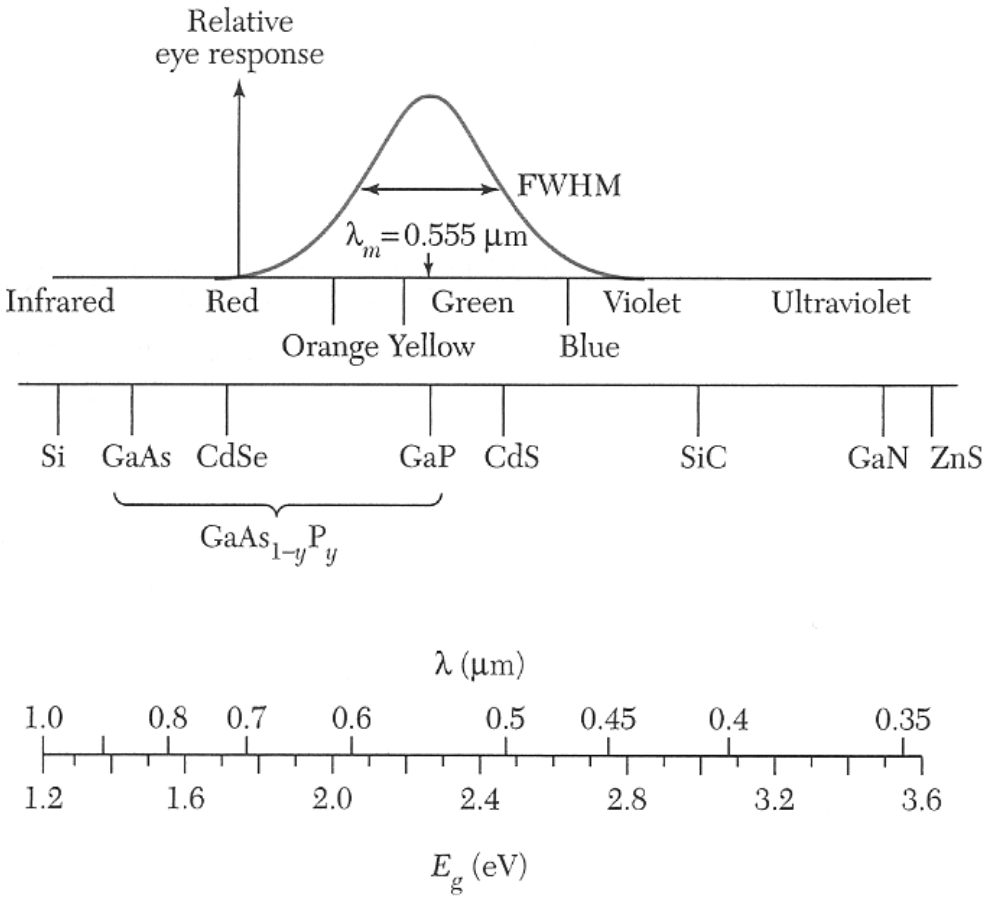


Momentum must be conserved when photons are absorbed or emitted.

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

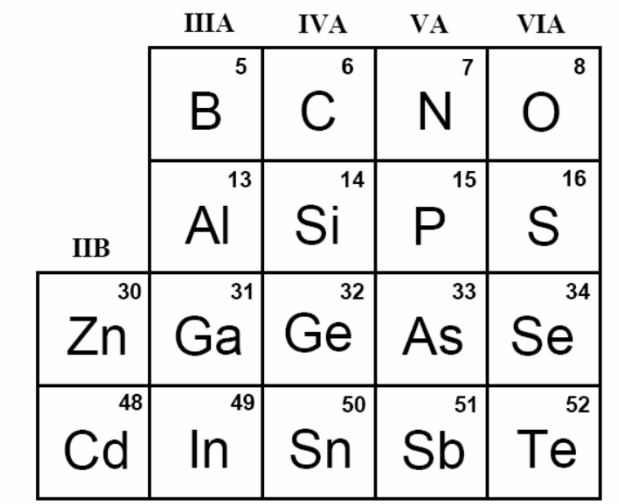


Extrinsic semiconductors

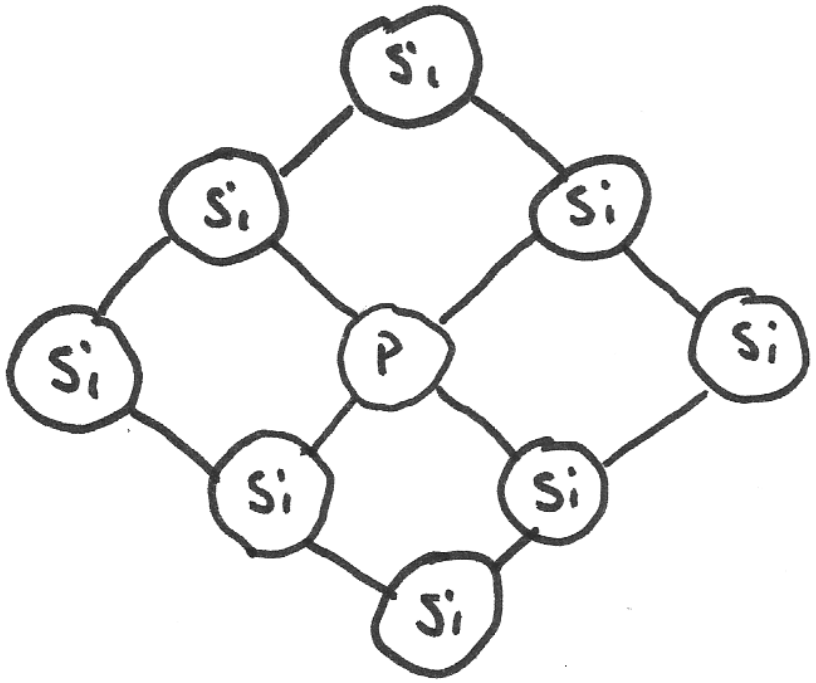
The introduction of impurity atoms that can and electrons or holes is called doping.

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

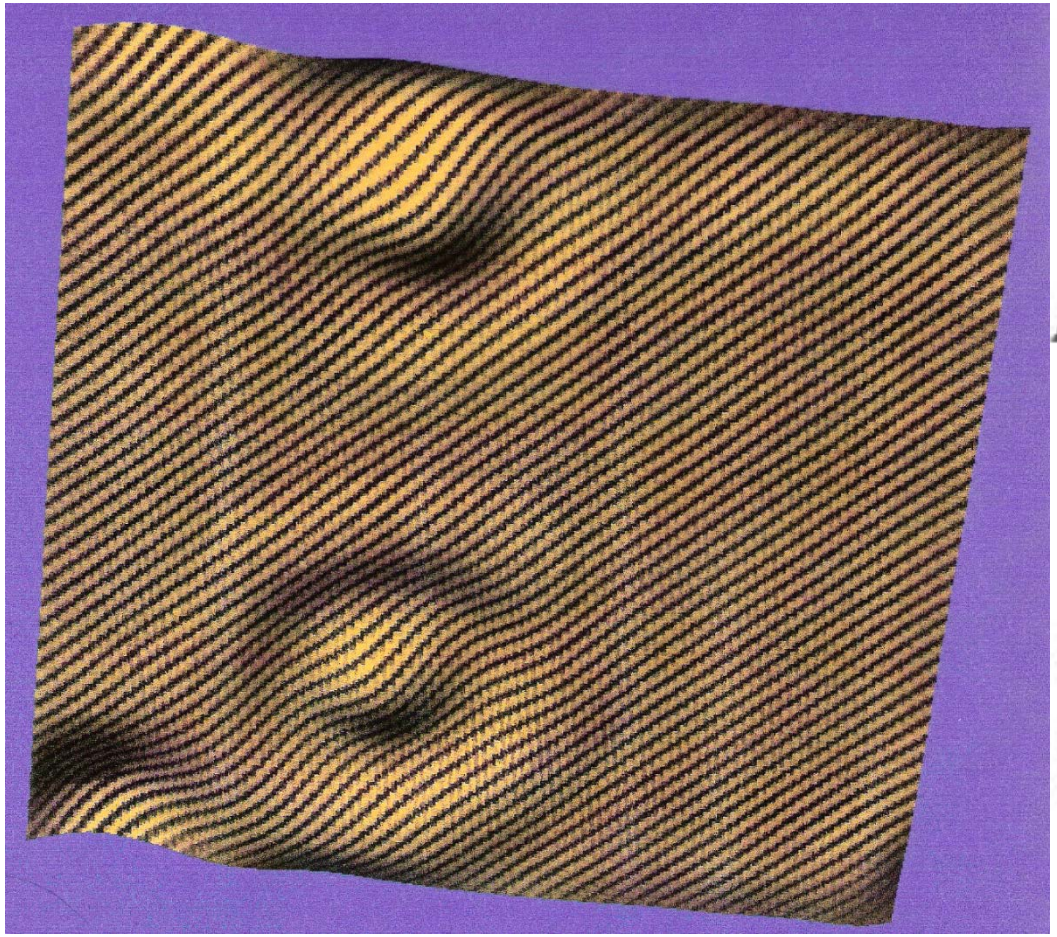
$$E_n = -\frac{me^4}{8\varepsilon_0^2 h^2 n^2}$$

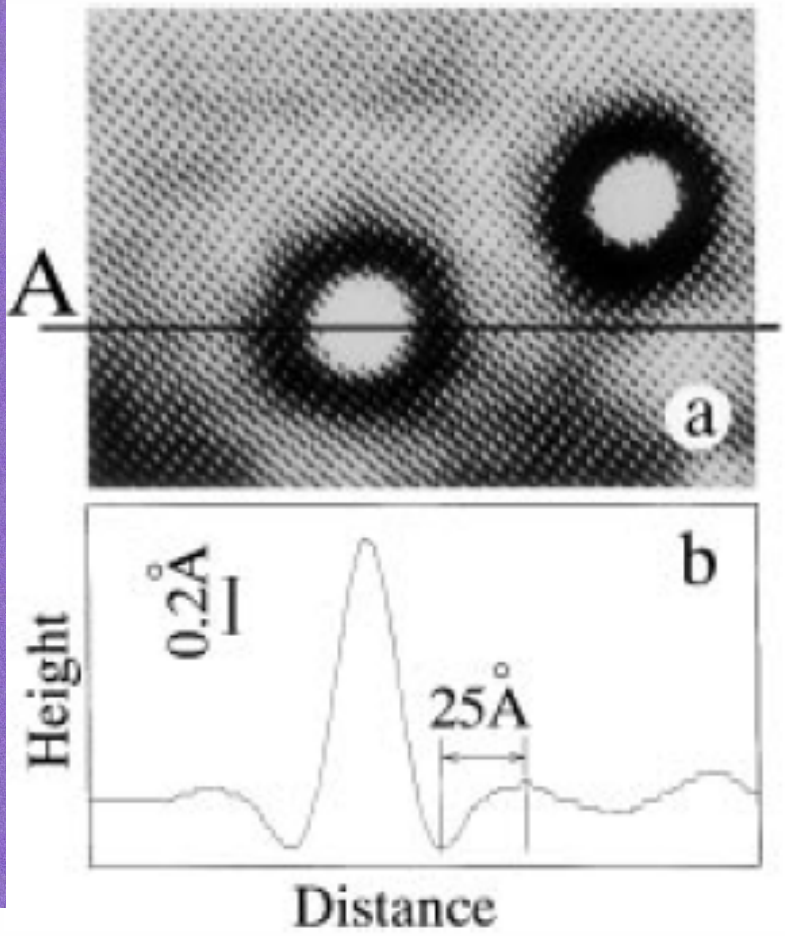
Ionization energy is smaller by a factor: $\frac{m^*}{m}\left(\frac{\varepsilon_0}{\varepsilon_r \varepsilon_0}\right)^2$

Ionization energy ~ 25 meV

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

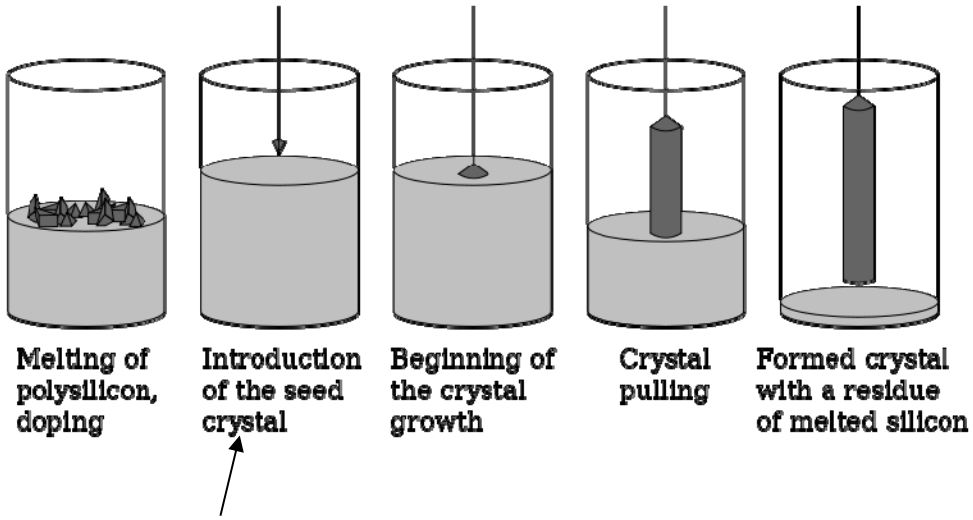
M. C. M. M. van der Wielen, A. J. A. van Roij, and H. van Kempen
Research Institute for Materials, University of Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands
(Received 25 July 1995)





Crystal growth

Czochralski Process



add dopants to the melt

images from wikipedia

Crystal growth

Float zone Process

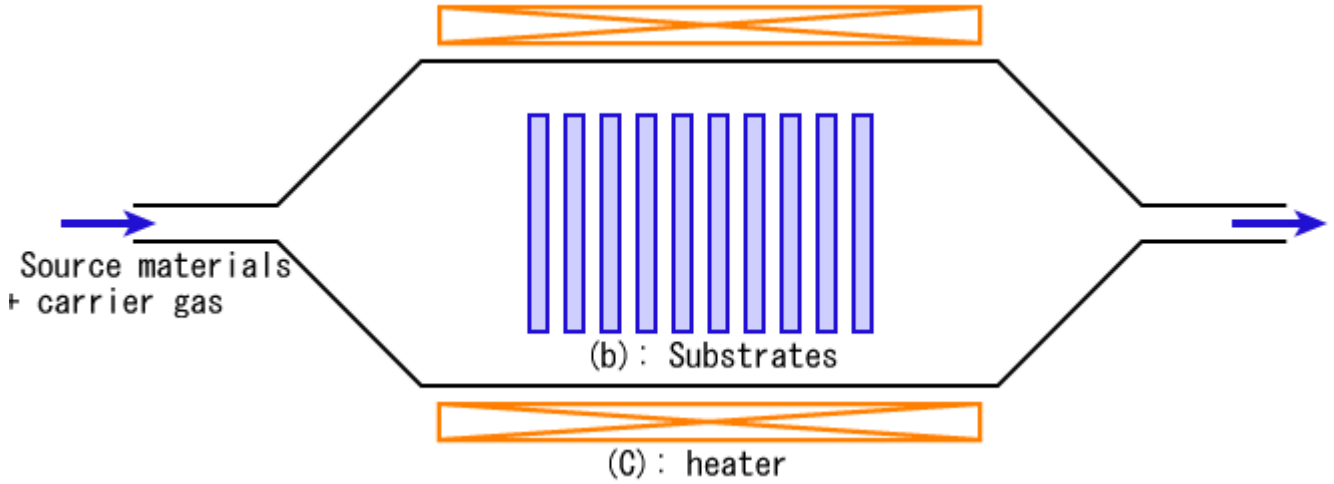
Neutron transmutation

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

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

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.

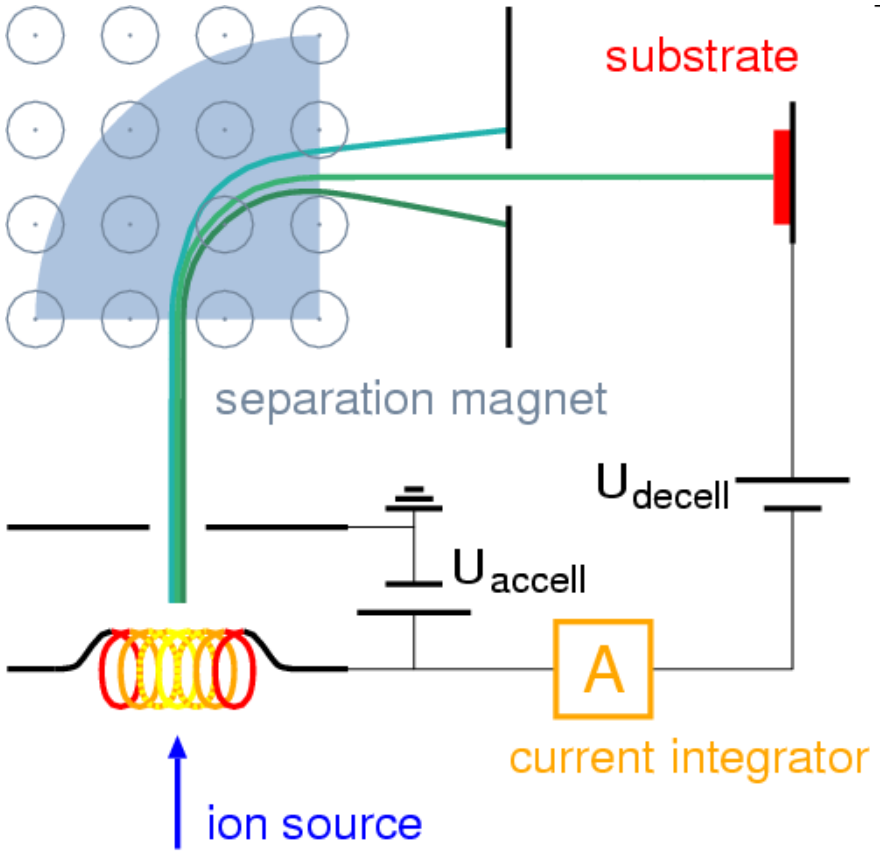
image from wikipedia

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

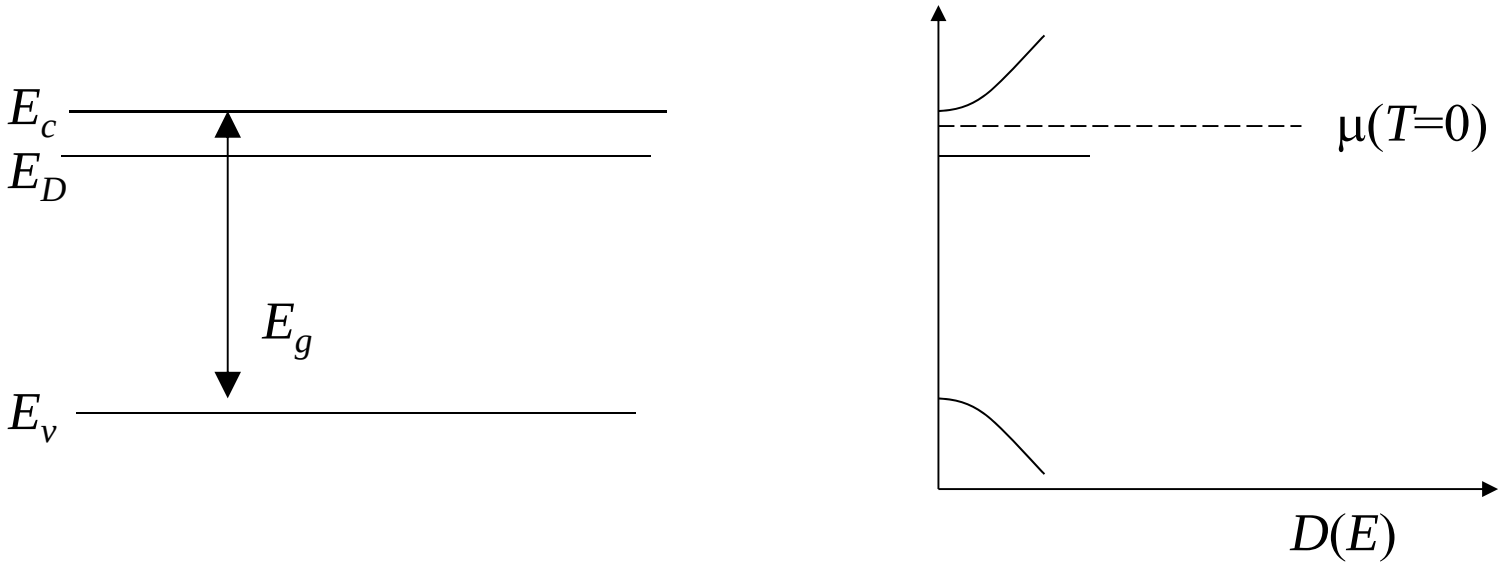


Implant at 7º to avoid channeling

Donors

Five valence electrons: P, As

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



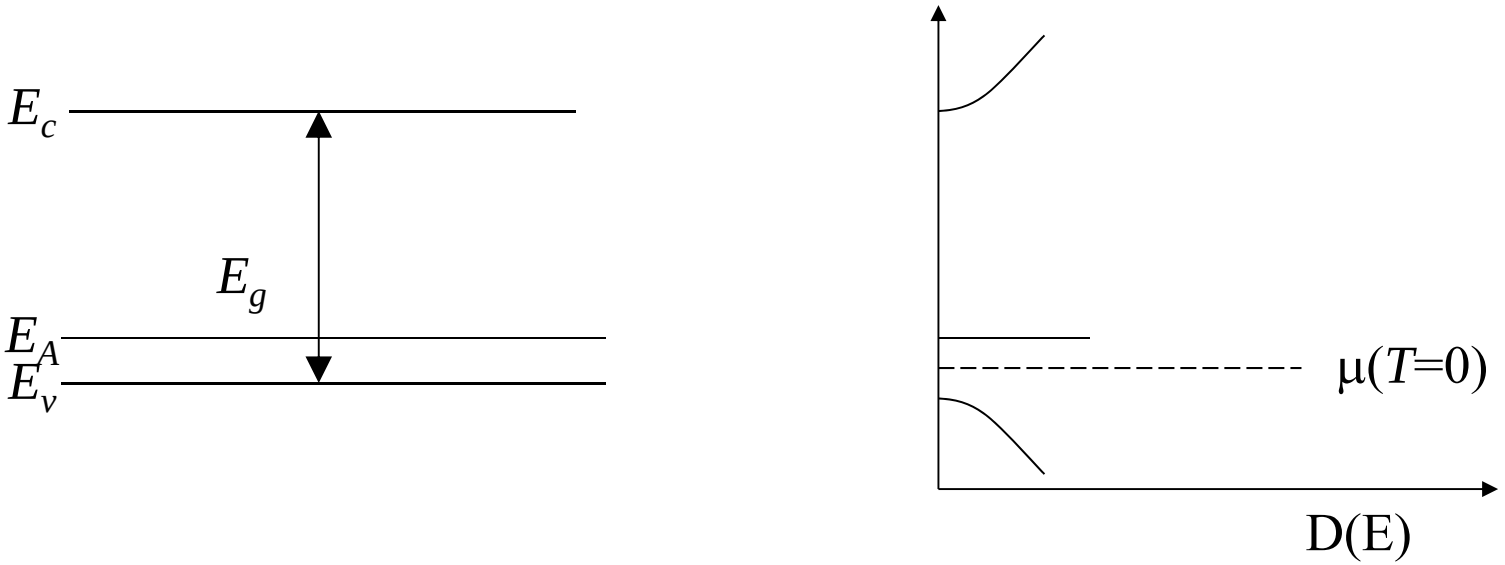
n-type: $n \sim N_D$ Many more electrons in the conduction band than holes in the valence band.

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

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

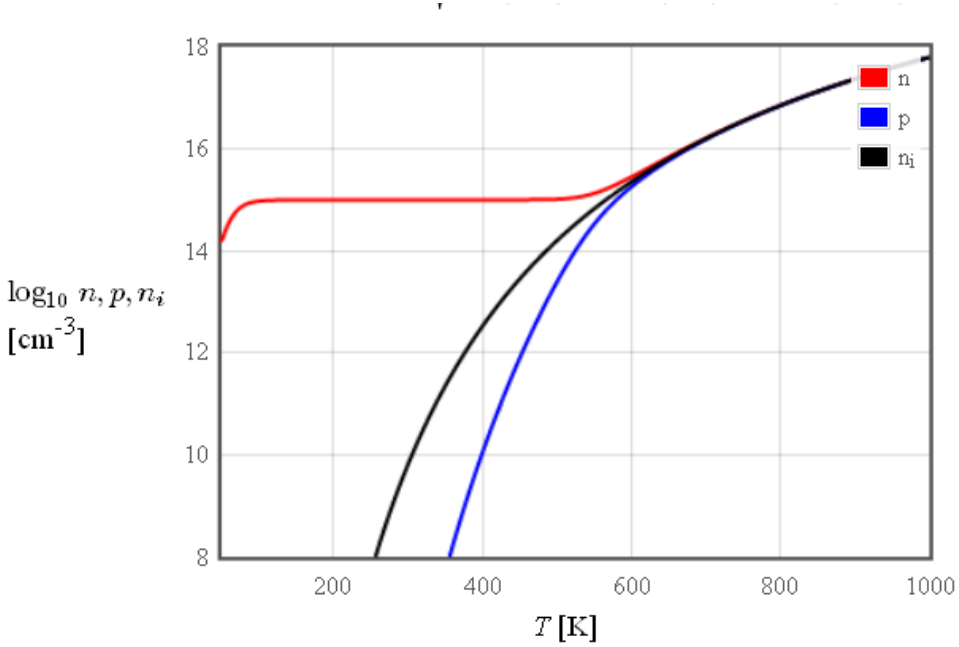
n-type

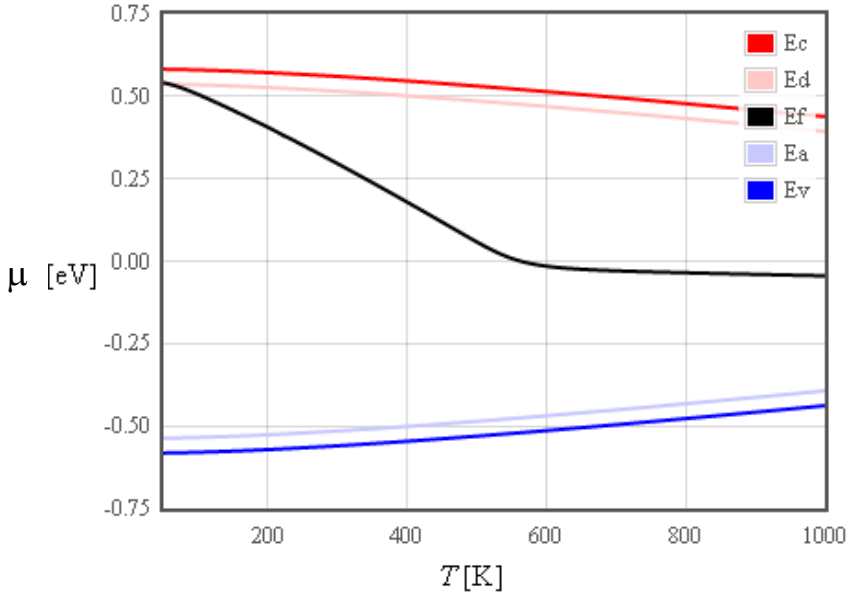
n-type $N_D > N_A$, $p \sim 0$

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

$$\mu = E_c - k_B T \ln\left(\frac{N_c}{N_D}\right)$$

For n-type, $n \sim$ density of donors,
$p = n_i^2 / n$





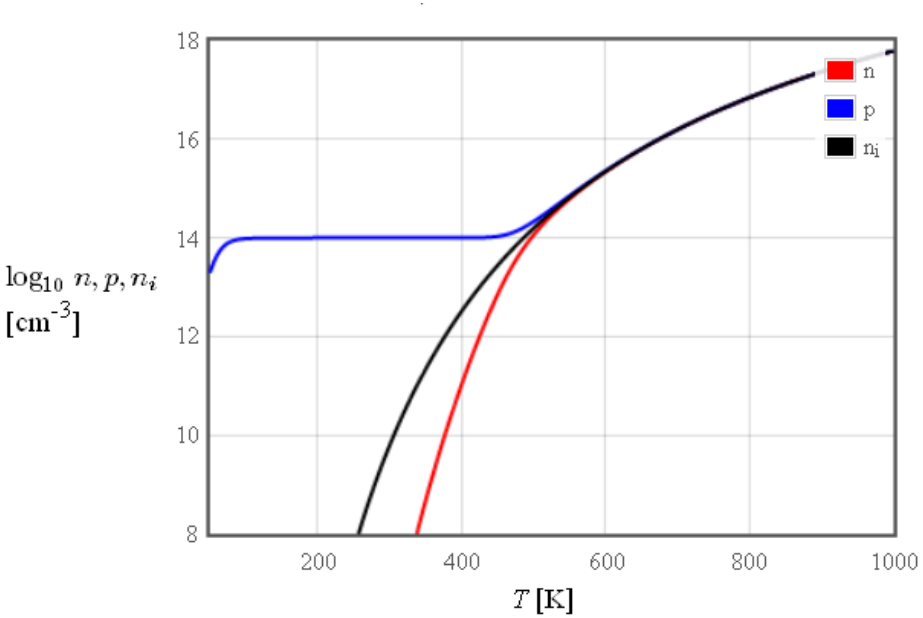
p-type

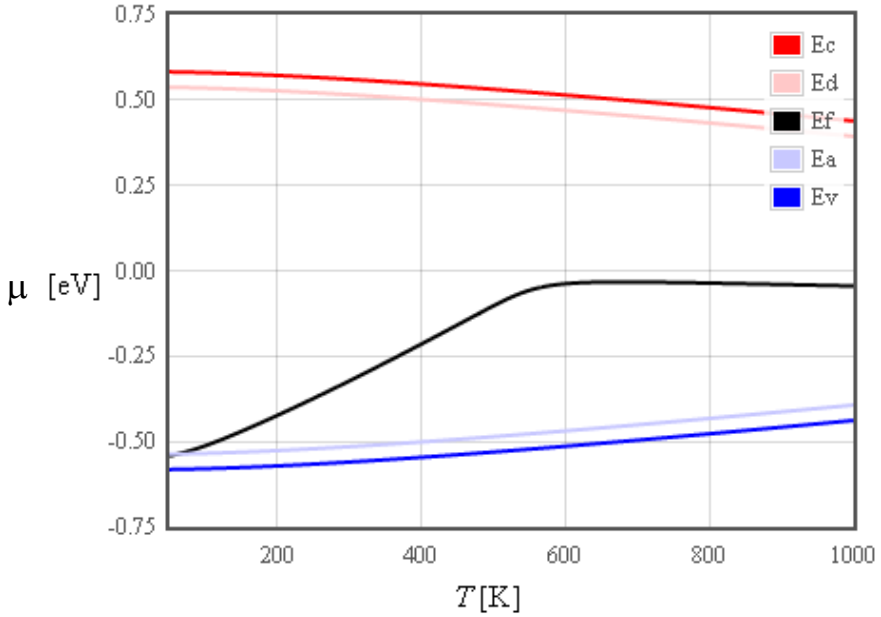
p-type $N_A > N_D$, $n \sim 0$

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

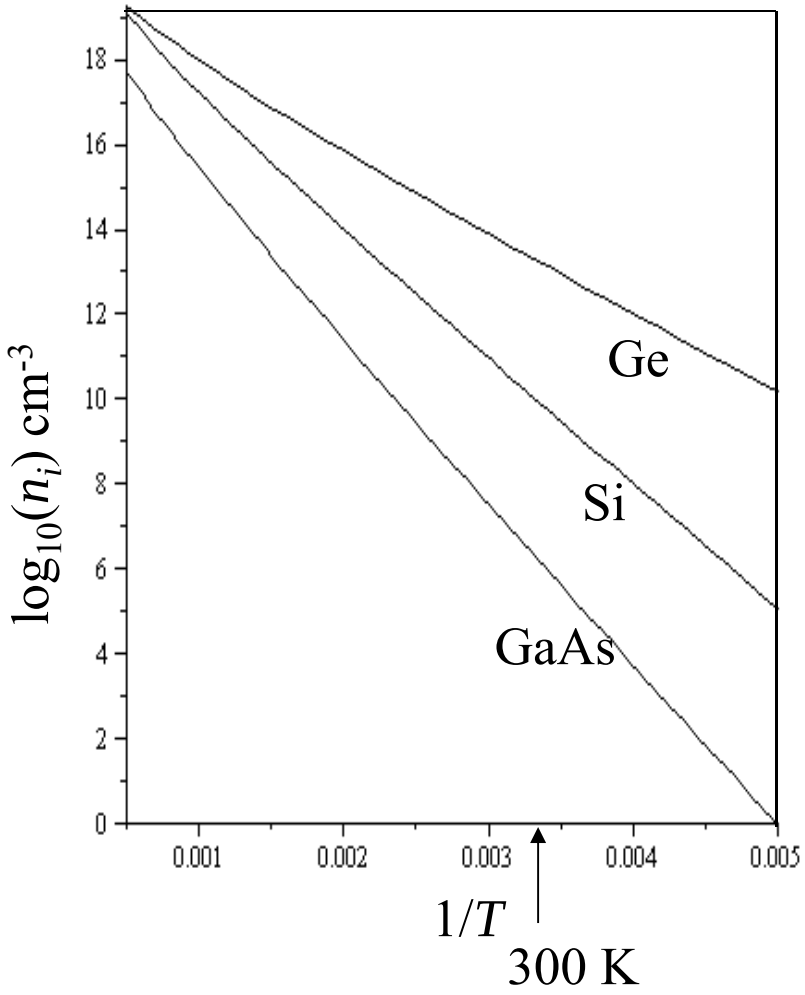
$$\mu = E_v + k_B T \ln\left(\frac{N_v}{N_A}\right)$$

For p-type, $p \sim$ density of acceptors, $n = n_i^2/p$



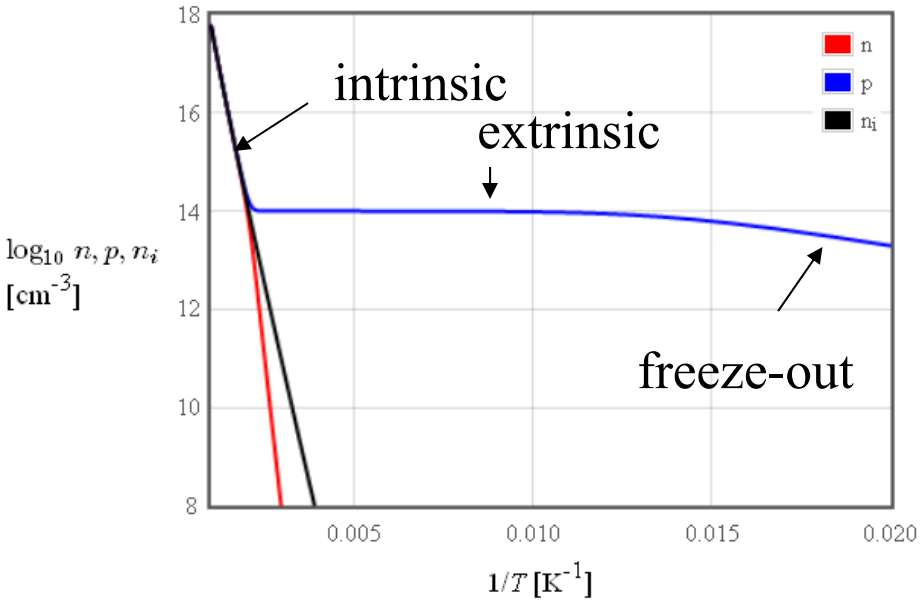


Intrinsic semiconductors



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

Extrinsic semiconductors



At high temperatures, extrinsic semiconductors have the same temperature dependence as intrincic semiconductors.

Energy spectra of donors in silicon

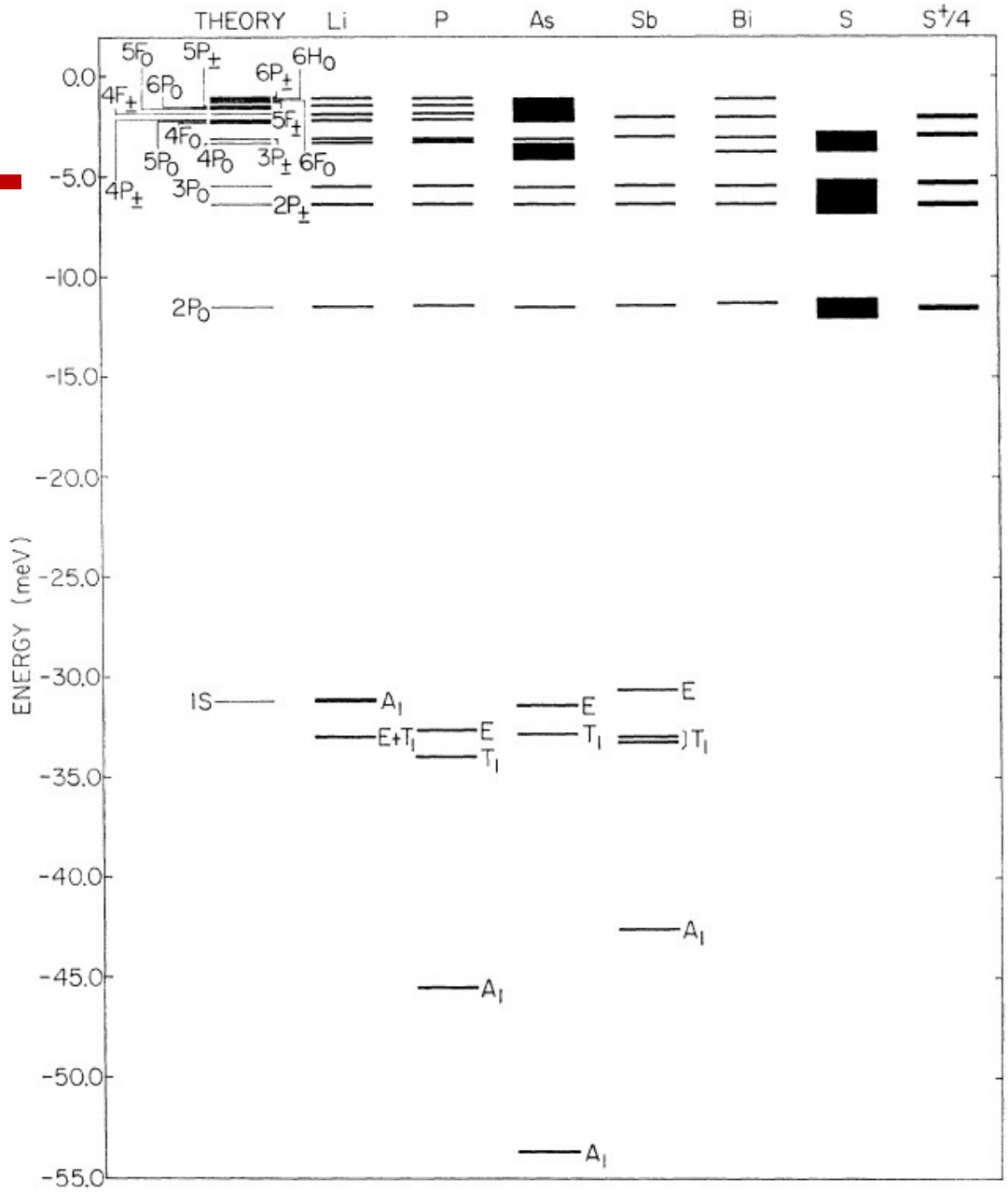


FIG. 6. Energy levels of donors in silicon. The theoretical spectrum is based on the dielectric constant appropriate for liquid-helium temperature, $K=11.40$. The experimental spectra have all been arranged so that the $2P_{\pm}$ level in each is lined up with the theoretical $2P_{\pm}$ level. The width of each level represents its experimental uncertainty, with the exception of Bi, for which no experimental error was quoted.

Ionized donors and acceptors

For $E_v + 3k_BT < \mu < E_c - 3k_BT$ Boltzmann approximation

$$N_D^+ = \frac{N_D}{1 + 2\exp\left(\frac{\mu - E_D}{k_BT}\right)}$$

$$N_A^- = \frac{N_A}{1 + 4\exp\left(\frac{E_A - \mu}{k_BT}\right)}$$

4 for materials with light holes and heavy holes (Si)
2 otherwise

N_D = donor density cm^{-3} N_D^+ = ionized donor density cm^{-3}

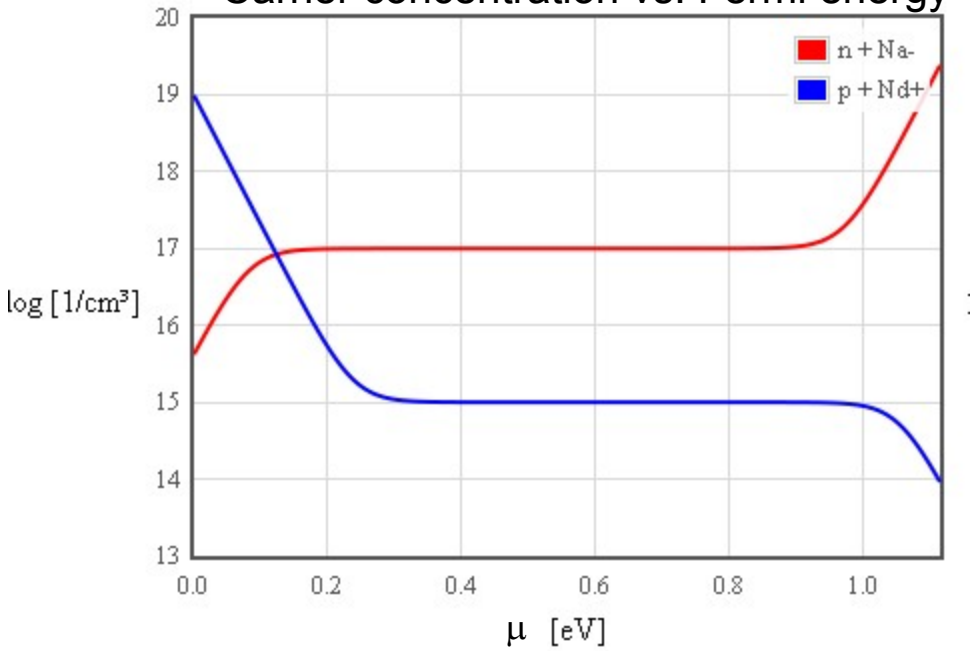
N_A = donor density cm^{-3} N_A^- = ionized donor density cm^{-3}

Mostly, $N_D^+ = N_D$ and $N_A^- = N_A$

Charge neutrality

$$n + N_A^- = p + N_D^+$$

Carrier concentration vs. Fermi energy

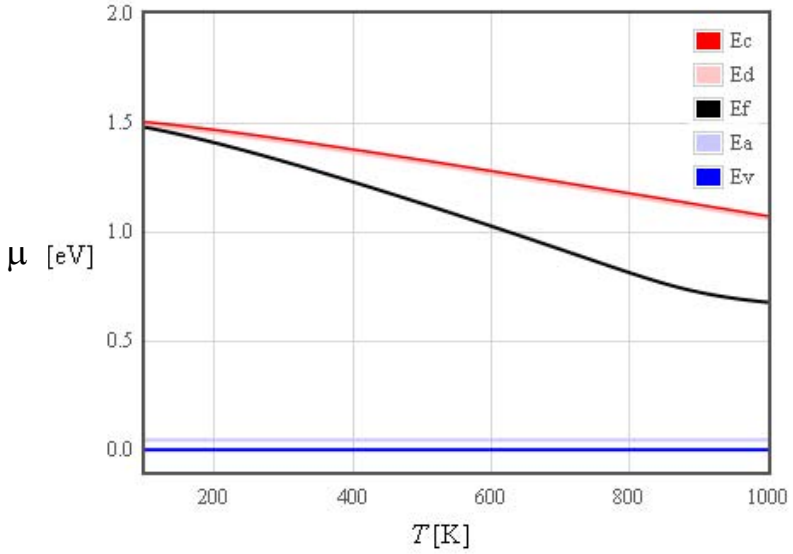



```
for ($i=0; $i<500; $i++) {
  $Ef = $i*$Eg/500;
  $n=$Nc*pow($T/300,1.5)*exp(1.6022E-19*($Ef-$Eg)/(1.38E-23*$T));
  $p=$Nv*pow($T/300,1.5)*exp(1.6022E-19*(-$Ef)/(1.38E-23*$T));
  $Namin = $Na/(1+4*exp(1.6022E-19*($Ea-$Ef)/(1.38E-23*$T)));
  $Ndplus = $Nd/(1+2*exp(1.6022E-19*($Ef-$Ed)/(1.38E-23*$T)));
}
```

E_f	n	p	N_d^+	N_a^-	$\log(n+N_a^-)$	$\log(p+N_d^+)$
0	4.16629283405	9.84E+18	1E+15	4.19743393218E+15	15.622983869	18.9930392318
0.00224	4.54358211887	9.0229075682E+18	1E+15	4.56020949614E+15	15.6589847946	18.9553946382
0.00448	4.95503779816	8.27366473417E+18	1E+15	4.95271809535E+15	15.694843609	18.9177504064
0.00672	5.40375389699	7.58663741327E+18	1E+15	5.37710747619E+15	15.7305487171	18.8801065693
0.00896	5.89210462781	6.95665036315E+18	1E+15	5.83569092025E+15	15.7660876057	18.8424631625

Fermi energy vs. temperature

Fermi energy of an extrinsic semiconductor is plotted as a function of temperature. At each temperature the Fermi energy was calculated by requiring that charge neutrality be satisfied.



N_c(300 K) =	4.45E17	1/cm³
N_v(300 K) =	7.72E18	1/cm³
E_g =	1.519-5.41E-4*T*T/(T+204)	eV
N_d =	1E16	1/cm³
E_c - E_d =	0.012	eV
N_a =	1E12	1/cm³
E_a - E_v =	0.045	eV
T_1 =	100	K
T_2 =	1000	K

Replot

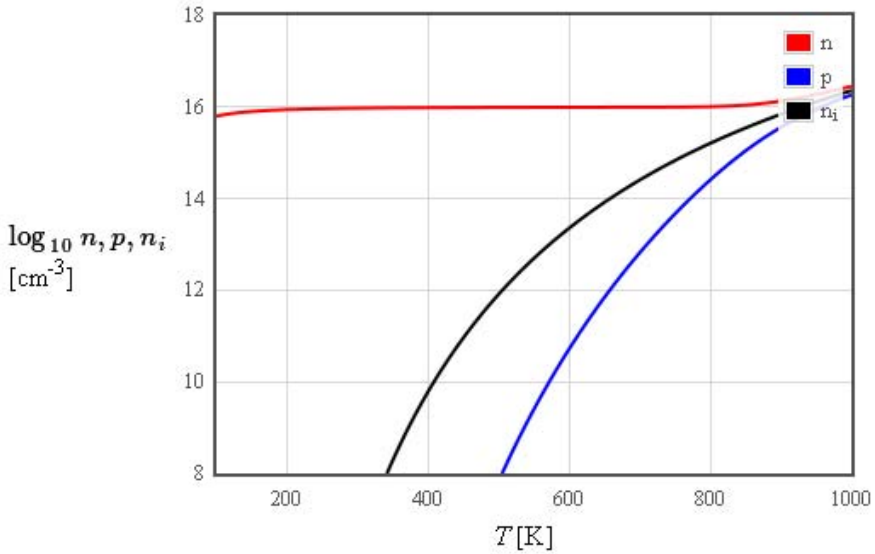
Semiconductor: Si | Ge | GaAs

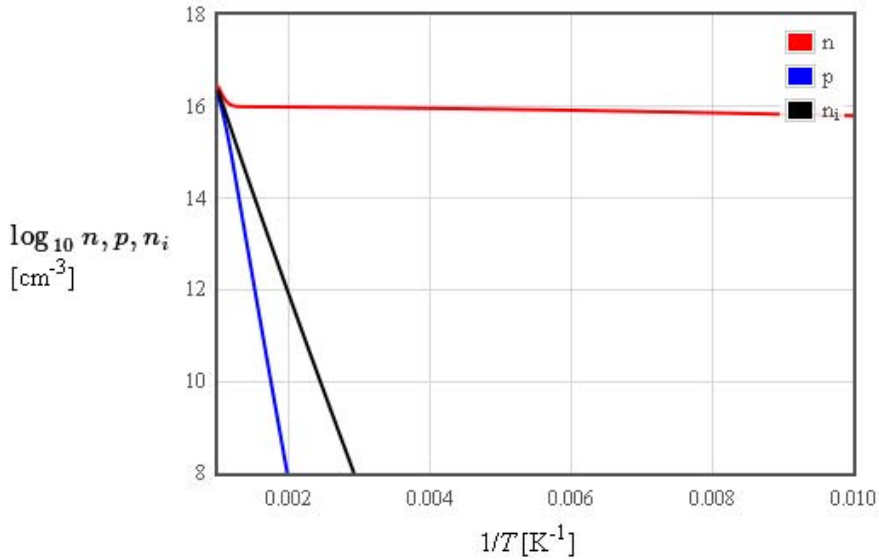
Donor: P in Si | P in Ge | Si in GaAs

Acceptor: B in Si | B in Ge | Si in GaAs

Once the Fermi energy is known, the carrier densities n and p can be calculated from the formulas, $n = N_c \left(\frac{T}{300}\right)^{3/2} \exp\left(\frac{E_F - E_c}{k_B T}\right)$ and $p = N_v \left(\frac{T}{300}\right)^{3/2} \exp\left(\frac{E_v - E_F}{k_B T}\right)$.

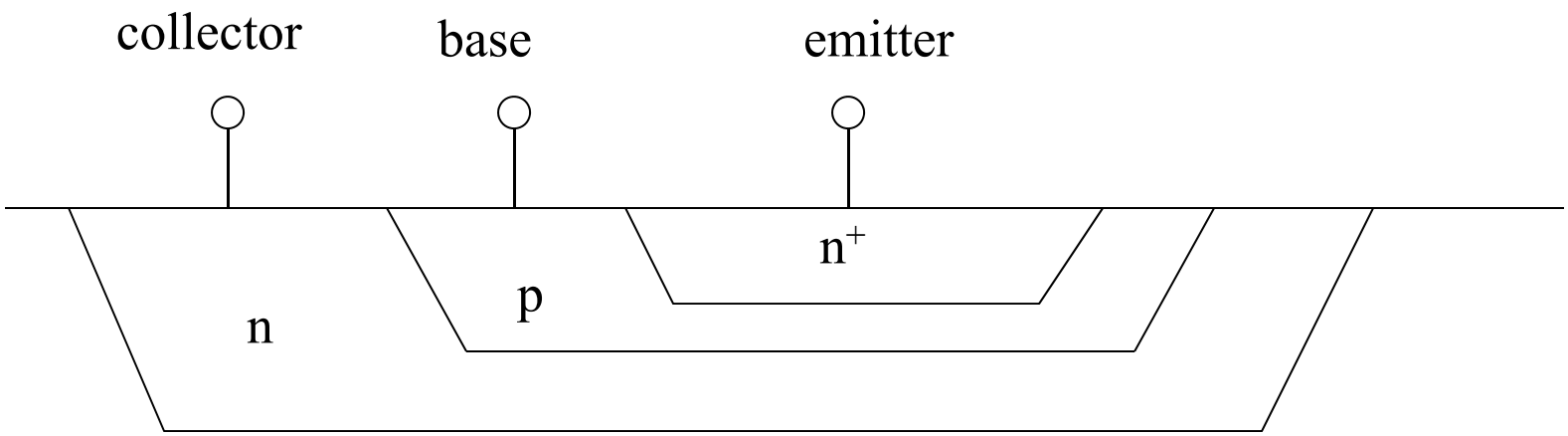
The intrinsic carrier density is $n_i = \sqrt{N_c \left(\frac{T}{300}\right)^{3/2} N_v \left(\frac{T}{300}\right)^{3/2}} \exp\left(\frac{-E_g}{2k_B T}\right)$.





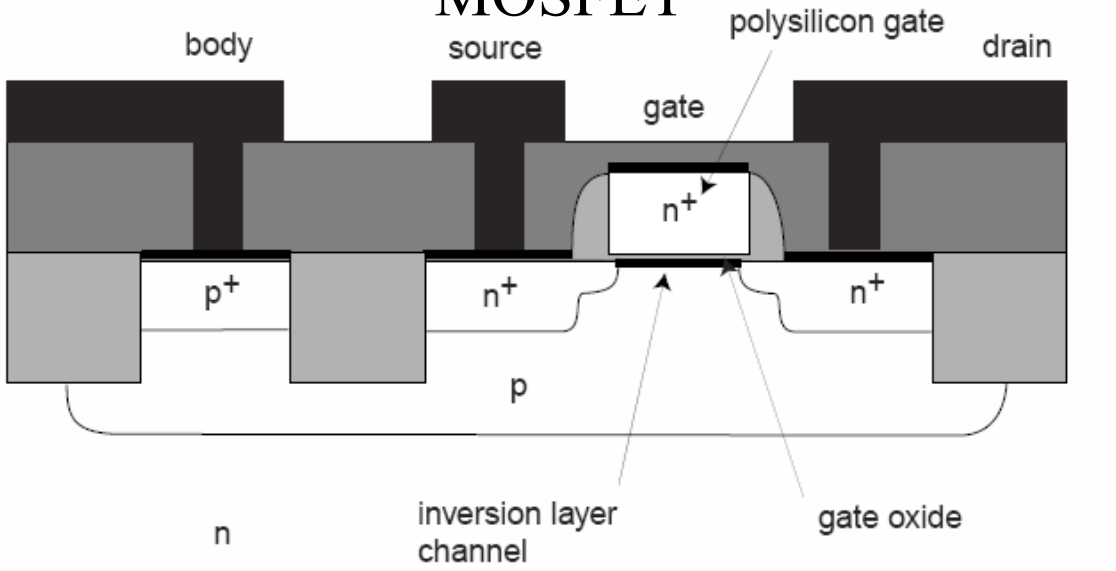
Why dope with donors AND acceptors?

Bipolar transistor

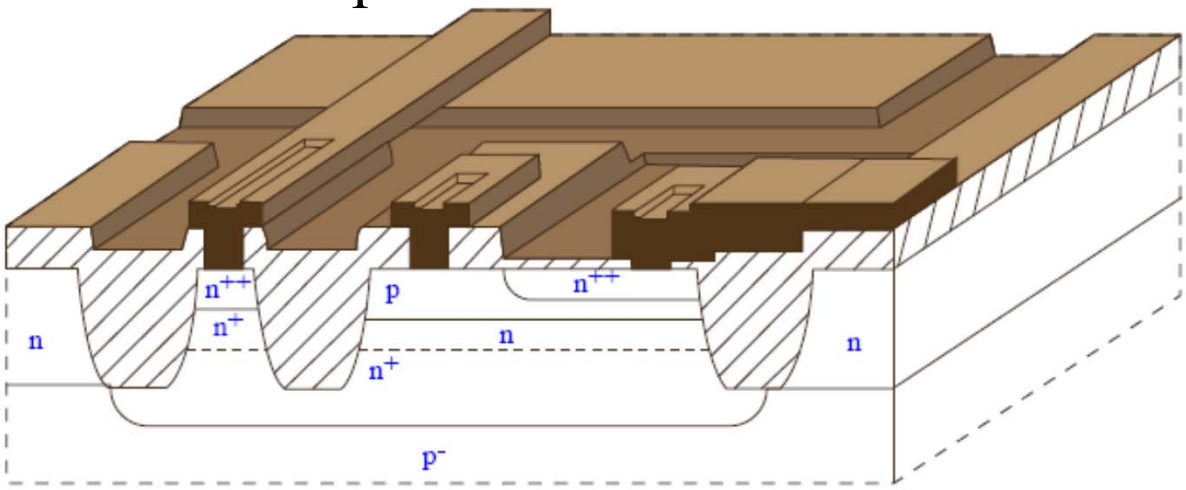


lightly doped p substrate

MOSFET



Bipolar Junction Transistor



Oxide isolated integrated BJT - a modern process