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

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,

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

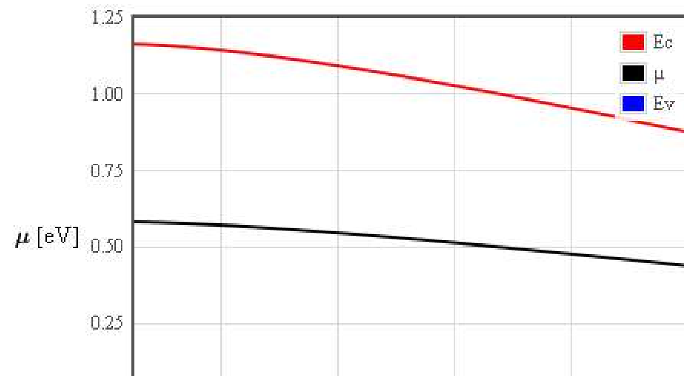
$$m_e^*=\frac{\pi\hbar^2}{300k_B}\left(\sqrt{2}N_c(300)\right)^{2/3}$$

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 K) =	2.78E19	1/cm³
N_v(300 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

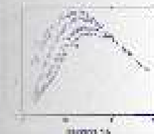
Si Ge GaAs

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

www.ioffe.rssi.ru/SVA/NSM/Semicond/index.html

d Getting Started Latest Headlines English to German

Semiconductors on NSM



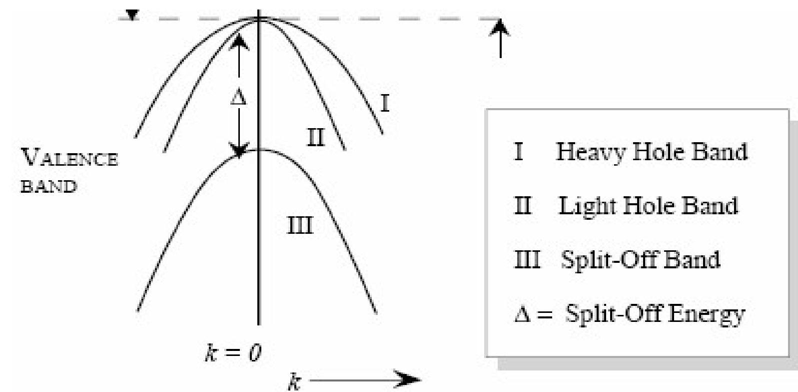
Semiconductors | n, k database | InGaAsP | Equivalents

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.

$m_l = 0.98 m_o$

$m_t = 0.19 m_o$

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

There are 6 equivalent valleys in the conduction band.

$m_{cc} = 0.26 m_o$

Holes:

Heavy $m_h = 0.49 m_o$

Light $m_{lp} = 0.16 m_o$

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

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

Intrinsic semiconductors with a split-off band

Many common semiconductors such as Si, Ge, and GaAs have a split-off band just below the valence band. The states in the split-off band change the temperature dependence of the concentration of holes. In the Boltzmann approximation, the density of states of a semiconductor with a split-off band just below the valence band is,

$$D(E)=\begin{cases}\frac{(2m_h^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{E_v-E}+\frac{(2m_{so}^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{E_{so}-E}, & \text{for } E<E_{so}\\ \frac{(2m_h^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{E_v-E}, & \text{for } E_{so}<E<E_v\\ 0, & \text{for } E_v<E<E_c\\ \frac{(2m_e^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{E-E_c}, & \text{for } E_c<E\end{cases}$$

Here m_e^*, m_h^*, and m_{so}^* are the 'density of states effective masses'. Often 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,

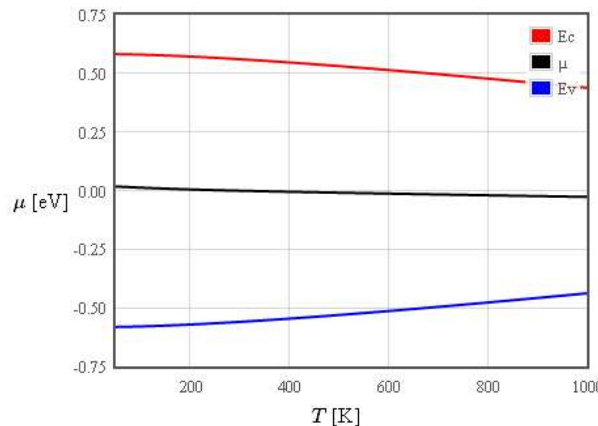
$$m_{so}^*=\frac{\pi\hbar^2}{300k_B}\left(\sqrt{2}\,N_{so}(300)\right)^{2/3}$$

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

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

The density of states can therefore also be written as,

$$D(E)=\begin{cases}\frac{2N_v(300)}{\sqrt{\pi}}\left(\frac{1}{300k_B}\right)^{3/2}\sqrt{E_v-E}+\frac{2N_{so}(300)}{\sqrt{\pi}}\left(\frac{1}{300k_B}\right)^{3/2}\sqrt{E_{so}-E}, & \text{for } E<E_{so}\\ \frac{2N_v(300)}{\sqrt{\pi}}\left(\frac{1}{300k_B}\right)^{3/2}\sqrt{E_v-E}, & \text{for } E_{so}<E<E_v\end{cases}$$



N_c(300 K) =	2.78E19	1/cm³
N_v(300 K) =	9.84E18	1/cm³
N_{so}(300 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

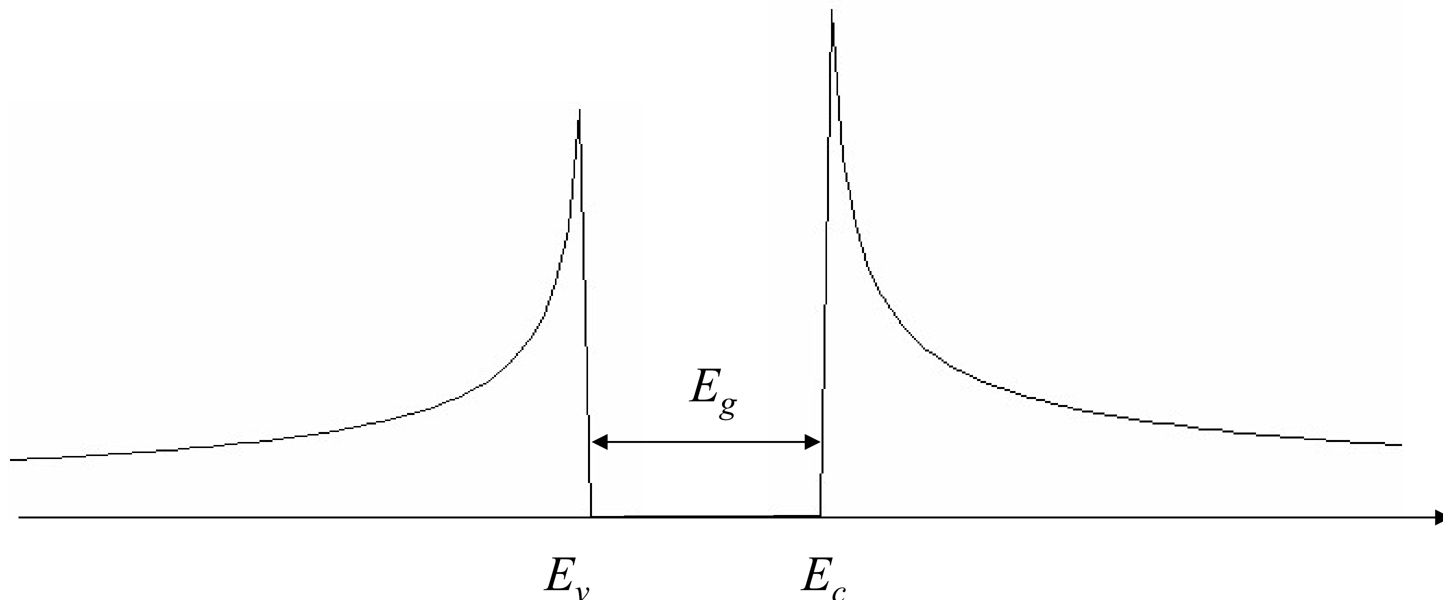
In an intrinsic semiconductor, tl ... ndgap, E_g. For most semiconductors the bandgap is

$n = p =$ ...).

Semiconductors and insulators - 1d

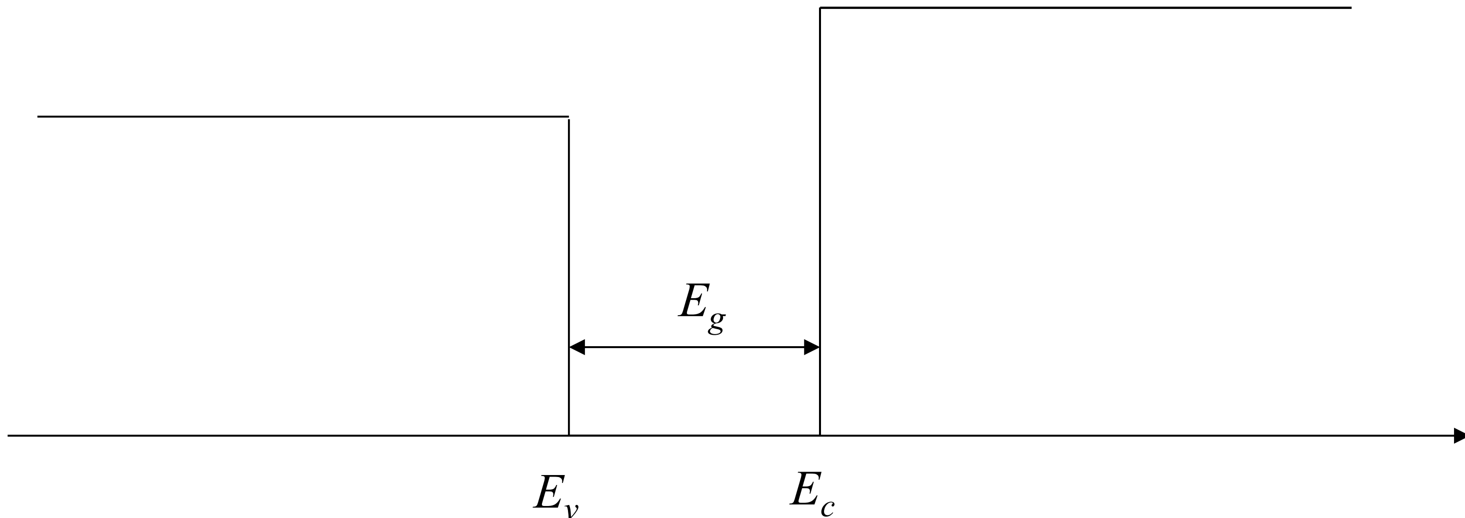
$$E = \frac{\hbar^2(\vec{k}-\vec{k}_0)^2}{2m^*}$$

$$D(E) = \begin{cases} \sqrt{\dfrac{2m_h^*}{\hbar^2\pi^2(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \sqrt{\dfrac{2m_e^*}{\hbar^2\pi^2(E - E_c)}} & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$



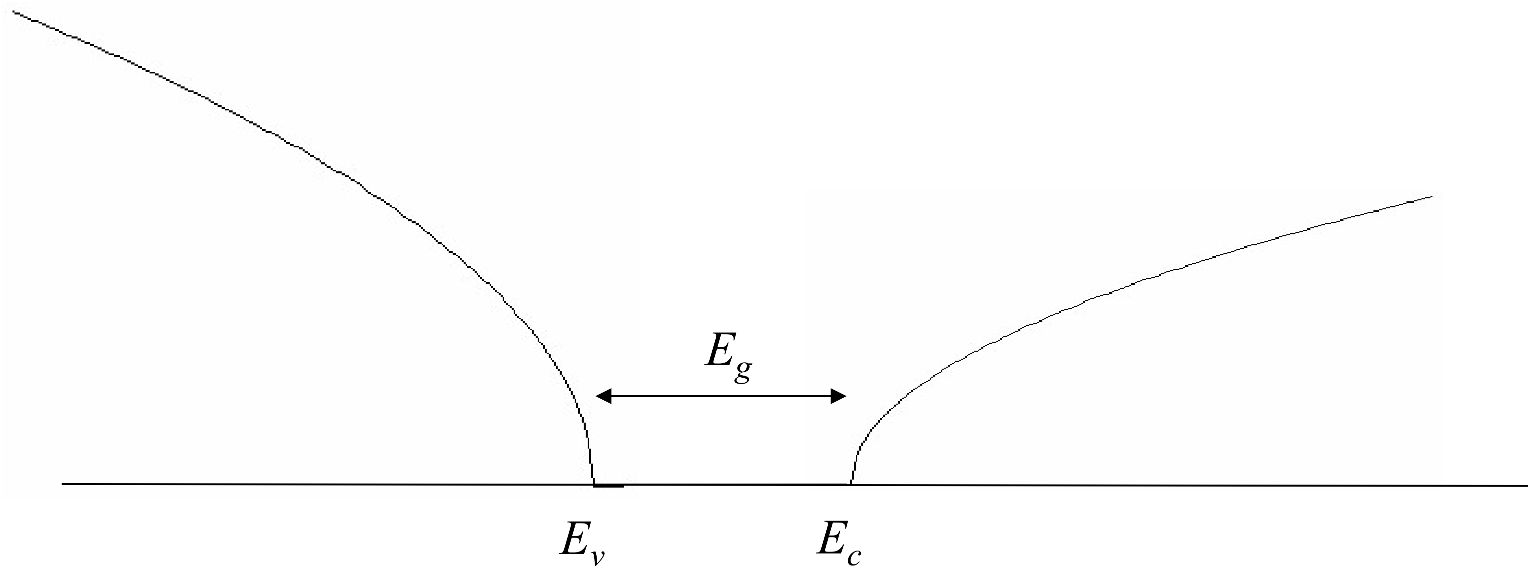
Semiconductors and insulators - 2d

$$D(E) = \begin{cases} \dfrac{m_h^*}{\hbar^2 \pi} & E < E_v \\ 0 & E_v < E < E_c \\ \dfrac{m_e^*}{\hbar^2 \pi} & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$



Semiconductors and insulators - 3d

$$D(E) = \begin{cases} \dfrac{\left(2m_h^*\right)^{\frac{3}{2}}}{2\pi^2\hbar^3}\sqrt{E_v - E} & E < E_v \\ 0 & E_v < E < E_c \\ \dfrac{\left(2m_e^*\right)^{\frac{3}{2}}}{2\pi^2\hbar^3}\sqrt{E - E_c} & E_c < E \end{cases} \quad \text{J}^{-1}\text{m}^{-3}$$

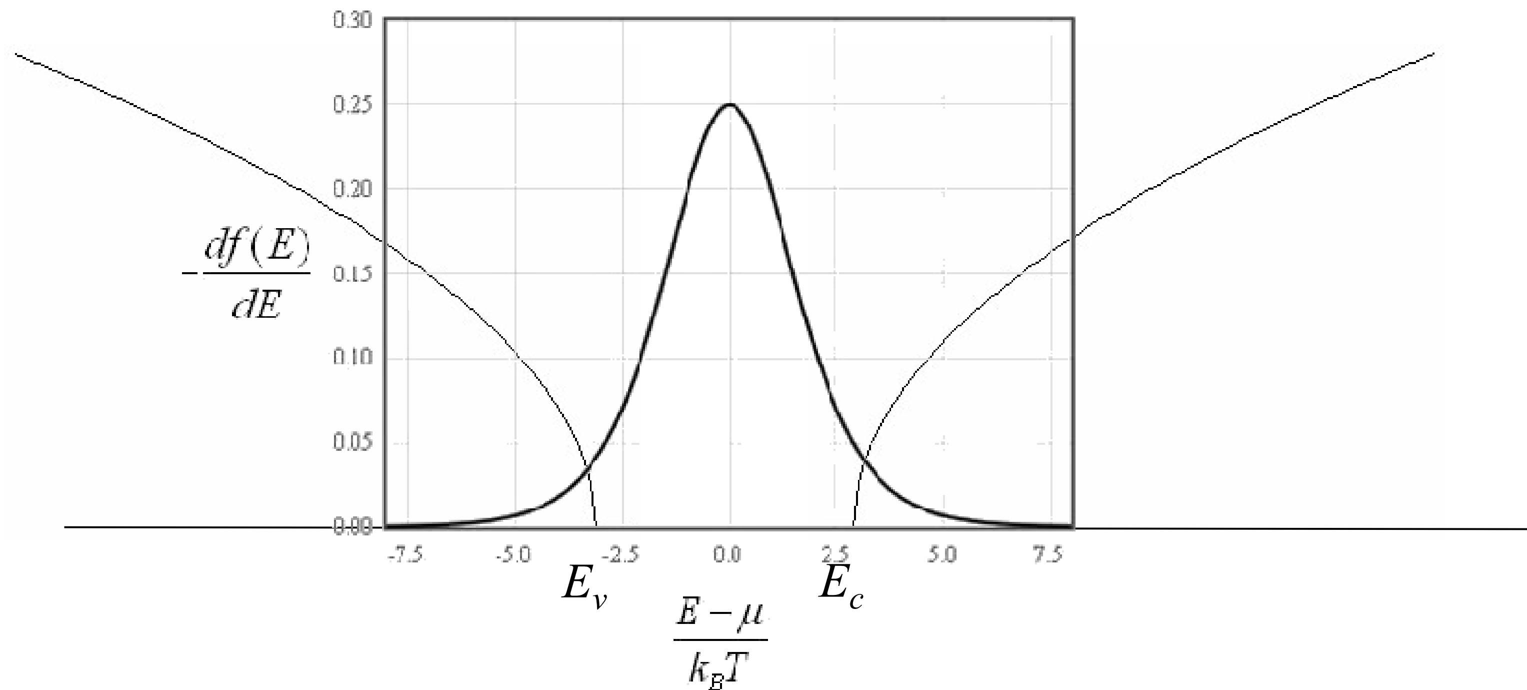


Boltzmann approximation

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.

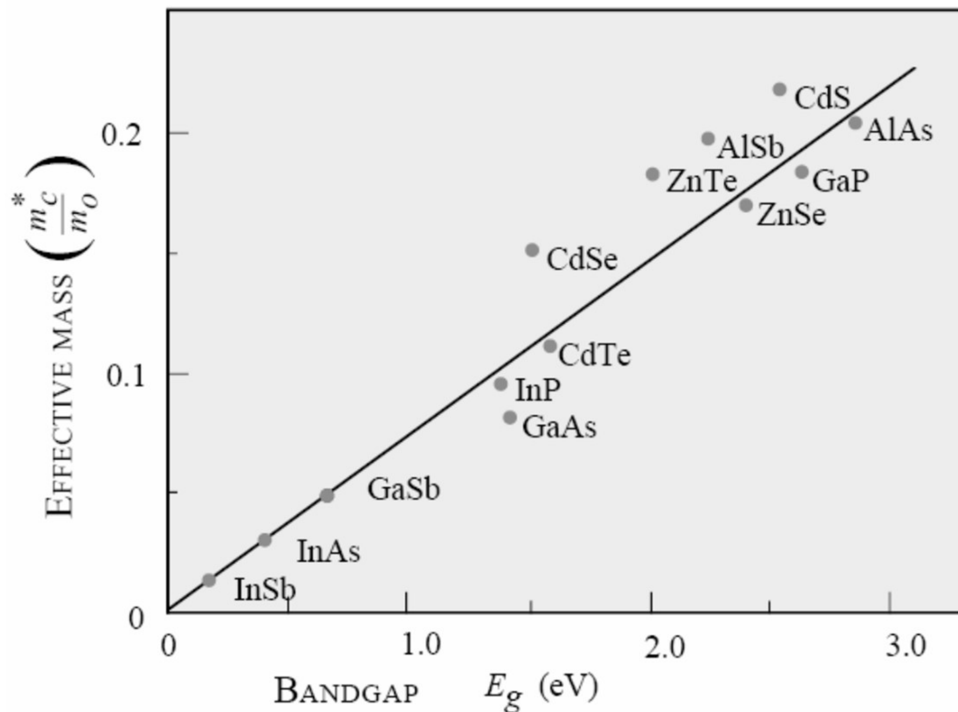
	1-d	2-d	3-d
Density of states	$D(E)=\begin{cases}\frac{1}{\hbar\pi}\sqrt{\frac{2m_h^*}{(E_v-E)}} & E<E_v\\ 0 & E_v<E<E_c\\ \frac{1}{\hbar\pi}\sqrt{\frac{2m_e^*}{(E-E_c)}} & E>E_c\end{cases}$ $\text{J}^{-1}\,\text{m}^{-1}$	$D(E)=\begin{cases}\frac{m_h^*}{\hbar^2\pi}H(E_v-E) & E<E_v\\ 0 & E_v<E<E_c\\ \frac{m_e^*}{\hbar^2\pi}H(E-E_c) & E>E_c\end{cases}$ $\text{J}^{-1}\,\text{m}^{-2}$ $H(x)=0$ for $x<0$ and $H(x)=1$ for $x>0$	$D(E)=\begin{cases}\frac{(2m_h^*)^{\frac{3}{2}}}{2\pi^2\hbar^3}\sqrt{E_v-E} & E<\\ 0 & E_v<E<E\\ \frac{(2m_e^*)^{\frac{3}{2}}}{2\pi^2\hbar^3}\sqrt{E-E_c} & E>\end{cases}$
Density of electrons in the conduction band $n=\int_{E_c}^{\infty}D(E)f(E)dE$	$n=\sqrt{\frac{m_e^*k_BT}{\hbar^2\pi}}\exp\left(\frac{\mu-E_c}{k_BT}\right)$ m^{-1}	$n=\frac{m_e^*k_BT}{\hbar^2\pi}\exp\left(\frac{\mu-E_c}{k_BT}\right)$ m^{-2}	$n=\frac{1}{\sqrt{2}}\left(\frac{m_e^*k_BT}{\pi\hbar^2}\right)^{3/2}\exp\left(\frac{\mu-E}{k_BT}\right.$
Density of holes in the valence band $p=\int_{-\infty}^{E_v}D(E)(1-f(E))dE$	$p=\sqrt{\frac{m_h^*k_BT}{\hbar^2\pi}}\exp\left(\frac{E_v-\mu}{k_BT}\right)$ m^{-1}	$p=\frac{m_h^*k_BT}{\hbar^2\pi}\exp\left(\frac{E_v-\mu}{k_BT}\right)$ m^{-2}	$p=\frac{1}{\sqrt{2}}\left(\frac{m_h^*k_BT}{\pi\hbar^2}\right)^{3/2}\exp\left(\frac{E_v-}{k_BT}\right.$
Law of mass action	$np=\frac{k_BT}{\hbar^2\pi}\sqrt{m_e^*m_h^*}\exp\left(\frac{-E_g}{k_BT}\right)$ m^{-2}	$np=\left(\frac{k_BT}{\pi\hbar^2}\right)^2 m_e^*m_h^*\exp\left(\frac{-E_g}{k_BT}\right)$ m^{-4}	$np=\frac{1}{2}\left(\frac{k_BT}{\pi\hbar^2}\right)^3(m_e^*m_h^*)^{3/2}\exp\left(\right.$
Intrisic carrier density $n_i=\sqrt{np}$	$n_i=\sqrt{\frac{k_BT}{\hbar^2\pi}}(m_e^*m_h^*)^{1/4}\exp\left(\frac{-E_g}{2k_BT}\right)$ m^{-1}	$n_i=\frac{k_BT}{\pi\hbar^2}\sqrt{m_e^*m_h^*}\exp\left(\frac{-E_g}{2k_BT}\right)$ m^{-2}	$n_i=\frac{1}{\sqrt{2}}\left(\frac{k_BT}{\pi\hbar^2}\right)^{3/2}(m_e^*m_h^*)^{3/4}\exp\left(\right.$
Chemical potential Set $n=p$, solve for μ.	$\mu=\frac{E_v+E_c}{2}-\frac{k_BT}{4}\ln\left(\frac{m_e^*}{m_h^*}\right)$ J	$\mu=\frac{E_v+E_c}{2}-\frac{k_BT}{2}\ln\left(\frac{m_e^*}{m_h^*}\right)$ J	$\mu=\frac{E_v+E_c}{2}-\frac{3}{4}k_BT\ln\left(\frac{m_e^*}{m_h^*}\right.$
Internal energy density $u=\int_{-\infty}^{\infty}ED(E)f(E)dE$	$u=u(T=0)+\sqrt{\frac{2k_BT}{\hbar^2\pi}}(m_e^*m_h^*)^{1/4}\exp\left(\frac{-E_g}{2k_BT}\right)(E_g+k_BT)$ J m^{-1}	$u=u(T=0)+\frac{k_BT}{\hbar^2\pi}\sqrt{m_e^*m_h^*}\exp\left(\frac{-E_g}{2k_BT}\right)(E_g+2k_BT)$ J m^{-2}	$u=u(T=0)+\frac{\sqrt{2\pi}}{2\pi^2\hbar^3}(m_e^*m_h^*)^{3/4}\exp\left(\frac{-E_g}{2k_BT}\right)(k_B$
Helmholtz free energy $f=u-Ts$	$f=u(T=0)-2\sqrt{\frac{2k_B}{\hbar^2\pi}}(m_e^*m_h^*)^{1/4}\exp\left(\frac{-E_g}{2k_BT}\right)k_BT^{3/2}$ J m^{-1}	$f=u(T=0)-\frac{2\sqrt{m_e^*m_h^*}}{\hbar^2\pi}k_B^2T^2\exp\left(\frac{-E_g}{2k_BT}\right)$ J m^{-2}	$f=u(T=0)-\frac{\sqrt{2\pi}}{\pi^2\hbar^3}(m_e^*m_h^*)^{3/4}(k_BT)^{5/2}$ e
Specific heat $c_v=\left(\frac{\partial u}{\partial T}\right)_{V=const}$	$c_v=\sqrt{\frac{2k_B}{\hbar^2\pi}}(m_e^*m_h^*)^{1/4}\exp\left(\frac{-E_g}{2k_BT}\right)\left(\frac{E_g^2\sqrt{T}}{2k_BT^2}+\frac{E_g}{\sqrt{T}}+\frac{3k_B\sqrt{T}}{2}\right)$ $\text{J K}^{-1}\,\text{m}^{-1}$	$c_v=\frac{\sqrt{m_e^*m_h^*}}{\hbar^2\pi}\exp\left(\frac{-E_g}{2k_BT}\right)\left(\frac{E_g^2}{2T}+2k_BE_g+4k_B^2T\right)$ $\text{J K}^{-1}\,\text{m}^{-2}$	$c_v=\frac{\sqrt{2\pi}}{2\pi^2\hbar^3}(m_e^*m_h^*)^{3/4}\exp\left(\frac{-E_g}{2k_BT}\right)(k_BT)^{3/2}\left(\frac{15}{2}k_B\right.$
Entropy $s=\int\frac{c_v}{T}dT$	$s=\sqrt{\frac{2k_B}{\hbar^2\pi}}(m_e^*m_h^*)^{1/4}\exp\left(\frac{-E_g}{2k_BT}\right)\left(\frac{E_g}{\sqrt{T}}+3k_B\sqrt{T}\right)$ $\text{J K}^{-1}\,\text{m}^{-1}$	$s=\frac{\sqrt{m_e^*m_h^*}}{\hbar^2\pi}\exp\left(\frac{-E_g}{2k_BT}\right)(k_BE_g+4k_B^2T)$ $\text{J K}^{-1}\,\text{m}^{-2}$	$s=\frac{\sqrt{2\pi}}{2\pi^2\hbar^3}(m_e^*m_h^*)^{3/4}\exp\left(\frac{-E_g}{2k_BT}\right)(k_BT)^{3/2}\left(\right.$

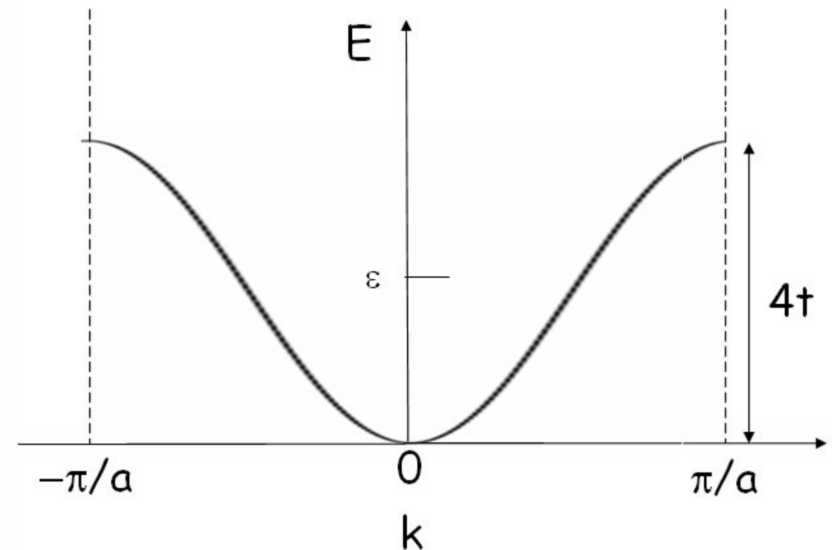
Narrow bandgap semiconductors



Use the programs for metals for small bandgap semiconductors.

Large gap -> large effective mass





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

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

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

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

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.

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

Extrinsic semiconductors

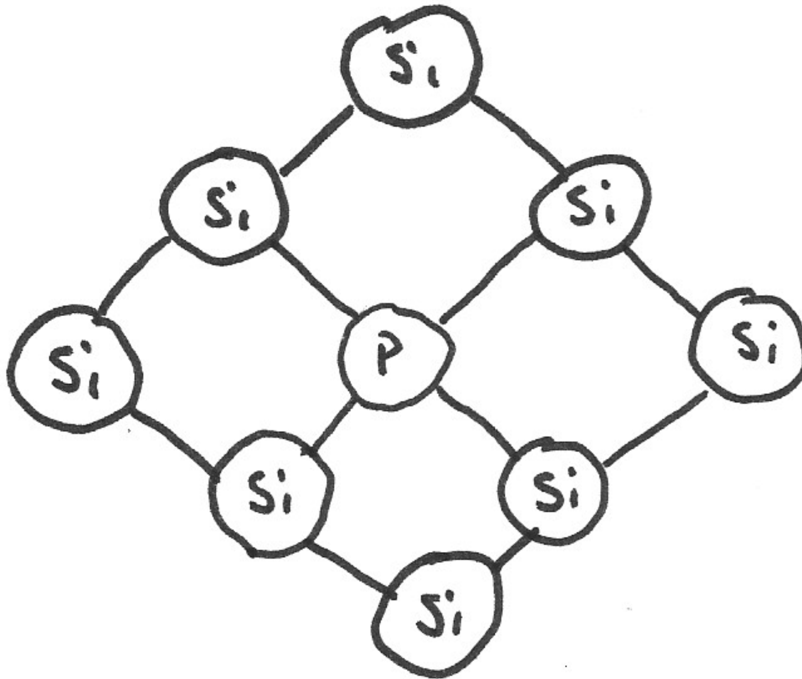
The introduction of impurity atoms that can and electrons or holes is called doping.

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.

IIB	IIIA	IVA	VA	VIA
	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

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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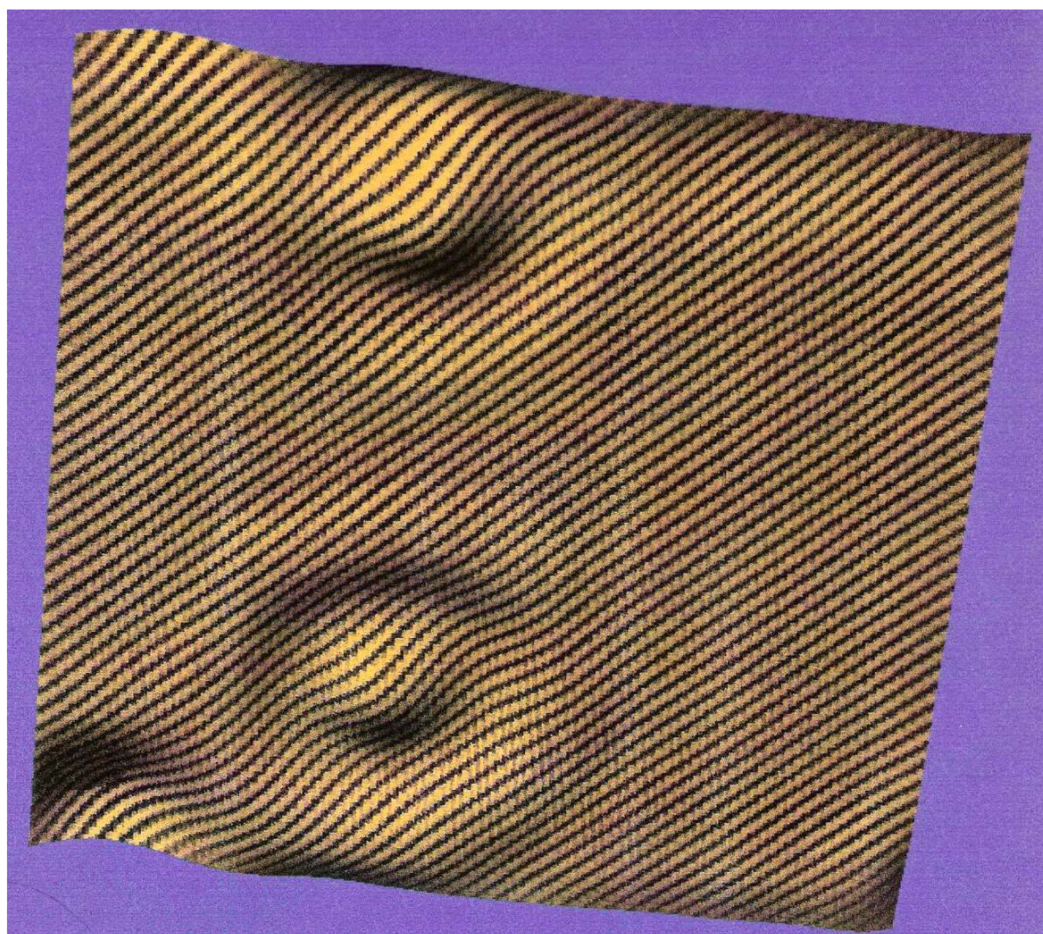
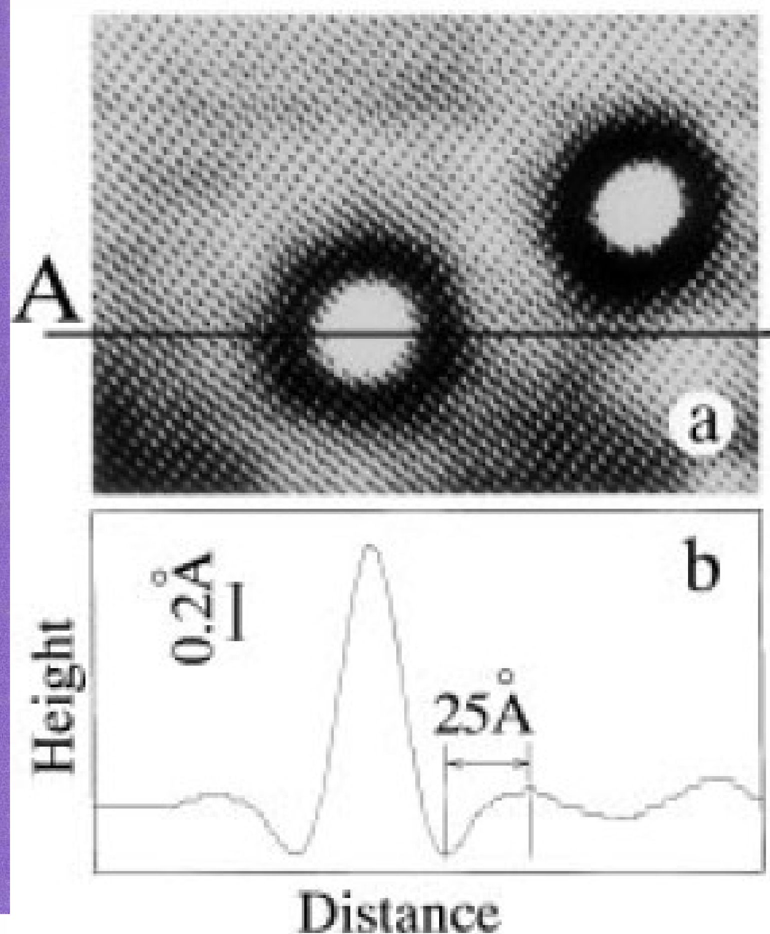
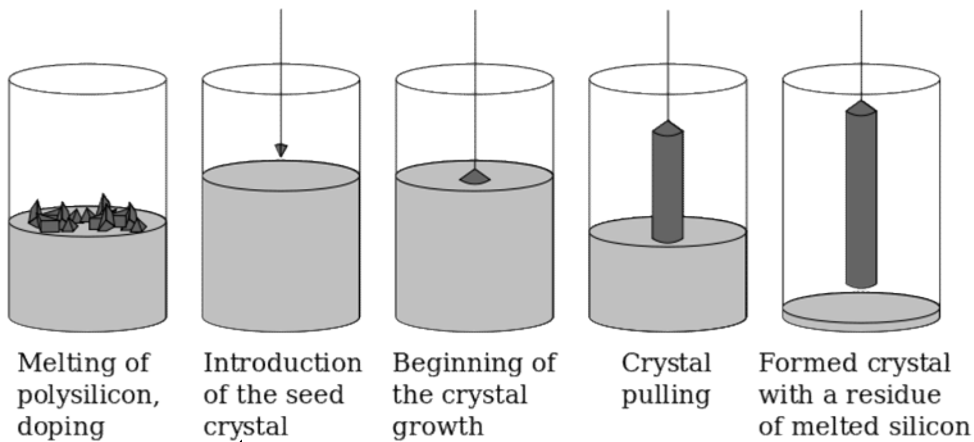
(Received 25 July 1995)





Crystal growth

Czochralski Process



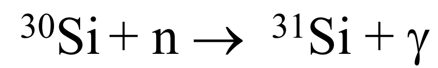
add dopants to the melt

images from wikipedia

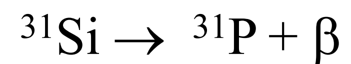
Crystal growth

Float zone Process

Neutron transmutation



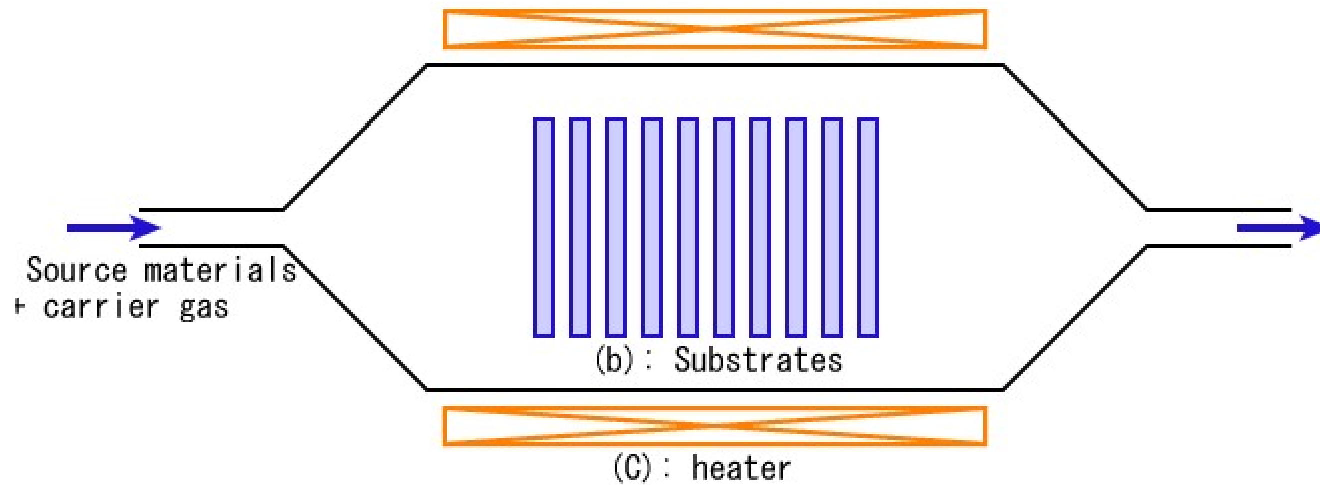
$$^{30}\mathrm{Si} + n \rightarrow {}^{31}\mathrm{Si} + \gamma$$



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

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.

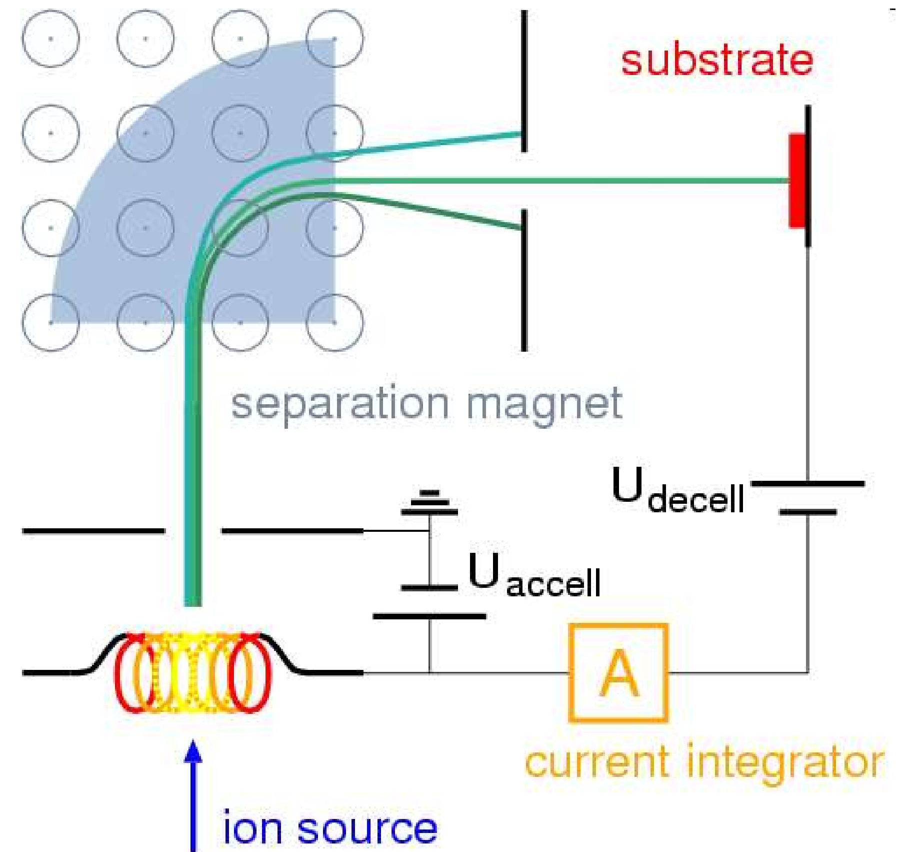
image from wikipedia

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

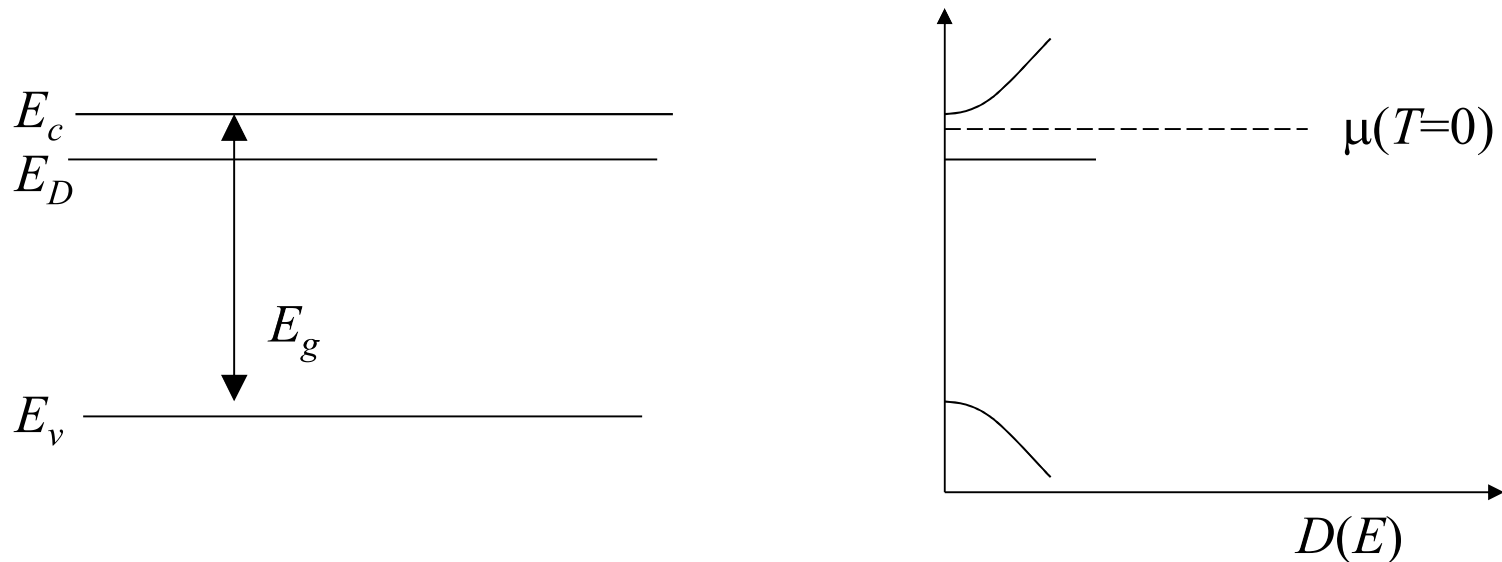


Implant at 7º to avoid channeling

Donors

Five valence electrons: P, As

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



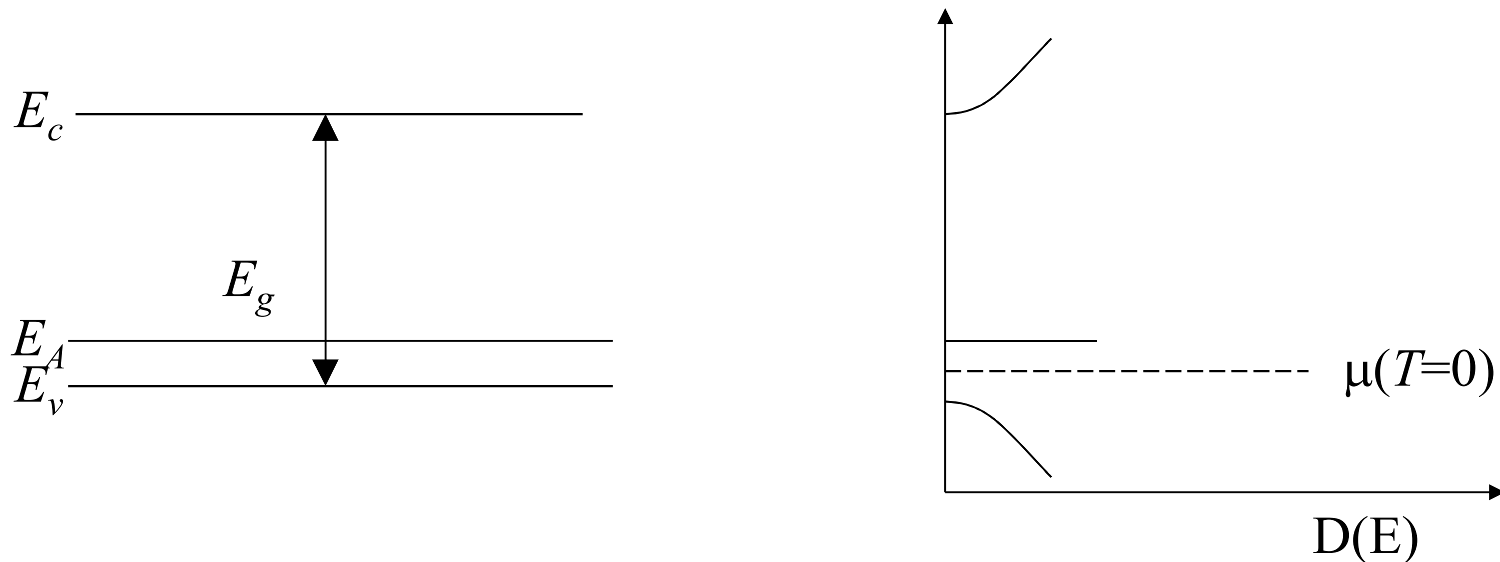
n-type: $n \sim N_D$ Many more electrons in the conduction band than holes in the valence band.

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

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

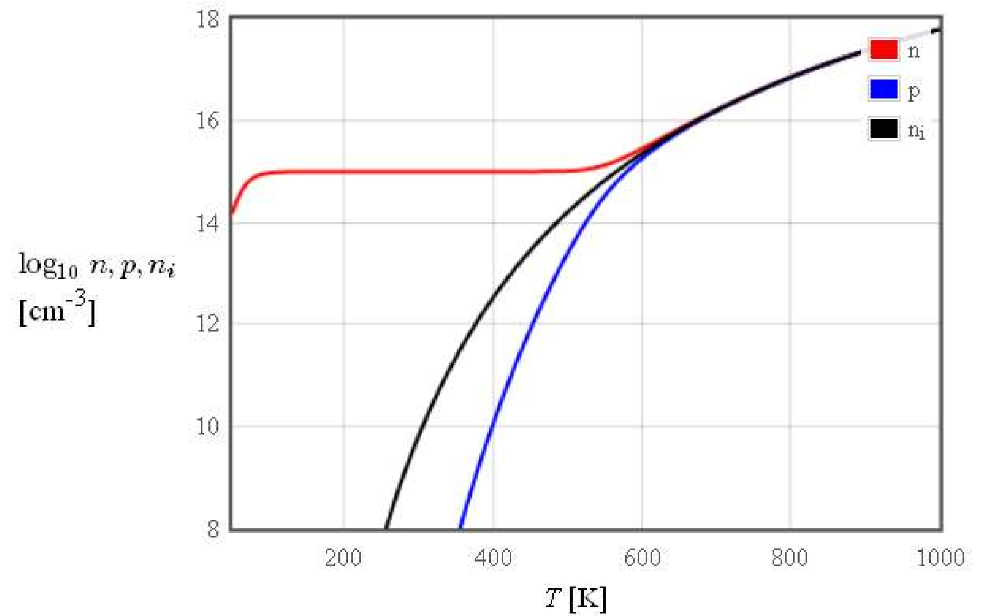
n-type

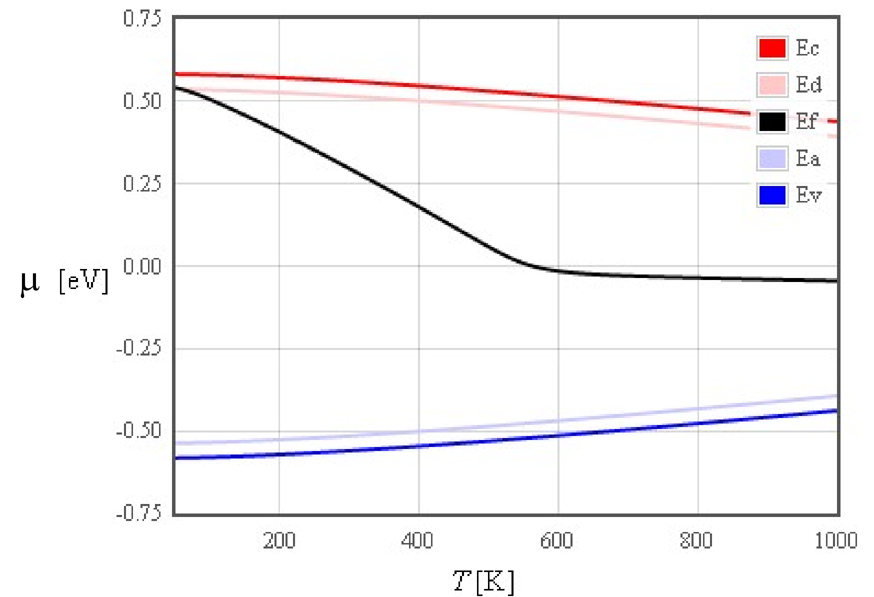
n-type $N_D > N_A$, $p \sim 0$

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

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

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





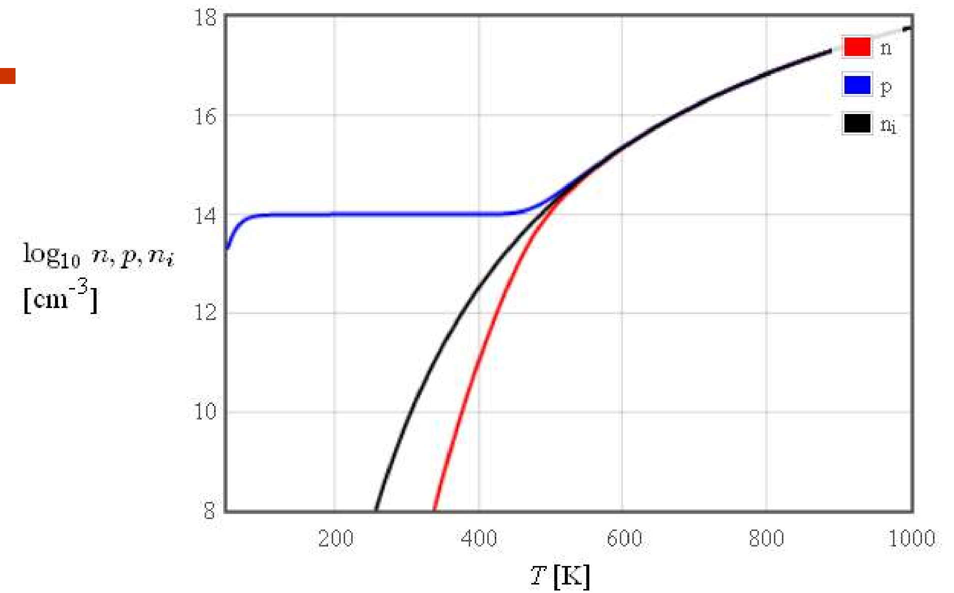
p-type

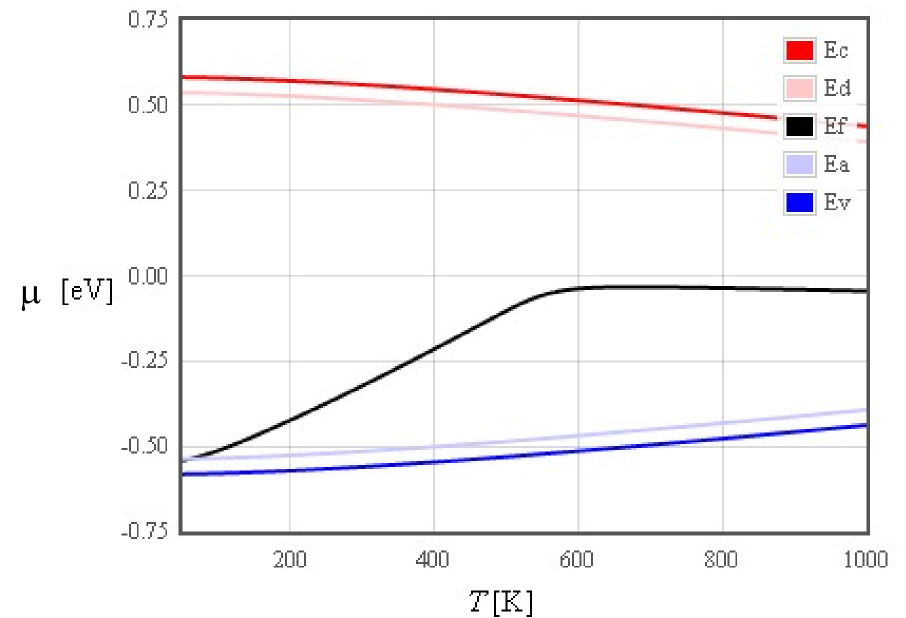
p-type $N_A > N_D$, $n \sim 0$

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

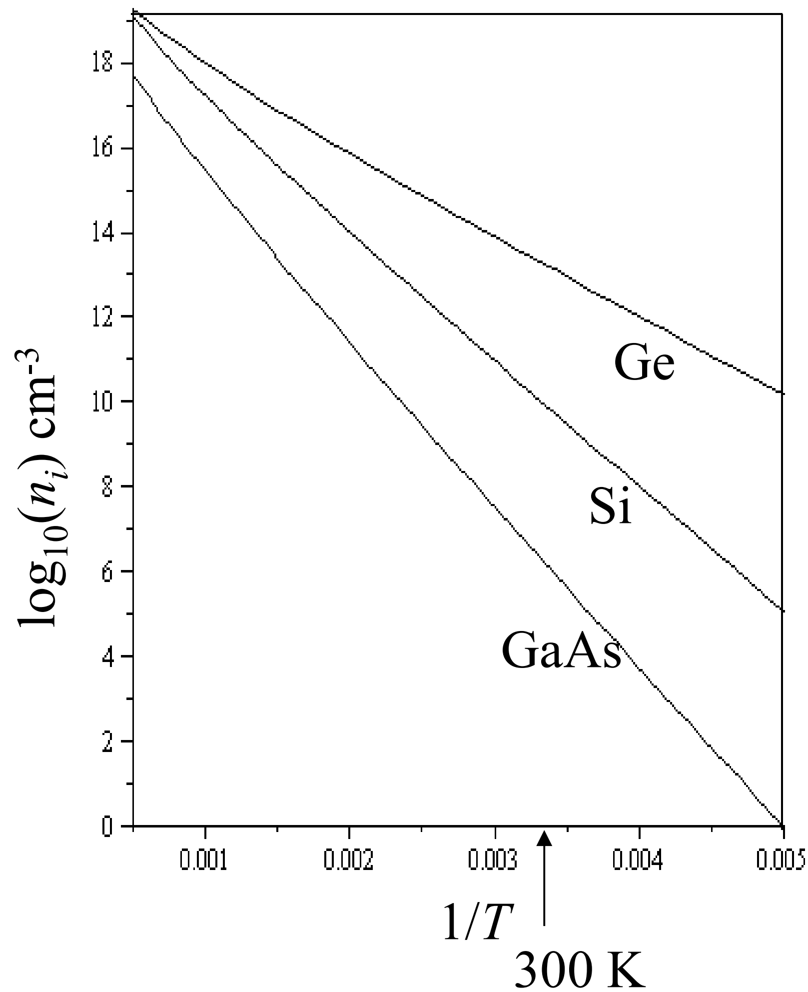
$$\mu = E_v + k_B T \ln\left(\frac{N_v}{N_A}\right)$$

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



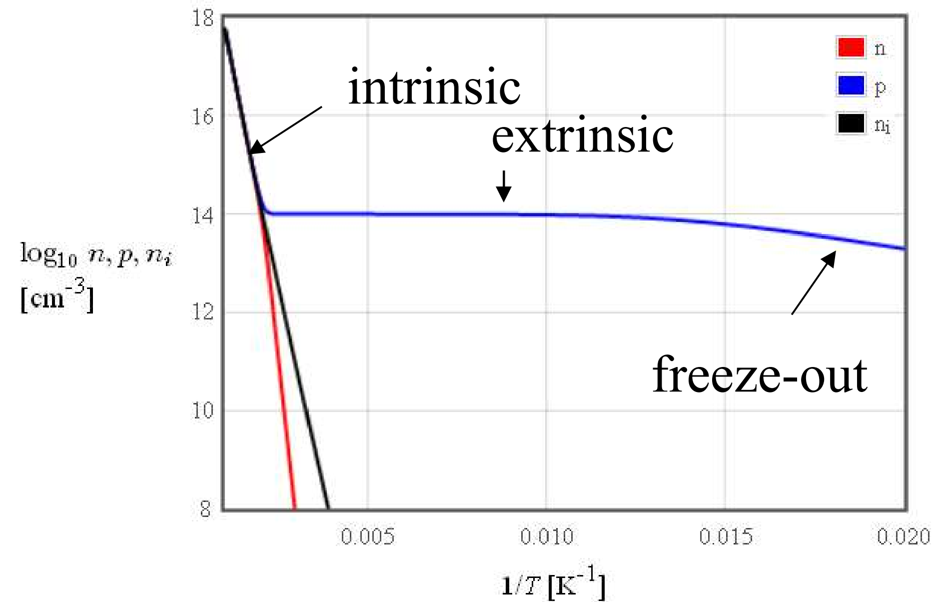


Intrinsic semiconductors



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

Extrinsic semiconductors



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

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

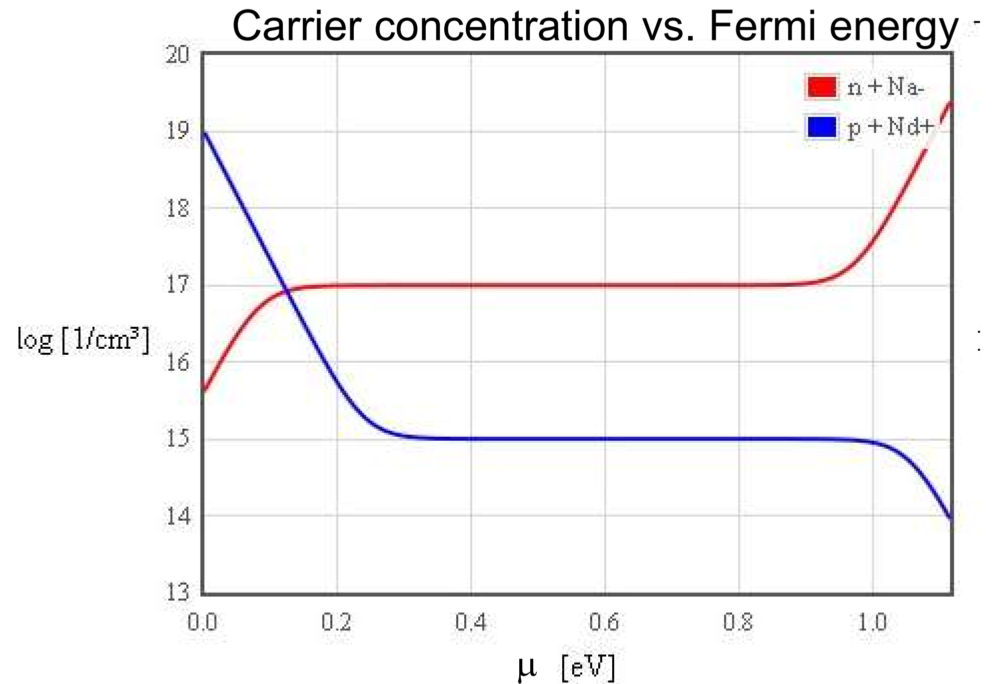
N_D = donor density cm^{-3} N_D^+ = ionized donor density cm^{-3}

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

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

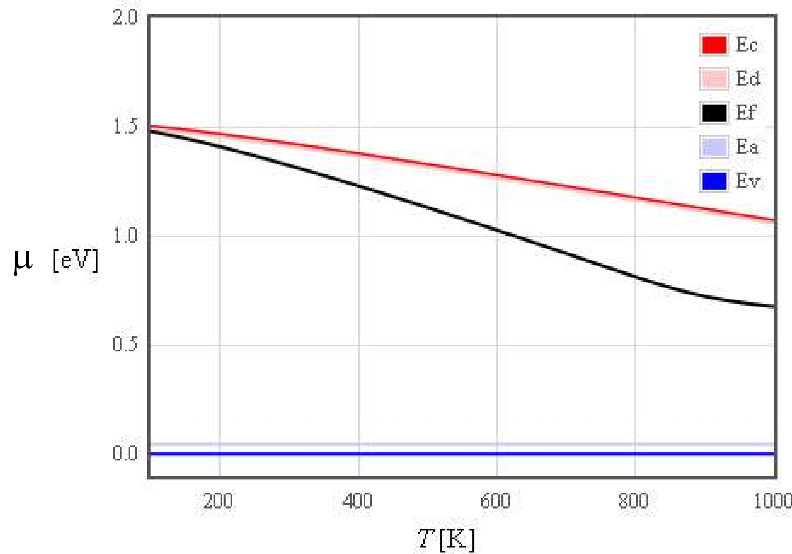



```
for ($i=0; $i<500; $i++) {
  $Ef = $i*$Eg/500;
  $n=$Nc*pow($T/300,1.5)*exp(1.6022E-19*($Ef-$Eg)/(1.38E-23*$T));
  $p=$Nv*pow($T/300,1.5)*exp(1.6022E-19*(-$Ef)/(1.38E-23*$T));
  $Namin = $Na/(1+4*exp(1.6022E-19*($Ea-$Ef)/(1.38E-23*$T)));
  $Ndplus = $Nd/(1+2*exp(1.6022E-19*($Ef-$Ed)/(1.38E-23*$T)));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

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

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

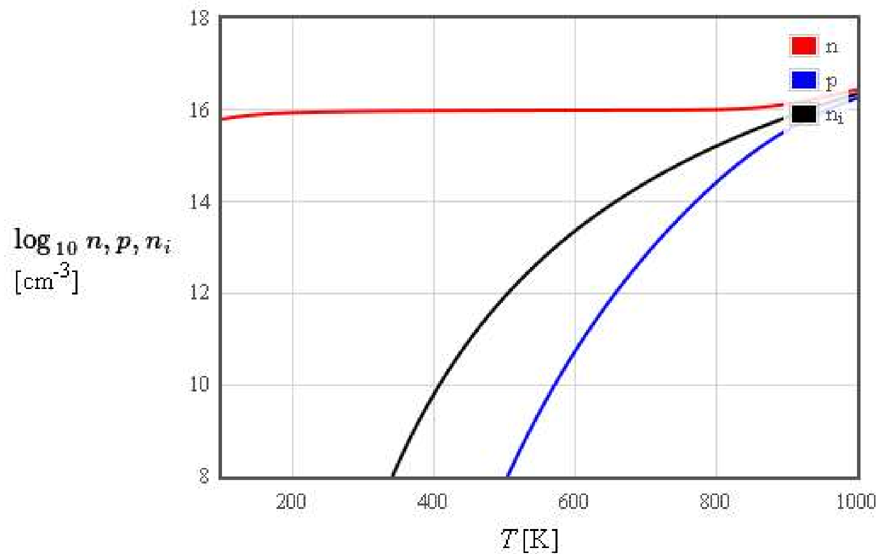
Semiconductor: Si | Ge | GaAs

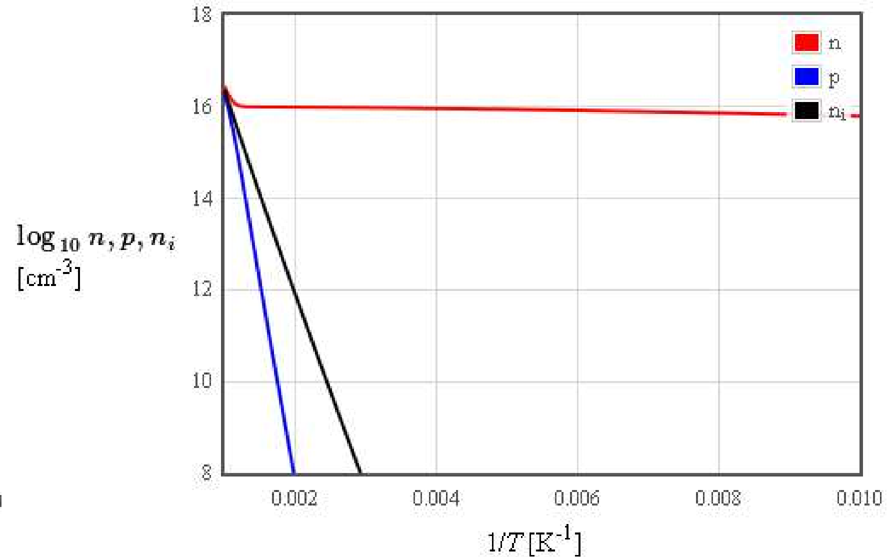
Donor: P in Si | P in Ge | Si in GaAs

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, $n = N_c\left(\frac{T}{300}\right)^{3/2}\exp\left(\frac{E_F-E_c}{k_BT}\right)$ and $p = N_v\left(\frac{T}{300}\right)^{3/2}\exp\left(\frac{E_v-E_F}{k_BT}\right)$.

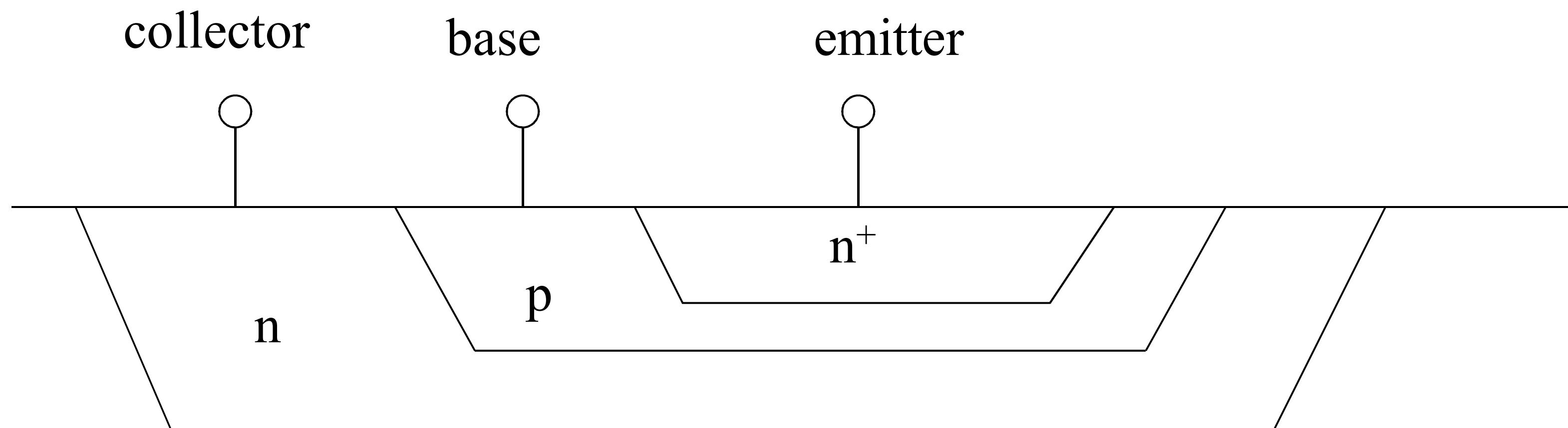
The intrinsic carrier density is $n_i = \sqrt{N_c\left(\frac{T}{300}\right)^{3/2}N_v\left(\frac{T}{300}\right)^{3/2}}\exp\left(\frac{-E_g}{2k_BT}\right)$.





Why dope with donors AND acceptors?

Bipolar transistor



lightly doped p substrate