

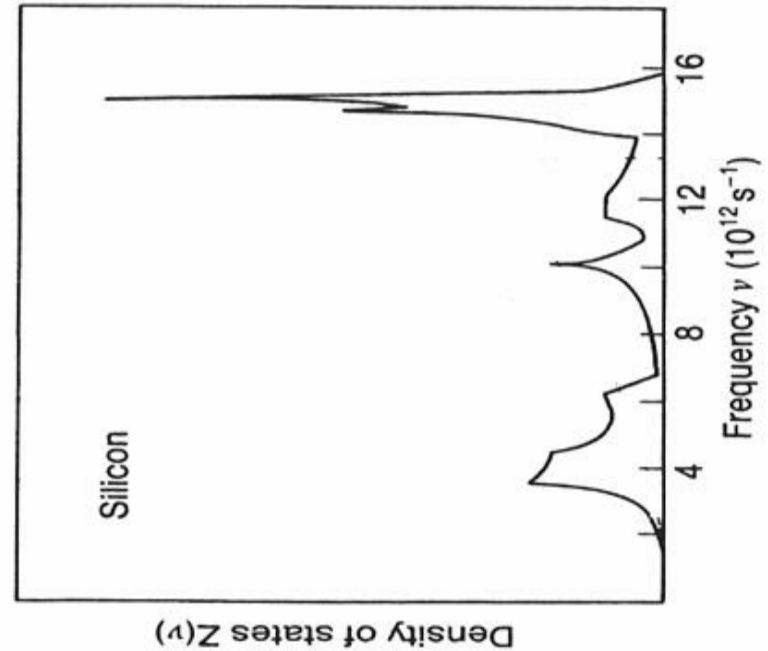
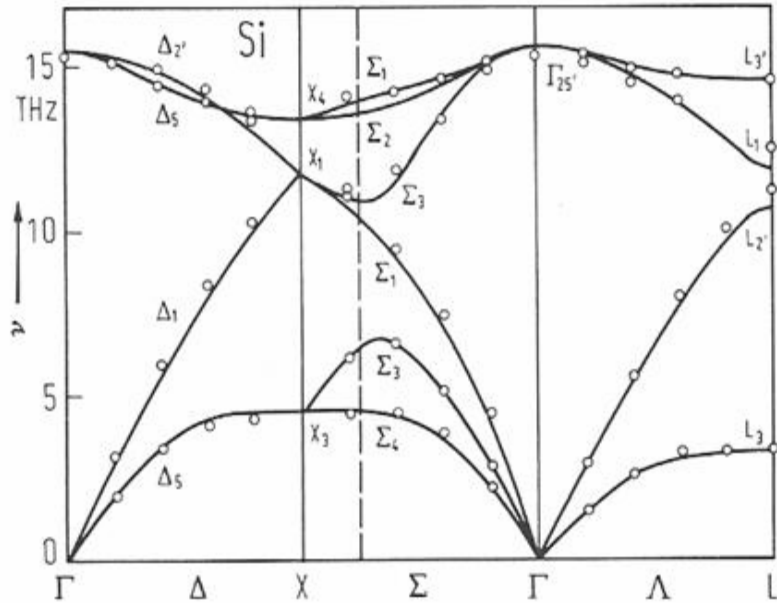
Silicon thermal properties

Thermal

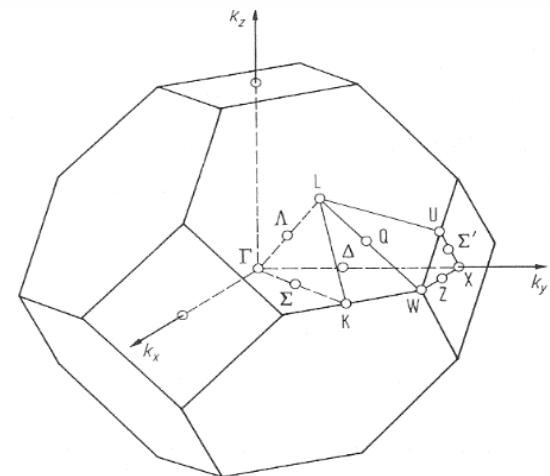
Coefficient of thermal expansion ($^{\circ}\text{C}^{-1}$)	2.6×10^{-6}
Melting point ($^{\circ}\text{C}$)	1421
Specific heat (J/kg-K)	700
Thermal conductivity (W/m-K)	150
Thermal diffusivity	$0.8 \text{ cm}^2/\text{s}$

Thermal properties are dominated by phonons

Silicon phonon dispersion, DOS



Different speeds of sound for different directions and polarizations causes dispersion of pulses.



Density of states → Specific heat

The specific heat is the derivative of the internal energy with respect to the temperature.

$$c_v = \left(\frac{\partial u}{\partial T} \right)_{V,N}$$

This can be expressed in terms of an integral over the frequency ω .

$$c_v = \frac{\partial}{\partial T} \int u(\omega) d\omega = \frac{\partial}{\partial T} \int \hbar\omega D(\omega) \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1} d\omega$$

The [Leibniz integral rule](#) can be used to bring the differentiation inside the integral. If the phonon density of states $D(\omega)$ is temperature independent, the result is,

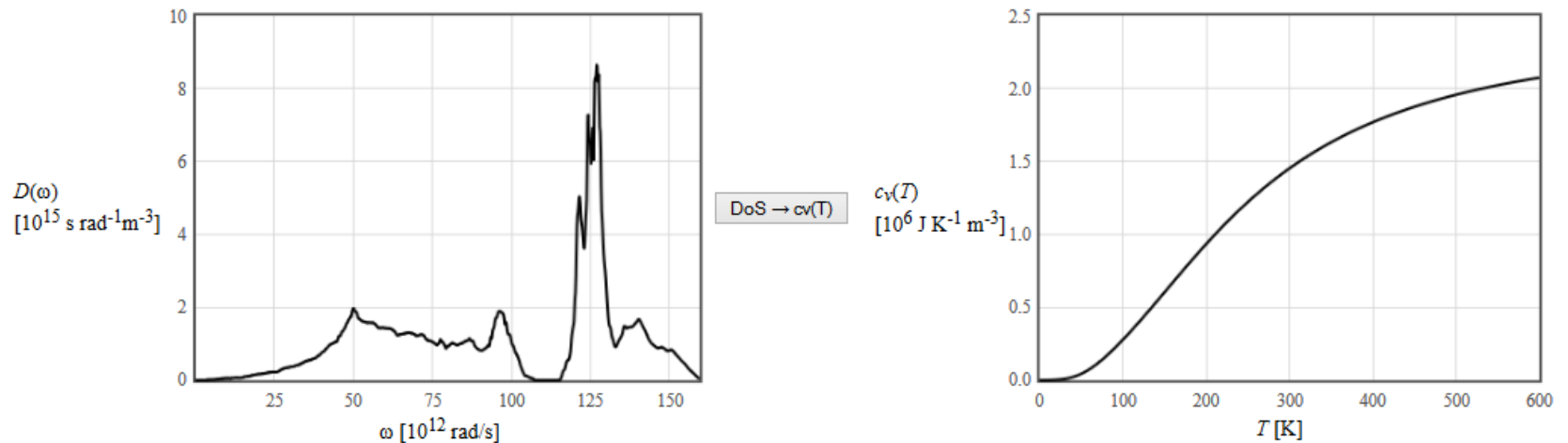
$$c_v = \int \hbar\omega D(\omega) \frac{\partial}{\partial T} \left(\frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1} \right) d\omega$$

Since only the Bose-Einstein factor depends on temperature, the differentiation can be performed analytically and the expression for the specific heat is,

$$c_v = \int \left(\frac{\hbar\omega}{T} \right)^2 \frac{D(\omega) e^{\frac{\hbar\omega}{k_B T}}}{k_B \cdot \left(e^{\frac{\hbar\omega}{k_B T}} - 1 \right)^2} d\omega$$

The form below uses this formula to calculate the temperature dependence of the specific heat from tabulated data for the density of states. The density of states data is input as two columns in the text box at the lower left. The first column is the angular-frequency ω in rad/s. The second column is the density of states in units of $\text{s rad}^{-1} \text{m}^{-3}$.

After the 'DoS → cv(T)' button is pressed, the density of states is plotted on the left and $c_v(T)$ is plotted from temperature T_{\min} to temperature T_{\max} on the right. The data for the $c_v(T)$ plot also appears in tabular form in the lower right text box. The first column is the temperature in Kelvin and the second column is the specific heat in units of $\text{J K}^{-1} \text{m}^{-3}$.



Density of states → Helmholtz free energy density $f(T)$

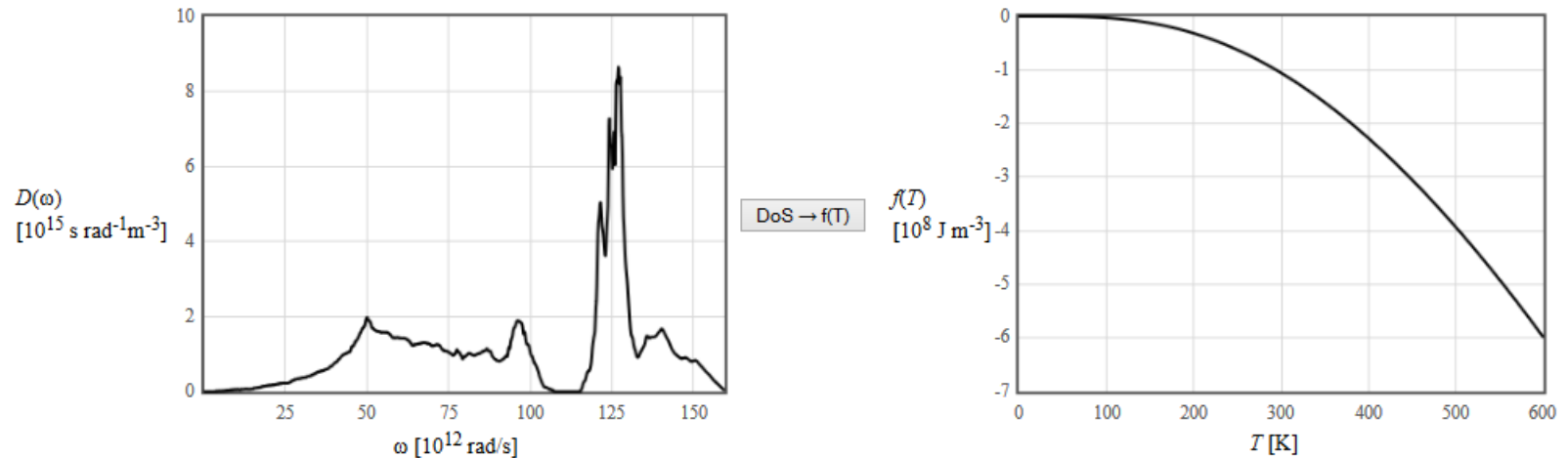
Using statistical mechanics, it can be shown that the Helmholtz free energy density $f(T)$ for bosons can be expressed as the following integral,

$$f(T) = k_B T \int_0^{\infty} D(\omega) \ln \left(1 - \exp \left(\frac{-\hbar \omega}{k_B T} \right) \right) d\omega$$

Here $\hbar \omega$ is the energy of phonons with frequency ω and $D(\omega)$ is the density of states. This result is discussed in *Statistical Physics, Part 1* by Landau and Lifshitz and in the [notes on the thermodynamic properties of non-interacting bosons](#).

The form below uses this formula to calculate the temperature dependence of the Helmholtz free energy density from tabulated data for the density of states. The density of states data is input as two columns in the textbox at the lower left. The first column is the angular-frequency ω in rad/s. The second column is the density of states in units of $\text{s rad}^{-1} \text{m}^{-3}$.

After the 'DoS → f(T)' button is pressed, the density of states is plotted on the left and $f(T)$ is plotted from temperature T_{\min} to temperature T_{\max} on the right. The data for the $f(T)$ plot also appears in tabular form in the lower right textbox. The first column is the temperature in Kelvin and the second column is the Helmholtz free energy density in units of J m^{-3} .

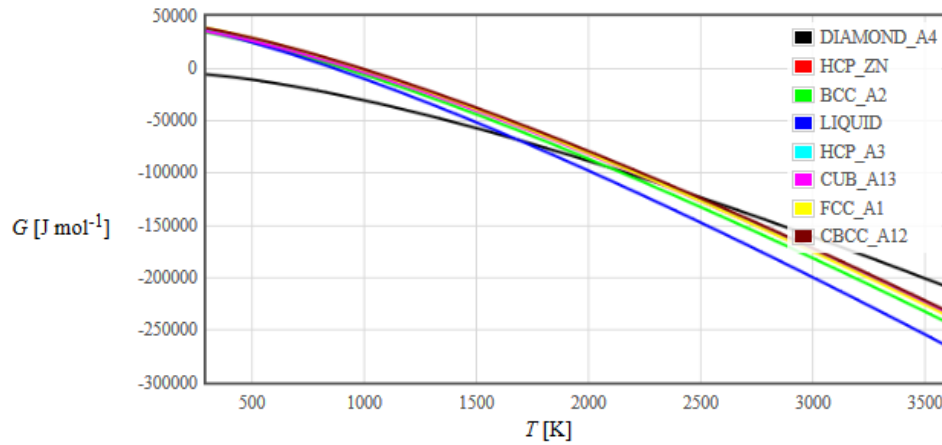


<http://lamp.tu-graz.ac.at/~hadley/ss1/phonons/table/dos2h.html>

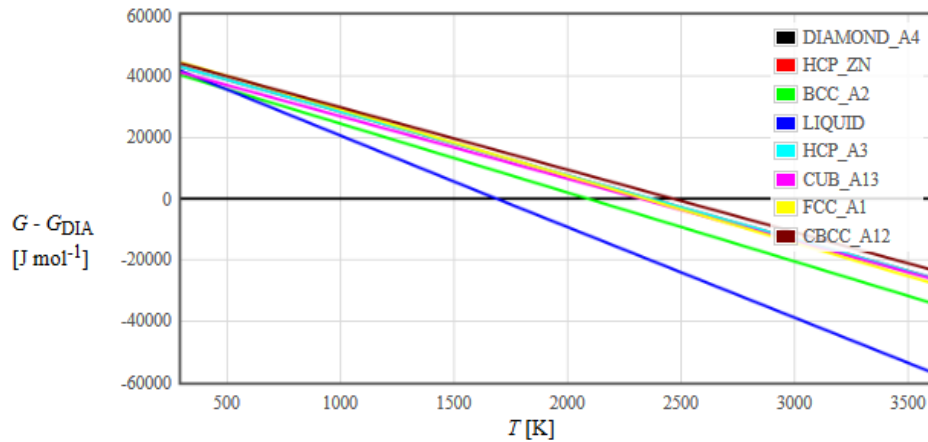
SGTE thermodynamic data

data Europe SGTE maintains [thermodynamic databanks for inorganic and metallurgical systems](#). Data from their 'pure element' performed at constant pressure p , temperature T , and number N . Under these conditions, the system will go to the minimum of the G , and S is the entropy. The top plot is the Gibbs energy per mole.

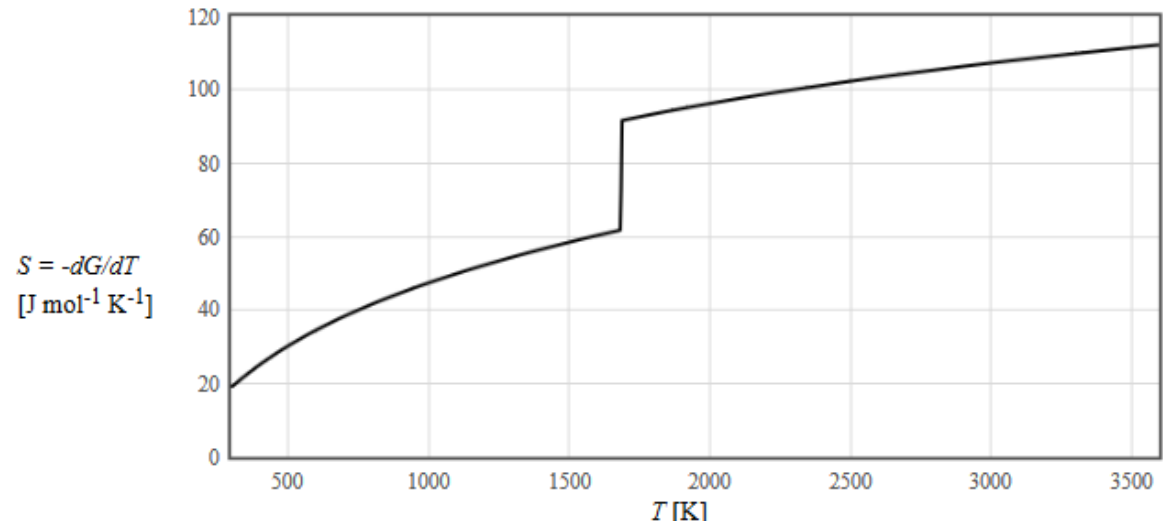
Si



Since the Gibbs energies of the different phases fall almost on top of each other, it is convenient to plot them relative to the temperature.



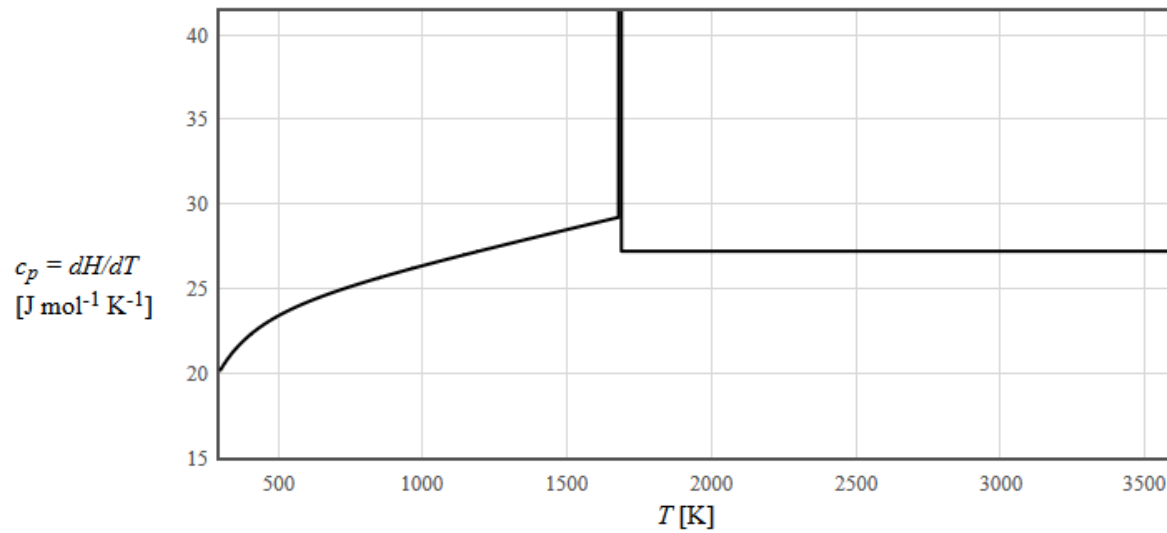
Melting point, latent heat, specific heat



$$S = -dG/dT$$

$[\text{J mol}^{-1} \text{K}^{-1}]$

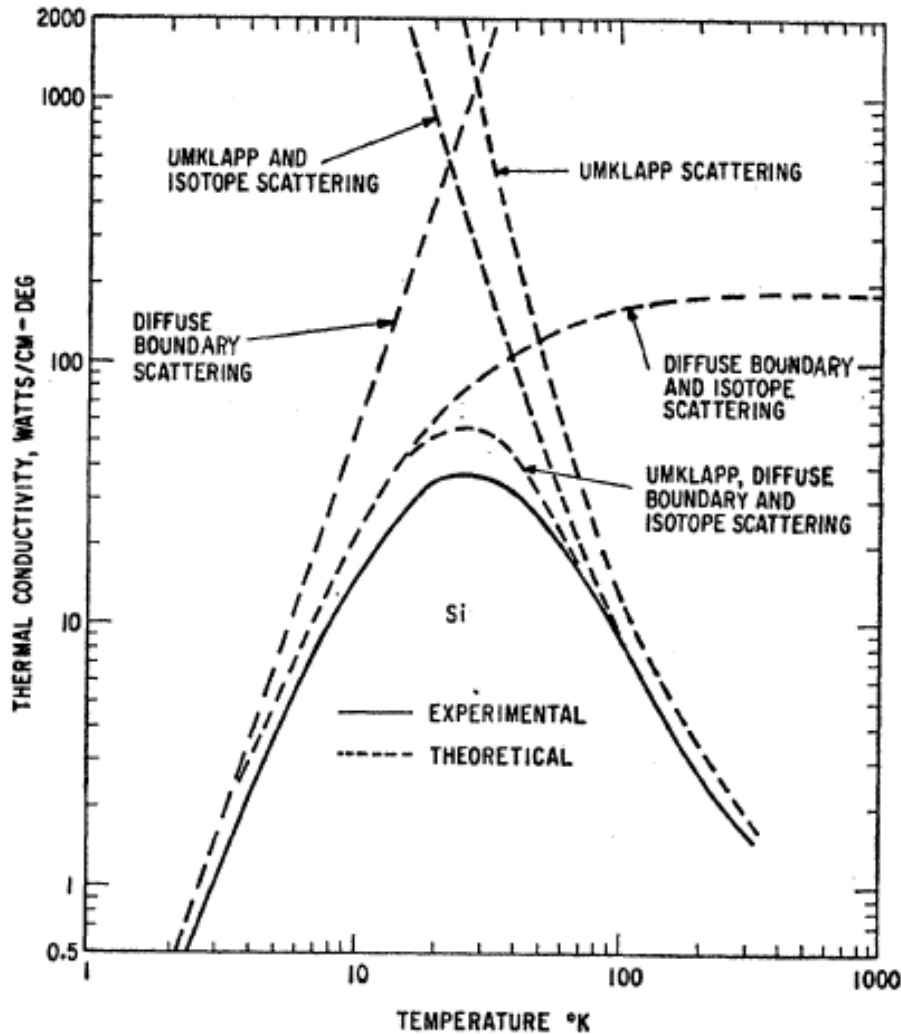
$$L = T(S(T^+) - S(T^-))$$



$$c_p = dH/dT$$

$[\text{J mol}^{-1} \text{K}^{-1}]$

Thermal conductivity $\vec{j}_U = -K\nabla T$



Imperfections in the crystal or grain boundaries decrease the mean free path and the thermal conductivity.

At high temperatures, the mean free path is limited by Umklapp processes. At low temperatures the Umklapp processes freeze out and the mean free path is limited by imperfections.

Student project

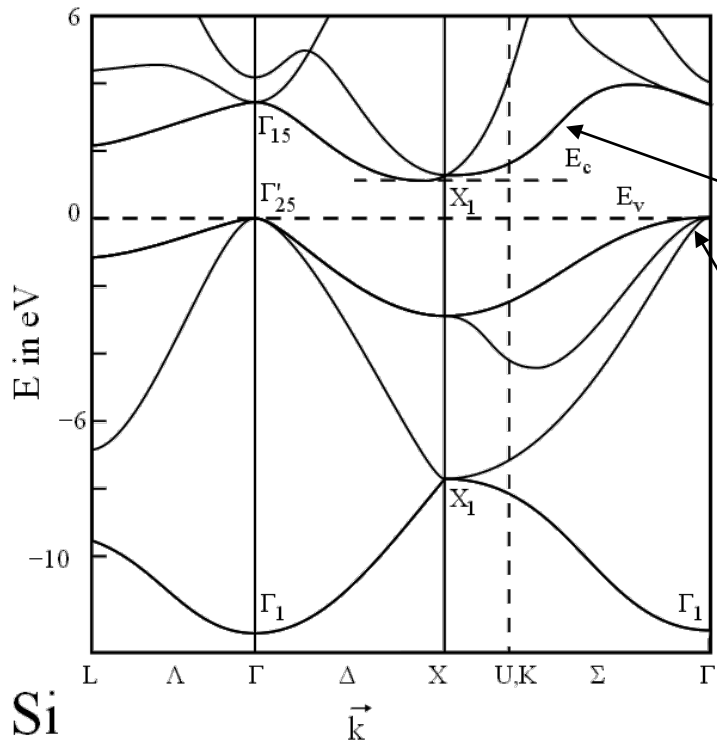
Help make the materials property page for Si.

Calculate the phonon dispersion relation for the diamond crystal structure.

Make table of the phonon density of states of silicon.

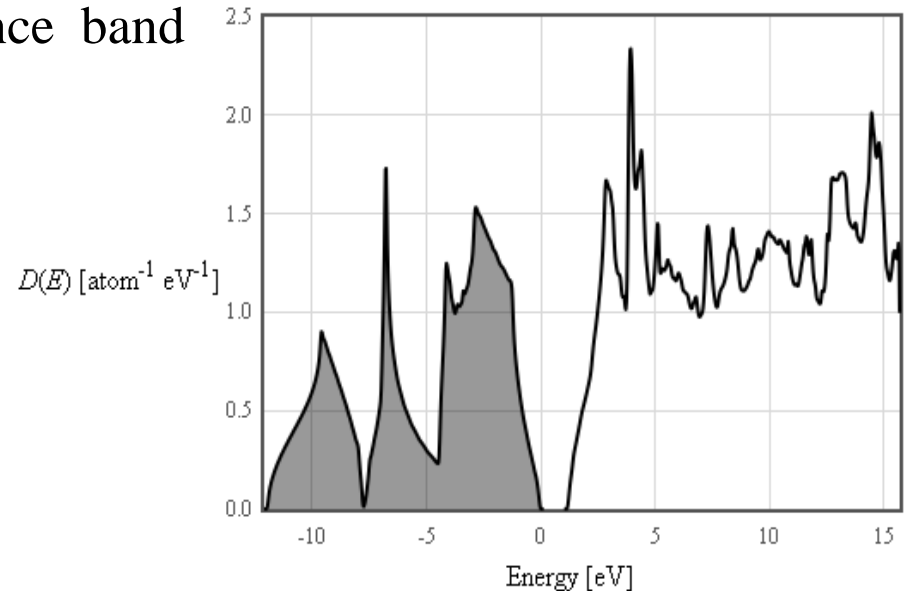
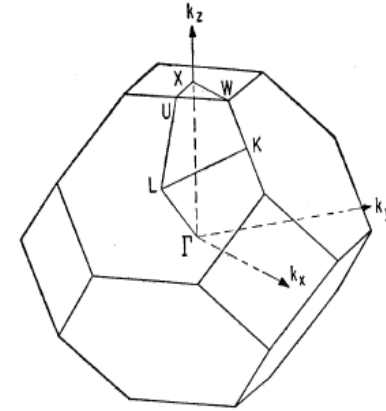
Plot the thermal properties as a function of temperature.

Silicon electronic structure

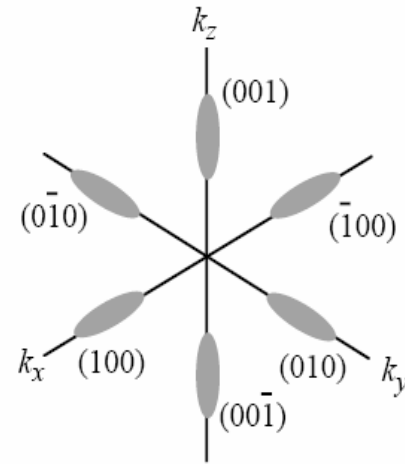
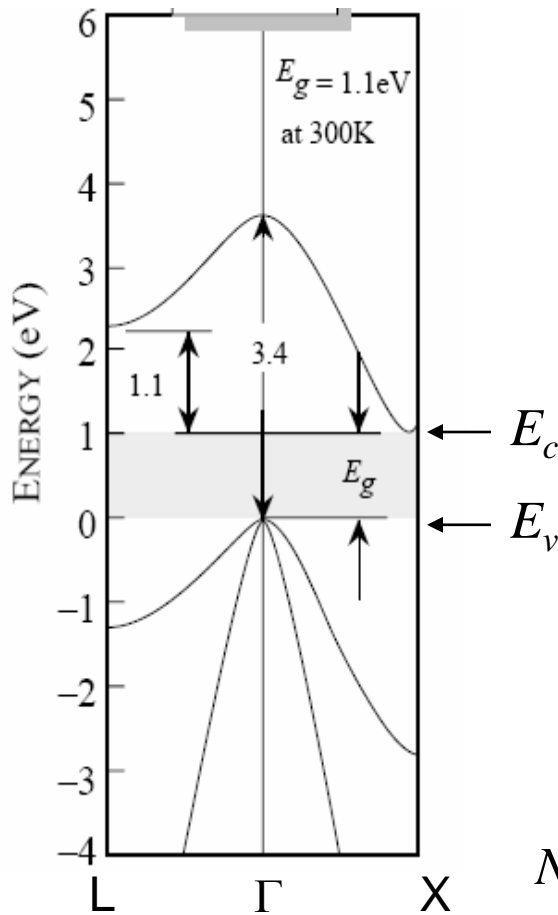


Conduction band

Valence band



Density of electrons in the conduction band



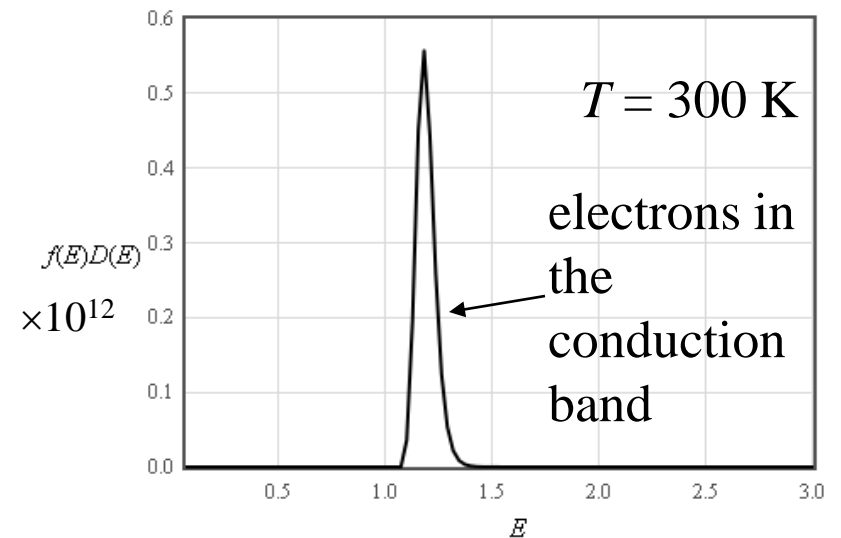
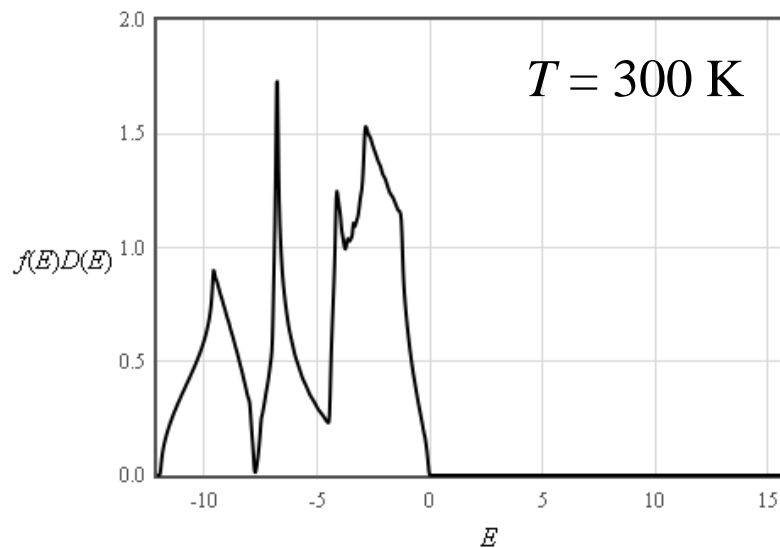
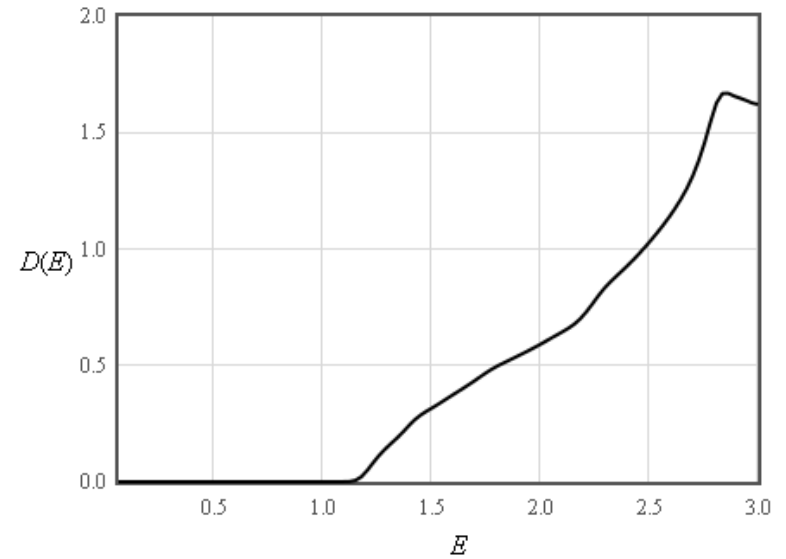
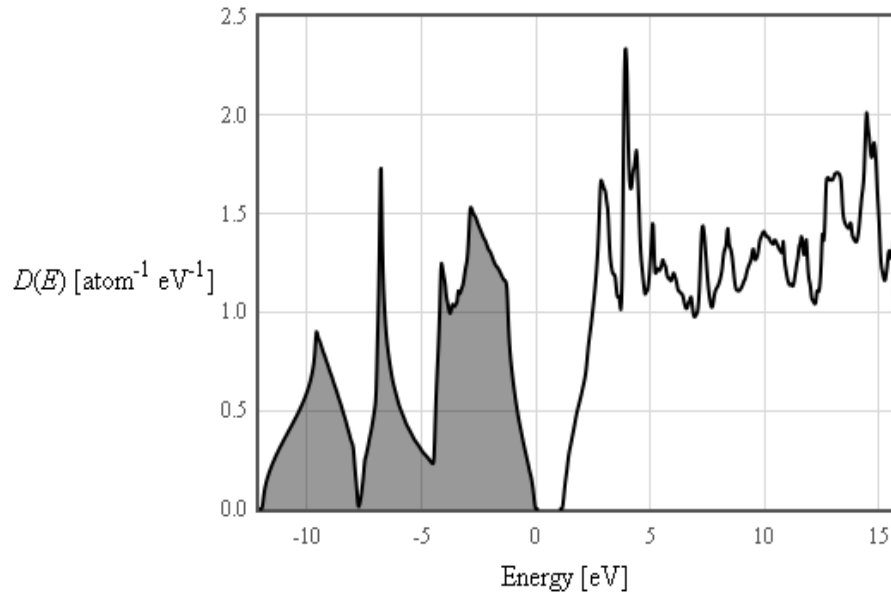
$$n = N_c \left(\frac{T}{300} \right)^{3/2} \exp \left(\frac{E_F - E_c}{k_B T} \right)$$

N_c = effective density of states in conduction band at 300 K

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	$2.78 \times 10^{25} \text{ m}^{-3}$	$1.04 \times 10^{25} \text{ m}^{-3}$	$4.45 \times 10^{23} \text{ m}^{-3}$

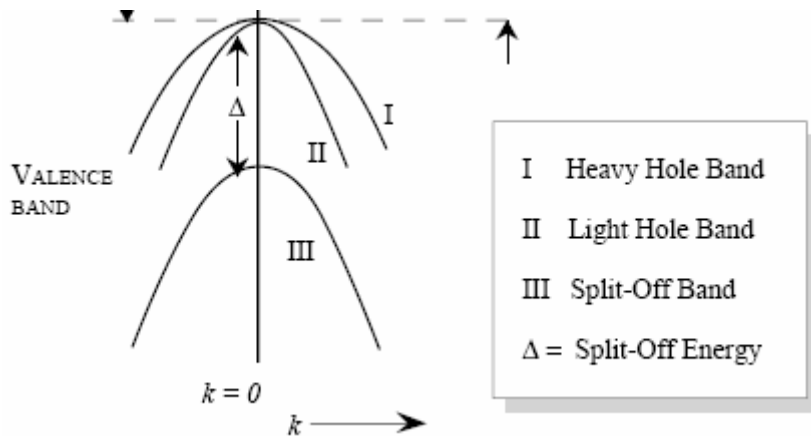
Electrons in the conduction band

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



Density of electrons in the conduction band

Density of holes in the valence band



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

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

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	$2.78 \times 10^{25} \text{ m}^{-3}$	$1.04 \times 10^{25} \text{ m}^{-3}$	$4.45 \times 10^{23} \text{ m}^{-3}$
Effective density of states in valence band (300 K) N_v	$9.84 \times 10^{24} \text{ m}^{-3}$	$6.0 \times 10^{24} \text{ m}^{-3}$	$7.72 \times 10^{24} \text{ m}^{-3}$
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/cm ³	5.3267 g/cm ³	5.32 g/cm ³
Atoms/m ³	5.0×10^{28}	4.42×10^{28}	4.42×10^{28}

Conduction bands

The six 6 conduction band minima can be approximated by the paraboloids,

$$E_{c100} = E_g + \frac{\hbar^2}{2m_l} \left(k_x - \frac{1.7\pi}{a} \right)^2 + \frac{\hbar^2}{2m_t} k_y^2 + \frac{\hbar^2}{2m_t} k_z^2,$$

$$E_{c\bar{1}00} = E_g + \frac{\hbar^2}{2m_l} \left(k_x + \frac{1.7\pi}{a} \right)^2 + \frac{\hbar^2}{2m_t} k_y^2 + \frac{\hbar^2}{2m_t} k_z^2,$$

$$E_{c010} = E_g + \frac{\hbar^2}{2m_t} k_x^2 + \frac{\hbar^2}{2m_l} \left(k_y - \frac{1.7\pi}{a} \right)^2 + \frac{\hbar^2}{2m_t} k_z^2,$$

$$E_{c0\bar{1}0} = E_g + \frac{\hbar^2}{2m_t} k_x^2 + \frac{\hbar^2}{2m_l} \left(k_y + \frac{1.7\pi}{a} \right)^2 + \frac{\hbar^2}{2m_t} k_z^2,$$

$$E_{c001} = E_g + \frac{\hbar^2}{2m_t} k_x^2 + \frac{\hbar^2}{2m_t} k_y^2 + \frac{\hbar^2}{2m_l} \left(k_z - \frac{1.7\pi}{a} \right)^2,$$

$$E_{c00\bar{1}} = E_g + \frac{\hbar^2}{2m_t} k_x^2 + \frac{\hbar^2}{2m_t} k_y^2 + \frac{\hbar^2}{2m_l} \left(k_z + \frac{1.7\pi}{a} \right)^2.$$

Valence bands

The valence bands can be approximated by paraboloids for the light holes,

$$E_{v,lh} = -\frac{\hbar^2}{2m_{lh}} (k_x^2 + k_y^2 + k_z^2),$$

the heavy holes,

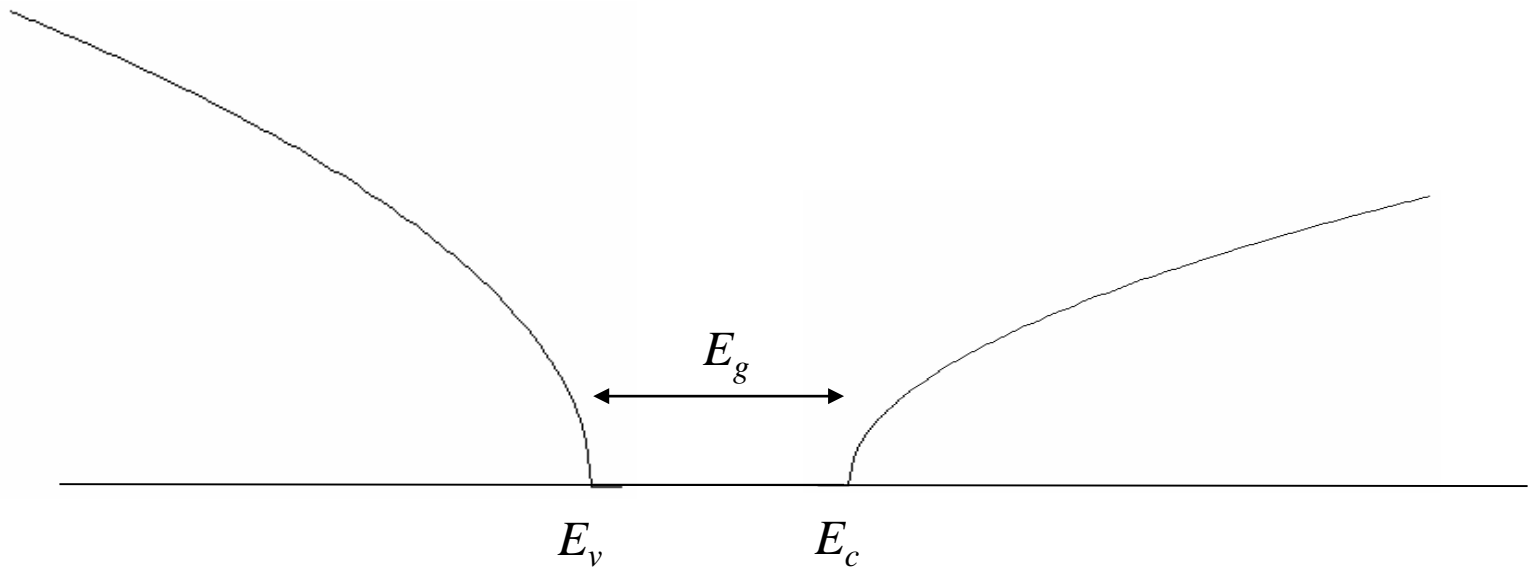
$$E_{v,hh} = -\frac{\hbar^2}{2m_{hh}} (k_x^2 + k_y^2 + k_z^2),$$

and the split-off band,

$$E_{v,so} = -E_{so} - \frac{\hbar^2}{2m_{so}} (k_x^2 + k_y^2 + k_z^2).$$

Density of states

$$D(E) = \begin{cases} \frac{2N_v(300)}{\sqrt{\pi}} \left(\frac{1}{300k_B} \right)^{3/2} \sqrt{E_v - E}, & \text{for } E < E_v \\ 0, & \text{for } E_v < E < E_c \\ \frac{2N_c(300)}{\sqrt{\pi}} \left(\frac{1}{300k_B} \right)^{3/2} \sqrt{E - E_c}, & \text{for } E_c < E \end{cases}$$

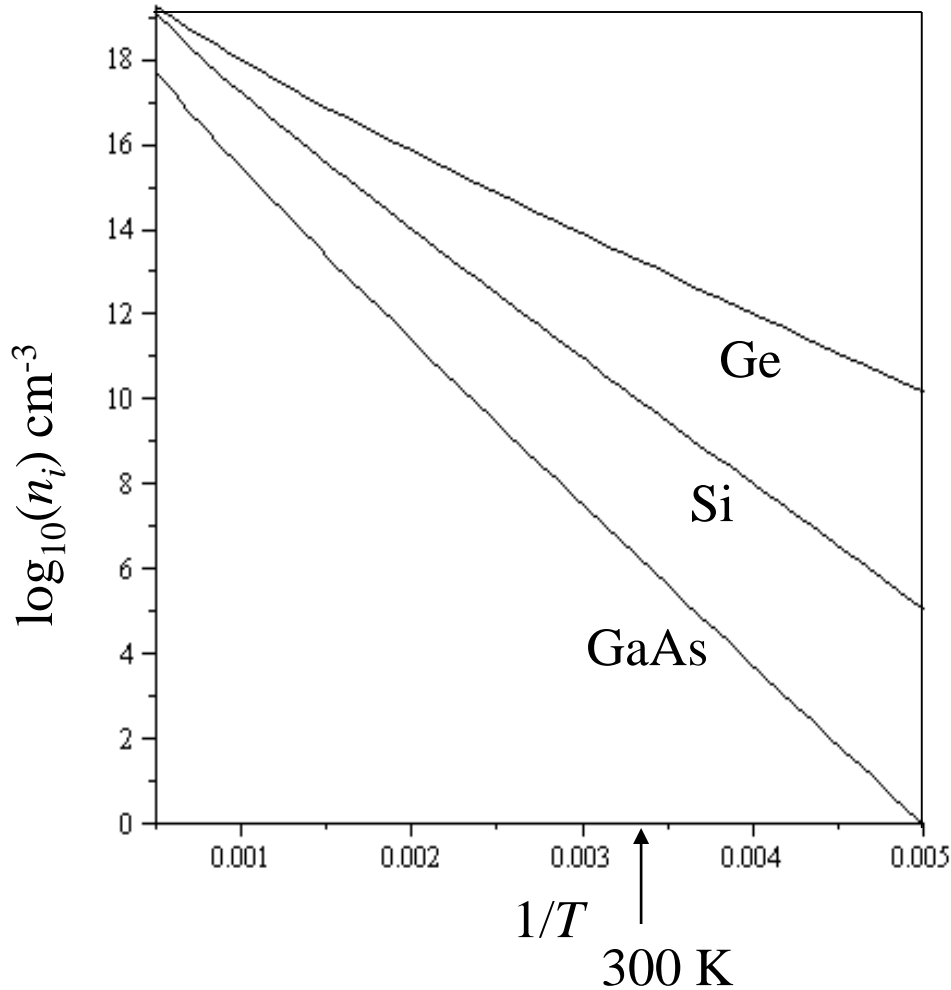


Boltzmann approximation

The table below gives the contribution of electrons in intrinsic semiconductors and insulators to some thermodynamic quantities. These results were calculated in the Boltzmann approximation where it is assumed that the chemical potential lies in the band gap more than $3k_B T$ 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	$D(E) = \begin{cases} \frac{1}{\hbar\pi} \sqrt{\frac{2m_h^*}{(E_v - E)}} & E < E_v \\ 0 & E_v < E < E_c \\ \frac{1}{\hbar\pi} \sqrt{\frac{2m_e^*}{(E - E_c)}} & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-1}$	$D(E) = \begin{cases} \frac{m_h^*}{\hbar^2\pi} H(E_v - E) & E < E_v \\ 0 & E_v < E < E_c \\ \frac{m_e^*}{\hbar^2\pi} H(E - E_c) & E > E_c \end{cases} \quad \text{J}^{-1} \text{m}^{-2}$ $H(x) = 0 \text{ for } x < 0 \text{ and } H(x) = 1 \text{ for } x > 0$	$D(E) = \begin{cases} \frac{(2m_h^*)^{\frac{3}{2}}}{2\pi^2\hbar^3} \sqrt{E_v - E} & E < E_v \\ 0 & E_v < E < E_c \\ \frac{(2m_e^*)^{\frac{3}{2}}}{2\pi^2\hbar^3} \sqrt{E - E_c} & E > E_c \end{cases}$
Density of electrons in the conduction band $n = \int_{E_c}^{\infty} D(E) f(E) dE$	$n = \sqrt{\frac{m_e^* k_B T}{\hbar^2 \pi}} \exp\left(\frac{\mu - E_c}{k_B T}\right) \quad \text{m}^{-1}$	$n = \frac{m_e^* k_B T}{\hbar^2 \pi} \exp\left(\frac{\mu - E_c}{k_B T}\right) \quad \text{m}^{-2}$	$n = \frac{1}{\sqrt{2}} \left(\frac{m_e^* k_B T}{\pi \hbar^2}\right)^{3/2} \exp\left(\frac{\mu - E_c}{k_B T}\right)$
Density of holes in the valence band $p = \int_{-\infty}^{E_v} D(E) (1 - f(E)) dE$	$p = \sqrt{\frac{m_h^* k_B T}{\hbar^2 \pi}} \exp\left(\frac{E_v - \mu}{k_B T}\right) \quad \text{m}^{-1}$	$p = \frac{m_h^* k_B T}{\hbar^2 \pi} \exp\left(\frac{E_v - \mu}{k_B T}\right) \quad \text{m}^{-2}$	$p = \frac{1}{\sqrt{2}} \left(\frac{m_h^* k_B T}{\pi \hbar^2}\right)^{3/2} \exp\left(\frac{E_v - \mu}{k_B T}\right)$
Law of mass action	$np = \frac{k_B T}{\hbar^2 \pi} \sqrt{m_e^* m_h^*} \exp\left(\frac{-E_g}{k_B T}\right) \quad \text{m}^{-2}$	$np = \left(\frac{k_B T}{\pi \hbar^2}\right)^2 m_e^* m_h^* \exp\left(\frac{-E_g}{k_B T}\right) \quad \text{m}^{-4}$	$np = \frac{1}{2} \left(\frac{k_B T}{\pi \hbar^2}\right)^3 (m_e^* m_h^*)^{3/2} \exp\left(\frac{-E_g}{k_B T}\right)$
Intrinsic carrier density $n_i = \sqrt{np}$	$n_i = \sqrt{\frac{k_B T}{\hbar^2 \pi}} (m_e^* m_h^*)^{1/4} \exp\left(\frac{-E_g}{2k_B T}\right) \quad \text{m}^{-1}$	$n_i = \frac{k_B T}{\pi \hbar^2} \sqrt{m_e^* m_h^*} \exp\left(\frac{-E_g}{2k_B T}\right) \quad \text{m}^{-2}$	$n_i = \frac{1}{\sqrt{2}} \left(\frac{k_B T}{\pi \hbar^2}\right)^{3/2} (m_e^* m_h^*)^{3/4} \exp\left(\frac{-E_g}{2k_B T}\right)$
Chemical potential Set $n = p$, solve for μ	$\mu = \frac{E_v + E_c}{2} - \frac{k_B T}{4} \ln\left(\frac{m_e^*}{m_h^*}\right) \quad \text{J}$	$\mu = \frac{E_v + E_c}{2} - \frac{k_B T}{2} \ln\left(\frac{m_e^*}{m_h^*}\right) \quad \text{J}$	$\mu = \frac{E_v + E_c}{2} - \frac{3}{4} k_B T \ln\left(\frac{m_e^*}{m_h^*}\right)$
Internal energy density $u = \int_{-\infty}^{\infty} E D(E) f(E) dE$	$u = u(T=0) + \sqrt{\frac{2k_B T}{\hbar^2 \pi}} (m_e^* m_h^*)^{1/4} \exp\left(\frac{-E_g}{2k_B T}\right) (E_g + k_B T) \quad \text{J m}^{-1}$	$u = u(T=0) + \frac{k_B T}{\hbar^2 \pi} \sqrt{m_e^* m_h^*} \exp\left(\frac{-E_g}{2k_B T}\right) (E_g + 2k_B T) \quad \text{J m}^{-2}$	$u = u(T=0) + \frac{\sqrt{2\pi}}{2\pi^2 \hbar^3} (m_e^* m_h^*)^{3/4} \exp\left(\frac{-E_g}{2k_B T}\right) (k_B T)^{3/2}$
Hehnholtz free energy $f = u - Ts$	$f = u(T=0) - 2\sqrt{\frac{2k_B}{\hbar^2 \pi}} (m_e^* m_h^*)^{1/4} \exp\left(\frac{-E_g}{2k_B T}\right) k_B T^{3/2} \quad \text{J m}^{-1}$	$f = u(T=0) - \frac{2\sqrt{m_e^* m_h^*}}{\hbar^2 \pi} k_B^2 T^2 \exp\left(\frac{-E_g}{2k_B T}\right) \quad \text{J m}^{-2}$	$f = u(T=0) - \frac{\sqrt{2\pi}}{\pi^2 \hbar^3} (m_e^* m_h^*)^{3/4} (k_B T)^{5/2} \exp\left(\frac{-E_g}{2k_B T}\right)$
Specific heat $C_v = \left(\frac{\partial u}{\partial T}\right)_{V=const}$	$C_v = \sqrt{\frac{2k_B}{\hbar^2 \pi}} (m_e^* m_h^*)^{1/4} \exp\left(\frac{-E_g}{2k_B T}\right) \left(\frac{E_g^2 \sqrt{T}}{2k_B T^2} + \frac{E_g}{\sqrt{T}} + \frac{3k_B \sqrt{T}}{2}\right) \quad \text{J K}^{-1} \text{m}^{-1}$	$C_v = \frac{\sqrt{m_e^* m_h^*}}{\hbar^2 \pi} \exp\left(\frac{-E_g}{2k_B T}\right) \left(\frac{E_g^2}{2T} + 2k_B E_g + 4k_B^2 T\right) \quad \text{J K}^{-1} \text{m}^{-2}$	$C_v = \frac{\sqrt{2\pi}}{2\pi^2 \hbar^3} (m_e^* m_h^*)^{3/4} \exp\left(\frac{-E_g}{2k_B T}\right) (k_B T)^{3/2} \left(\frac{15}{2} k_B + \frac{E_g}{T}\right)$
Entropy $s = \int \frac{C_v}{T} dT$	$s = \sqrt{\frac{2k_B}{\hbar^2 \pi}} (m_e^* m_h^*)^{1/4} \exp\left(\frac{-E_g}{2k_B T}\right) \left(\frac{E_g}{\sqrt{T}} + 3k_B \sqrt{T}\right) \quad \text{J K}^{-1} \text{m}^{-1}$	$s = \frac{\sqrt{m_e^* m_h^*}}{\hbar^2 \pi} \exp\left(\frac{-E_g}{2k_B T}\right) (k_B E_g + 4k_B^2 T) \quad \text{J K}^{-1} \text{m}^{-2}$	$s = \frac{\sqrt{2\pi}}{2\pi^2 \hbar^3} (m_e^* m_h^*)^{3/4} \exp\left(\frac{-E_g}{2k_B T}\right) (k_B T)^{3/2} \left(\frac{15}{2} k_B + \frac{E_g}{T}\right)$

Intrinsic carrier concentration



$$n = p = n_i$$

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

$$\sim 5 \times 10^{22} \text{ atoms/cm}^3$$

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,

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

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

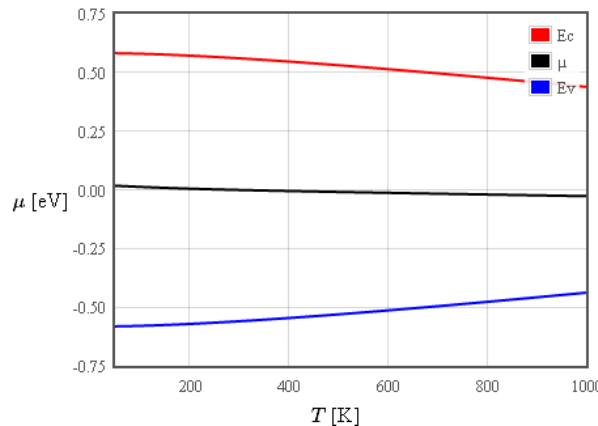
$$m_e^* = \frac{\pi \hbar^3}{300k_B} (\sqrt{2} N_c(300))^{2/3}$$

The density of states can therefore also be written as,

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

In an intrinsic semiconductor, the concentration of electrons and holes is equal, $n = p =$

$$n = p =$$



$N_c(300 \text{ K}) =$	<input type="text" value="2.78E19"/>	$1/\text{cm}^3$
$N_v(300 \text{ K}) =$	<input type="text" value="9.84E18"/>	$1/\text{cm}^3$
$N_{so}(300 \text{ K}) =$	<input type="text" value="2.98E18"/>	$1/\text{cm}^3$
$E_g =$	<input type="text" value="1.166-4.73E-4*T*(T+636)"/>	eV
$E_v - E_{so} =$	<input type="text" value="0.044"/>	eV
$T_1 =$	<input type="text" value="50"/>	K
$T_2 =$	<input type="text" value="1000"/>	K
<input type="button" value="Replot"/>		

Semiconductor bandgap, E_g . For most

$\left(\frac{1}{\sqrt{\pi}}\right)$

Extrinsic semiconductors

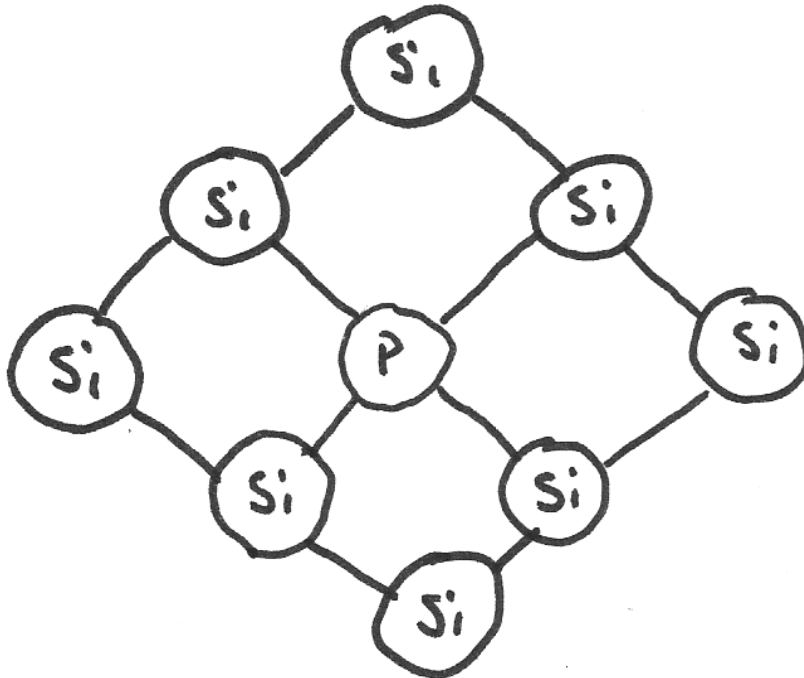
The introduction of impurity atoms that can add electrons or holes is called doping.

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.

	IIIA	IVA	VA	VIA	
	5 B	6 C	7 N	8 O	
	13 Al	14 Si	15 P	16 S	
IIB	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

$$E_n = -\frac{me^4}{8\epsilon_0^2 h^2 n^2}$$

Ionization energy is smaller by a factor: $\frac{m^*}{m} \left(\frac{\epsilon_0}{\epsilon_r \epsilon_0} \right)^2$

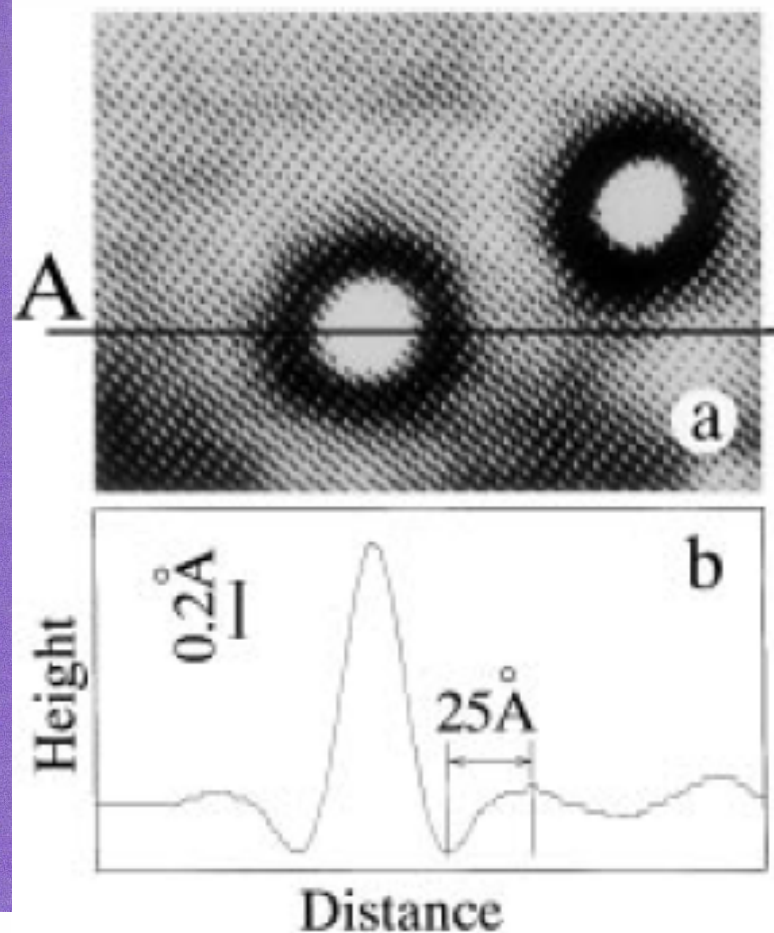
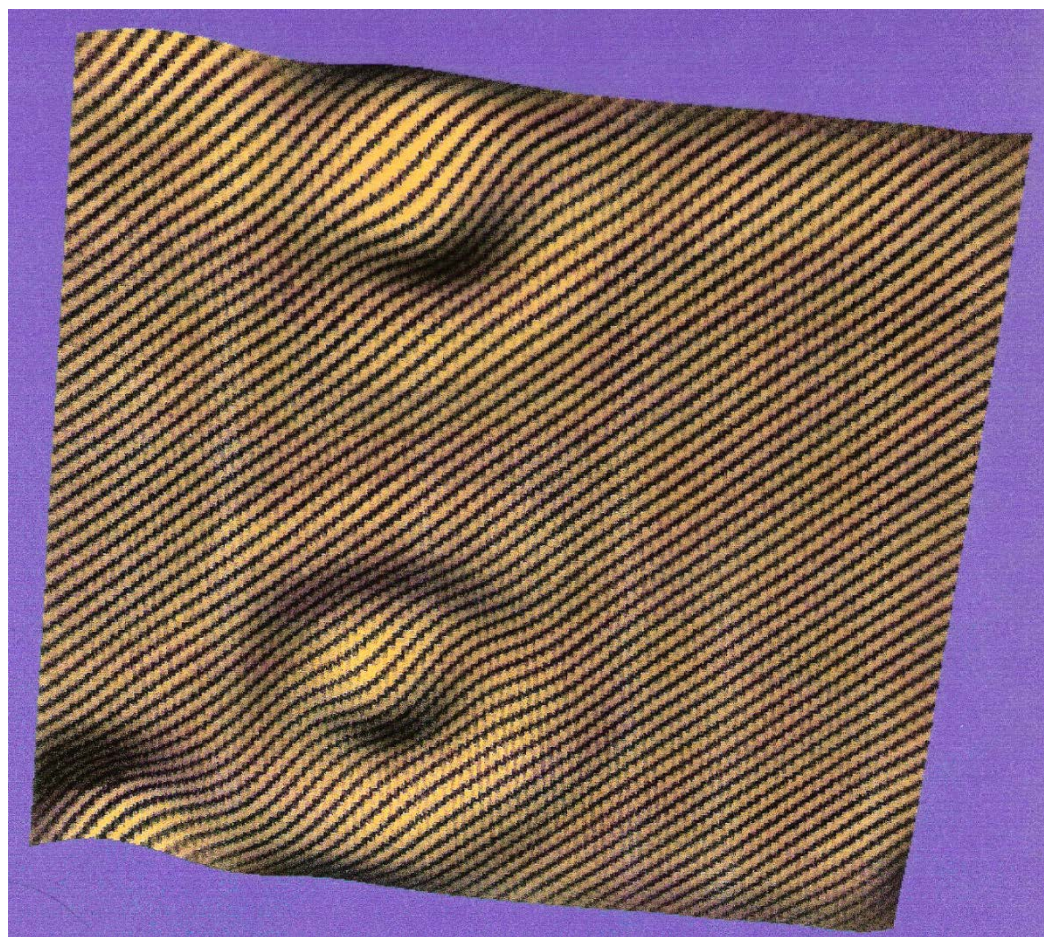
Ionization energy ~ 25 meV

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

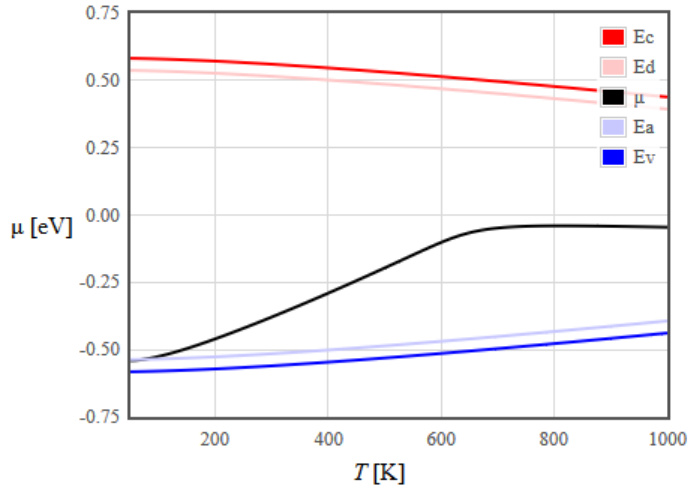
Research Institute for Materials, University of Nijmegen, Toernooiveld 1, 6525 ED Nijmegen, The Netherlands

(Received 25 July 1995)



Extrinsic semiconductors (Boltzmann approximation)

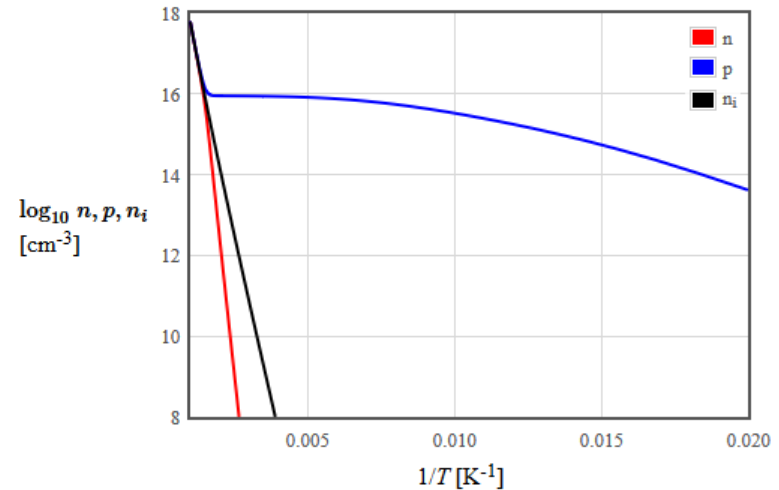
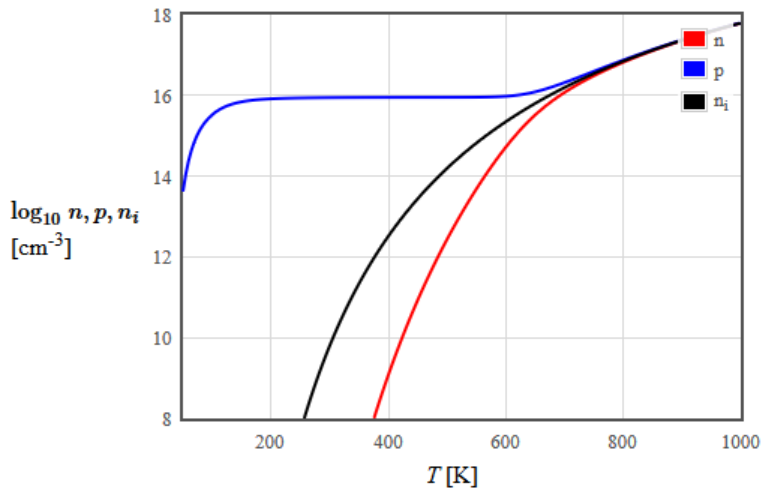
The chemical potential μ of an extrinsic semiconductor is plotted as a function of temperature. At each temperature the chemical potential was calculated by requiring that [charge neutrality](#) be satisfied.



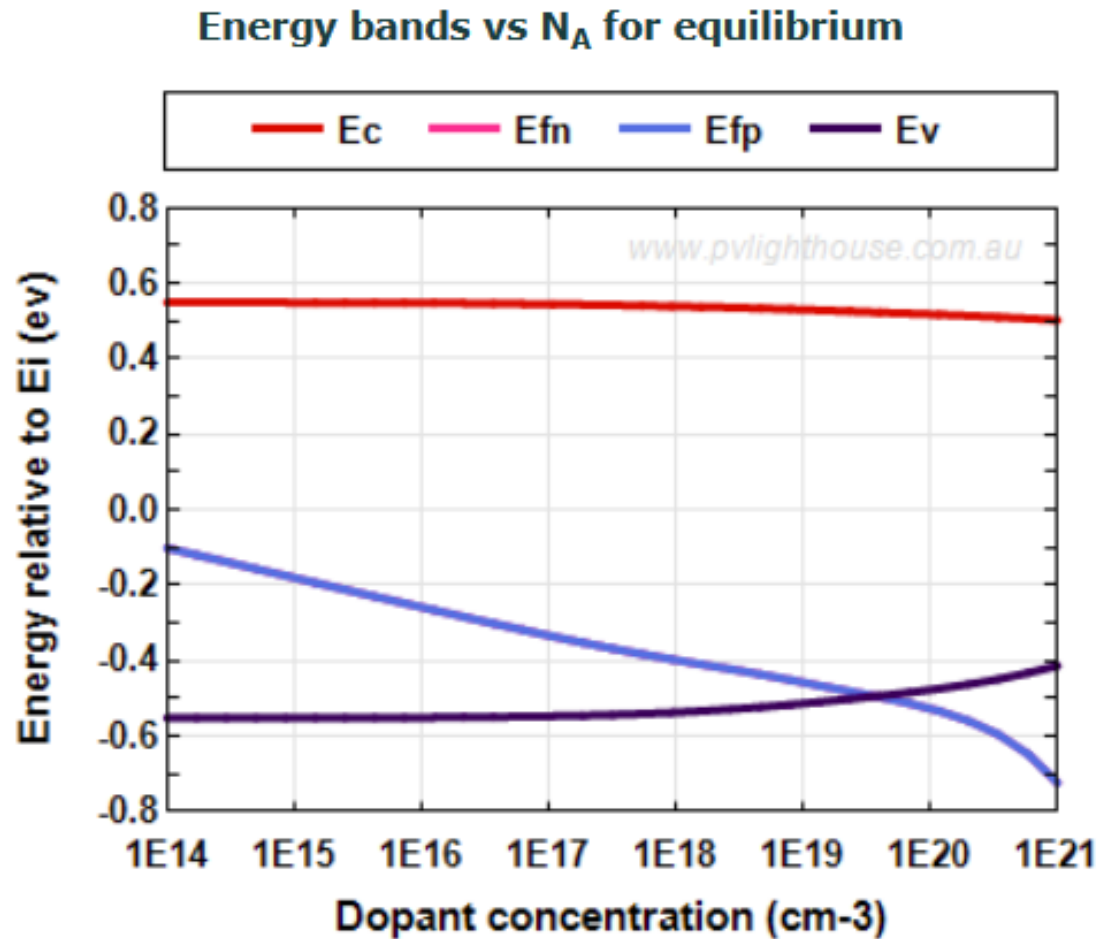
$N_c(300\text{ K}) = 2.78\text{E}19$	1/cm ³	Semiconductor <input type="button" value="Si"/> <input type="button" value="Ge"/> <input type="button" value="GaAs"/>
$N_v(300\text{ K}) = 9.84\text{E}18$	1/cm ³	
$E_g = 1.166-4.73\text{E-}4*T*(T+636)$	eV	
$N_d = 1\text{E}15$	1/cm ³	Donor <input type="button" value="P in Si"/> <input type="button" value="P in Ge"/> <input type="button" value="Si in GaAs"/>
$E_c - E_d = 0.045$	eV	
$N_a = 1\text{E}16$	1/cm ³	Acceptor <input type="button" value="B in Si"/> <input type="button" value="B in Ge"/> <input type="button" value="Si in GaAs"/>
$E_a - E_v = 0.045$	eV	
$T_1 = 50$	K	
$T_2 = 1000$	K	
<input type="button" value="Replot"/>		

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

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



Bandgap narrowing



Drift

drift velocity: $\vec{v}_{d,n} = -\mu_n \vec{E}$ $\vec{v}_{d,p} = \mu_p \vec{E}$

$$\vec{j} = -ne\vec{v}_{d,n} + pe\vec{v}_{d,p} = (ne\mu_n + pe\mu_p) \vec{E} = \sigma \vec{E}$$

$$\mu = \frac{-e\tau_{sc}}{m^*} = \frac{-e\ell}{m^* v}$$

for Si: $\mu_n = 1500 \text{ cm}^2/\text{Vs}$
 $\mu_p = 450 \text{ cm}^2/\text{Vs}$

For $E = 1000 \text{ V/cm}$ $v_d = 10^6 \text{ cm/s}$

Drift

		E_g (eV)	μ_n (cm ² /V-s)	μ_p (cm ² /V-s)	m_n^*/m_0 (m_l, m_t)	m_p^*/m_0 (m_{lh}, m_{hh})	a (Å)	ϵ_r	Density (g/cm ³)	Melting point (°C)
Si	(i/D)	1.11	1350	480	0.98, 0.19	0.16, 0.49	5.43	11.8	2.33	1415
Ge	(i/D)	0.67	3900	1900	1.64, 0.082	0.04, 0.28	5.65	16	5.32	936
SiC (α)	(i/W)	2.86	500	—	0.6	1.0	3.08	10.2	3.21	2830
AlP	(i/Z)	2.45	80	—	—	0.2, 0.63	5.46	9.8	2.40	2000
AlAs	(i/Z)	2.16	1200	420	2.0	0.15, 0.76	5.66	10.9	3.60	1740
AlSb	(i/Z)	1.6	200	300	0.12	0.98	6.14	11	4.26	1080
GaP	(i/Z)	2.26	300	150	1.12, 0.22	0.14, 0.79	5.45	11.1	4.13	1467
GaAs	(d/Z)	1.43	8500	400	0.067	0.074, 0.50	5.65	13.2	5.31	1238
GaN	(d/Z, W)	3.4	380	—	0.19	0.60	4.5	12.2	6.1	2530
GaSb	(d/Z)	0.7	5000	1000	0.042	0.06, 0.23	6.09	15.7	5.61	712
InP	(d/Z)	1.35	4000	100	0.077	0.089, 0.85	5.87	12.4	4.79	1070
InAs	(d/Z)	0.36	22600	200	0.023	0.025, 0.41	6.06	14.6	5.67	943
InSb	(d/Z)	0.18	10 ⁵	1700	0.014	0.015, 0.40	6.48	17.7	5.78	525
ZnS	(d/Z, W)	3.6	180	10	0.28	—	5.409	8.9	4.09	1650*
ZnSe	(d/Z)	2.7	600	28	0.14	0.60	5.671	9.2	5.65	1100*
ZnTe	(d/Z)	2.25	530	100	0.18	0.65	6.101	10.4	5.51	1238*
CdS	(d/W, Z)	2.42	250	15	0.21	0.80	4.137	8.9	4.82	1475
CdSe	(d/W)	1.73	800	—	0.13	0.45	4.30	10.2	5.81	1258
CdTe	(d/Z)	1.58	1050	100	0.10	0.37	6.482	10.2	6.20	1098
PbS	(i/H)	0.37	575	200	0.22	0.29	5.936	17.0	7.6	1119
PbSe	(i/H)	0.27	1500	1500	—	—	6.147	23.6	8.73	1081
PbTe	(i/H)	0.29	6000	4000	0.17	0.20	6.452	30	8.16	925

$$\vec{v}_{d,n} = -\mu_n \vec{E} \quad \vec{v}_{d,p} = \mu_p \vec{E}$$

$$\vec{j} = -ne\vec{v}_{d,n} + pe\vec{v}_{d,p} = (ne\mu_n + pe\mu_p) \vec{E} = \sigma \vec{E}$$

Mobility calculator

INPUTS

Semiconductor material	c-silicon	Excess electron conc. Δn	1	cm ⁻³
Dopant atom	boron	Excess hole conc. Δp	1	cm ⁻³
Ionised dopant conc. N_{dop}	1E+16	Electron eff. lifetime $\tau_{eff\ e}$	1E-4	s
Temperature T	300	Hole eff. lifetime $\tau_{eff\ h}$	1E-4	s

OUTPUTS

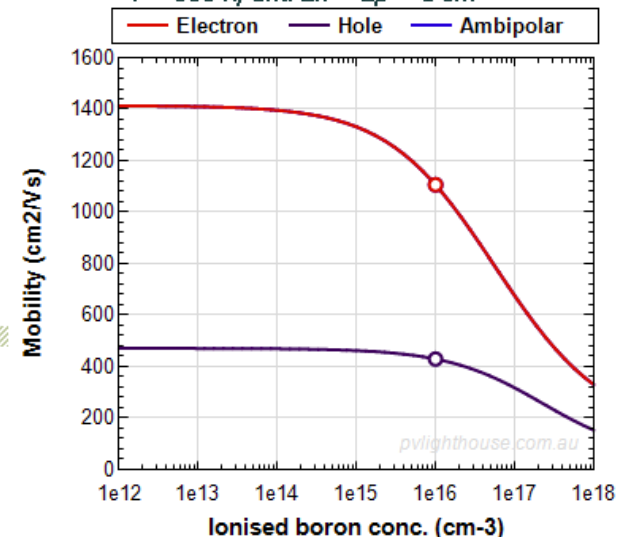
	Carrier concentrations			Carrier mobility etc.		
	Equilibrium n_0, p_0 (cm ⁻³)	Excess $\Delta n, \Delta p$ (cm ⁻³)	Net n, p (cm ⁻³)	Mobility μ_e, μ_h, μ_a (cm ² V ⁻¹ s ⁻¹)	Diffusivity D_e, D_h, D_a (cm ² s ⁻¹)	Diff Length L_e, L_h, L_a (cm)
Electrons	9300	1.0	9300	1107	28.61	5.349E-2
Holes	1.0E+16	1.0	1.0E+16	429.3	11.10	3.331E-2
Ambipolar				1107	28.61	5.349E-2

	Resistivity (Ω -cm)	
Equilibrium ρ_0		1.454
Steady-state ρ		1.454

Figure inputs

Y-axis	Mobility
X-axis	Ionised dopant conc.
First x	1E+12 cm ⁻³
Last x	1E+18 cm ⁻³
Data points	50

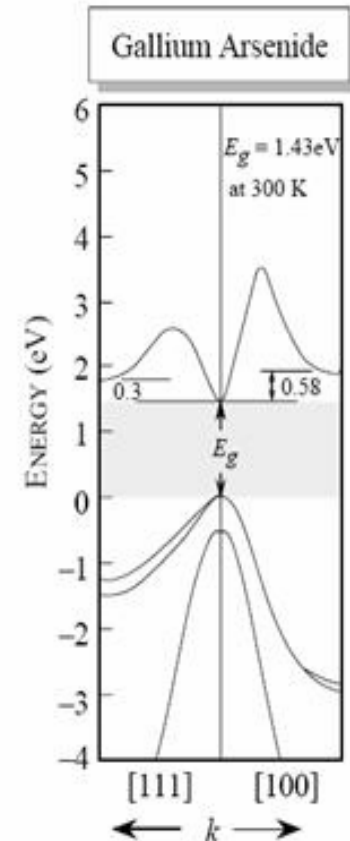
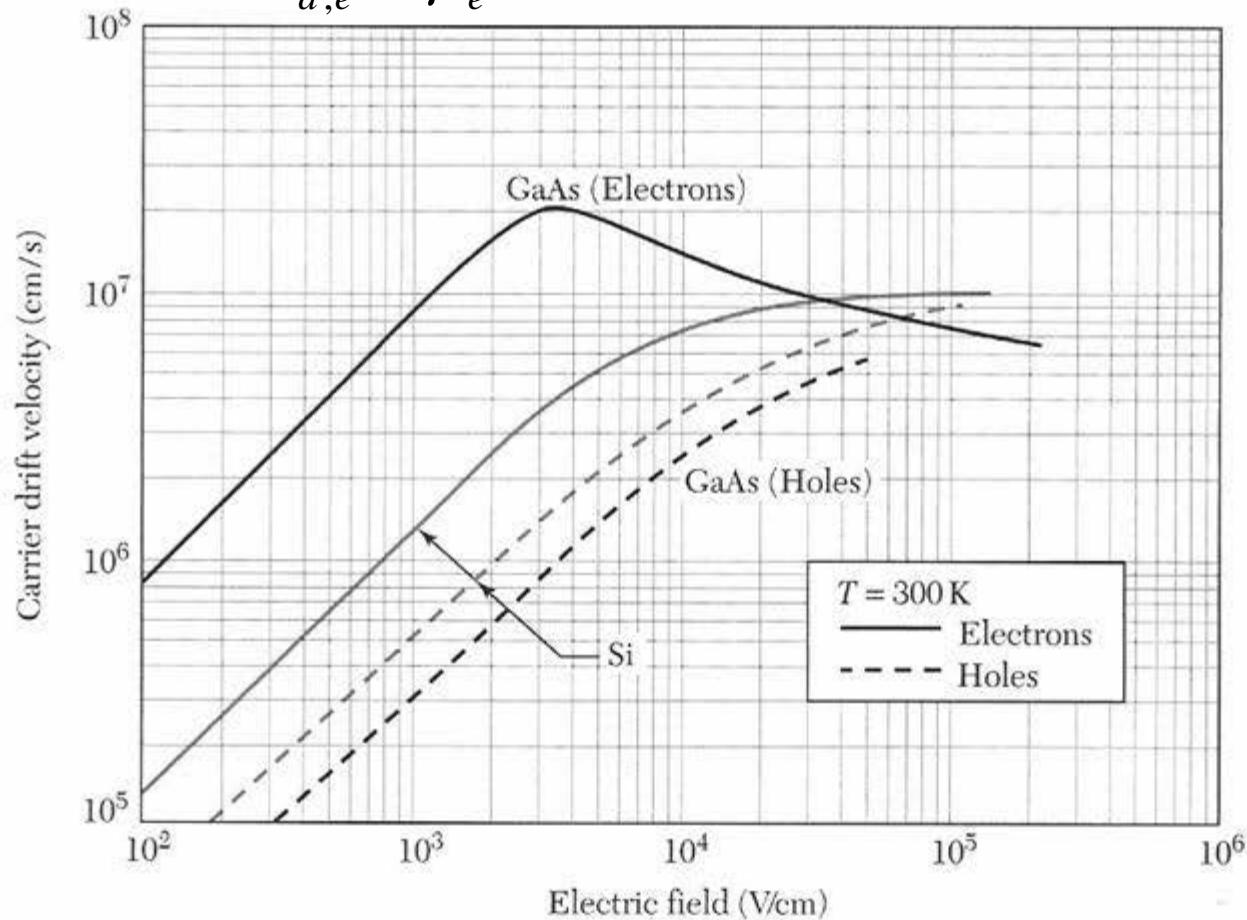
Mobility vs ionised dopant concentration for boron-doped c-silicon with $T = 300\text{ K}$, and $\Delta n = \Delta p = 1\text{ cm}^{-3}$



High fields

$$\vec{v}_{d,e} = \mu_e \vec{E}$$

$$\vec{v}_{d,h} = \mu_h \vec{E}$$



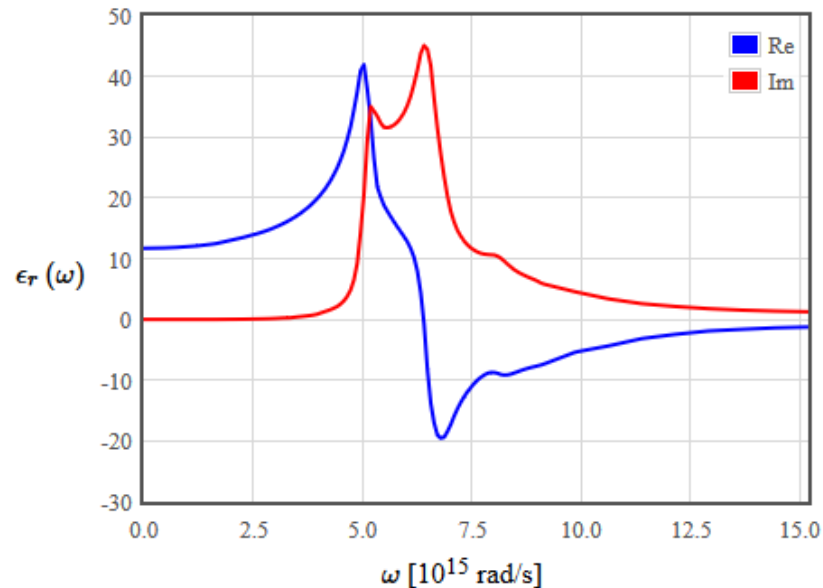
Emission of optical phonons causes the saturation of electron velocity. There are no semiconductors without optical phonons.

The optical properties of silicon

D. E. Aspnes and A. A. Studna, Phys. Rev. B 27, 985-1009 (1983) nanophotonics.csic.es

Dielectric function

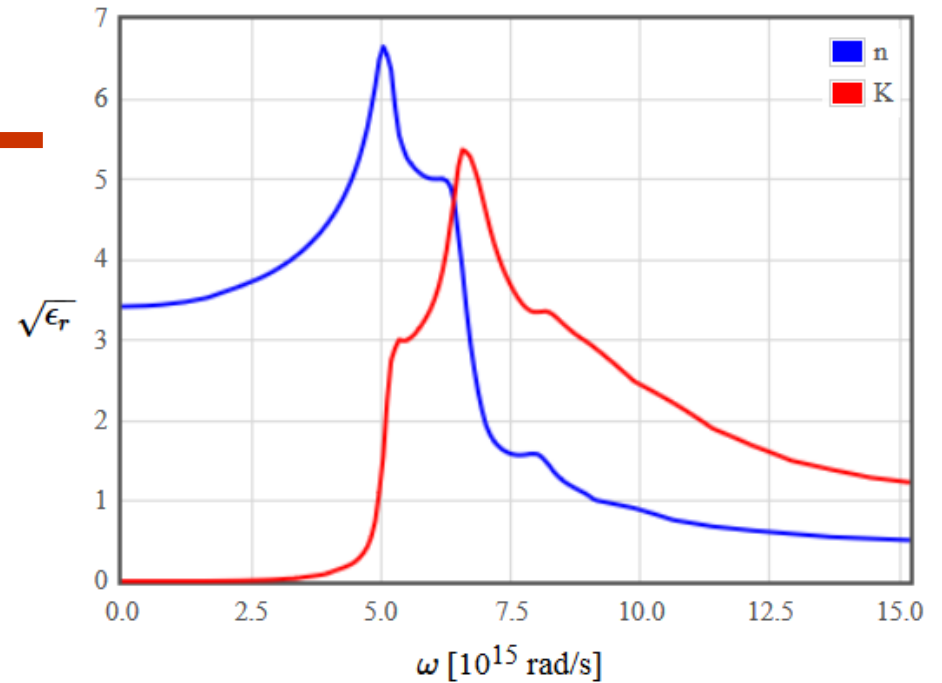
The relative dielectric function describes the relationship between the electric displacement \vec{D} and the electric field \vec{E} , $\vec{D} = \epsilon_r \epsilon_0 \vec{E} = \vec{P} + \epsilon_0 \vec{E}$.



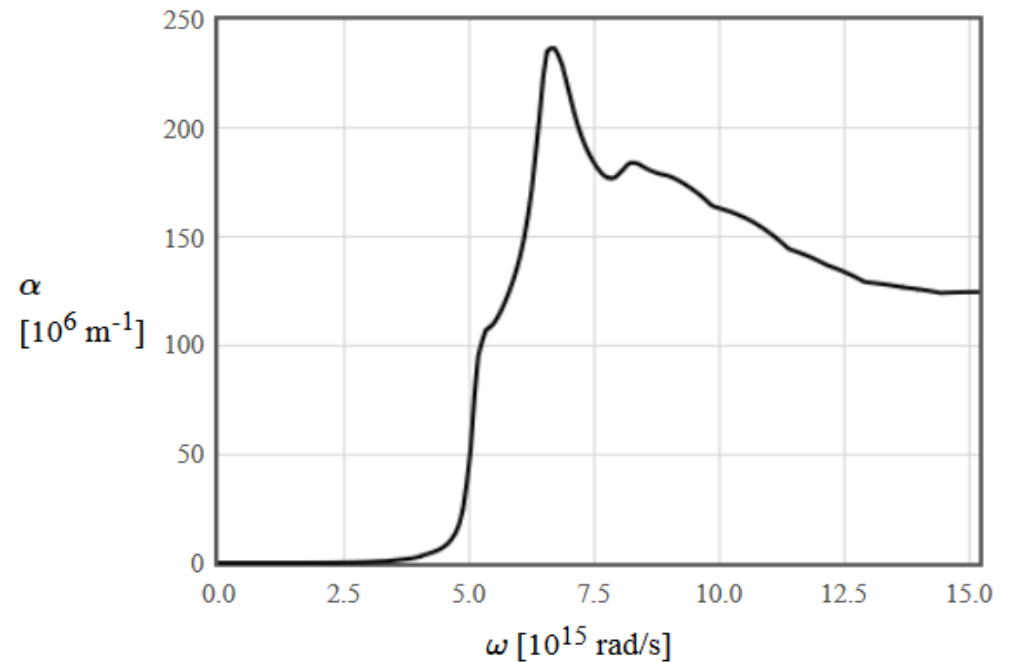
There are two conventions for dielectric function. Either it is assumed that the time dependence of \vec{D} , \vec{P} , and \vec{E} is $\exp(-i\omega t)$ and the plot of the dielectric function looks as it is shown above, or it is assumed that the time dependence of \vec{D} , \vec{P} , and \vec{E} is $\exp(i\omega t)$ and the imaginary part of the has the opposite sign as in the plot above. Here we will assume a time dependence of $\exp(-i\omega t)$.

Optical properties

Index of refraction
Extinction coefficient

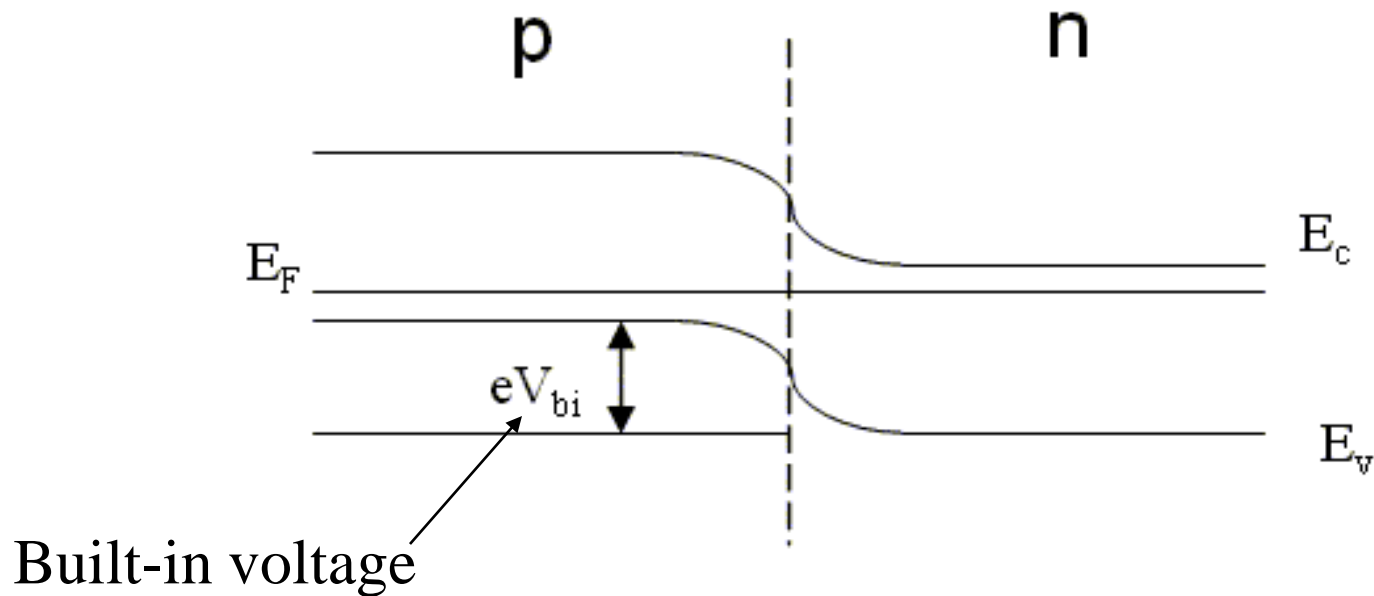


Absorption coefficient



pn junction

semiconductors in contact



Abrupt junction: the doping changes abruptly from p to n

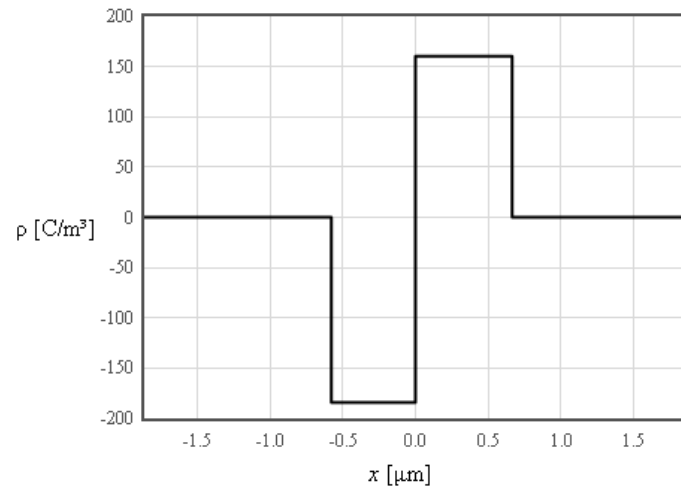
$$eV_{bi} = k_B T \ln \left(\frac{N_D N_A}{n_i^2} \right)$$

Abrupt pn junctions in the depletion approximation

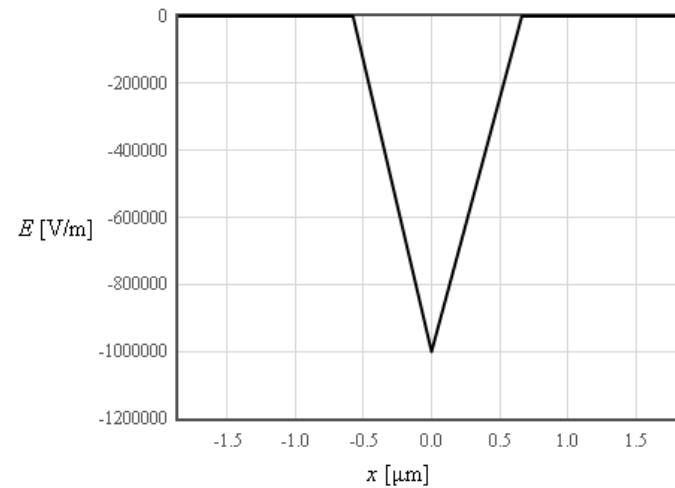
In an abrupt pn junction, the doping changes abruptly from p to n. It is common to solve for the band bending, the local electric field, the carrier concentration profiles, and the local conductivity in the depletion approximation. In this approximation it is assumed that there is a depletion width W around the transition from p to n where the charge carrier densities are negligible. Outside the depletion width the charge carrier densities are equal to the doping densities so that the semiconductor is electrically neutral outside the depletion width. Using this approximation it is possible to calculate the important properties of the pn junction.

$N_A =$ $1/\text{cm}^3$ $N_D =$ $1/\text{cm}^3$ $T =$ K

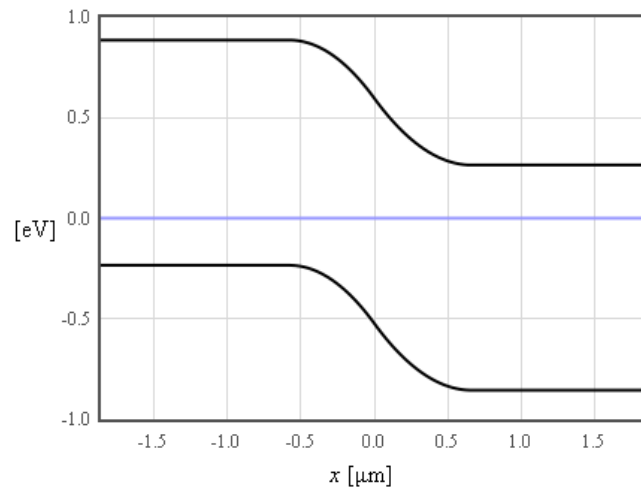
Charge density



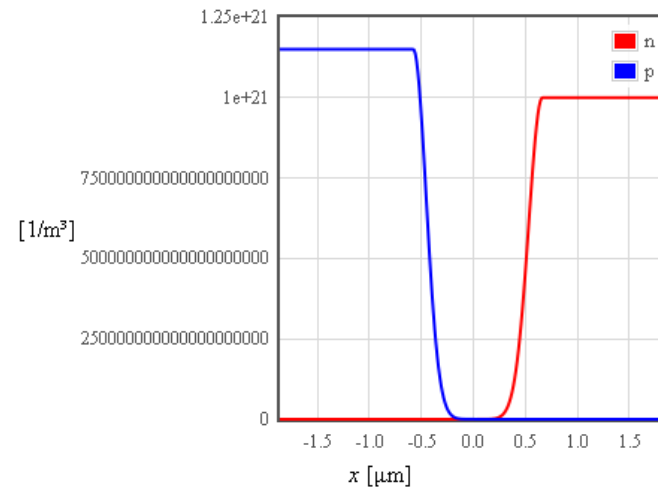
Electric field



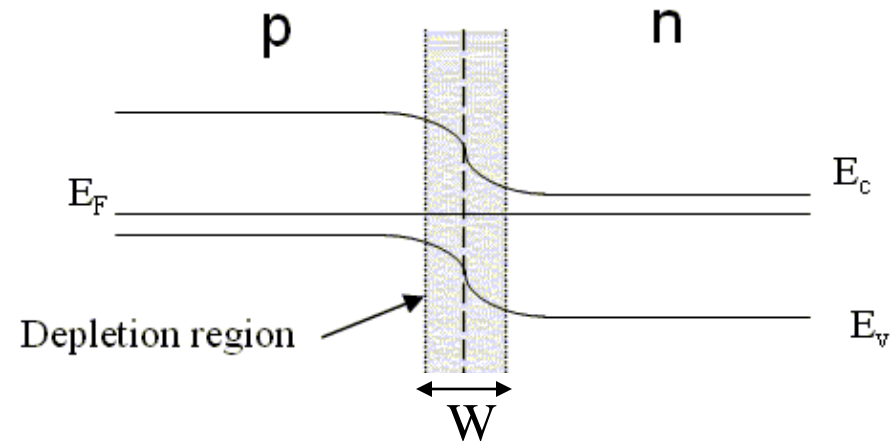
Band diagram



Carrier densities



Depletion width



$$V_{bi} \sim 1\text{V}$$

$$W \sim 1\mu\text{m}$$

$$E_{max} \sim 10^4\text{ V/cm}$$

$$v_{sat} \sim 10^7\text{ cm/sec}$$

The electric field pushes the electrons towards the n-region and the holes towards the p-region.

Diffusion sends electrons towards the p-region and holes towards the n-region.

Diodes

solar cells

Photodetectors

LEDs

laser diodes (CD, AFM, bar code)

signal diodes

surge protection

Zener diodes

thermometers

variable capacitors

$$I = I_s \left(\exp\left(\frac{eV}{k_B T}\right) - 1 \right)$$

