Carrier density of intrinsic semiconductors

Calculation result & code

$$n_i = \sqrt{N_c N_p}\exp(-\frac{\epsilon_g}{2k_B T})$$

n_i: carrier density

ϵ_g: band gap

$N_c = \frac{2(2\pi m_e^* k_B T)^{3/2}}{h^3}$: effective density of electron state

$N_p = \frac{2(2\pi m_p^* k_B T)^{3/2}}{h^3}$: effective density of hole state

m_e^*: effective mass of the electron

m_p^*: effective mass of the hole

In [1]:
```
%matplotlib inline
import math
import numpy as np
from __future__ import division
import matplotlib.pyplot as plt
import scipy.signal as sig
import scipy.constants as const
from IPython.display import display, Image, display_jpeg
import scipy.optimize as optim

# Update the matplotlib configuration parameters:
plt.rcParams.update({'font.size': 22, 'font.family': 'serif'})
plt.rc('ytick.major', size=8)
plt.rc('ytick.minor', size=4)
plt.rc('xtick.major', size=8)
plt.rc('xtick.minor', size=4)
```

In [2]:
```
# Physical constants

h  = 6.626e-34 # Planck constant
m0 = 9.109e-31 # electron mass
e  = 1.602e-19 # electron charge
kb = 1.381e-23 # Boltzman constant
```

In [3]:
```
# empirical function of bandgap as a function of the temperature
# http://ecee.colorado.edu/~bart/book/eband5.htm
# Justification Appl Phys Lett 58 (1991) 2924-2926 http://dx.doi.org/10.1063/
1.104723

def eg(T, eg0, a, b):
    y = eg0 - a*T*T/(T+b)

    return y
```

In [4]:
```
# Silicon bandgap parameters
# http://ecee.colorado.edu/~bart/book/eband5.htm
eg0Si = 1.166   # eV
aSi   = 4.73e-4 # eV/K
bSi   = 636     # K

# Temperature
T = np.array([120, 300])

egSi = eg(T, eg0Si, aSi, bSi)
```

In [5]:
```
# Effective masses
# http://ecee.colorado.edu/~bart/book/effmass.htm
me = 1.08*m0   # effective mass of the electron
mp = 0.81*m0   # effective mass of the hole

Nc = (2*pow(2*np.pi*me*kb*T,3/2))/pow(h,3)
Np = (2*pow(2*np.pi*mp*kb*T,3/2))/pow(h,3)
```

In [6]:
```
ni = np.sqrt(Nc*Np)*np.exp(-egSi*e/(2*kb*T)) # number per m^3
ni_cm3 = ni/1e6
```

In [7]:
```
print ni_cm3

# Carrier density of intrinsic Silicon [/cm^3]
# at 120K and 300K
```

```
[  2.96734315e-06   8.86416411e+09]
```

Limitation

Here the calculation has been done with the fixed m_e^* and m_p^*. There is some temperature dependence of them on the temperature. However, it is outside of the exponential, it only has a small effect. About the temperature dependence of the electron/hall effective mass, refer the following paper

Intrinsic concentration, effective densities of states, and effective mass in silicon, Martin A. Green, J. Appl. Phys. 67, 2944 (1990); http://dx.doi.org/10.1063/1.345414 (http://dx.doi.org/10.1063/1.345414)

Derivation

State density, Fermi distribution, Fermi energy

State density of free electrons (number of states in a unit volme) is expressed as

$$\rho(\epsilon) = \frac{\pi}{2}\left(\frac{8m_e}{h^2}\right)^{3/2}\sqrt{\epsilon}$$

where, ϵ: state energy, m_e: electron mass, h: Planck constant

Fermi distribution: Electrons follow Fermi distribution $f(\epsilon)$

$$f(\epsilon) = \frac{1}{1+\exp(\frac{\epsilon-\epsilon_F}{k_B T})}$$

where, ϵ_F: Fermi energy, k_B: Boltzman constant, T: temperature of the system

Fermi level ϵ: $f(\epsilon)$ describes how much fraction of the states are occupied for the given temperature T. When T is zero, $f(\epsilon)$ becomes a step function and the states are occupied from the bottom.

i.e. for a given number of electron number density of N, the Fermi level ϵ_F becomes

$$\epsilon_F = \frac{h^2}{8m_e}\left(\frac{3N}{\pi}\right)^{2/3}$$

It is said that metal has $N = 10^{22} \sim 10^{23}$. This yields $\epsilon_F = 1.7 \sim 7.9eV$, while $k_B T$ is much lower (0.026eV@300K). Therefore we can assume that almost all conductve electrons for metals are degenerate.

Electron/hole density of intrinsic semiconductors

In a semiconductor crystal, the electron behaves like unbound once it is excited from the valence band. So the effective energy of electron is $\epsilon - \epsilon_c$ where ϵ_c is the bottom energy of the conduction band. The mass of the electron m_e must be replaced with an effective mass of the electon m_e^*. The carrier elecron state density can be written as:

$$\rho_e(\epsilon) = \frac{\pi}{2}\left(\frac{8m_e^*}{h^2}\right)^{3/2}\sqrt{\epsilon-\epsilon_c}$$

The hole where the excited electon is lost behaves like a free carrier too. e-k relationship is just flipped upside down. The top energy of the valence band ϵ_V behaves as the ''bottom'' of the band for holes. Also holes behave as Fermion ($f_p(\epsilon) = 1 - f(\epsilon)$ has the Fermi distribution). The carrier hole state density can be written as:

$$\rho_p(\epsilon) = \frac{\pi}{2}\left(\frac{8m_p^*}{h^2}\right)^{3/2}\sqrt{\epsilon_v-\epsilon}$$

The carrier electron and hole density n and n_p can be obtained by the following integrals:

$$n = \int_{\epsilon_C}^{\infty} \rho(\epsilon)f(\epsilon)d\epsilon,\ f(\epsilon) = \frac{1}{1+\exp(\frac{\epsilon-\epsilon_F}{k_B T})}$$

$$n_p = \int_{-\infty}^{\epsilon_V} \rho_p(\epsilon)f_P(\epsilon)d\epsilon,\ f_p(\epsilon) = \frac{1}{1+\exp(\frac{\epsilon_F-\epsilon}{k_B T})}$$

For intrinsic semiconductors, the band gap is the order of 1eV. Therefore we can use the low temperature approximation. i.e. if $\epsilon - \epsilon_F \gg k_B T, f(\epsilon) = \exp(-\frac{\epsilon - \epsilon_F}{k_B T})$ (Boltzman distribution). This makes the integration easier.

$$n = \int_{\epsilon_c}^{\infty} \frac{\pi}{2}\left(\frac{8m_e^*}{h^2}\right)^{3/2} \sqrt{\epsilon - \epsilon_c}\, \exp\left(-\frac{\epsilon - \epsilon_F}{k_B T}\right) d\epsilon$$

$$= N_c \exp\left(-\frac{\epsilon_c - \epsilon_F}{k_B T}\right), \ N_c = \frac{2(2\pi m_e^* k_B T)^{3/2}}{h^3}$$

Similarly, n_p is given as

$$n_p = N_p \exp\left(-\frac{\epsilon_F - \epsilon_v}{k_B T}\right), \ N_p = \frac{2(2\pi m_p^* k_B T)^{3/2}}{h^3}$$

N_c and N_p are called effective density of electron (or hole) state, respectively.

Using the fact $n_p = n(\equiv n_i)$, we can figure out the carrier density of an intrinsic semiconductor n_i without knowing the Fermi level.

$$n_i = \sqrt{N_c N_p}\, \exp(-\frac{\epsilon_g}{2k_B T}), \quad (\epsilon_g = \epsilon_c - \epsilon_v)$$

Fermi level: By taking logarithmic of $n = n_p$, we obtain

$$\epsilon_F = \frac{\epsilon_c + \epsilon_v}{2} + \frac{3k_B T}{4} \ln \frac{m_p^*}{m_e^*}$$

For the silicon case, temperature dependence is $-1.9 \times 10^{-5} T$ [eV], and it is negligible