Carrier density of doped semiconductors

Conclusion

The conclusion is simple:

With lightly doped ($< 10^{16}/\mathrm{cm}^3$) n-type Silicon down to 120K, we can assume all of the doping sites are ionized, and therefore $n = n_d$.

Introduction

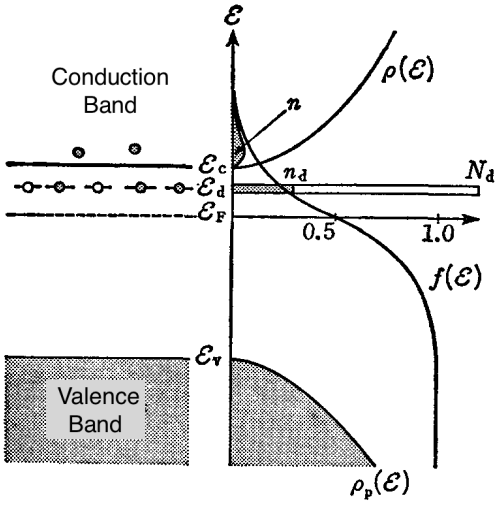
The calculation of the carrier density is similar to the case of instrinsic semiconductors. For doped semiconductors, however, the donor level (or the acceptor level) is too close to the conduction band (or the valence band) to use the approximation of the state distribution with the Boltzman distribution. Therefore, we need numerical integration (or polylog function) for the calculation of the carrier density and the Fermi level.

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
```

N-type semiconductor

In [2]:
```
fig1 = Image('./Notebook_figures/doped_silicon_N.png', width ='50%')
fig1
```

Out[2]:



Assume an N-type semiconductor. The dopant concentration is N_d. i.e. There are N_d sites.

A single site can accept only one electron whose spin can be up or down. This situation is different from the case of the usual state which is occupied by an electron with a certain spin. Therefore the distribution of the electron for the donor level is modified as follows (refer http://ecee.colorado.edu/~bart/book/distrib.htm#impurity (http://ecee.colorado.edu/~bart/book/distrib.htm#impurity) section 2.4.4)

$$f_d(\epsilon_D) = \frac{1}{1 + \frac{1}{2} e^{(\epsilon_d - \epsilon_F)/(k_B T)}}$$

Here the Fermi level ϵ_F is to be determined later.

The number of the electrons n_d that stay on the donor level is

$$n_d = N_d \frac{1}{1 + \frac{1}{2} e^{(\epsilon_d - \epsilon_F)/(k_B T)}}$$

Note: this factor 1/2 seems to be modified to 4 for the case of the acceptor. Refer the same link above.

Concequently, **the number of excited electrons in the conduction band** is

$$n \equiv N_d - n_d = \frac{N_d}{1 + 2e^{(\epsilon_F - \epsilon_d)/(k_B T)}} \quad \cdots (\mathrm{A})$$

Now we consider the distribution of the electrons in the conduction band:

This can be done similarly to the case for intrinsic semiconductors.

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

$$n = \int_{\epsilon_c}^{\infty} \frac{\pi}{2}\left(\frac{8m_e^*}{h^2}\right)^{3/2} \sqrt{\epsilon-\epsilon_c}\, \frac{1}{1+\exp(\frac{\epsilon-\epsilon_F}{k_B T})} d\epsilon$$

$$= \int_{0}^{\infty} \frac{\pi}{2}\left(\frac{8m_e^*}{h^2}\right)^{3/2} \sqrt{\epsilon}\, \frac{1}{1+\exp(\frac{\epsilon+(\epsilon_c-\epsilon_F)}{k_B T})} d\epsilon$$

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

where $\mathrm{Li}_n(x)$ is a polylogarithm function:

$$\mathrm{Li}_n(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^n}$$

The Fermi level is determined by the relationship (A) = (B), and the n for this Fermi level is the carrier concentration.

First order approximation: i.e. when $|\epsilon_c - \epsilon_F| \gg k_B T$

$$\frac{N_d}{1+2e^{-(\epsilon_d-\epsilon_F)/(k_B T)}} = N_c\ \exp(-\frac{\epsilon_c-\epsilon_F}{k_B T})$$

$$\frac{N_d}{N_c} = e^{-(\epsilon_c-\epsilon_F)/(k_B T)} + 2e^{-(\epsilon_d+\epsilon_c-2\epsilon_F)/(k_B T)}$$

By solving this we obtain ϵ_F. Then this leads us to calculate n. With the same approximation, the first term approaches to the unity and can be ignored. Therefore $epsilon_F$ at the low temperature can be expressed as:

$$\epsilon_F = \frac{\epsilon_c+\epsilon_d}{2} - \frac{k_B T}{2}\ln\frac{2N_c}{N_d}$$

This yield the carrier density of

$$n = \frac{N_d}{1+\sqrt{2N_d/N_c}\exp(\epsilon_g/(2k_B T))},\quad \epsilon_g = \epsilon_c - \epsilon_d$$

When the approximation is not applicable (i.e. at the room temp), the equation (A)=(B) needs to be solved numerically.

Numerical evaluation

Actual calculation is done with the mathematica file in the same folder.

Assumptions:

N_c: $2.8 \times 10^{19} \left(\frac{T}{300} \right)^{3/2} [1/\text{cm}^3]$

k_B: 0.026/300eV/K

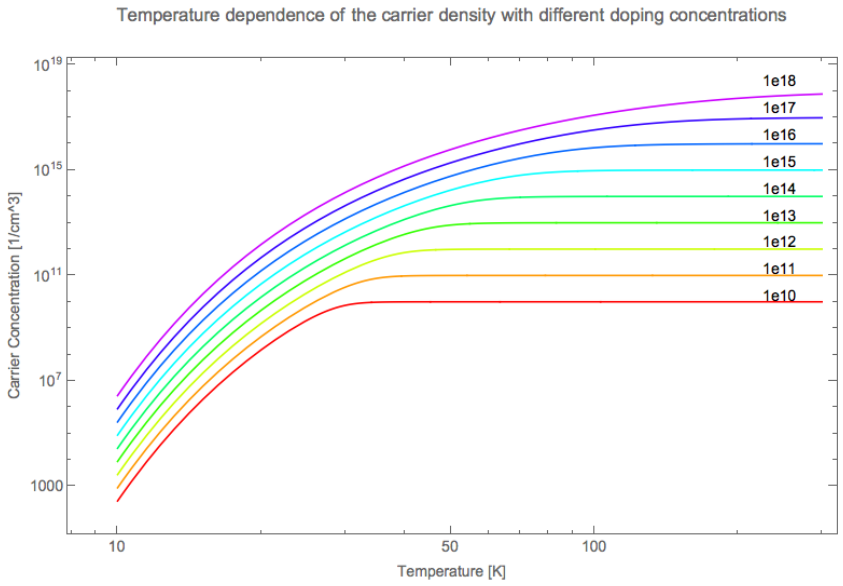
$\epsilon_c = \epsilon_g/2$

$\epsilon_d = -\epsilon_g/2$

$\epsilon_g = 0.044[\text{eV}]$ --- typical donor level of P doped silicon

In [3]:
```
fig2 = Image('./Notebook_figures/CarrierFreezeOut_CarrierDensity.png', width
='80%')
fig2
```

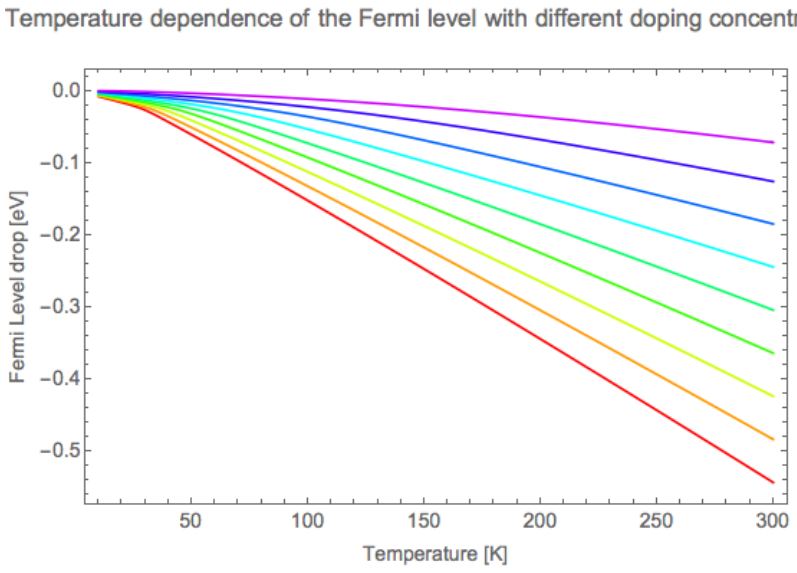
Out[3]:



The above plot shows the temperature dependence of the carrier concentration as a function of the temperature for different doping concentration levels. The numbers in the plot shows the doping concentration. As the concentration is larger, the carrier freeze out temperature goes higher. For the doping concentration less than $10^{16}/\text{cm}^3$, we can assume that all dopants are ionized i.e. $n = n_d$ at 120K.

In [4]:
```
fig3 = Image('./Notebook_figures/CarrierFreezeOut_FermiLevel.png', width ='80
%')
fig3
```

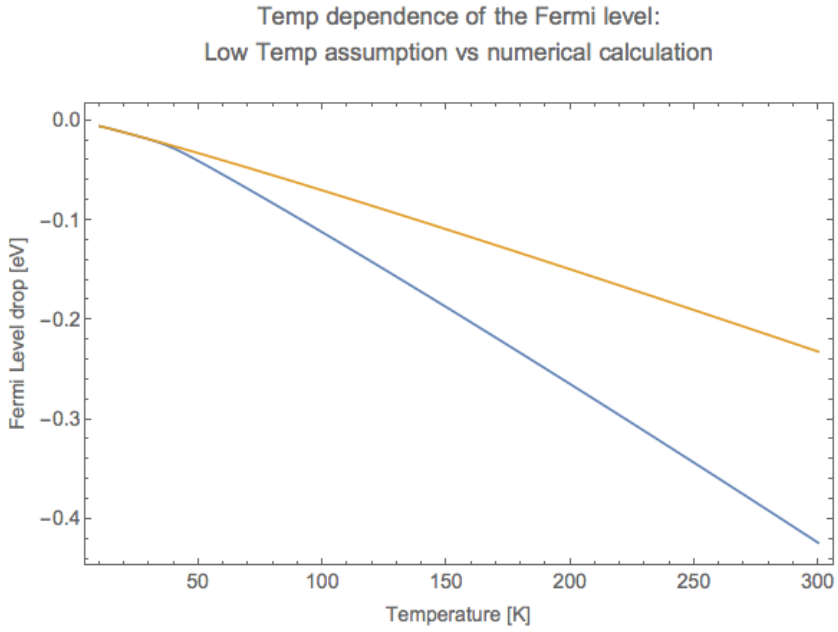
Out[4]:



For some curiosity, dependence of the Fermi level as a fuction of the doping level and temperature is plotted in the above figure. The color of the curves are assigned in the same way as the previous carrier density plot. The vertical axis shows how much the Fermi level drops from the average energy between the donor level and the bottom energy of the conduction band. As the doping concentration gets lower, the bending of the linear region of the curve comes at a lower temperature.

In [5]:
```
fig4 = Image('./Notebook_figures/CarrierFreezeOut_FermiLevel_Assumption.png',
 width ='80%')
fig4
```

Out[5]:



The above plot shows the comparison of the Fermi level as a function of the temperature for the doping concentration of $10^{12}/\mathrm{cm}^3$. The low temperature approximation is valid upto 40K. At 120K we definitely need to solve the equation including the polylog function.