Homework Set #1:

1. If for silicon at 27°C the effective densities of states at the conduction and valence band edges are $N_C=3.28\times(10^{19})$ cm^{-3} and $N_V=1.47\times(10^{19})$ cm^{-3}, respectively, and if at any temperature, the effective densities of states are proportional to $T^{3/2}$, calculate the intrinsic Fermi energy, E_i, relative to the midgap energy at −73°C, 27°C, and 127°C. Is it reasonable to approximate E_i as simply the midgap energy for all of these temperatures? At what temperature would the intrinsic Fermi energy differ from the midgap energy by 0.30 eV? Is this a physically realizable condition for crystalline silicon? (Boltzmann's constant$=8.61735\times(10^{-5})$ eV/°K)

The intrinsic Fermi energy is given by the expression:

$$E_i = \frac{1}{2}(E_C + E_V) + \frac{1}{2}kT\ln\frac{N_V}{N_C}$$

The midgap energy is just the average of the energies of the valence and conduction band edges. Hence, the first term on the right hand side is just the midgap energy. Now, if one defines ΔE_i as the difference between the intrinsic Fermi energy and midgap, one has:

$$\Delta E_i = \frac{1}{2}kT\ln\frac{N_V}{N_C}$$

The densities of states are assumed to be both proportional to $T^{3/2}$, therefore, the ratio is independent of temperature. Thus, one finds that:

$$\frac{N_V}{N_C} = \frac{1.47(10^{19})}{3.28(10^{19})} = 0.4482$$

$$\ln\frac{N_V}{N_C} = -0.8026$$

$$\frac{k}{2}\ln\frac{N_V}{N_C} = -3.459(10^{-5}) \text{ eV/°K}$$

Accordingly, it immediately follows that:
at −73°C(200°K), ΔE_F equals −0.0069 eV
at   27°C(300°K), ΔE_F equals −0.0104 eV
at 127°C(400°K), ΔE_F equals −0.0138 eV

The Fermi energy falls slightly below midgap because the density of conduction band states is more than twice as large as the density of valence band states. However, the band gap in silicon is more than 1 eV, therefore, even at relatively high temperature, the Fermi energy is less than 2% below the middle of the gap. Thus, it is reasonable for all of these temperatures to assume that the Fermi energy is in the middle of the gap.

Now, since the intrinsic Fermi energy always lies below midgap, if one assumes that ΔE_i is -0.30 eV, then one can solve for the corresponding temperature:

$$T = \frac{\Delta E_i}{\dfrac{k}{2}\ln\dfrac{N_V}{N_C}} = \frac{-0.30}{-3.459(10^{-5})} = 8673°\text{K}$$

Silicon melts at 1687°K and boils at 3528°K and, thus, <u>vaporizes</u> long before this temperature is reached, therefore, this is not a physically realizable situation.

2. Assuming that over the ambient temperature range –200°-500°C, the band gap energy for silicon is a function of absolute temperature according to the empirical formula:

$$E_g = -3(10^{-4})\times T + 1.20$$

where energy is in eV's, use data given in the preceding problem to find the intrinsic carrier concentration in silicon at –73°C, 27°C, and 127°C. Would you expect the conductivity of undoped silicon to increase or decrease as a function of temperature?

The intrinsic carrier concentration is given by the formula:

$$n_i^{\,2} = N_V N_C e^{-E_g/kT}$$

One takes the square root to obtain:

$$n_i = \sqrt{N_V N_C}\, e^{-E_g/2kT}$$

Again, the densities of states are proportional to $T^{\,3/2}$, however, the temperature dependence does not disappear since it is the <u>product</u> of the densities of states that enters into the equation. One can substitute to obtain:

$$n_i = \sqrt{1.47(10^{19})\times 3.28(10^{19})}\left(\frac{T}{300}\right)^{3/2} e^{-[-3(10^{-4})\times T+1.20]/2kT} = 4.226(10^{15})T^{3/2}e^{-[-3(10^{-4})\times T+1.20]/2kT}$$

Therefore, it immediately follows that:
  at –73°C(200°K), n_i equals $5.18(10^4)$ cm^{-3}

at 27°C(300°K), n_i equals 1.04(10¹⁰) cm⁻³
at 127°C(400°K), n_i equals 5.31(10¹²) cm⁻³

One expects that, as temperature increases the conductivity of <u>intrinsic</u> silicon will also increase just due to a large increase in the concentration of mobile carriers generated by thermal excitation alone. Naturally, a corresponding decrease in mobility due to lattice scattering must somewhat reduce this effect. However, for intrinsic silicon the exponential dependence of carrier concentration as a function of temperature dominates the relatively weak, power law dependence of mobility on temperature. In contrast, for <u>extrinsic</u> silicon, temperature does not increase mobile carrier concentrations significantly (until very high temperatures are reached) and mobility effects will dominate conductivity.

3a. Using the value of n_i obtained in the last problem and assuming complete impurity ionization, at 27°C determine the actual Fermi energy relative to the intrinsic Fermi energy for silicon doped with 2×(10¹³), 10¹⁶, and 5×(10¹⁸) acceptor atoms/cm³. Then, using the results obtained, check if this assumption is justifiable in all three cases.

Assuming Maxwell-Boltzmann statistics, the ratio of mobile carrier concentrations can be written as follows:

$$\frac{p}{n} = \frac{N_v}{N_c} \frac{e^{(E_v - E_F)/kT}}{e^{-(E_c - E_F)/kT}}$$

If one takes the natural logarithm of both sides of this expression, one obtains:

$$\frac{kT}{2} \ln \frac{p}{n} = \frac{E_c + E_v}{2} + \frac{kT}{2} \ln \frac{N_v}{N_c} - E_F$$

The first two terms are immediately recognizable as the Fermi energy for an intrinsic semiconductor, hence:

$$\frac{kT}{2} \ln \frac{p}{n} = E_i - E_F$$

Of course, as was found previously, E_i lies very close to the middle of the band gap. This expression is valid for extrinsically doped as well as intrinsic semiconductors. Thus, for fully ionized acceptor dopant of concentration, N_A:

$$p = N_A \qquad n = \frac{n_i^2}{N_A}$$

hence:

$$E_i - E_F = kT \ln \frac{N_A}{n_i}$$

Using the intrinsic carrier concentration value of $1.04(10^{10})$ *cm*$^{-3}$ *obtained in the preceding problem, one finds:*

for $2\times(10^{13})$ *acceptors* cm^{-3} $E_i - E_F$ *is 0.1955 eV*
for 10^{16} *acceptors* cm^{-3} $E_i - E_F$ *is 0.3561 eV*
for $5\times(10^{18})$ *acceptors* cm^{-3} $E_i - E_F$ *is 0.5168 eV*

At 27°C *according to the previous empirical formula, the bandgap in silicon is 1.11 eV, hence, half of the bandgap is 0.555 eV. Furthermore, it was shown previously that* E_i *lies 0.0104 eV below midgap, therefore, the difference between* E_i *and the valence band edge is 0.545 eV. Clearly, this implies that at the highest doping concentration, the Fermi level lies just 0.0282 eV above the valence band edge. Therefore, in this case the assumption of Maxwell-Boltzmann statistics for mobile carriers becomes suspect and the full Fermi-Dirac distribution function must give a much better description of carrier density. In contrast, Maxwell-Boltzmann statistics can be used for the two lower doping concentrations. To understand if complete ionization is a valid assumption consider part* **b**.

b. If the Fermi energy coincides exactly with the energy of the shallow acceptor states, what is the occupation probability and can dopant impurities be assumed to be completely ionized as in part **a**? Be sure to explain your reasoning clearly and take the acceptor states to lie 0.05 eV above the valence band edge.

If the Fermi level coincides exactly with the shallow acceptor states, then the Fermi-Dirac distribution implies that the occupation probability for these states should be exactly one half, i.e., shallow acceptor states are 50% occupied. Therefore, in this case the dopant atoms cannot be completely ionized.

Accordingly, in part **a** *for concentrations of* $2(10^{13})$ *and* 10^{16} *acceptor atoms/cm³ the Fermi level lies 0.2995 and 0.1389 eV above the acceptor states, respectively. Moreover, at* 27°C *kT has a nominal value of 0.0259 eV; hence for these dopant concentrations acceptor states are essentially fully occupied and the assumption of complete ionization remains applicable. However, for the highest concentration since the Fermi level lies 0.0218 eV* <u>below</u> *the acceptor states, they must be less than 50% occupied and, thus, the assumption of complete ionization cannot be valid for dopant concentration as high as* $5(10^{18})$ *acceptor atoms/cm³. In practice, a semiconductor doped at such a high concentration is said to be* <u>degenerate</u>.

c. What atomic species is the most practical acceptor dopant?

As a practical matter, boron is the most practical acceptor dopant. In principle, any Group III element substituted into the silicon lattice would work, viz., aluminum, gallium, indium, etc.; however, all other alternatives suffer from undesirable characteristics such as low solubility, high diffusivity, etc.

4. Consider a pure silicon crystal uniformly doped with $5\times(10^{15})$ boron atoms/cm³. What is the doping type (*n* or *p*)? If the lattice scattering contribution to carrier mobilities has the explicit absolute temperature dependence:

$$\mu_L = \mu_{300}\left(\frac{300}{T}\right)^{\nu}$$

where ν equals exactly 1.5 and μ_{300} is 480 cm²/volt sec for holes and 1400 cm²/volt sec for electrons and if the ionized impurity contribution to carrier mobilities has the explicit absolute temperature dependence:

$$\mu_I = \frac{\alpha}{C_I}\left(\frac{T}{300}\right)^{3/2}$$

where $\alpha=2.0\times(10^{20})$ per cm volt sec for holes and $4.5\times(10^{20})$ per cm volt sec for electrons and C_I is the *total* ionized impurity concentration, what, then is the resistivity of the silicon crystal at −73°C, 27°C, and 127°C? If an additional $2.5\times(10^{17})$ boron atoms/cm³ and $2.5(10^{17})$ phosphorus atoms/cm³ together are uniformly added to the crystal, what happens to carrier concentrations, mobilities, and resistivities at the three temperatures?

Clearly, this silicon is extrinsically doped p-type. The expression for the resistivity of a silicon crystal is given by the formula:

$$\rho = \frac{1}{q(n\mu_e + p\mu_h)}$$

At all of the temperatures but, perhaps, the highest one, the carrier concentration is completely dominated by the extrinsic doping and, therefore, since holes are the majority carriers, the resistivity is just determined by the hole mobility. Now, one can use the given formulae to calculate the hole mobilities at the three temperatures. First, one notes that the total hole or electron mobility is given by the formula:

$$\mu = \frac{1}{\mu_L^{-1} + \mu_I^{-1}}$$

hence:

$$\mu = \cfrac{1}{\cfrac{1}{\mu_{300}}\left(\cfrac{T}{300}\right)^{3/2} + \cfrac{C_I}{\alpha}\left(\cfrac{300}{T}\right)^{3/2}}$$

Thus, substituting the above parameters yield lattice and impurity contributions to the hole mobility as follows:
  at −73°C(200°K), μ_L *equals* 882 cm²/V sec; μ_I *equals* 21773 cm²/V sec
  at 27°C(300°K), μ_L *equals* 480 cm²/V sec; μ_I *equals* 40000 cm²/V sec
  at 127°C(400°K), μ_L *equals* 312 cm²/V sec; μ_I *equals* 61584 cm²/V sec
Clearly, at this doping level, the mobility is dominated by the lattice scattering mechanism.

The above results can be combined to give total hole mobilities:
  at −73°C(200°K), μ *equals* 847 cm²/V sec
  at 27°C(300°K), μ *equals* 474 cm²/V sec
  at 127°C(400°K), μ *equals* 310 cm²/V sec

Using q equal to 1.602(10⁻¹⁹) C, *and the extrinsic carrier concentration, one finds resistivities:*
  at −73°C(200°K), ρ *equals* 1.47 Ω cm
  at 27°C(300°K), ρ *equals* 2.63 Ω cm
  at 127°C(400°K), ρ *equals* 4.02 Ω cm

In this case, only majority carriers (holes) have been considered. Indeed, if one calculates the contribution due to minority carriers (electrons) one finds that it is negligible.

If one adds equal amounts of acceptor and donor type dopants to the crystal, the doping is unchanged. However, the impurity contribution to the mobility is greatly increased because the total ionized impurity concentration is the sum of all dopant concentrations irrespective of type. Thus, C_I is 5.05×(10¹⁷) cm⁻³ *instead of* 5×(10¹⁵) cm⁻³. *The contribution to hole mobility from lattice scattering remains unchanged, however, the contribution from ionized impurity scattering changes as follows:*
  at −73°C(200°K), μ_I *equals* 216 cm²/V sec
  at 27°C(300°K), μ_I *equals* 396 cm²/V sec
  at 127°C(400°K), μ_I *equals* 610 cm²/V sec
and, thus, the total hole mobilities are:
  at −73°C(200°K), μ *equals* 173 cm²/V sec
  at 27°C(300°K), μ *equals* 217 cm²/V sec
  at 127°C(400°K), μ *equals* 206 cm²/V sec

Clearly, under these conditions, mobility is substantially reduced by the ionized impurity scattering mechanism.

Again, resistivities are immediately obtained considering only holes:
  at −73°C(200°K), ρ equals 7.21 Ω cm
  at   27°C(300°K), ρ equals 5.75 Ω cm
  at 127°C(400°K), ρ equals 6.05 Ω cm

These two results illustrate that lightly doped silicon has a normal, positive TCR, i.e., resistivity increases with temperature. In contrast, heavily doped silicon, even if compensated, can have a negative TCR. (Note the behavior of resistivities at −73° and 27°C.) This kind of behavior has important implications for the operation and reliability of real devices in real circuits.

b. If the exponent, ν, for lattice scattering is 2 instead of 1.5, repeat part **a** and explain why results are either the same or different.

If ν has a value of 2, then the expression for overall mobility must be modified as follows:

$$\mu = \cfrac{1}{\cfrac{1}{\mu_{300}}\left(\cfrac{T}{300}\right)^2 + \cfrac{C_I}{\alpha}\left(\cfrac{300}{T}\right)^{3/2}}$$

Clearly, only the contribution due to lattice scattering has changed, thus these values need to be redetermined as follows
  at −73°C(200°K), μ_L equals 1080 cm²/V sec
  at   27°C(300°K), μ_L equals   480 cm²/V sec
  at 127°C(400°K), μ_L equals   270 cm²/V sec

Thus, for the uncompensated case:
  at −73°C(200°K), μ equals 1028 cm²/V sec
  at   27°C(300°K), μ equals   474 cm²/V sec
  at 127°C(400°K), μ equals   268 cm²/V sec

  at −73°C(200°K), ρ equals 0.823 Ω cm
  at   27°C(300°K), ρ equals 2.63 Ω cm
  at 127°C(400°K), ρ equals 4.66 Ω cm

Likewise, for the compensated case

  at −73°C(200°K), μ equals 180 cm²/V sec
  at   27°C(300°K), μ equals 217 cm²/V sec
  at 127°C(400°K), μ equals 187 cm²/V sec

at −73°C(200°K), ρ equals 6.93 Ω cm
at   27°C(300°K), ρ equals 5.75 Ω cm
at 127°C(400°K), ρ *equals* 6.68 Ω cm

Clearly, temperature dependence remains broadly similar to the previous case showing that qualitative behavior of mobility and resistivity is much more sensitive to concentration rather than temperature.