Solution 4

Exercise 1: Valence band tail states

The density of states is defined as number of states with respect to space and energy. The spatial density of states is thus obtained by integrating over the whole energy range. With $E_V = 0$, we get:

$$\begin{aligned} N &= N_V \int_0^\infty e^{-\frac{E}{E_0}} dE \\ &= N_V \cdot \left[-E_0 \cdot e^{-\frac{E}{E_0}} \right]_0^\infty \\ &= N_V \cdot E_0 \\ &= 0.05 \cdot 2 \times 10^{21}\,\mathrm{cm}^{-3} \\ &= 10^{20}\,\mathrm{cm}^{-3} \end{aligned}$$

Exercise 2: Equilibrium defect density

a) The number of possible arrangements W is given by:

$$W = \binom{N_0}{N_D} = \frac{N_0!}{(N_0 - N_D)! N_D!}\,.$$

b) Using the previous result for W, the entropy S is obtained by:

$$\begin{aligned} S &= k \ln W \\ &= k \ln N_0! - k \left[\ln (N_0 - N_D)! + \ln N_D! \right] \\ &\overset{\text{Stirling}}{\approx} k \left[N_0 \ln N_0 - (N_0 - N_D) \ln (N_0 - N_D) - N_D \ln N_D \right]. \end{aligned}$$

c) To minimize F with respect to N_D, $\frac{\partial F}{\partial N_D} \overset{!}{=} 0$.

$$\begin{aligned} F &= N_D \cdot U - TS \\ &= N_D \cdot U - kT \left[N_0 \ln N_0 - (N_0 - N_D) \ln (N_0 - N_D) - N_D \ln N_D \right] \\ &= N_D \cdot U - kT \left[N_0 \ln N_0 - N_0 \ln (N_0 - N_D) + N_D \ln (N_0 - N_D) - N_D \ln N_D \right] \end{aligned}$$

By differentiating F with respect to N_D, we obtain:

$$\begin{aligned} \frac{\partial F}{\partial N_D} &= U - kT \left[0 - N_0 \frac{(-1)}{N_0 - N_D} + \ln (N_0 - N_D) + N_D \frac{(-1)}{N_0 - N_D} - \ln N_D - 1 \right] \\ &= U - kT \left[\ln (N_0 - N_D) - \ln N_D \right] \\ &= U - kT \ln \frac{N_0 - N_D}{N_D} \overset{!}{=} 0. \end{aligned}$$

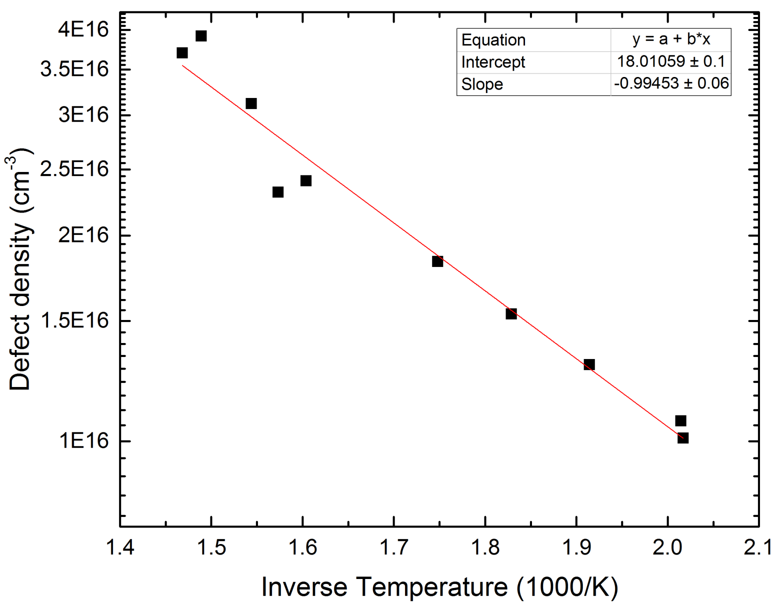
Thus,

$$\frac{U}{kT} = \ln \frac{N_0 - N_D}{N_D}$$

and

$$e^{\frac{U}{kT}} = \frac{N_0 - N_D}{N_D} = \frac{N_0}{N_D} - 1,$$

from which the desired result for $N_D(T)$ follows directly.



d) Use the Arrhenius plot with a linear fit to find a Boltzmann like defect density distribution. Boltzmann constant $k = 8.6 \cdot 10^{-5}$ eV/K

$$\begin{aligned}
logN_D &= -0.99\,(1000/T) + 18 \\
N_D &= 10^{-0.99(1000/T)+18} \\
N_D &= 10^{18} \cdot 10^{-0.99(1000/T)} \\
N_D &= 10^{18} \cdot e^{2.303\cdot(-0.99\cdot 1000/T)} \\
N_D &= 10^{18} \cdot e^{-2.28(1000/T)} \\
N_D &= 10^{18} \cdot e^{-0.20/kT}
\end{aligned}$$

Exercise 3: Ionization of donor impurities

a) Using the given hints (replacing ϵ_0 by $\epsilon_0\epsilon_{\mathrm{Si}}$ and using the effective mass of the electron in silicon), one gets a value of about 35 meV, which is much lower that the Rydberg energy of an electron bonded to a proton (13.6 eV) in the hydrogen atom model of Bohr.

b) Remembering that kT is equal to about 25.8 meV at room temperature, one can conclude that the donors are ionized at room temperature with this "hydrogen atom-like model", a fact which is of tremendous importance for the semiconductor industry! The measured donor level for phosphorous in silicon lies 46 meV below E_C[1], meaning that this model gives a good estimation!

[1] S. M. Sze, *Physics of Semiconductor Devices*, Wiley, 2007, p.23.