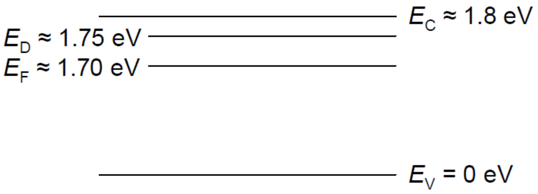
Solution 3

Exercise 1: Occupation function of a donor state

a) In the figure below you can see the band diagram of n-type doped amorphous silicon with approximative values for the requested energy levels. The position of these levels — namely E_D and E_F — depend on various parameters such as the dopant concentration and shall only give an idea of the order of magnitude.



The choice of $E_\mathrm{V} = 0$ as reference is absolutely arbitrary.

b) With only one energy level between the valence and the conduction band at E_D close to E_F, an electron will occupy most likely that level. As a fermion, the electron can occupy this level in two different spin configurations (spin up and down) with the same probability, we call these states $\mathrm{D_{up}}$ and $\mathrm{D_{down}}$. The next probable state is with an electron at the conduction band edge, we call it C.

When the system is in thermal equilibrium (i.e. the probability that a hypothetical state at E_F is occupied is exactly 50 %, we consider the energy of the system to be 0. Therefore, the system with an electron at $E_{\mathrm{D_{up}}} = E_{\mathrm{D_{down}}}$ has the energy $E_\mathrm{D} - E_\mathrm{F}$, the system with an electron at E_C has the energy $E_\mathrm{C} - E_\mathrm{F}$.

c) In a system with j states that have the energy E_j, the probability that the system is in state i is given by

$$p_i = \frac{e^{-\frac{E_i}{k_\mathrm{B}T}}}{\sum\limits_j e^{-\frac{E_j}{k_\mathrm{B}T}}}. \tag{1}$$

For the states $\mathrm{D_{up}}$ and $\mathrm{D_{down}}$, this is

$$p_{\mathrm{D_{up}}} = p_{\mathrm{D_{down}}} = \frac{e^{-\frac{E_\mathrm{D}-E_\mathrm{F}}{k_\mathrm{B}T}}}{2 \cdot e^{-\frac{E_\mathrm{D}-E_\mathrm{F}}{k_\mathrm{B}T}} + e^{-\frac{E_\mathrm{C}-E_\mathrm{F}}{k_\mathrm{B}T}}}. \tag{2}$$

The probability that the system is in the state D — be it spin up or down — is therefore

$$\begin{aligned}
p_\mathrm{D} = 2 \cdot p_{\mathrm{D}_\mathrm{down}} &= \frac{2 \cdot e^{-\frac{E_\mathrm{D}-E_\mathrm{F}}{k_\mathrm{B}T}}}{2 \cdot e^{-\frac{E_\mathrm{D}-E_\mathrm{F}}{k_\mathrm{B}T}} + e^{-\frac{E_\mathrm{C}-E_\mathrm{F}}{k_\mathrm{B}T}}} && (3) \\
&= \frac{1}{1 + \frac{1}{2} \cdot e^{-\frac{E_\mathrm{C}-E_\mathrm{F}}{k_\mathrm{B}T} + \frac{E_\mathrm{D}-E_\mathrm{F}}{k_\mathrm{B}T}}} && (4) \\
&= \frac{1}{1 + \frac{1}{2} \cdot e^{-\frac{E_\mathrm{C}-E_\mathrm{D}}{k_\mathrm{B}T}}} && (5) \\
&= 93\% \quad \text{with} \quad k_\mathrm{B}T = 0.026\,\mathrm{eV} \quad \text{at room temperature.} && (6)
\end{aligned}$$

The probability that the system is in the state C is

$$\begin{aligned}
p_\mathrm{C} &= 1 - p_\mathrm{D} = 7\% \quad \text{or} && (7) \\
&= \frac{e^{-\frac{E_\mathrm{C}-E_\mathrm{F}}{k_\mathrm{B}T}}}{2 \cdot e^{-\frac{E_\mathrm{D}-E_\mathrm{F}}{k_\mathrm{B}T}} + e^{-\frac{E_\mathrm{C}-E_\mathrm{F}}{k_\mathrm{B}T}}} && (8) \\
&= \frac{1}{2 \cdot e^{-\frac{E_\mathrm{D}-E_\mathrm{F}}{k_\mathrm{B}T} + \frac{E_\mathrm{C}-E_\mathrm{F}}{k_\mathrm{B}T}} + 1} && (9) \\
&= \frac{1}{2 \cdot e^{-\frac{E_\mathrm{D}-E_\mathrm{C}}{k_\mathrm{B}T}} + 1} && (10) \\
&= 7\% && (11)
\end{aligned}$$

d) Under the assumptions that

- the phosphorus concentration is $c_\mathrm{P} = 10^{-6}$ which corresponds to $N_\mathrm{P} = c_\mathrm{P} \cdot N_\mathrm{Si} = 5 \times 10^{16}\,\mathrm{cm}^{-3}$,
- the doping efficiency is 100% (i.e. all dopants substitute a silicon atom in the ≪lattice≫and can contribute an electron to the conduction band),
- the formula derived above is still valid for a multi-state system, and
- thermal excitation from other energy levels than the dopant level (e.g. from the valence band) into the conduction band is negligible.

the electron density in the conduction band is $N_\mathrm{e} = p_\mathrm{C} \cdot N_\mathrm{P} = 4.3 \times 10^{15}\,\mathrm{cm}^{-3}$.

e) The derived equation is nothing else than the occupation function of energy states introduced by impurities or dopants. The Fermi-Dirac distribution

$$F_\text{F-D}(E) = \frac{1}{1 + e^{\frac{E-E_\mathrm{F}}{k_\mathrm{B}T}}} \tag{12}$$

can be derived exactly the same way but for states that can be occupied only once. To do so, we consider a state at energy E, either filled (1) or empty (0), in exchange with a “reservoir” at E_F:

$$F_\text{F-D}(E) = p_\mathrm{E} = \frac{e^{-\frac{E-E_\mathrm{F}}{k_\mathrm{B}T}}}{e^{-\frac{0\cdot(E-E_\mathrm{F})}{k_\mathrm{B}T}} + e^{-\frac{1\cdot(E-E_\mathrm{F})}{k_\mathrm{B}T}}} = \frac{1}{1 + e^{\frac{E-E_\mathrm{F}}{k_\mathrm{B}T}}} \tag{13}$$

Exercise 2: Meyer-Neldel behaviour in the conductivity of a-Si:H

We assume that $T \neq 0$, i.e. $\alpha \neq 1$.

a) We compute

$$\begin{aligned} L &= \frac{\mu_{00}E}{\omega^\alpha}\int_0^{t_L} t^{-\alpha}dt \\ &= \frac{\mu_{00}E}{\omega^\alpha}\frac{t_L^{1-\alpha}}{1-\alpha}. \end{aligned}$$

Thus we get:

$$t_L^{1-\alpha} = \frac{L\omega^\alpha\left(1-\alpha\right)}{\mu_{00}E} \tag{14}$$

and

$$t_L = \left(\frac{L\omega^\alpha\left(1-\alpha\right)}{\mu_{00}E}\right)^{\frac{1}{1-\alpha}}. \tag{15}$$

b) In the following, we'll use the fact that $\omega^\alpha = \frac{\omega}{\omega^{1-\alpha}}$, and hence (with (14))

$$\left(\omega t_L\right)^{1-\alpha} = \frac{L\omega\left(1-\alpha\right)}{\mu_{00}E}.$$

Thus,

$$\omega t_L = \left(\frac{L\omega\left(1-\alpha\right)}{\mu_{00}E}\right)^{\frac{1}{1-\alpha}}. \tag{16}$$

We now calculate

$$\begin{aligned} \mu(t_L) &= \mu_{00}(\omega t_L)^{-\alpha} \overset{(16)}{=} \mu_{00}\left(\frac{L\omega\left(1-\alpha\right)}{\mu_{00}E}\right)^{-\frac{\alpha}{1-\alpha}} \\ &= \mu_{00}\left(\frac{L\omega\left(1-\alpha\right)}{\mu_{00}E}\right)^{\left(\frac{1-\alpha}{1-\alpha}-\frac{1}{1-\alpha}\right)} \\ &= \mu_{00}\left(\frac{L\omega\left(1-\alpha\right)}{\mu_{00}E}\right)\cdot\underbrace{\left(\frac{L\omega\left(1-\alpha\right)}{\mu_{00}E}\right)^{-\frac{1}{1-\alpha}}}_{(\omega t_L)^{-1}} \\ &= \underbrace{\frac{Lw(1-\alpha)}{E}}_{\mu_0}\frac{1}{\omega t_L}. \end{aligned}$$

c) Using (16) and the definition of μ_0, we start with the previous result and calculate:

$$
\begin{aligned}
\mu(t_L) &= \mu_0 \frac{1}{\omega t_L} \\
&= \mu_0 \left(\frac{\mu_0}{\mu_{00}}\right)^{-\frac{1}{1-\alpha}} \\
&= \mu_0 \left(\frac{\mu_0}{\mu_{00}}\right)^{-\frac{T_0}{T}} \\
&= \mu_0 \exp\left[-\frac{T_0}{T} \ln\left(\frac{\mu_0}{\mu_{00}}\right)\right] \\
&= \mu_0 \exp\left[-\frac{kT_0 \ln\left(\frac{\mu_0}{\mu_{00}}\right)}{kT}\right] \\
&\overset{\text{def}}{=} \mu_0 \exp\left(-\frac{E_{\text{mob}}}{kT}\right) \\
&= \mu(T).
\end{aligned}
$$