Exercise 4

Exercise 1: Valence band tail states

Disorder in the bond structure blurs the band edges. Even in single crystal semiconductors the edges are not sharp because of thermal fluctuations at non-zero temperatures. This disorder in amorphous silicon will also blur the band edges, only much stronger. We assume exponential tails of states that extend from the band edges into the gap, e.g. for the valence band:

$$g(E) = N_V \cdot e^{-\frac{E-E_V}{E_0}}.$$

Refer the energy scale to the valence band energy ($E_V = 0$) and calculate the total spatial density of tail states, assuming $N_V = 2 \times 10^{21}\,\mathrm{cm}^{-3}\,\mathrm{eV}^{-1}$ and a band edge parameter $E_0 = 50\,\mathrm{meV}$.

Exercise 2: Equilibrium defect density

Assume that the formation of a defect by breaking a bond requires an energy U per defect. Calculate the equilibrium density of defects at a temperature T by minimizing the free energy of the system.

a) Determine the number W of possible arrangements of N_D defect states within an ensemble of N_0 states.

b) Calculate the entropy $S = k \ln W$, using the Stirling approximation for the factorials:

$$\ln N! \approx N \ln N.$$

c) Minimize the free energy $F = N_D \cdot U - TS$ with respect to the number of defects N_D, and show that the result is given by:

$$N_D(T) = \frac{N_0}{1 + e^{\frac{U}{kT}}}.$$

d) Plot the measurement data given in the following table. Derive the expression for $N_D(T)$

Temperature T $°C$	Defect density N_D cm^{-3}
407.8897	3.702E16
398.39127	3.92E16
374.48201	3.121E16
362.41372	2.316E16
350.31186	2.407E16
298.90062	1.834E16
273.68043	1.536E16
249.25382	1.295E16
223.27792	1.071E16
222.6766	1.011E16

Exercise 3: Ionization of donor impurities

a) Calculate the binding energy of an electron to a donor (e.g phosphorus dopant) in the silicon lattice. For this, you can use the fact that an electron in the presence of a donor impurity within a semiconductor can be approximated as a electron with effective mass m^*, moving in free space in the presence of an attractive center of charge $\frac{e}{\epsilon}$, where ϵ is the static dielectric constant of the semiconductor[1]. You could need the following for the calculation:

- The first energy level of an electron in the Bohr model of the hydrogen atom is given by $E = \frac{me^4}{8\epsilon_0^2 h^2}$;
- The effective mass of an electron in silicon is $m^*_{\mathrm{Si}} = 0.3m_e$;
- The static dielectric constant of silicon is $\epsilon_{\mathrm{Si}} = 11.7$.

b) Compare it with the thermal energy at room temperature.

[1] N. W. Ashcroft, N. D. Mermin, *Solid State Physics*, Thomoson Learning, 1976.