Module 4

Candidate number: 27

24. august 2017

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GaAs Has a direct bandgap of $1.42\,\text{eV}$ at room temperature. From experiments three effective masses of 0.067,0.082 and 0.45 for electrons in the conduction band, light, and heavy holes respectively has been found. The corresponding energy dispersion relations can be computed from these values and a band diagram can be drawn.
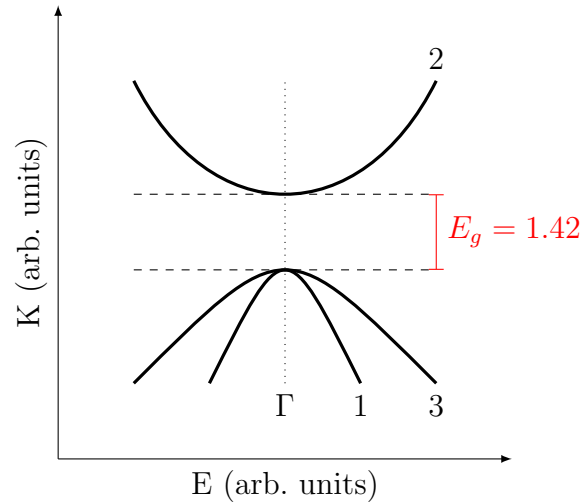

Figur 1: tikz illustration of the energy dispersion relation for 1. light holes, 2. electrons and 3. heavy holes. NB this is just a sketch, not a plot. The trends will be correct but the scale is not correct

The energy dispersion relation from the lectures can be written as:

$$E'(k) = E(k_0) + \frac{\hbar^2}{2m^*}(k - \Gamma)^2$$

Here effective mass ,$\frac{1}{m^*}$, is defined as $\frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k^2}$.
Inserting the given values for the effective mass gives:

$$E(k)_3 = E(k_0) - 0.47(k - \Gamma)^2$$
$$E(k)_2 = E(k_0) + 0.57(k - \Gamma)^2$$
$$E(k)_1 = E(k_0) - 0.09(k - \Gamma)^2$$

These energy dispersions has been plotted above.

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a

From the lectures the energy of a electron in a hydrogen-like impurity is defined as:

$$E_H = -\frac{me^4}{2(4\pi\hbar\epsilon)^2}\frac{1}{n^2} = 13.6\,\text{eV}$$

This model does not take into account that the hydrogen-like impurities has varying amounts of protons in the core, which will result in a factor not considered in this expression. Here it is assumed that the sceening from the core results in a total coverage and that the only factor left is e^4.

A phosphor atom in the silisium crystal will have one too many electrons for the lattice. This results in one loosely bound electron that can be viewed as a hydrogen-like defect. In the approximation one has to exchange the mass for the effective mass and the dielectric constant for the relative dielectric constant $K_s = 11.8$. This is because both of these values are relative to the surrounding environment.
Assuming the effective mass approximation gives:

$$E_d = E_H \cdot \frac{m_n^*}{m_0}\left(\frac{1}{K_S}\right)^2 = -13.6\,\text{eV} \cdot \frac{m_n^*}{m_0}\left(\frac{1}{K_S}\right)^2$$

The task does not give any numbers for the effective mass or the dielectric constant. If one uses the same numbers as in the lecture, with $K_S = 11.8$ and a effective mass of around $m_n = 0.5m_0$, one gets an energy of approximately $-0.05\,\text{eV}$. This number is negative because it gives the state of the electron relative to the conduction band. This means that the energy needed to excite the phosphorus electron is $0.05\,\text{eV}$.

b

The radius in which the electrons are from the nucleus is called the Bohr radius and is defined as

$$r_H = 4\pi\frac{\epsilon\hbar^2}{me^2}n^2$$

for a hydrogen atom. In a similar fashion as in the case for the energy this expression has to be manipulated to consider the environment of the impurity.

$$r_d = 4\pi\frac{\epsilon_0\epsilon_d\hbar^2}{m^*e^2}n^2$$

Which in a similar manner as for the energy becomes:

$$r_d = r_H\frac{m}{m^*}\epsilon_d$$

By using the same constants as in **a** one gets a Bohr orbit of approximately $\approx 5\,\text{nm}$.
Given that one wants to estimate the doping concentration to estimate when the localized states transforms into an impurity band
The second part of this question was a bit unclear. In the lectures there were no mention of a criterea for there to be formed a new impurity-band in the semiconductor. From my understanding this would

need some more thought due to us never mentioning any correlation between a band being formed and the distance or energy for the impurities. If one introduce a impurity-band i would think that the semiconductor behaves in a very different manner than before due to electrons and holes ability to move in the new band. To answer this question i decided to put aside my questions and talk to some of my class colleagues. Thought discussion we decided to give the following criterea:

For the defects to create a band the electron "orbitals"(its not really a orbital, its more of a approximate distance from the core) has to have the ability to move from one defect to another without breaking the bond resulting in a excitation. Thus the limit will be when the hydrogen like impurities radius overlaps. This can be calculated easily for a concentration in cubic centimeters, by dividing on the volume one impurity has.

$$\frac{1 \, \text{cm}^3}{V_{impurity}} = \frac{1 \, \text{cm}^3}{\frac{4}{3}\pi (r_d)^3} \approx 4 \cdot 10^{18}$$

The validity of this number is questionable. I think i recall from the lectures in semiconducting components(halvlederkurset 2210) that one could dope a silisium chip with more than 10^{18} phosphor atoms, without the properties changing too much.

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a

From the plot in lecture 21 and the different intervals here i have chosen a low temperature of $20 \, \text{K}$, a intermediate temperature of $300 \, \text{K}$ and a high temperature of $1200 \, \text{K}$. Full plot of all the values for the n concentrations at different temperatures follows in c.

For low temperatures the carrier concentration is dominated by the extrinsic phosphor atom donors. This is due to their loosely bound excess electron. In this region the carrier concentration can be approximated to only extrinsic effects, formula from the lectures:

$$n = N_C e^{-E_{donor}/k_b T} = 2.62 \cdot 10^7 \tag{1}$$

The hole concentration is found by using the law of mass action:

$$p = \frac{n_i^2}{n} \tag{2}$$

For energies in an intermediate range there will be two contributing effects. Assuming that the crystal has enough energy to excite all extrinsic electrons this will have reached a maximum value, the value equal to the amount of doped atoms. The other effect is the intrinsic electrons that can contribute to the charge carrier concentration. This is somewhat unimportant at these temperatures but will become essensial at higher temperatures. The energy at these temperatures is too low to make the intrinsic carrier concentration become in the same order of magnitude as the extrinsic. So there will exist a saturatedlevel for a temperature range, where the increase in carrier concentration will be almost nothing:

$$n = N_d \tag{3}$$

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The hole concentration is found by using the law of mass action:

$$p = \frac{n_i^2}{n} = 2.25 \cdot 10^3 \tag{4}$$

Note here that i have assumed a perfectly doped Si crystal, where there exists no other impurities then the phosphor. Is there had existed impurities like bor or iron the only adjustment to the formula would be to subtract/add the amount of electrons associated with the impurity.

For high temperatures the intrinsic effects would take over and become of a greater magnitude that the extrinsic effects. For these temperatures one can approximate the carrier concentration to the intrinsic carrier concentration, formula from the lecture.

$$n = N_i e^{-E_g/2k_b T} \simeq 2 \cdot 10^{19} \tag{5}$$

This number, which is higher than the doping concentration is in the range of what is expected for this temperature interval.

$$p = \frac{n_i^2}{n} \tag{6}$$

b

The formula to find the fermielevel relative to the intrinsic level is $E_f - E_i = kT \ln(n_0/n_i)$. At 0K the fermie level will be at the highest occupied state. Increasing the temperature will result in more electrons in the conduction band than before. This leads to a shift downwards in the fermielevel relative to the conduction band. For the low temperature it becomes:

$$E_f - E_i = kT \ln(n_0/n_i) = k \cdot T \ln \frac{n_0}{n_i} = 0.0121 \, \text{eV}$$

When this reaches the intermediate temperatire state the fermie level will become:

$$E_f - E_i = kT \ln(n_0/n_i) = 0.407 \, \text{eV}$$

Which is the same value obtained in the lecture.

For high temperatures intrinsic effects overtakes. For this value one does not need to do the calculation. This is because when the intrinsic effects overtakes the difference between $E_f - E_i$ goes to zero. Since E_f for a intrinsic semiconductor goes towards E_i. so for temperatures above the high temperature, 1200 K, there is no difference between $E_f - E_i$.

c
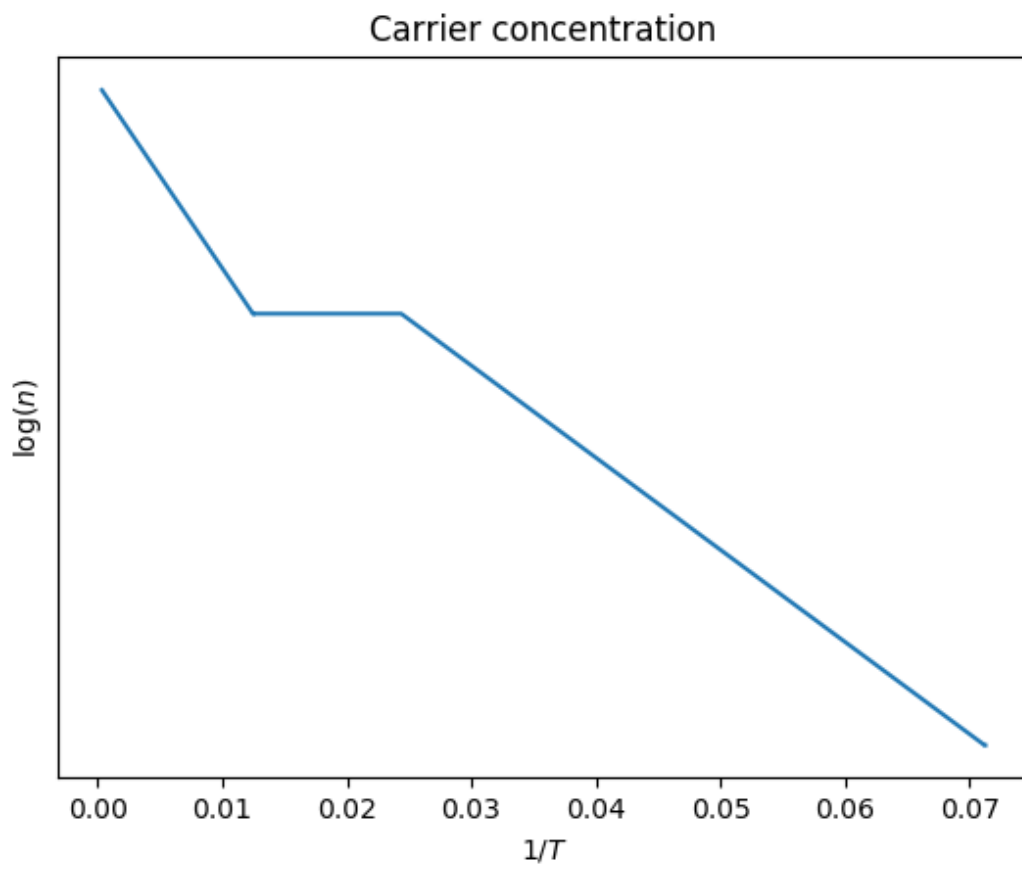
Figur 2: tikz plot of the charge carrier concentration plottet against the inverse of temperature.