Series - Electronic and optical semiconductor devices

Series 5 Density of states, ionization and activation energies, statistics of donor levels

Exercise 1- Two-dimensional and one-dimensional density of states (DOS)

1- We consider an isotropic band structure so that $E(k) = E_1 + \frac{\hbar^2 k^2}{2m^*}$ (1.1)

The surface occupied by each k value is $\frac{4\pi^2}{S}$ where $S = N^2 a^2$ is the surface associated with the two-dimensional layer.

The DOS being a constant in k-space, the number of states which are in a disk of radius k is given by:

$$N_{2D} = \underbrace{\pi k^2}_{S_{disk}} \times \underbrace{\frac{S}{4\pi^2}}_{\text{surface density}} \times \underbrace{2}_{\text{spin degeneracy}} \qquad (1.2)$$

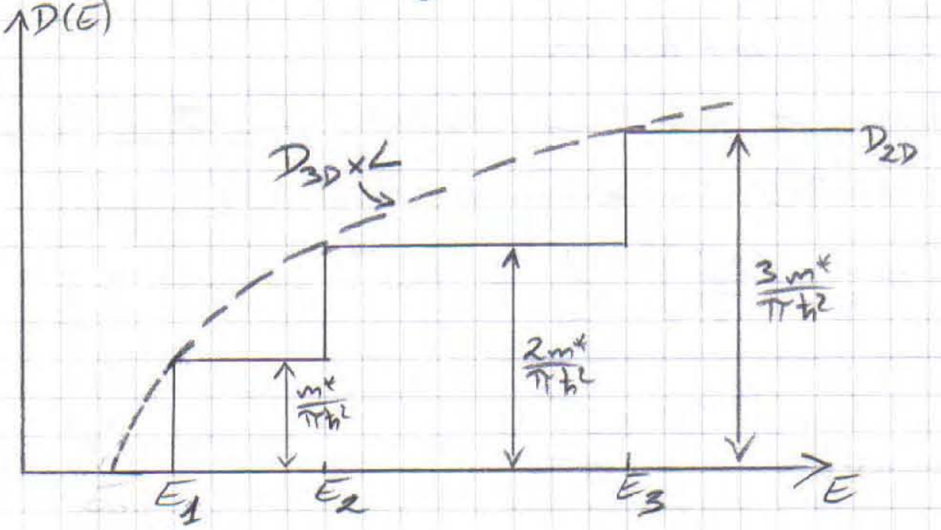
From (1.2) we get: $k^2 = \frac{2m^*}{\hbar^2}(E - E_1)$ (1.3)

As a result $N_{2D} = \frac{m^*}{\pi\hbar^2} S(E - E_1)$ and the DOS per energy and surface unit will express as:

$$\boxed{D_{2D}(E) = \frac{1}{S}\frac{dN_{2D}}{dE} = \frac{m^*}{\pi\hbar^2} H(E - E_1)} \quad (1.4)$$

where H is the Heaviside function.

2-



2D case : staircase density of states

3D case : DOS $\propto E^{1/2}$

Comparison between the 2D-DOS of an infinitely deep potential well and the 3D-DOS of a bulk layer whose thickness is identical to that of the well (thickness L).

Note here that the energy spacing between the quantized levels increases when moving toward excited states as expected from the infinitely deep square potential well problem. Indeed, in this latter case

$V(x) = 0$ for $0 \leqslant x \leqslant a$

$V(x) = +\infty$ for $x \in]-\infty, 0[\cup]a, +\infty[$

The dispersion relation is such that $k = \left(\frac{2m^*E}{\hbar^2}\right)^{1/2}$ and the wave function is equal to $\varphi(x) = 0$ for x values $\notin [0,a]$ and $\varphi(x) = Ae^{ikx} + A'e^{-ikx}$ for $x \in [0,a]$. In addition, $\varphi(0) = 0$ (as $\varphi(x)$ is a continuous function in $x = 0$) so that $A' = -A$, hence $\varphi(x) = 2iA\sin kx$. For continuity reasons in $x = a$, $\varphi(a) = 0$ which implies that $k = \frac{n\pi}{a}$ with $n \in \mathbb{N}^*$. Moreover, $\varphi(x)$ is a normalized function so that

$$\boxed{\varphi_n(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right)} \quad \text{and} \quad \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2m^*a^2}}$$

The energetic dependence is proportional to n^2.

3- By analogy with the 2D case, the "length" occupied by each value of k is equal to $\frac{2\pi}{L}$ where $L = Na$. The number of states which are lying on a $2k$ length portion will express as:

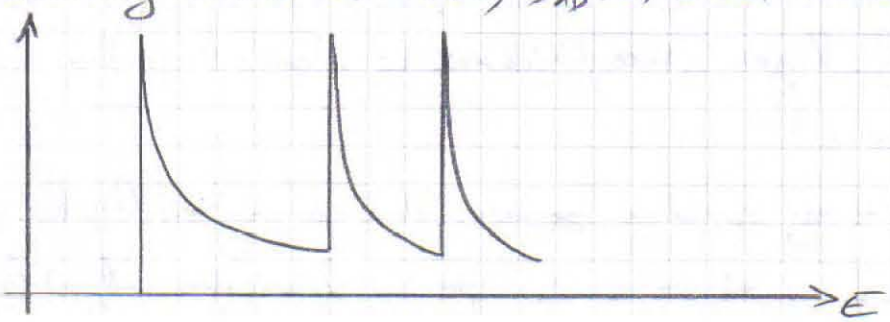
$$N_{1D} = 2k \times \underbrace{\frac{L}{2\pi}}_{\text{linear density}} \times \underbrace{2}_{\text{spin degeneracy}} = \frac{2kL}{\pi}$$

As we still consider an isotropic band structure $k^2 = \frac{2m^*}{\hbar^2}(E - E_0)$ which lead to the 1D-DOS per energy and length unit:

$$D_{1D}(E) = \frac{1}{L}\frac{dN_{1D}}{dE} = \frac{2}{\pi} \times \left(\frac{2m^*}{\hbar^2}\right)^{1/2} \times \frac{1}{2}(E - E_0)^{-1/2}$$

i.e. $$\boxed{D_{1D}(E) = \left(\frac{8m^*}{h^2}\right)^{1/2}(E - E_0)^{-1/2}}$$

Contrary to the 2D case, $D_{1D}(E)$ is not a constant.



Exercise 2 - Ionization energies

1_ The situation is identical to that of the hydrogen atom except the fact that acceptors (or donors) lie in a layer characterized by a large dielectric constant. The ionization energy will express as $\boxed{\mathcal{E}_i = \frac{\hbar^2}{2ma_0^2}\,\frac{m_r^*}{\varepsilon_r^2}\,\frac{1}{n^2}}$ (2.1)

which resumes to $\mathcal{E}_i = 13.6\,\frac{m_r^*}{\varepsilon_r^2}\,\frac{1}{n^2}$ if we want to get energies in eV. $m_r^* = \frac{m}{m_0}$ is the reduced mass of the carrier under consideration and $\varepsilon_r = \varepsilon/\varepsilon_0$ is the relative dielectric constant of the semiconductor and n is the principal quantum number of the orbital of interest. (a_0 is the hydrogen Bohr radius, $a_0 = \frac{\hbar}{me^2} = 0.53\,\text{Å}$).

The ionization energy is the energy difference between the $n = 1$ energy state ($n = 1$, energetic level of the acceptor) and the top of the valence band ($n = +\infty$). We will thus have $\mathcal{E}_{\text{ionization}} = 13600 \times \frac{0.53}{(11.9)^2} \times \frac{1}{(1)^2} \sim 50.9\,\text{meV}$

The various peaks seen in figure 1 correspond to transitions between the level $n = 1$ and levels $n = 2$ to 4.

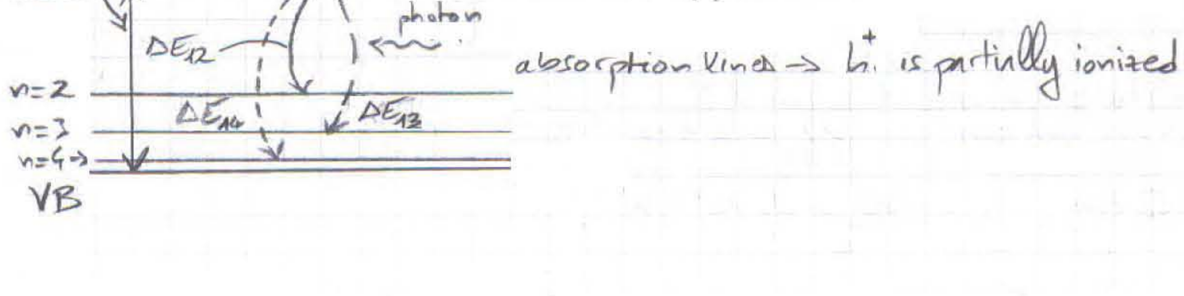
$$\Delta\mathcal{E}_{12} = \mathcal{E}_{\text{ionization}} \times \left(1 - \frac{1}{(2)^2}\right) = \frac{3}{4}\,\mathcal{E}_{\text{ionization}} = 38.2\,\text{meV}$$

$$\Delta\mathcal{E}_{13} = \mathcal{E}_{\text{ionization}} \times \left(1 - \frac{1}{(3)^2}\right) = \frac{8}{9}\,\mathcal{E}_{\text{ionization}} = 45.2\,\text{meV}$$

$$\Delta\mathcal{E}_{14} = \mathcal{E}_{\text{ionization}} \times \left(1 - \frac{1}{(4)^2}\right) = \frac{15}{16}\,\mathcal{E}_{\text{ionization}} = 47.7\,\text{meV}$$

Graphically, we deduce the following energies:
33.8 meV, 39 meV, 42.9 meV and 51.9 meV

We see here the limits of the hydrogen-like model as the effective masses change considerably in the vicinity of impurities



absorption lines → h_i^+ is partially ionized

Such a measurement can only be carried out at low temperature, i.e. when donors and acceptors are neutral. It will also limit the impact of phonons. The decrease of the absorption coefficient for energies superior to the broad peak at ~ 51meV results from the strong decrease of the transition probability away from the top of the valence band. The limited extent of the acceptor in momentum space is then responsible for the declining absorption at photon energies greater than the binding energy of the acceptor state.

Exercise 3 - Activation energies

Data are plotted on a semilogarithmic scale.

↳ ① linear slopes ⇒ exponential dependence

② $\rho\,(\Omega\,\text{cm})$ vs. $1/T$

③ when T increases, ρ decreases

$$① + ② + ③ \Rightarrow \rho \propto \exp\left(\frac{E}{k_B T}\right)$$

Low temperature range (curve A)

$\rho_1 = 0.05\,\Omega\,\text{cm} \qquad 1/T_1 = 3\times10^{-3}\,K^{-1}$

$\rho_2 = 8\,\Omega\,\text{cm} \qquad 1/T_2 = 1.2\times10^{-2}\,K^{-1}$

$$E_{LT} = k_B\left(\frac{1}{T_1} - \frac{1}{T_2}\right)^{-1} \ln\left(\frac{\rho_1}{\rho_2}\right) \sim 7.78\times10^{-21}\,\text{J} \quad \text{i.e.} \sim 48.6\,\text{meV}$$

This value has to be compared to the ionization energy of phosphorus atoms in silicon (donor state) ~ 45 meV given in the lecture (idem in the article by G.L. Pearson and J. Bardeen, Phys. Rev. 75, 865 (1949)).

High temperature range (curve A)

$\rho_3 = 2.1\times10^{-3}\,\Omega\,\text{cm} \qquad 1/T_3 = 5\times10^{-4}\,K^{-1}$

$\rho_4 = 0.07\,\Omega\,\text{cm} \qquad 1/T_4 = 1\times10^{-3}\,K^{-1}$

$E_{HT} \sim 0.604$ eV , this value has to be compared to the band gap of Si ($E_g(Si) \sim 1.12$ eV at 300K). It is thus seen that at "high" temperature the transport properties (electrical properties to be more precised) are governed by the intrinsic density of free carriers as $\rho \propto \exp\left(\frac{E_g}{2k_BT}\right)$ and $n_c = p_v = n_i = (N_c(T)N_v(T))^{1/2}\exp\left(-\frac{E_g}{2k_BT}\right)$

Exercise 4

1) Let's take the 3rd row of the matrix formalism relationship:

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{pmatrix} = \begin{pmatrix} C_{33} & C_{13} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{33} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{zx} \\ \varepsilon_{xy} \end{pmatrix}$$

$$\sigma_{zz} = C_{13}\, \varepsilon_{xx} + C_{13}\, \varepsilon_{yy} + C_{33}\, \varepsilon_{zz}$$

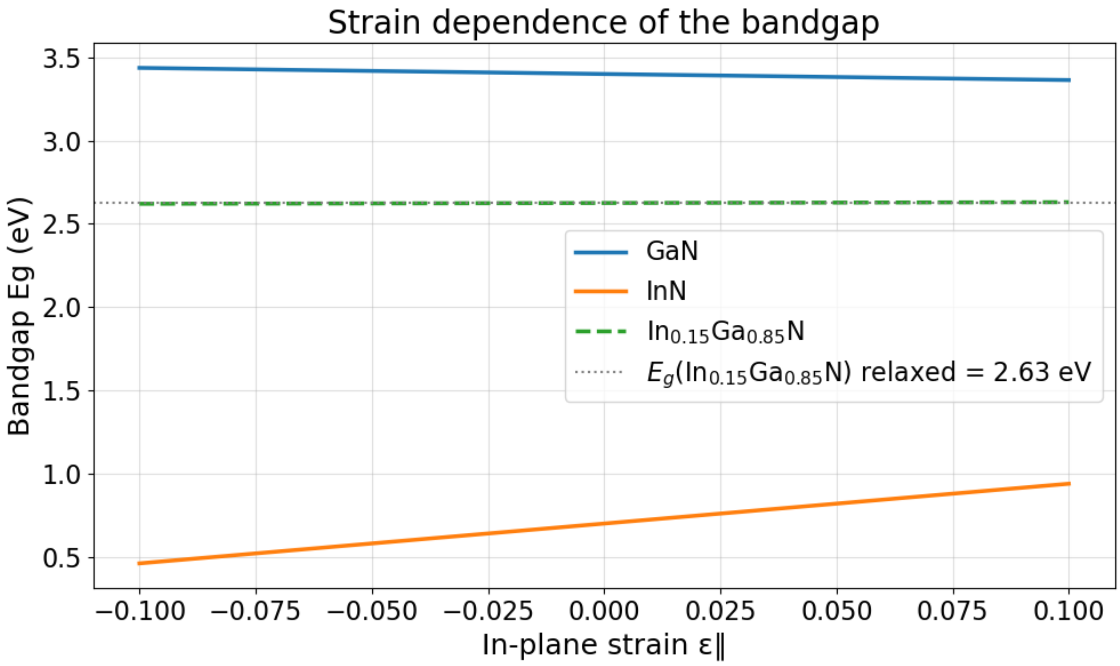
In an epilayer oriented on the xy plane we can say that:

a. ε_{xx} and ε_{yy} are equal due to symmetry reasons.

b. $\sigma_{zz} = 0$ because the top surface is free, so no stress is applied on the epilayer in the z direction

Therefore, by reverting the formula we get $\varepsilon_{zz} = -2\frac{C_{13}}{C33}\varepsilon_{xx}$

2) See Jupyter notebook for the code. You should get a graph like this:



Comments:

a) For GaN, we see that for $\varepsilon_{\|} > 0$ (in-plane tensile strain), the bandgap is expected to decrease, compared to the relaxed case $\varepsilon_{\|} = 0$

b) On the contrary, using the given parameters, we get an opposite trend for InN: the bandgap is expected to increase with increasing in-plane strain

c) The bandgap of relaxed $In_{0.15}Ga_{0.85}N$ can be obtained from Vegard's law:

$$E_{g,(\mathrm{In_xGa_{1-x}N})} = x\, E_{g,\mathrm{InN}} + (1-x)E_{g,\mathrm{GaN}} - b \cdot x \cdot (1-x)$$

Where $x = 0.15$ and $b = 2.9$ eV. You should get $E_{g,(\mathrm{In_{0.15}Ga_{0.85}N})} = 2.63$ eV

d) To find the evolution of $E_{g,(\mathrm{In_{0.15}Ga_{0.85}N})}$ with strain, we can use the same approach as for GaN and InN. From the table, we only have the deformation potential and elasticity coefficients for GaN and InN. However, we can use a linear interpolation to find the approximated values for $In_xGa_{(1-x)}N$ for any given alloy concentration. For example:

$$D_{3,(\mathrm{In_{0.15}Ga_{0.85}N})} = 0.15 \cdot D_{3,\mathrm{InN}} + 0.85 \cdot D_{3,\mathrm{GaN}},$$

and so on, for the other parameters.

From the plot, we can observe that the graph is fairly flat, meaning that for $\mathrm{In_{0.15}Ga_{0.85}N}$ the opposite contributions of GaN and InN almost cancel each other, causing negligible variations of the bangap with strain.

As an extra exercise, we also can calculate the alloy concentration for which we have almost zero derivative of bandgap with respect to strain, which is expected to be around $x = 0.13$ (see Jupyter notebook).