Series - Electronic and optical semiconductor devices

Series 4 - Band structure, strain effect, magneto-transport and Hall effect

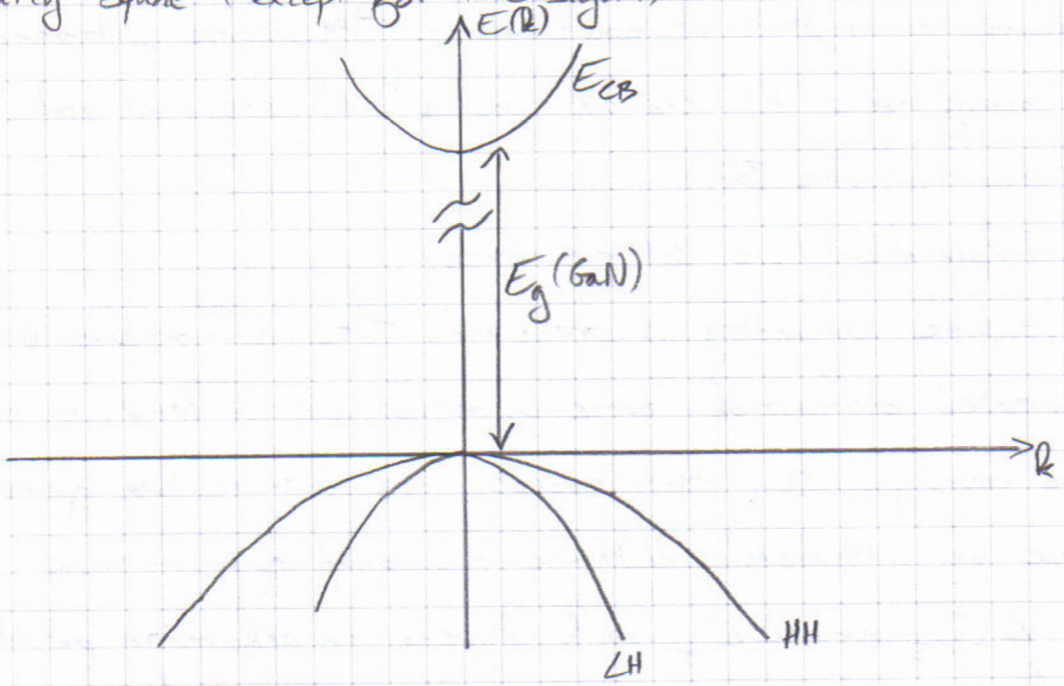
Exercise 1 - Band structure

1- We consider isotropic effective masses so that we can use the general expression $E(k) = E_0 + \frac{\hbar^2 k^2}{2m^*}$ for each band (corrected for the energy E_0). For the sake of simplicity, we choose the top of the valence as the origin of energies. We then get:

$$E_{CB} = E_g(\text{GaN}) + \frac{\hbar^2 k^2}{2m_e}$$

$$E_{HH} = -\frac{\hbar^2 k^2}{2m_{hh}} \quad \text{and} \quad E_{LH} = -\frac{\hbar^2 k^2}{2m_{lh}}$$

Note that the band curvatures associated with electrons and light holes are nearly equal (except for the sign!).

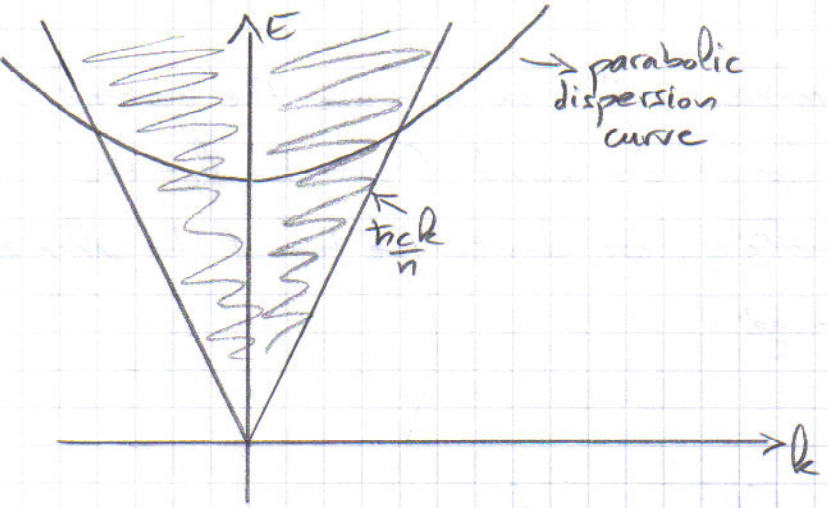


2- $|\vec{k}| = 5\times 10^6\ \text{cm}^{-1}$

$$\Delta E = E_{CB}(\vec{k}) - E_{HH}(\vec{k}) = E_g(\text{GaN}) + \frac{\hbar^2 k^2 (m_e + m_{hh})}{2\, m_e m_{hh}}$$

so that $\Delta E = E_g(\text{GaN}) + \frac{1.32}{0.242}\frac{\hbar^2 k^2}{2m_0} \sim 3.462\,\text{eV}$ $(\lambda \sim 358\,\text{nm})$

Note that optical transitions are considered to be vertical transitions in the $(E-k)$ space. In addition owing to the very steep dispersion of photons ($E_{photon} = \hbar \frac{c}{n} k$ where n is the real part of the refractive index of the propagating medium), optical transitions will only involve carriers with a small wave vector => momentum conservation will imply that only carriers with a k lower than that of the intersect between the photon dispersion and the dispersion curve of carriers (here it is assumed to be parabolic for the sake of simplicity) can recombine radiatively, hence the denomination "light cone".



Exercise 2 - Band structure scheme - strain effect

(a) Bulk semiconductor crystal at equilibrium. The valence subbands associated with heavy holes (HH) and light holes (LH) are degenerate in $\vec{k} = \vec{0}$ (Γ point of the BZ).

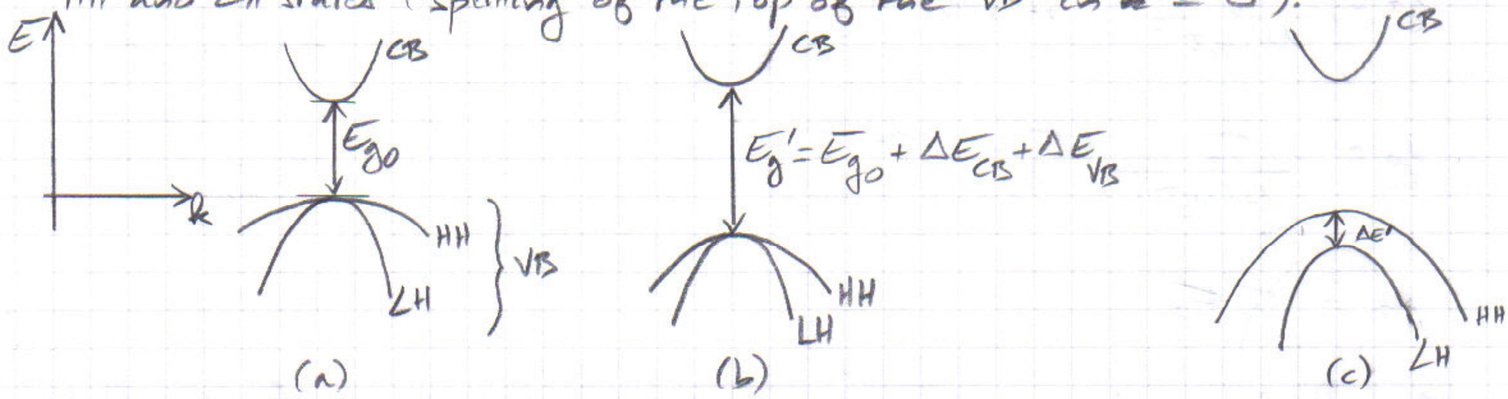
(b) Hydrostatic deformation (i.e. isotropic stress).

The whole crystal symmetry is preserved. The compressive stress induces an increased overlap of atomic orbitals which leads to an increase of the bandgap. In other words, we observe the general trend: decrease of interatomic distance => band gap increase. The energy shifts ΔE_{CB} and ΔE_{VB} will depend on deformation potentials which vary from one band to the other (and from one semiconductor to the other).

(c) A shear stress is added (anisotropic stress).

This time the crystal deformation is anisotropic. The top of the VB consists of electronic states with sp^3 hybridization whereas the bottom of the CB consists of states having s type orbitals. The latter are much less sensitive than p states to shear stress.

The anisotropic stress will induce a lift of degeneracy between HH and LH states (splitting of the top of the VB in $\vec{k} = \vec{0}$).



Exercise 3 - Magneto-transport and Hall effect

I - Magneto-conductivity tensor

1 - Under steady-state conditions as $\frac{d\vec{v}}{dt} = \vec{0}$ the Lorentz equation reduces to $\frac{m^*}{\tau}\vec{v_d} = -e[\vec{F} + (\vec{v_d} \wedge \vec{B}/c)]$. When projecting on the x, y and z axes we get:

$$\begin{cases} \frac{m^*}{\tau} v_{d,x} = -e[F_x + (v_{d,y} B_z/c)] \\ \frac{m^*}{\tau} v_{d,y} = -e[F_y - (v_{d,x} B_z/c)] \\ \frac{m^*}{\tau} v_{d,z} = -e F_z \end{cases}$$

By multiplying the previous set of equations by the electron density n and the charge $-e$ and knowing that $\vec{j} = -ne\vec{v_d}$, we obtain:

$$\boxed{\begin{cases} j_x = \frac{ne^2\tau}{m^*} F_x - (eB_z/m^*c)\tau j_y \\ j_y = \frac{ne^2\tau}{m^*} F_y + (eB_z/m^*c)\tau j_x \\ j_z = \frac{ne^2\tau}{m^*} F_z \end{cases}} \qquad (1.2)$$

2 - As $\sigma_0 = \frac{ne^2\tau}{m^*}$ and $\omega_c = \frac{eB_z}{m^*c}$ we deduce that

$$\begin{cases} j_x = \sigma_0 F_x - \omega_c \tau j_y \\ j_y = \sigma_0 F_y + \omega_c \tau j_x \\ j_z = \sigma_0 F_z \end{cases}$$

The previous set of equations can be rearranged so as to give:

$$j_x = \frac{\sigma_0}{1+(\omega_c\tau)^2}\left(F_x - \omega_c\tau F_y\right)$$

$$j_y = \frac{\sigma_0}{1+(\omega_c\tau)^2}\left(F_y + \omega_c\tau F_x\right)$$

$$j_z = \sigma_0 F_z$$

This leads to the generalized magneto-conductivity tensor for the electrons:

$$\boxed{\sigma(B) = \frac{\sigma_0}{1+(\omega_c\tau)^2}\begin{pmatrix} 1 & -\omega_c\tau & 0 \\ \omega_c\tau & 1 & 0 \\ 0 & 0 & 1+(\omega_c\tau)^2 \end{pmatrix} \qquad (1.3)}$$

3- From (1.3) we conclude that the effects of the magnetic field on the charge transport are twofold. First, the conductivity perpendicular to the magnetic field is decreased by the factor $[1+(\omega_c\tau)^2]^{-1}$. The corresponding increase in the sample resistance induced by a magnetic field is known as magnetoresistance (for small values of B it is proportional to B^2 because $\rho \propto 1/\sigma$). Second, the magnetic field also generates a current transverse to the applied electric field, resulting in off-diagonal elements in the conductivity tensor. These are linearly proportional to the magnetic field whereas the diagonal elements are quadratic in the magnetic field.

II- Hall effect

4- $j_y = 0$ so that from question 2 we get:

$$j_x = \sigma_0 F_x \quad \text{and} \quad F_y = -\frac{\omega_c\tau}{\sigma_0} j_x$$

Since R_H is defined by the relationship $R_H = \dfrac{F_y}{j_x B_z}$, we obtain:

$$R_H = -\frac{\omega_c\tau}{\sigma_0 B_z} = -\frac{eB_z\cancel{\tau}}{\cancel{m^*}c} \times \frac{\cancel{m^*}}{ne^{\cancel{2}}\cancel{\tau}} \times \frac{1}{\cancel{B_z}}$$

i.e. $\boxed{R_H = \dfrac{-1}{nec}}$

It is thus seen that the Hall effect allows determining both the concentration and the sign of charged carriers in a sample.

Supplementary information on Exercise 1

The light cone is defined by the condition of total internal reflection.
$\vec{k} = \vec{k}_{//} + \vec{k}_{\perp}$ where $\vec{k}_{//}$ corresponds to the in-plane wavevector and $\vec{k}_{\perp}$ corresponds to the component of the total wavevector along the growth axis. It can be shown that $|\vec{k}_{//}| = \frac{\omega}{c} \sin\theta$ where θ is the external angle with respect to the normal to the sample.
Photons escaping from the sample will have a maximum in-plane component equal to $\frac{\omega}{c}$ ($= k_{//max}$). The corresponding internal angle is given by Snell law $\theta_{int,max} = \arcsin(1/n_{sc})$ where n_{sc} is the refractive index of the dielectric medium.

Supplementary information on the origin of light-hole and heavy-hole subbands

The top of the valence band is characterized by p-type like orbitals: p_x, p_y and p_z in the specific case of semiconductors (for the sake of simplicity we will restrict ourselves to the case of diamond- (Si, Ge) and zincblende-type (GaAs, InAs, InP, GaP, InSb ...) semiconductors). Due to spin effects, one could believe that at $\vec{k} = \vec{0}$ the top of the valence band is 3×2 degenerate. However, due to the spin-orbit interaction there is a lift of the 3×2 degeneracy in two levels, one fourfold degenerate and one twofold degenerate at an energy Δ_0 below the first one (this is the split-off valence band due to the spin-orbit interaction between $j = l+s = 3/2$ and $j = l-s = 1/2$ states, i.e. p states characterized by an orbital angular momentum $l=1$, the interaction Hamiltonian being equal as a first approximation to $H_{so} = \lambda \vec{l}.\vec{s}$ with λ the spin-orbit coupling constant).
The $j = 3/2$ state is fourfold degenerate with $j_z = \pm 3/2, \pm 1/2$ and the new eigenstates are identified using the notation $|j, j_z\rangle$. Heavy calculations carried out in the $|3/2, \pm 3/2\rangle$ and $|3/2, \pm 1/2\rangle$ basis for the effective

Hamiltonian leads to two energies which are doubly degenerate. One of those energies will be associated with an heavier mass (hence the denomination heavy hole) and the second one will correspond to a lighter mass (→ light hole).

As far as deformation potentials are concerned, it is usually found that the Γ_1 conduction band deformation potential is about ten times larger than that of the Γ_{15} (or $\Gamma_{25'}$) valence bands. Note however that in an optical experiment under hydrostatic stress only the relative volume deformation potentials $a(\Gamma_{1c}) - a(\Gamma_{15v})$ between the conduction and valence bands are measured.

More information on the above-mentioned phenomena can be found in:

Fundamentals of Semiconductors, physics and materials properties by Peter Y. Yu and Manuel Cardona, 2nd edition (Springer, Berlin, 1999).