Series_ Electronic and optical semiconductor devices

Series 12_ Absorption in semiconductors

I. Case of allowed direct transitions

1_ We make use of the usual approximation of parabolic bands. Consequently,

$$E_c(k) = E_g + \frac{\hbar^2 k^2}{2m_c} \quad \text{and} \quad E_v = -\frac{\hbar^2 k^2}{2m_v}$$

As a result we get $\hbar\omega_{vc} = E_c(k) - E_v(k) = E_g + \frac{\hbar^2 k^2}{2}\left(\frac{1}{m_c} + \frac{1}{m_v}\right)$

From the expression of the reduced effective mass we deduce that:

$$\boxed{\hbar\omega_{vc} = E_g + \frac{\hbar^2 k^2}{2m_r}}$$

2_ The Lorentzian distribution $\frac{1/\pi T_2}{(\omega - \omega_{vc})^2 + (1/T_2)^2}$ can be replaced by a Dirac distribution function centered on ω_{vc}. As a result, equation (I.1) can be simplified to:

$$\alpha(\omega) = \frac{\pi e^2 x_{vc}^2 \omega}{\varepsilon_0 \hbar n_{op} c} \int_{\omega_g}^{+\infty} \rho_j(\omega_{vc}) [f_v(E_v) - f_c(E_c)]\, \delta(\omega_{vc} - \omega)\, d\omega_{vc}$$

i.e. $$\boxed{\alpha(\omega) \approx \frac{\pi e^2 x_{vc}^2 \omega}{\varepsilon_0 \hbar n_{op} c}\, \rho_j(\omega) [f_v(\hbar\omega) - f_c(\hbar\omega)]}$$

At this stage we can give several useful comments.

a_ The Lorentzian distribution found in equation (I.1) originated from the derivation of the expression of the linear optical susceptibility $\chi(\omega) = \chi_R(\omega) + i\chi_I(\omega)$ in the framework of the density matrix (quantum optics). A detailed description is given in Chapter 3 of the book "Optoelectronics" by E. Rosencher & B. Vinter. For semiconductors, $T_2 \approx 100$ fs

b_ The joint density of states corresponds to the density of states belonging to the valence and conduction bands which are effectively linked/connected by photons of energy $\hbar\omega$. It is thus easily understandable that $\rho_j(\omega)$ will be equal to

zero for $\hbar\omega < E_g$ since no states corresponding to an interband transition will be connected!

As it is often the case in such a situation, to derive $\rho_j(\omega)$ we make use of the approximation of an isotropic effective mass (→ parabolic bands) as most of the physics remains unaffected while letting the problem fully tractable analytically.

c- $x_{vc} = \left(\frac{2}{3}\right)^{1/2} |\vec{r}_{vc}|$ where $\vec{r}_{vc}$ enters in the expression of the dipolar matrix element describing valence band to conduction band transitions:

$$W_{vc}(\vec{k}) = -q\vec{E}.\vec{r}_{vc}\,\delta(\vec{k}'-\vec{k}_{op}-\vec{k})$$

and $$\vec{r}_{vc} = \frac{1}{V_i}\iiint_{cell} u^*_{c,\vec{k}}(\vec{R})\,\vec{R}\,u_{v,\vec{k}}(\vec{R})\,d^3\vec{R}$$

($u^*_{c,\vec{k}}$: Bloch functions; $u_{v,\vec{k}}$: Bloch functions)

b- The joint energies E_v and E_c can be written as a function of $\hbar\omega$ using expressions derived in question 1 so that in the expression of $\alpha(\omega)$ we can directly switch from $f_v(E_v(k))$, $f_c(E_c(k))$ to $f_v(\hbar\omega)$ and $f_c(\hbar\omega)$.

Thus $$f_c(\hbar\omega) = \left[1+\exp\left(\frac{E_c(\hbar\omega)-E_{F_c}}{k_B T}\right)\right]^{-1}$$

with $$E_c(\hbar\omega) = E_g + \frac{m_r}{m_c}(\hbar\omega - E_g)$$

$$f_v(\hbar\omega) = \left[1+\exp\left(\frac{E_v(\hbar\omega)-E_{F_v}}{k_B T}\right)\right]^{-1}$$

$$E_v(\hbar\omega) = -\frac{m_r}{m_v}(\hbar\omega - E_g)$$

e- It is seen that $\alpha(\omega) = \alpha_0(\omega)[f_v(\hbar\omega) - f_c(\hbar\omega)]$.

The condition required to get optical gain, i.e. $\alpha(\omega) < 0$ is given by $f_c(\hbar\omega) - f_v(\hbar\omega) > 0$, which means that, taking into account the expressions of Fermi-Dirac distribution functions: $E_{F_c} - E_{F_v} > \hbar\omega$. This is the so-called Bernard-Durrafourg condition. The latter implies that only photons with an energy smaller than the energy separation between quasi-Fermi levels can be amplified (at the same time, we must have $\hbar\omega > E_g$).

3- First, we shall derive the expression of the density of states for a single isotropic band (case of a bulk semiconductor).

The density of states in k space when adopting periodic boundary conditions (first without considering the spin of electron) can be written as:

$$\rho(k) = \frac{V}{8\pi^3} = \frac{1}{8\pi^3} \quad \text{(we have } V=1\text{)}$$

The number of states dN contained in a volume sandwiched between 2 spheres of radius k and $k+dk$ is expressed as: $dN = \frac{V(=1)}{8\pi^3} 4\pi k^2 dk = \frac{1}{2\pi^2} k^2 dk$

To this elementary volume $k^2 dk$ in k space will correspond an elementary volume in the energy space. In the conduction band's case, we get:

$$E_c(k) = E_c + \frac{\hbar^2 k^2}{2m_c} \quad \text{so that} \quad k^2 = \frac{2m_c}{\hbar^2}(E - E_c)$$

$$dk = \left(\frac{2m_c}{\hbar^2}\right)^{1/2} \frac{1}{2} (E-E_c)^{-1/2} dE$$

which leads to $k^2 dk = \frac{1}{2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2} (E-E_c)^{1/2} dE$ and when introducing the spin degeneracy

$$dN = \frac{1}{2\pi^2} \times 2 \times \frac{1}{2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2} (E-E_c)^{1/2} dE \quad \text{and} \quad \rho_c(E) = \frac{dN}{dE}$$

(↑ spin)

so that $\boxed{\rho_c(E) = \frac{1}{2\pi^2}\left(\frac{2m_c}{\hbar^2}\right)^{3/2} (E-E_c)^{1/2}}$

To derive the joint density of states $\rho_j(\omega)$, we use the expression $\hbar\omega = E_g + \frac{\hbar^2 k^2}{2m_r}$ which leads to $\boxed{\rho_j(E) = \frac{1}{2\pi^2}\left(\frac{2m_r}{\hbar^2}\right)^{3/2} (E-E_g)^{1/2}}$

In addition, $\rho_j(\omega) = \rho_j(E)\frac{dE}{d\omega}$ i.e. $\rho_j(\omega) = \hbar\rho_j(E)$ and thus we get

$$\boxed{\rho_j(\omega) = \frac{1}{2\pi^2}\left(\frac{2m_r}{\hbar}\right)^{3/2} (\omega - E_g/\hbar)^{1/2}}$$

4- From previous questions we can thus write

$$\alpha_0(\omega) = \frac{\pi e^2 x_{vc}^2 \omega}{\varepsilon_0 n_{op} c} \times \frac{1}{2\pi^2}\left(\frac{2m_r}{\hbar}\right)^{3/2} (\omega - E_g/\hbar)^{1/2}$$

i.e. $\alpha_0(\omega) = \frac{e^2 x_{vc}^2 \omega}{2\pi\varepsilon_0 n_{op} c}\left(\frac{2m_r}{\hbar^2}\right)^{3/2}\sqrt{\hbar\omega - E_g}$. It is thus seen that

$$\alpha_0(\omega) = A(\hbar\omega - E_g)^{1/2} \quad \text{where} \quad \boxed{A = \frac{e^2 x_{vc}^2}{\lambda \varepsilon_0 n_{op}} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2}}$$

(i) Case of GaAs

$E = 1.464\,eV \rightarrow \lambda \sim 846.7\,nm$

We determine the value of A using the international system units. As energies are usually expressed in eV when dealing with semiconductors, we will then convert the prefactor A from $J^{-1/2} m^{-1}$ to $eV^{-1/2} cm^{-1}$

$$A = \frac{(1.6\times10^{-19}\times 5\times10^{-10})^2}{846.7\times10^{-9}\times 8.85\times10^{-12}\times 3.6} \times \left(\frac{2\times 0.059\times 9.1\times10^{-31}}{(1.05\times10^{-34})^2}\right)^{3/2} \approx 7.2\times10^{15}\,J^{-1/2} m^{-1}$$

i.e. $A \approx 28846\,eV^{-1/2} cm^{-1}$ so that $\alpha_0(E = 1.464\,eV) \approx 5769\,cm^{-1}$

(ii) Case of GaN

$$A = \frac{(1.6\times10^{-19}\times 2.1\times10^{-10})^2}{358.2\times10^{-9}\times 8.85\times10^{-12}\times 2.6} \times \left(\frac{2\times 0.169\times 9.1\times10^{-31}}{(1.05\times10^{-34})^2}\right)^{3/2} \approx 2.02\times10^{16}\,J^{-1/2} m^{-1}$$

i.e. $A \approx 80736\,eV^{-1/2} cm^{-1}$ so that $\alpha_0(E = 3.46\,eV) \approx 16147\,cm^{-1}$

We thus have an illustration of the high absorption of direct semiconductors above the band gap. We can observe the much larger absorption coefficient of GaN 40 meV above the band gap compared with GaAs. Such a behavior will have a significant impact when realizing optoelectronic devices (optical confinement layers: compromise between stress and optical absorption (lasers)).

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