# THEORETICAL ANALYSIS OF OPTICAL GAIN IN QUANTUM WELL LASERS INCLUDING VALENCE-BAND MIXING EFFECT

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The linear optical gain in the AlGaAs/GaAs quantum well lasers is studied theoretically, taking into account the valence-band mixing effect. Our approach is based on the multiband effective-mass theory ($k\,p$ method) and the density-matrix formalism. In order to obtain the valence bands' structure we employ the $4 \times 4$ Luttinger–Kohn Hamiltonian, neglecting the coupling to the split-off band. The spectral dependence of the linear optical gain is calculated using the density-matrix method with interband relaxation. Finally, we analyse the spatial distribution of the optical gain in the quantum well region for the photon energy corresponding to the peak value of the linear gain.

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## 1. Introduction

The quantum well (QW) lasers are presently the key components of many optical and communication systems. Although the beginnings of QW lasers reach the late seventies, they are still the subject of intense research due to their promise as a compact, efficient lasers sources for a number of important applications [1, 2]. In order to better understand the physical processes taking place in the QW lasers, as well as to optimise the technological parameters of their manufacturing process, a great number of numerical modelling approaches has been undertaken [1, 2]. The fundamental data used in the numerical simulations of the electro-optical phenomena taking place in the QW lasers is the optical gain, which determines the laser threshold and affects the lasing mode structure [1, 2]. Therefore, the optical gain has been studied extensively, for the various types of quantum wells including strained and unstrained structures [3–5]. The first step in calculating the spectral dependence of the optical gain is to determine the QW band structure. The conduction band is usually treated as a parabolic and decoupled from the valence bands, thus the quantized energies and envelope functions for electrons can be found from the single effective-mass equation for a nondegenerate band. The nonparabolic valence band structure is calculated employing the Luttinger–Kohn (L–K) Hamiltonian derived from the multi-band effective-mass theory ($k\,p$ method) [3, 4]. In

order to obtain the spectral dependence of the optical gain in the QW laser we apply the density matrix formalism with the interband relaxation [3, 4]. We do not consider here the electrostatic deformation of QW band profile caused by the inhomogeneous space charge distribution, since it plays a less important role in AlGaAs/GaAs wells [5]. Besides the analysis of the spectral dependence of the optical gain in this paper we present the position dependent distribution of the optical gain in the QW region for the chosen photon energy. Our results show the significant variations in the distribution of optical gain in the direction perpendicular to the QW which can have important consequences for the modelling of QW lasers.

## 2. The band structure of quantum well

Applying the multiband effective-mass theory ($k$ $p$ method) we calculate the band structure of the QW region. First, considering the conduction band as parabolic and decoupled from the valence bands, we find the quantized energies $E_n^e$ and the envelope functions for electrons $F_n(z)$ solving the single effective-mass equation for a nondegenerate energy band. We assume that the QW potential profile for electrons as well as for holes depends only on the difference in the energy band-gap of the materials used in the QW structure. In other words, we do not consider the influence of the external electrical potential on the band structure which is quite reasonable in the analysis of the optical gain in QW lasers because of the fact that for the lasing condition the external electrostatic field is practically compensated by the built-in potential of the $p-n$ junction. Analysing the valence band structure, we employ the 4 × 4 Luttinger–Kohn Hamiltonian, which takes into account the coupling between the heavy and the light hole bands, but neglects the coupling to the split-off band. The valence band envelope functions satisfy the multiband effective-mass equations written below

$$\sum_{j=1}^{4} \left[ \widehat{H}_{i,j}(k_\perp, k_z) + V_h(z)\delta_{i,j} \right] G_m^j(k_\perp, z)$$

$$= E_m^h(k_\perp)G_m^i(k_\perp, z), \qquad i = 1, \ldots, 4, \tag{2}$$

where $\widehat{H}_{i,j}(k_\perp, k_z)$ is the L–K Hamiltonian [3]. The L–K Hamiltonian can be transformed by the unitary transformation into two 2 × 2 decoupled Hamiltonians [3] resulting in block effective-mass equations

$$\sum_{j=1}^{2} \left[ \widehat{H}_{i,j}^U(k_\perp, k_z) + V_h(z)\delta_{i,j} \right] g_m^j(k_\perp, z) = E_m^{hU}(k_\perp)g_m^i(k_\perp, z), \quad i = 1, 2, \tag{3a}$$

$$\sum_{j=1}^{2} \left[ \widehat{H}_{i,j}^L(k_\perp, k_z) + V_h(z)\delta_{i,j} \right] g_m^{j+2}(k_\perp, z) = E_m^{hL}(k_\perp)g_m^{i+2}(k_\perp, z), \quad i = 1, 2. \tag{3b}$$

Equations (3a) and (3b) describe upper 2 × 2 and lower 2 × 2 Hamiltonians. The appropriate solutions for upper and lower Hamiltonians, for each subband $m$ are degenerate. The effective-mass equations are solved using the finite element method. For different values of $k_\perp = \sqrt{k_x^2 + k_y^2}$, we obtain the block envelope

functions $g_m^i(k_\perp, z)$ and discrete energy levels $E_m^h(k_\perp)$, which form the valence band structure of QW [3, 4].

### 3. The linear optical gain in the quantum well structure

Having established the band structure, we are able to calculate the linear optical gain using the density-matrix formulation with the interband relaxation [3]. To calculate the linear optical susceptibility distribution in the QW region we define the $z$-dependent optical dipole matrix elements which for the TE mode have the following form:

$$\left|\hat{\varepsilon} M_{n,m}^{s,\mathrm{U}}(k_\perp, z)\right|^2 = \frac{1}{4}\langle S|ex|X\rangle^2$$

$$\times \left[\langle F_n|g_m^1\rangle^2 L^2 |F_n(z)|^2 \left|g_m^1(k_\perp, z)\right|^2 + \frac{1}{3}\langle F_n|g_m^2\rangle^2 L^2 |F_n(z)|^2 \left|g_m^2(k_\perp, z)\right|^2\right], \quad (4a)$$

$$\left|\hat{\varepsilon} M_{n,m}^{s,\mathrm{L}}(k_\perp, z)\right|^2 = \frac{1}{4}\langle S|ex|X\rangle^2$$

$$\times \left[\langle F_n|g_m^4\rangle^2 L^2 |F_n(z)|^2 \left|g_m^4(k_\perp, z)\right|^2 + \frac{1}{3}\langle F_n|g_m^3\rangle^2 L^2 |F_n(z)|^2 \left|g_m^3(k_\perp, z)\right|^2\right], \quad (4b)$$

where $\langle S|ex|X\rangle^2$ is the transition matrix element for the bulk GaAs, $F_n(z)$ are the envelope functions for the conduction band, $L$ is the thickness of the QW layer. In expressions (4a)–(4b) we have omitted terms containing the angular depend- ence since they average to zero after integration. Calculating the average value of the optical dipole matrix elements in the QW region we obtain the well-known formulas [3, 4]. The $z$-dependent susceptibility is given by

$$\varepsilon_0 \chi^{(1)}(w, z) = \frac{1}{V} \sum_s \sum_{in} \sum_{mk_\perp} \left|\hat{\varepsilon} M_{n,m}^{s,i}(k_\perp, z)\right|^2$$

$$\times \frac{f_e^n - f_{h,i}^m}{E_n^e(k_\perp) - E_m^h(k_\perp) + E_\mathrm{G} - \Delta E_\mathrm{G} - \hbar w - i\hbar/\tau_\mathrm{in}}, \quad (5)$$

where $f_e^n$ and $f_{h,i}^m$ are the Fermi functions for the $n$-th subband in the conduction band and the $m$-th subband (with the $i$-th spin state) in the valence band, $E_\mathrm{G}$ is the band-gap energy, $\omega$ is the angular frequency of photons, $V$ is the volume and $\tau_\mathrm{in}$ is the intraband relaxation time. The many-body effects have been taken into account by adding the band-gap renormalization term, $\Delta E_\mathrm{G}$, whose values, for different carrier densities, have been estimated from the experimental data [6]. The linear gain distribution in QW is given by

$$g(\omega, z) = \frac{\omega \mu c}{n_\mathrm{r}} \mathrm{Im}[\varepsilon_0 \chi^{(1)}(\omega, z)], \quad (6)$$

where $\mu$ is the permeability, $n_\mathrm{r}$ is the refractive index and $\varepsilon_0$ is the permittivity of free space.

## 4. Results

We performed analysis of the optical gain for the AlGaAs/GaAs unstrained QW structure with a well width $L = 80$ Å. For the conduction band we obtained two discrete levels with energies: 0.0337 eV and 0.1158 eV measured with respect to the bottom of the well. The calculated valence band structure is shown in Fig. 1. The optical gain was calculated for different values of the quasi Fermi level for electrons and holes which were obtained from the solution of the drift-diffusion equations for the chosen QW laser structure [7]. For different densities of carriers injected into the active region of the QW laser, the spectral dependences of the optical gain and the optical gain distributions in the QW region corresponding to the photon energy equal to 1.45 eV are shown in Fig. 2.
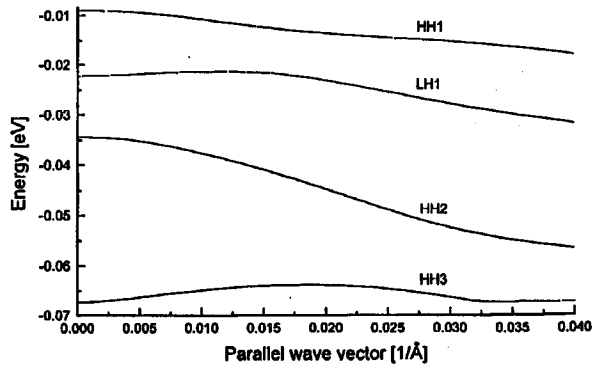
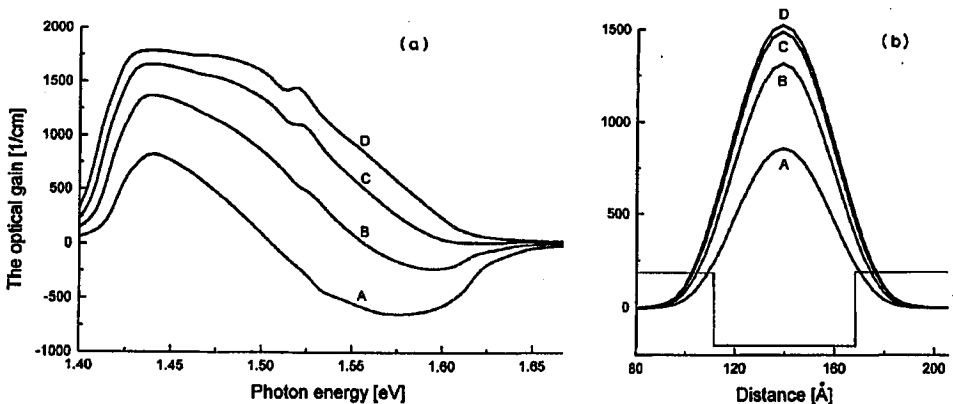Fig. 1.   The valence-band structure for a 80 Å thick GaAs–Al$_{0.15}$Ga$_{0.85}$As quantum well.

Fig. 2.   (a) The spectral dependence of the optical gain. (b) The optical gain distribution in the quantum well layer. $A - N = 3 \times 10^{18}$ cm$^{-3}$, $B - N = 4 \times 10^{18}$ cm$^{-3}$, $C - N = 5 \times 10^{18}$ cm$^{-3}$, $D - N = 6 \times 10^{18}$ cm$^{-3}$.

## 5. Conclusion

In this paper we present the spectral and position dependent distribution of the optical gain in the AlGaAs/GaAs QW lasers. In order to calculate the distribution of the optical gain in QW region the $z$-dependent optical matrix elements were proposed. The valence band mixing effects with the band-gap renormalization due to the many-body interactions were taken into account.

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