Numerical simulation of a nitride single quantum well laser

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Abstract. Numerical simulation of a quantum well on nitrides, optical interband transitions in low dimensional semiconductor structures (semiconductor quantum wells), conduction-heavy hole and transitions in quantum wells, refinement of the gain for a quantum well on nitride materials with allowance for the overlap integral and approximate this.

1. Introduction

The optical gain is a key parameter in the design of quantum well lasers. The design optimization necessitates a large degree of numerical computation because there are a large number of laser parameters involved, such as the quantum well barrier composition, the number of QW’s, the cavity length, and the facet reflectivity. In the dynamic performance of QW lasers, the differential gain and the line width enhancement factor are key parameters in addition to the gain. The efficiency of numerical calculations becomes a serious factor when analyzing the structures of 2D or 3D quantum-well lasers, such as nitride lasers, in which medium deformations due to polarization effects play a significant role. Furthermore, in the design optimization, some of the important physics becomes obscured because of the large number of laser parameters. Therefore, simple analytical formulas are desired that can clearly delineate the relations between design parameters and predict device performance characteristics.

2. Analytical approach

Alloys of GaN, which are discussed in our modeling, are mainly used to achieve increased device performance or to achieve a certain radiation wavelength, but many important parameters, such as energy of the forbidden zone, depend on the composition of the alloy. In our work, this parameter was also one of the most important. For the calculation, Vegard’s law was used, with which most of the experimental results for the width of the forbidden zone of solid solutions recently agree. Vegard’s law for $In_xGa_{1-x}N$:

$$E_g(In_xGa_{1-x}N) = xE_g(InGa) + (1 - x)E_g(InN) - bx(1 - x),$$

where $b$ is the bending parameter determined by the structure.
Nitride materials, as already noted above, are of particular interest because of their internal spontaneous $P_s$ and external $P_{pz}$ piezoelectric effect. For example, the piezoelectric field ($E_{pz}$), induced by voltage, along the axis [0001], in the absence of free charges, is then defined as:

$$E_{pz}^x = -\frac{P_z}{\varepsilon_0} = -\frac{2d_{44}}{\varepsilon_0} \left[ C_{11} + C_{12} - 2 C_{13}^2 \right] e_{xx},$$

where $\varepsilon_r$ and $\varepsilon_0$ are the dielectric constant of the material and the dielectric constant of the vacuum, $e_{xx}$ is the deformation component along the x axis, which can be defined in terms of lattice constants as $e_{xx} = (a_e - a_c) / a_c$, where $a_c$ and $a_e$ are the lattice constants of the epitaxial layer and bulk material, respectively. Thus, the direction of the piezoelectric field depends on whether the epitaxial layer is in a state of compression or tension, which determine the variable $e_{xx}$.

To check the results obtained by other scientific groups when trying to verify the truth of the study, we attach a table with structural parameters used in our research (Table 1). The parameters of the crystal structure of these compounds are given in the Table. 1, where $a,c$ - constants of the hexagonal lattice, and $P_s$ - spontaneous polarization.

| Table 1. Structural parameters and calculated spontaneous polarization of nitrides of elements of the nitride group. |
|---|---|---|---|
| | GaN | InN | AlN |
| $a$, Å | 3.189 | 3.54 | 3.112 |
| $c$, Å | 5.185 | 5.705 | 4.982 |
| $a / c$ | 1.627 | 1.612 | 1.601 |
| $P_s$, C/m2 | $-0.029$ | $-0.032$ | $-0.081$ |

A numerical model was developed for solving the one-dimensional stationary Schrödinger equation and the search for allowable energy values for a quantum well on nitrides. During the calculations, spontaneous and piezoelectric polarizations of nitrides were taken into account, leading to a distortion of the profile of the quantum well on nitrides (in particular, GaN/In$_{0.7}$Ga$_{0.2}$N/GaN). The overlap integral of the wave functions was calculated, which makes it possible to more accurately calculate the characteristics of nitride lasers (including amplification, the probability of spontaneous emission and absorption, spontaneous emission).

The rate of stimulated absorption $R^\uparrow$ and emission $R^\downarrow$ can be calculated by the formulas below:

$$R^\uparrow,\downarrow = \left( \frac{q}{m} \right) \left( \begin{array}{c} m_p \\ n_{n_g}^M \end{array} \right) \int d\chi \phi_e^* \psi_{hh} = \frac{2mE_p}{q} \left( n_x^2 + n_y^2 \right) f_{e,c} \left( 1 - f_{e,v} \right) \frac{m_r^2}{\hbar^2} \delta (E - E_c)$$

Where $\int d\chi \phi_e^* \psi_{hh}$ is integral of overlap $I$, $n_x, n_y$ - components of the electric polarization vector, $f_{e,c,v}$ - Fermi function for electrons and holes, $E_c, E_p$ - quantization energy level for electrons and holes, $n_{p}$ - photon density, $m$ - electron mass, $n, n_{n_g}^M, E_p$ - determined by the material parameters, $m_r$ - reduced mass, $q$ - electron charge, $\varepsilon_r$ - dielectric constant, $\hbar$ - 'h-bar' Planck’s constant.

We take the traditional model, the optical gain $g(\omega)$ model of Asada et al. [1]. It is assumed that all levels are parabolic and that the optical transitions obey the $k$-selection rules. In order to have a general idea of the nature of gain, we write the empirical expression for optical gain without taking into account spontaneous radiation for single QW, which is expressed as:

$$g(\omega) = \frac{R^\downarrow(\omega) - R^\uparrow(\omega)}{n_p v_g M}$$
The absorption coefficient of a pure photon is the difference between the speed of stimulated absorption and the speed of stimulated emission. The semiconductor absorption coefficient can then be associated with the photon group velocity \( v_g^M \) and with the photon density \( n_p \). Through the values of the stimulated emission and absorption rates in this paper, we have calculated the attenuation and other laser characteristics. The work echoes the themes that affect the articles in the list of references [2]-[4]. The numerical simulation results are presented in Figure 1-3.

**Figure 1. (a,b)** The potential well profile (dependence of the quantum well energy on the coordinate) is distorted by the polarization in the GaN/In\(_{0.7}\)Ga\(_{0.3}\)N/GaN structure. By the shooting method, the wave functions for electrons \( \Psi_e \) and heavy holes \( \Psi_{hh} \) are calculated. (a) - is in equilibrium (\( E_f \) - the equilibrium Fermi level), Integral of overlap \( I=0.124 \), (b) - at an applied voltage of 1.6V (\( E_{fc}, E_{fv} \) - the quasi-Fermi level), \( I=0.103 \).

For a better understanding of the configuration of the drawings Figure 1 (a, b), Figure 2 is also attached. with the image of a simulated zone diagram without calculating the Schrödinger equation, which is calculated taking into account information on the internal and external piezoelectric effect of the nitride. The figure shows the regions of the quantum well (radiating region), and the p, n-doped regions (mirrors) doped out along the bottom of the conduction band and the valence band top.

**Figure 2.** The energy diagram of a nitride laser with a quantum well, taking into account the distortion of the diagram under the action of polarization of nitrides.
3. Result

An analytical expression was obtained for optical amplification in nitride quantum-well lasers using explicit quadratic approximations of approximations of the parabolic optical gain part. It was shown that approximate formulas provide not only an efficient way to calculate the parameters associated with the gain, but also a convenient way to obtain physical information for the general interaction of the SQW parameters. It is expected that the presented analytical approach will demonstrate its significant advantage, especially in terms of optimizing the design of practical SQW nitride lasers, which require consideration of material deformation parameters.

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