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# Modeling and simulation of $Zn_xCd_{1-x}Te/ZnTe$ quantum well structure for laser applications



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#### 1. Introduction

#### ABSTRACT

In this work, we modeled and simulated  $aZn_xCd_{1-x}Te/ZnTe$  based single quantum well structure. We have taken into account the effect of carrier density, alloy composition, temperature and wells width on the optical gain as well as threshold current density. The use of ZnTe as a barrier leads to the improvement of the carrier confinement such as  $Q_c$  (83%)/ $Q_v$  (17%). Then, we have optimized the quantum well structure that allows obtaining a threshold current density  $J_{th}$  = 500 A/cm<sup>2</sup>. This study allowed us to achieve laser diodes VCSEL quantum well reliable and emitting around 0.740 µm.

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one of the semiconductor materials to get a short wave laser is the  $Zn_xCd_{1-x}Te$  compounds [8–10]. This last is the alloy of two binary materials which are ZnTe and CdTe that have direct band gap at room temperature to Eg(ZnTe)=2.26 eV and Eg(CdTe)=1.51 eV, this material has the cubic crystal structure (Zinc blend) [11]. It should be known that the optical confinement studied of the unstrained  $Zn_xCd_{1-x}Te/ZnTe$  quantum well (QW) structure is important that in low Zn concentration x = (0.1-0.3). In this paper, our objectives are the improving the optical gain of this quantum well structure comparing to a previous

During the last years, the II–VI compound semiconductors were frequently used in the manufacture of optoelectronic devices such as light-emitting diodes (LED), laser diodes (LDs), and the physical sensors because of their bandwidths prohibited which can emit the laser light in the visible spectrum [1–5]. The efforts accomplished by several scientists and the advancement in the II–VI materials growth technology such as the molecular beam epitaxy (MBE) and metal–organic vapor phase epitaxy (MOVPE) [6]. They allow the production of high-quality heterostructures with a reduction of substantive impurities and doping levels ranging from 10<sup>17</sup> to 10<sup>18</sup> cm<sup>-3</sup> [7]. The II–VI materials are still valid as advanced materials,

In this paper, our objectives are the improving the optical gain of this quantum well structure comparing to a previous study [12], and additionally, the investigation of influences of the temperature, well width on the optical gain and the

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threshold current density that are not studied by the reference [12]. This investigation permits us to optimize the QW structure by choosing the parameters that allowed having a low threshold current density.

#### 2. The calculation model

#### 2.1. Energy quantification

The particles movement in a quantum well was described by the wave equation, except that this last it can be solved that for some energy values. The equation system that we allow to determine the eigenvalues of electron energy and that of the hole is described as following [13]:

$$\left[\frac{m_{cb}}{m_{cw}}\frac{\Delta E_c - E_{cn}}{E_{cn}}\right]^{1/2} = \left\{ \frac{\tan}{-\cot} \right\} \left[ \frac{L_w \sqrt{2m_{cw}E_{cn}}}{2\hbar} \right] \left\{ \frac{n; even}{n; odd} \right\}$$
(1)

$$\left[\frac{m_{cb}}{m_{cw}}\frac{\Delta E_{\nu} - E_{\nu m}}{E_{\nu m}}\right]^{1/2} = \left\{ \underset{-\text{cot}}{\tan} \right\} \left[\frac{L_w \sqrt{2m_{hw}E_c \nu m}}{2\hbar}\right] \left\{ \underset{m;odd}{m;odd} \right\}$$
(2)

where  $m_{cw}$ ,  $m_{cb}$  are the effective mass of the electrons in the well and in the barrier, respectively. While  $m_{hw}$  and  $m_{hb}$  represent the effective mass of holes in the well and the barrier,  $\Delta E_{c,v}$  is the depth of the well and  $E_{cn}$ ,  $E_{vm}$  are the eigenvalues for the energy of electron and that of the holes, respectively.  $L_z$  is the width of the well.

#### 2.2. Optical gain models

The optical gain is one of the significant parameters to investigate the quantum well laser structure because it is with him that can be determined the threshold current density. In this study, optical gain was calculated by the model of Asada as is showing in the following relationship [13]:

$$g(\omega) = \omega \sqrt{\frac{\mu}{\varepsilon}} \sum_{n=1} \left( \frac{m_r}{\pi \hbar^2 L_z} \right) \int_{E_g + E_{cn} + E_{vn}}^{\infty} \langle R_{cv}^2 \rangle (f_c - f_v) F_\tau (E_{cv}) dE_{cv}$$
(3)

where  $m_r$  is the reduced effective mass,  $E_{cv}$  is the transition energy [14].  $R_{cv}$  is the element of the optical matrix for the waves Transverse Electric (TE) modes [15].  $f_c$  and  $f_v$  are actual occupancy factors of each sub-band Considered.  $F_{\tau}$  ( $E_{cv}$ ) is the function that expresses the enlargement transition [16–18].

The energy transition of laser is:

$$E_{tr} = E_g + E_e + E_{hh} = \frac{1.24}{\lambda} \tag{4}$$

The calculation of the gap was determined by the using of Varshni model as is shown in the following empirical relationship [19]:

$$E_g(x,T) = E_g(x,0) - \alpha \frac{T^2}{\beta + T}$$
(5)

where  $\alpha$ ,  $\beta$  represents the Varshni coefficients.

2.3. The spontaneous emission rate - radiative current

The spontaneous emission rate  $r_{spon}(E)$  of a quantum well structure is given by:

$$r_{spon}(E) = \frac{8\pi n^2 E^2}{h^3 c^2} \frac{1}{\exp\left[\frac{E - (E_{FN} - E_{FP})}{kT}\right] - 1} (-g(E))$$
(6)

where g(E) is the optical gain.

 $\infty$ 

In the spontaneous emission regime, the total number of photons per volume unit and per second is:

$$R = \int_{0}^{\infty} r_{spon}(E) dE \tag{7}$$

As a result, if we consider that the excess carrier densities are homogeneous in a quantum well structure, the current density associated with spontaneous radiative recombination's that cross this structure is written [20,21]:

$$J_{spon} = qL_z R \tag{8}$$

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