

# Investigation of optical gain in ZnO/MgZnO quantum well incorporating piezoelectric polarization

H. P. BHADANE, E. P. SAMUEL, D. S. PATIL\*

*Department of Electronics, North Maharashtra University, Jalgaon [Maharashtra], India*

Quantum well heterostructures comprising ZnO wells sandwiched within MgZnO barriers have been investigated through Kronig Penny Model. The carrier density has been obtained through self consistent solutions of Schrödinger and Poisson equation. The optical gain obtained for ZnO/MgZnO quantum well structure was 4113 (cm<sup>-1</sup>) for Mg mole fraction of 30% with carrier density 3.9 × 10<sup>18</sup> cm<sup>-3</sup>. The probability density shows a good confinement in the quantum well region for well width of 5 nm considering 30% of Mg composition in the barrier. Peak value of optical gain was found to be maximum for higher value of carrier density as expected.

(Received January 30, 2009; accepted March 19, 2009)

**Keywords:** ZnO/MgZnO, Quantum well, Piezoelectric polarization

## 1. Introduction

Zinc oxide (ZnO) is II-VI compound semiconductor [1] with hexagonal wurtzite structure and a wide direct band gap similar to GaN and ZnSe. ZnO films have optical transparency, large piezoelectric constant and ultraviolet (UV) emission properties [2-6]. Over the past few decades, ZnO films have been generally used in UV light emitting diodes (LEDs), transparent conducting electrodes of laser diodes (LDs), photovoltaic devices, optical wave guides, gas sensors, etc. Therefore, wurtzite semiconductors GaN and ZnO are of great technological interest. GaN and its alloys are promising for wide band gap optoelectronic devices. However, nowadays wurtzite ZnO has attracted much attention due to its simple fabrication. In this work, we focus on the visible-ultraviolet properties of ZnO wide band gap material and present theoretically the electron probability density, optical gain and spontaneous emission of ZnO/MgZnO quantum well laser diode.

The Quantum Well Lasers are a class of semiconductor lasers that have ultra thin active layers forming narrow potential wells for injected carriers and giving rise to a size quantization of the electronic status. Today, researchers in quantum optics are interested in the physics of semiconductor lasers, which have cavity comparable to wavelengths and to improve laser characteristics by miniaturizing device structures. Light emitters such as light-emitting diodes (LEDs) and laser diodes convert electrical energy into optical energy. The development of light sources which emit only the desired part of the spectrum with higher efficiency and a longer lifetime than incandescent bulbs are very lucrative venture.

The developing of simulation tools for finite quantum well is, imposed by the necessity to avoid trial and error method in fabrication which is a complex process and too expensive. Therefore, the assistance of adequate programming tools is always welcome. In this present

paper we have solved the Schrödinger's equation applying appropriate boundary conditions using Kronig-Penney model to realize the E-K relation for different eigen energy states and electron probability density in quantum well region [7-10]. Further, the investigation has been extended to analyze the spontaneous emission and optical gain for different carrier concentration which has been obtained through self-consistent solution of Schrödinger-Poisson equation. The paper is organized in four main sections. The section 2 describes the theory involved in the analysis. Section 3 discusses the results obtained using the developed simulation tools and in last section the concluding remarks have been presented.

## 2. Theory

In this work, we have used the effective mass approximation (EMA) to calculate the electronic and optical properties of wurtzite ZnO/MgZnO. The Schrödinger equation (SE) which has been solved for our ZnO/MgZnO based quantum well heterostructures is given as follows,

$$\frac{\partial^2 \psi(x)}{\partial x^2} = \frac{2m}{\hbar^2} (E \psi(x) - V(x) \psi(x)) \quad (1)$$

This is the time-independent SE (TISE), which is an equation of a very special importance for analyzing quantum heterostructures. For energies  $E < V_0$  (where  $V_0$  is barrier height), the general solution of the 1D TISE in each of the three regions, is of the form:

$$\begin{aligned}\psi_1(x) &= Ae^{ikx} + Be^{-ikx} \\ \psi_2(x) &= Ce^{-\gamma x} + De^{\gamma x}, \\ \psi_3(x) &= Ee^{ikx} + Fe^{-ikx}\end{aligned}\quad (2)$$

where,

$$\begin{aligned}k &= \frac{\sqrt{2m_w^* E}}{\hbar} \\ \gamma &= \frac{\sqrt{2m_b^* (V-E)}}{\hbar}\end{aligned}\quad (3)$$

Here,  $k$  and  $\gamma$  are the wave vectors in  $x$  direction for barrier and well region respectively, while  $m_w$  and  $m_b$  are the effective mass of ZnO and MgZnO respectively.  $\psi_i(x)$ ,  $i = 1, 2$  and  $3$  are the general solutions of Schrödinger equation in barrier and well region, which are clearly depicted in Fig. 1.

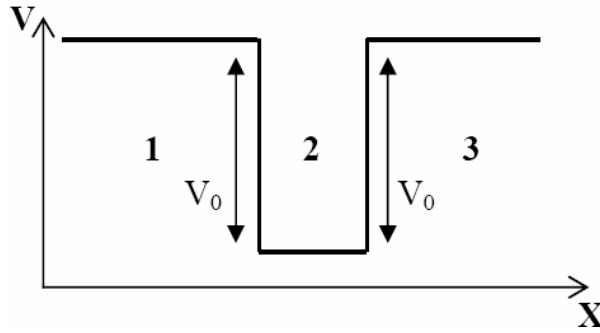


Fig. 1. MgZnO/ZnO/MgZnO quantum well structure.

The normalized solution of equation (2) with an appropriate conditions for the three regions as shown in Fig. 1, using Bloch theory in accordance with Kronig-Penny Model the Eigen equation have been obtained. By the  $k$ - $p$  model, we had obtained the three different Eigen energy states. Further, we had extended the study to obtain the variation of Eigen energy with varying wave vector ( $k$ ) for different states.

The optical gain can be achieved from equation (5). The electrostatic potential has been obtained from the self-consistent solution of Schrödinger-Poisson equation and the spontaneous polarization and the piezoelectric potential are included. The momentum matrix element has been obtained from

$$P_{cv} = i\sqrt{\frac{m_0^2}{m^*}}(E - E_v) \quad (4)$$

while, the optical gain as a function of spontaneous emission relation is given by

$$g = \frac{h}{2\pi} \left( \frac{\pi c}{n\omega} \right)^2 \left[ 1 - \exp\left( \frac{h\omega - 2\Delta\mu\pi}{2\pi k_B T} \right) \right] R_{sp} \quad (5)$$

In this formula,  $R_{sp}$  is the spontaneous emission rate, and other variables are having their usual meanings. In the following section, we had explored the variation of optical gain and spontaneous emission as a function of photon energy for different carrier concentrations. To determine the carrier concentration the Poisson equation as mentioned earlier is being solved self-consistently as reported by us in earlier paper [11].

### 3. Results and discussion

There is currently a lot of interest in the science and potential technological applications of spin-transport electronics (or spintronics), in which the spin of charge carriers are exploited to provide new functionality for microelectronic devices. By using the Kronig Penny Model, we have investigated the variation of Eigen energy as function of wave vector ( $k$ ). It has been observed from the result as shown in Fig. 2 that energy states E1 and E3 shows greater values of energy for the extreme values of wave vector while when  $k$  becomes zero the value of energy becomes minimum and found to be 1.60 and 9.92 meV, respectively.

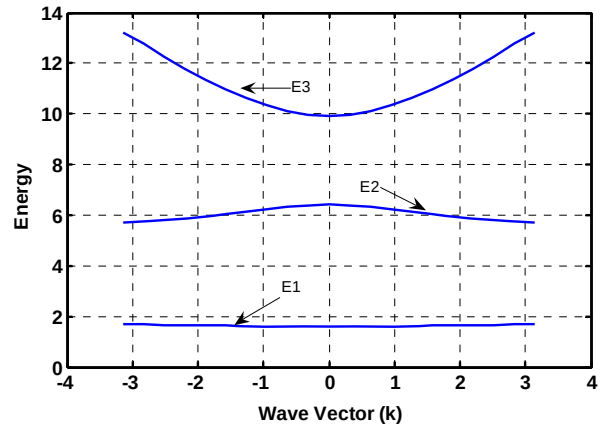


Fig. 2. Eigen energy states as a function of wavevector for 3 different levels.

The solution of the Schrödinger equation leads us to obtained the Eigen energy which has been utilized to investigate the probability of the electron to be present in the quantum well region under different Eigen energy states. We have shown in Fig. 3 and Fig. 4 the Probability density of electron in quantum well region of ZnO/MgZnO based quantum structure. We had studied the two cases of quantum structure one when the barrier region and well region are having same width, while the other case is barrier region are thicker then the quantum well layers. It is revealed from the results shown in the following Figs. 3 and 4, that electron having a better confinement in the

quantum well region for energy state E1 in both the cases. The minimum and maximum values of E1 when barrier region was thicker than well region was found to be 2.905 and 2.9145 meV respectively, while the minimum and maximum values of E1 was found to be 2.000 and 2.041 meV for the quantum periodic structure having equal thickness of barrier and well.

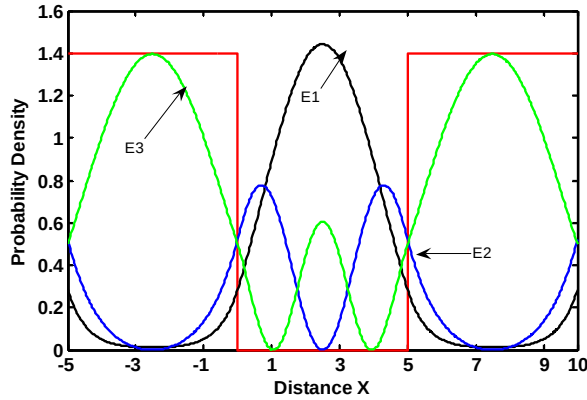


Fig. 3. Probability density with distance  $X$  (quantum well thickness and barrier width equal to 5 nm).

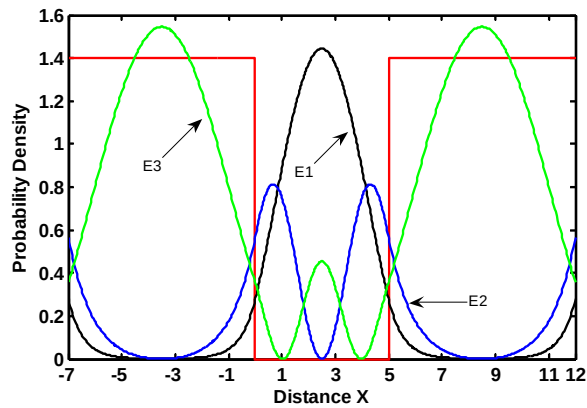


Fig. 4. Probability density with Distance  $X$  for quantum well (5 nm) thinner than barrier width.

The quantization effect is more advanced when the well region are thinner than the barrier regions. This effect is being attributed by the tunneling of the carriers from well region to barriers regions and due to the small variation in the wave vector dependent Eigen energy. Thus, from the results shown in Figs. 3 and 4, it has been realized that electron having higher energy states remains in barrier region while the ground state electrons confines in the well region only.

The full width at half maxima of the probability density was worked out and found increasing linearly with the well width. This linear relationship has been depicted in Fig. 5.

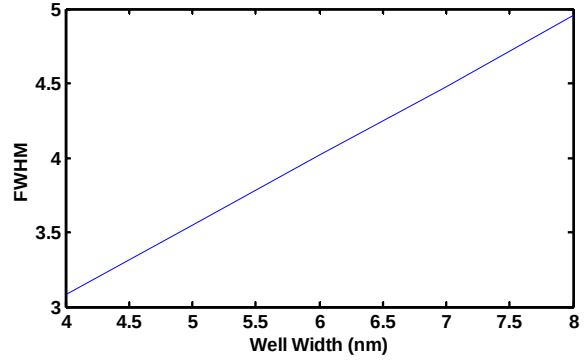


Fig. 5. Full width half maxima (FWHM) of probability density as function of quantum well width.

We have investigated the effect of carrier concentration on the optical gain and spontaneous emissions for ZnO based quantum well structures. To obtain the carrier density, we had solved Schrödinger and Poisson equation self-consistently. Optical gain were calculated for quantum well structure with carrier densities 3.07, 3.21, 3.48, 3.7 and 3.94 in multiples of  $10^{18}$  at  $T=300$  K, as shown in Fig. 6. Figs. 5 and 6 explore the variation of spontaneous and optical gain in accordance with photon energy and carrier concentration.

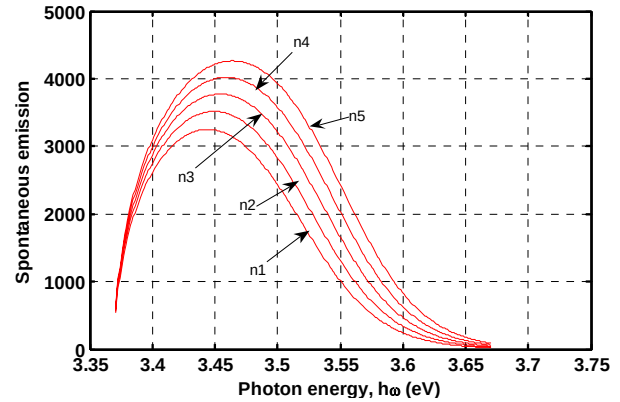


Fig. 6. Spontaneous emission as a function of photon energy.

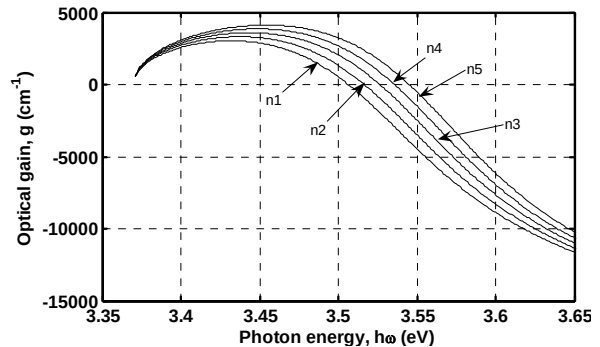


Fig. 7. Optical gain as a function of photon energy.

In Figs. 6 and 7, the spontaneous emission and optical gain has been shown as function of photon energy for different carrier concentrations. It has been observed that the spontaneous emission and optical gain initially increases with photon energy while after certain value of photon energy they decrease later on. In the following results, it has been observed that with an increase in carrier density the spontaneous emission and optical gain increases. This variation is attributed to the variation in effective mass with the increase in Magnesium concentration which is evident due to higher band offset and higher electron confinement in the well region.

#### 4. Conclusions

Detailed analysis of optical gain and spontaneous emission has been performed as function of photon energy for different carrier concentrations considering effect of piezoelectric polarization. Self consistent solutions of Schrödinger and Poisson equation provide accurate values of carrier concentration in the quantum structures. The study were extended to find the probability density and electron confinement in quantum well region using quasi transmitting boundary method. Higher optical gain and good electron confinement is obtained for 30% of Mg mole fraction in the barrier region and with well width of 5 nanometers.

#### References

- [1] M. P. Bhole, E. P. Samuel, D S Patil, J. of Modern Optics **55**(9), 1427 (2008).
- [2] X. W. Zhang, J. B. Xia, J. Phys.: Condens. Matter **18**, 3107 (2006).
- [3] C. Skierbiszewski<sup>1</sup>, P. Perlin, I. Grzegory, Z. R. Wasilewski, M. Siekacz, A. Feduniewicz, P. Wisniewski, J. Borysiuk, P. Prystawko, G. Kamler, T. Suski, S. Porowski, Semiconductor Science and Technology **20**, 809 (2005).
- [4] J.-Y. Chang, Y.-K. Kuo, J. of Applied Physics **93**(9), 4992 (2003).
- [5] E. P. Samuel, D. S. Patil, Optoelectronics Adv. Mater.-Rapid Comm. **1**(8), 394 (2007).
- [6] E. P. Samuel, M. P. Bhole, D. S. Patil, Semiconductor Science and Technology **21**, 993 (2006).
- [7] X. C. Zhang, K. Ortner, A. Pfeuffer-Jeschke, C. R. Becker, G. Landwehr, Physical Review B **69**, 115340 (2004).
- [8] S. Tomic, E. P. O'Reilly, P. J. Klar, H. Gruning, W. Heimbrodt, W. M. Chen, I. A. Buyanova, Physical Review B **69**, 245305 (2004).
- [9] L. Tsang, S. L. Chuang, IEEE J. Quantum Electronics **31**, 20 (1995).
- [10] A. V. Rodina, M. Dietrich, A. Goldner, et. al, Physical Review B **64**, 115204 (2001).
- [11] E. P. Samuel, D. S. Patil, Optoelectronics Adv. Mater.-Rapid Comm. **2**(8), 498 (2008).

\*Corresponding author: patildsp@rediffmail.com