Comparative study of single and multiple quantum wells of $In_{0.13}Ga_{0.87}N$ based LED by simulation method

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The emission efficiency of single and multiple quantum wells of InGaN based LED was compared by using standard industrial software, SILVACO/ATLAS. We found that the performance of multiple quantum LED decreases as the number of $In_{0.13}Ga_{0.87}N$ quantum wells is increases. The simulation results suggest that the inhomogeneous distribution of carriers, particularly holes in the entire quantum wells (at higher number of $In_{0.13}Ga_{0.87}N$ quantum well) is responsible for the reduction of the LED performance.

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1. Introduction

Rapid development of light emitting diode (LED) has lead to numerous research works being done in order to achieve high LED performance [1-5]. These include the optimization of some parameters of LED structure such as thickness of layers, doping level concentration, number of quantum wells and others. However, these objectives are difficult to achieve experimentally. For this reason, simulation has become important since it can offer an efficient way in attaining high performance LED. Simulation is an inexpensive, faster and relatively easy tool that can provide good insights based on simulated results.

The use of multiquantum wells in LED and laser diode (LD) designs are desirable to obtain multiple emission spots of the luminescent while maintaining efficiency. However, Nakamura et al. [6] found that, the lowest threshold current density was obtained for two InGaN quantum wells layer as the number of quantum well was varied from one to four for LDs. Other work by Nakamura et al. [7] realized that the lowest threshold current density was obtained at single InGaN quantum well compared to multiple quantum wells for LDs with emission wavelengths equal or longer than 435 nm. This phenomenon was due to a high InGaN dissociation pressure that caused the dissociation of the high indium content InGaN well layer at a high growth temperature of 750 °C [8]. Later, Chang *et al.,* 2002 [9], Chang *et al.,* 2003 [10] and Kuo *et al.,* 2004 [11] studied the performance of InGaN quantum wells as LD by using LASTIP simulation software. They found that the LD performance reduced as the number of quantum wells was increased. The inhomogeneity of holes within the quantum wells was found as the factor to this issue.

In this work, the emission efficiencies of single quantum well (SQW) and multiquantum wells (MQWs) of $In_{0.13}Ga_{0.87}N$ based LED designs are compared. This comparative study is implemented by using SILVACO/ATLAS simulation tool. The formation of energy band structures and carriers distribution of the entire LED structure for each design is observed. In the end, the factor which contributes to the lower efficiency for higher number of quantum wells is revealed.

2. Simulation procedures

As illustrated in Fig. 1, it is assumed that the LED has been grown on an n-type GaN cladding layer, which has a thickness of 3 µm with doping concentration of 5×10^{18} cm^{-3}. The active region consists of a 5 nm thick $In_{0.13}Ga_{0.87}N$ quantum well and it is sandwiched by 7.5 nm thick $In_{0.01}Ga_{0.99}N$ barriers. The active region is left undoped. The top cladding layer, GaN is doped p-type with doping level of 5×10^{18} cm^{-3}. The number of $In_{0.13}Ga_{0.87}N$ quantum well is varied from one to five. The emission efficiency for every single LED designs are simulated and investigated.

The structures are assumed to have emission at 435 nm since the active region is similar to the research work by Egawa et al. [12]. From Fig. 1, light emission is in the z-direction (normal to page). Hence, the luminescent power is in the form of emission in z-direction per µm width.

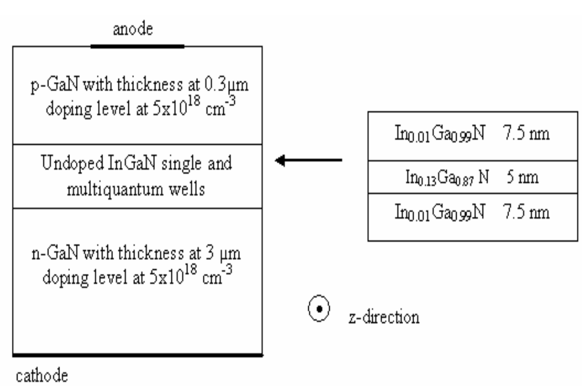


Fig. 1. The LEDs structures for single (SQW) and multi quantum wells (MQWs) in the active region.

The simulator takes into account Klaasen mobility model (applies separated mobility to majority and minority carrier and include doping concentration, temperature and carrier concentration dependence), Shockley-Read-Hall recombination model (calculates non-radiative recombination rate), bandgap narrowing model (enumerate the shrinkage of bandgap energy at higher doping level), optical recombination model (counts radiative recombination rate) and quantum moment model (applies quantum effect) to simulate the LEDs characteristics. The quantum model allows simulation of quantum confinement effect on carrier transport. This model is based on moments of the Wigner function equation of motion [13, 14] which consists of quantum correction to carrier temperature in the carrier current and energy flux equations [15].

The bandgap energy of the $In_xGa_{1-x}N$ [16] ternary alloy at room temperature is governed by the following equation in this study:

$$E_g(In_xGa_{1-x}N)\ [eV]=x\ E_g(InN)+(1-x)\ E_g(GaN)-3.8\times(1-x) \quad (1)$$

where E_g(InN) and E_g (GaN) are the bandgap energies at room temperature for Indium nitride (InN) and GaN respectively. The Shockley Read Hall recombination lifetime is assumed to be 1 ns [17]. The optical recombination (radiative recombination) is given by

$$R_{opt} = C_{opt}\,(np-n_i^2) \quad (2)$$

where C_{opt} is the radiative recombination coefficient and its value is assumed to be 3×10^{-11} cm^3/s [18].

3. Results and discussion

Fig. 2 shows the integrated radiative recombination rate per sec per μm width (which is attributed as the emission efficiency) as a function of the number of InGaN quantum wells. Apparently, the LED performance reduces as the number of InGaN quantum well layer is increased. Hence the single quantum well always has a better performance than those of multiquantum wells. This simulation result is similar to other research works by Chang *et al.,* 2002 [9], Chang *et al.,* 2003 [10] and Kuo *et al.,* 2004 [11], where the performance of LEDs decreased as the number of quantum wells increased.

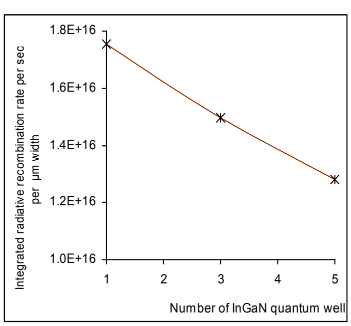


Fig. 2. Integrated radiative recombination rate versus for various number of quantum well.

Fig. 3 shows the energy band diagrams of simulated SQW and five quantum wells (5QWs) structures for comparison. Note that the barrier heights (at p-GaN/active region interface at the valence band and active region/n-GaN interface at the conduction band) for 5QWs structure are higher particularly at active region/n-GaN interface at the conduction band rather than the single quantum well structure. These result in the difficulty of electrons and holes to be transported into the active region.

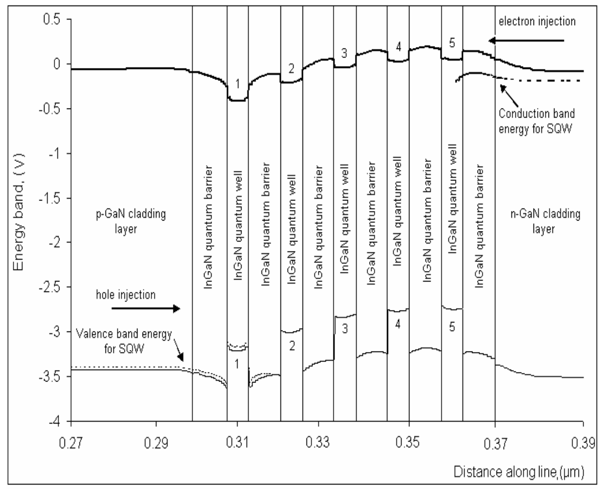
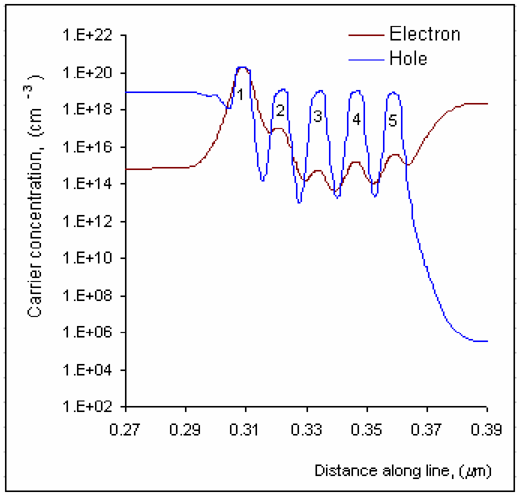


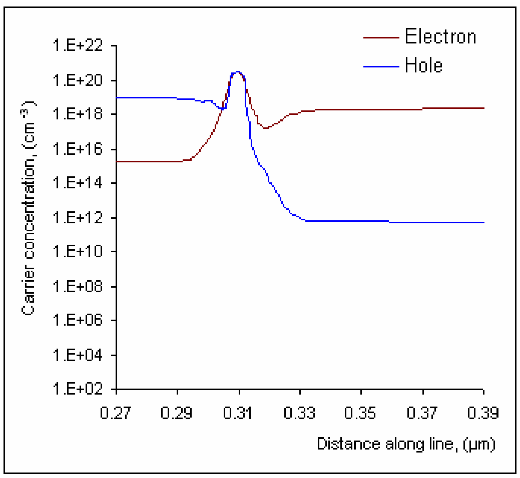
Fig. 3. The conduction and valence band for 5QWs and SQW at applied voltage of 3.5 V. Quantum wells are numbered as 1, 2, 3, 4 and 5.

The carriers' distribution in the 5QWs is found inhomogeneous as indicated in Fig. 4. This figure also indicates that most injected electrons and holes are present in the first quantum well (numbered as 1) for five quantum wells LED. Higher electron mobility and lower band offset helps the easy transfer of electrons to the furthest quantum well (numbered 1).

Moreover, higher confinement of electrons is found in the first quantum well due to higher band offset that had been formed within the well. Thus, the distribution of electrons increases towards the p-side GaN. The largest density of electron attracts more holes to be accumulated into the same well at valence band. Additionally, lower mobility of holes and high band offset formed at the valence band is responsible for the difficulty of hole to be transported to other wells. However, the holes distribution throughout the entire quantum wells is more homogeneous than the electrons distribution, which are differ from the results that had been obtained by Chang *et al.,* 2002 [9], Chang *et al.,* 2003 [10] and Kuo *et al.,* 2004 [11] where they found that the distribution of hole was more inhomogeneous than the electron distribution.



(a)



(b)

Fig. 4. (a) The distribution of electrons and holes concentration for 5QWs LED at an applied voltage of 3.5 V. (b) The distribution of electrons and holes concentration for SQW LED at the same applied voltage.

Fig. 5 illustrates the distribution of emission efficiency of the entire LED structure for 5QWs. It can be seen that the highest emission has been generated in the first quantum well, and the emission reduces in other quantum wells towards the n-GaN layer. In general understanding, higher number of electrons and holes promote higher emission of light. Therefore, higher number of carriers in the first quantum well produces higher radiative efficiency. Note that the last three quantum wells share almost similar emission rates. This result renders that the use of these three quantum wells are not productive and do not help to increase the LED performance.

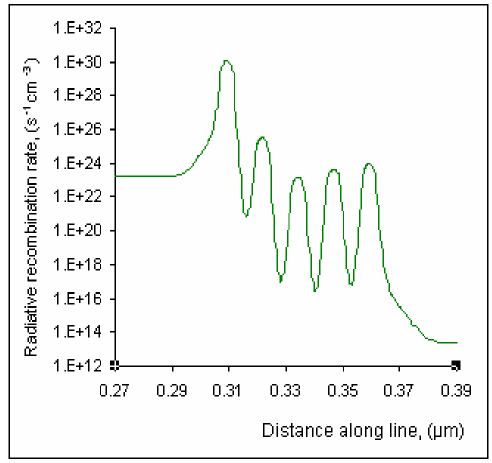


Fig. 5. The distribution of radiative recombination rate (emission efficiency) for 5 QWs LED at an applied voltage of 3.5 V.

4. Conclusion

Based on the simulation results, we found that the SQW LED always gives higher performance compared to MQWs LED. This phenomenon owing to the inhomogeneity of carriers especially for electrons in the entire quantum wells for higher number of $In_{0.13}Ga_{0.87}N$ quantum wells. The formation of conduction and valence bands for 5QWs LED structure has great influence on the transportation and distribution of carriers throughout the LED device. Due to its higher mobility and lower band offsets at conduction band, electrons were found higher in the first quantum well. This leads to higher accumulation of holes in the same quantum well. Moreover, higher band offsets at the valence band created difficulty for holes to be transported to further quantum wells towards the n-GaN region. However, the distribution of electrons particularly within the quantum wells is more inhomogeneous compared to holes distribution. As a result, the distribution of radiative efficiency was found to be inhomogeneous as well. This suggests that the last three quantum wells in 5QWs were unproductive since these quantum wells shared almost similar level of emission efficiency.

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