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Simulation on the Roles of the Number of Quantum Well and Doping in $In_xGa_{1-x}N$ Multiple Quantum Wells LEDs

(Simulasi Peranan Bilangan Telaga Kuantum dan Pendopan dalam Multi Telaga Kuantum $In_xGa_{1-x}N$ LEDs)

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ABSTRACT

In this work, the emission efficiency of $In_xGa_{1-x}N$ based light emitting diodes (LEDs) had been numerically investigated with the variation of the number of quantum well. From our calculation, we found that non-uniformity of carriers distribution (especially electron) in the wells leads to serious inhomogeneity of radiative recombination distribution that would degrade the efficiency of the LED with more wells. However, the problem was minimized when the selected quantum barriers were doped with a reasonable doping level. Comparison with other reported experimental works were also included. At the end of this work, we proposed several types of preferable LEDs designs with optimum structural parameters.

Keywords: Light emitting diodes; numerical simulation; optical properties; III-V semiconductors

ABSTRAK

Dalam kajian ini, kecekapan pancaran daripada diod pemancar cahaya (LED) berasaskan $In_xGa_{1-x}N$ telah dikaji secara berangka dengan variasi bilangan telaga kuantum. Daripada pengiraan kami, didapati bahawa ketidakseragaman taburan pembawa (terutamanya elektron) dalam telaga memberi kesan kepada ketidakseragaman taburan penggabungan semula menyinar yang serius dan mengurangkan kecekapan LED yang mempunyai bilangan telaga yang tinggi. Walau bagaimanapun, kecekapan diod tersebut dapat diperbaiki apabila sawar kuantum tertentu didopkan pada tahap yang berpatutan. Perbandingan dengan kerja-kerja experimen lain yang telah dilaporkan turut disertakan. Di akhir kajian ini, kami mencadangkan beberapa jenis reka bentuk LED yang lebih baik dengan parameter struktur yang optimum.

Kata kunci: Diod pemancar cahaya; semikonduktor III-V; sifat optikal; simulasi berangka

INTRODUCTION

So far, the information on III-V nitrides based LED is widely reported and documented. Nitride based blue LEDs with external quantum efficiency higher than 65% have been recently developed (Mueller-Mach et al. 2009) and also, a deeper UV emitting laser diode (LDs) with emission at 336 nm is now possible (Yoshida et al. 2009). While material quality remains an important issue for the optical devices, the main subject for achieving a high LED performance is to find an appropriate structure of the device, especially the active region that consists of well and barrier layers. This involves optimizing the thickness of the layers, doping level and the number of wells. Those works through experiment however is very complicated, time consuming and costly. Therefore, the numerical calculation is more preferable approach as it is much quicker and cheaper. Furthermore, it provides information that is difficult or impossible to measure experimentally.

The use of multi-quantum well in optical devices are desirable for achieving multiple emission spots of the luminescent while maintaining efficiency. For this reason, radiative emission distribution in the multi quantum wells structure should be homogenous. However, the inhomogeneity of the distribution of the radiative emission had been reported by Chang and Kuo (2003) in LDs structure. They found that the LDs efficiency degraded with the number of quantum wells. This problem was attributed to the inhomogeneity of holes distribution throughout the quantum wells structure, as holes in general having heavy mass and thus facing difficulty to move to further wells. Nevertheless, at certain applied voltage, electrons might be distributed inhomogeneously too, because the barriers at conduction band decreases with applied bias. This may lead to poor confinement in the wells that consequently produce inhomogeneity of radiative emission in the multi quantum well structure. The problem will be more significant as electrons can easily move to further wells due to their smaller mass. This issue therefore will be investigated and addressed in this work.

In our calculation, the emission efficiency of $In_xGa_{1-x}N$ quantum wells LEDs with the variation of the number of well layers was investigated using two-dimensional (2-D) simulation software, Silvaco with its device simulator, ATLAS. As the non-uniformity of electron distribution in the active region decreases the emission efficiency of the diode, we suggested applying n-type doping in the selected quantum barrier in order to improve the efficiency of the multiquantum well (MQWs) devices. This is considering the fact that in the fabrication work, n-type doping is easier to be achieved than p-type doping in the InGaN layer (Jenkins & Dow 1998; Mohammad et al. 1995). On top of that, we investigated the benefits of having triple quantum wells (3QWs) compared to five quantum wells (5QWs) LEDs with n-type doping in the selected quantum barriers. The reliability of some simulated results will be seen by comparing them to other reported experimental works. Finally, we proposed few types of preferable LEDs designs that could be used as a starting point for device growth.

SIMULATION PROCEDURES

The structure of $In_xGa_{1-x}N$ quantum wells LEDs, as shown in Figure 1 is designed with undoped $In_xGa_{1-x}N$ active region in between two doped GaN layers, which act as cladding layers of the device. The active region consists of $In_{0.13}Ga_{0.87}N$ quantum well with thickness, d_w of 5 nm, sandwiched with two $In_{0.01}Ga_{0.99}N$ barriers of equal width, d_b=7.5 nm. The $In_xGa_{1-x}N$ quantum barriers are chosen instead of GaN as they can reduce the polarization effect and subsequently lower the turn-on voltage of the device (Chang et al. 2011). In this work, the number of $In_{0.13}Ga_{0.87}N$ well is changed to observe its influence on the efficiency of the LEDs device.

The emission efficiency of the device is found by numerically calculating the radiative emission rate per μm width in z-direction (Figure 1), while the luminescent power is calculated using the following equation (ATLAS Manual 2003):

$$P = \frac{hc}{\lambda_{emission}} \int R_{RAD} dA,$$

where $\lambda_{emission}$ is the emission wavelength of the device and the integration term is referred to the radiative emission rate of the device. We assume that our devices have an emission of 435 nm as the active region in our device is similar to that of Egawa et al. (2002). It should be noted that, the more electrons and holes in the active region, the higher is the radiative recombination. All devices were assumed to be operated at an applied voltage of 3.5V.

In our calculation, we included the Klaasen mobility model (applies separated mobility to majority and minority carriers and include doping concentration, temperature and carrier concentration dependence), Shockley-Read-Hall recombination model (calculates non-radiative recombination rate), bandgap narrowing model (enumerates the shrinkage of bandgap energy at higher doping level), optical recombination model (counts radiative recombination rate) and quantum moment model (applies quantum effect) to determine the efficiency of the device. 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 (Zhou & Ferry 1992a, 1992b) which consists of quantum correction to carrier temperature in the carrier current and energy flux equations (ATLAS Manual 2003). The parameter values used in these models are defined by default.

RESULTS AND DISCUSSION

Figure 2 shows the dependence of luminescence efficiency of $In_xGa_{1-x}N$ LEDs with different number of quantum well. As been mentioned before, the use of MQWs in LEDs structure would enhance the brightness of the device. When the electrons and holes in the wells are uniformly distributed, there would be more radiative recombinations that subsequently lead to multiple radiative emissions from the MWQs device. However, our calculation showed that the brightness of the device decreases linearly as the number of the quantum well increases, suggesting the single quantum well LEDs always has a better performance than those of multi quantum wells devices. This is similar to what had been reported in Chang et al. (2011).

To explain this behavior further, we present a model of energy band diagram for a single and 5QWs LEDs in Figure 3. Note that 5QWs diode has higher barrier height as compared with the single quantum well (SQW). The higher the barrier height, the less are the electrons and

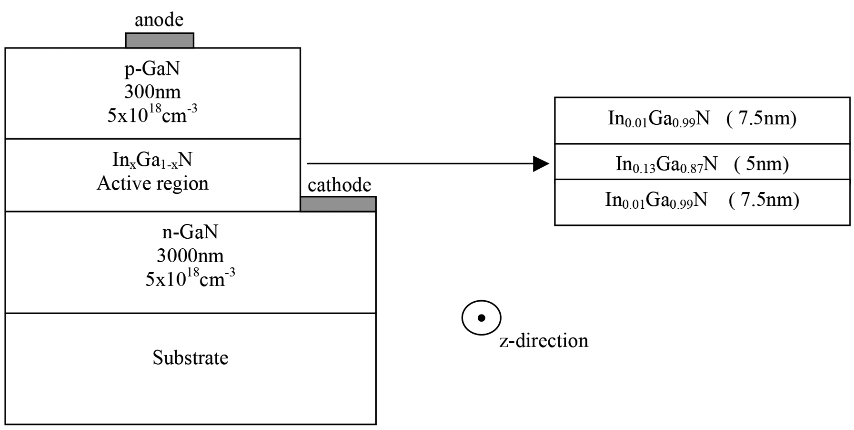

FIGURE 1. LEDs structures for single (SQW) and multi quantum wells (MQWs) in the active region

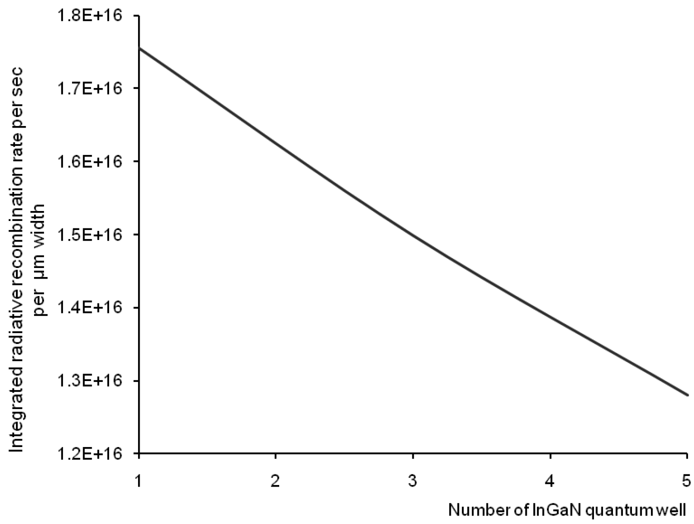

FIGURE 2. The dependence of radiative recombination in LED with different number of quantum well

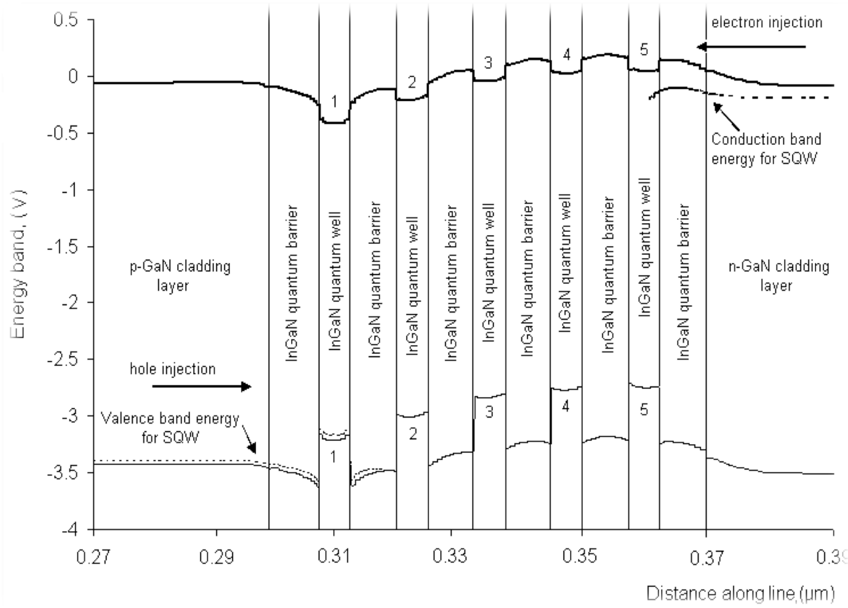

FIGURE 3. The conduction and valence band for 5QWs and SQW at applied voltage of 3.5 V. Quantum wells are numbered as 1, 2, 3, 4 and 5

holes being injected into the active region. Therefore, these carriers are non-uniformly distributed in the wells. Such behavior can be clearly seen in Figure 4. The distribution of holes is about uniform throughout the wells, which is not the case for electrons distribution. It is not clear to explain this behavior as electrons have higher mobility and therefore, they should be easily transported and have uniform distribution in the wells. However, we need to consider that the band offsets at valence band is higher than that at conduction band. With this regard, we suggest that those band offsets provide sufficient confinement for the holes within the wells while allow those holes to transport to the subsequent wells.

Unlike holes, electrons have higher mobility and the band offsets at the conduction band are smaller. These effects give higher possibility for the electrons to transport to further wells. After all, they lead to poor confinement of electrons within the wells and consequently cause the electrons non-uniformly distributed throughout the wells. From the diagram, more carriers are accumulated in the first well (numbered as 1). This is due to more holes are concentrated in the well which leads to attract more electrons to be accumulated in the same well.

From this observation, we propose to apply n-type doping for the third, fourth, fifth and sixth quantum barriers at reasonable doping level so that the distribution

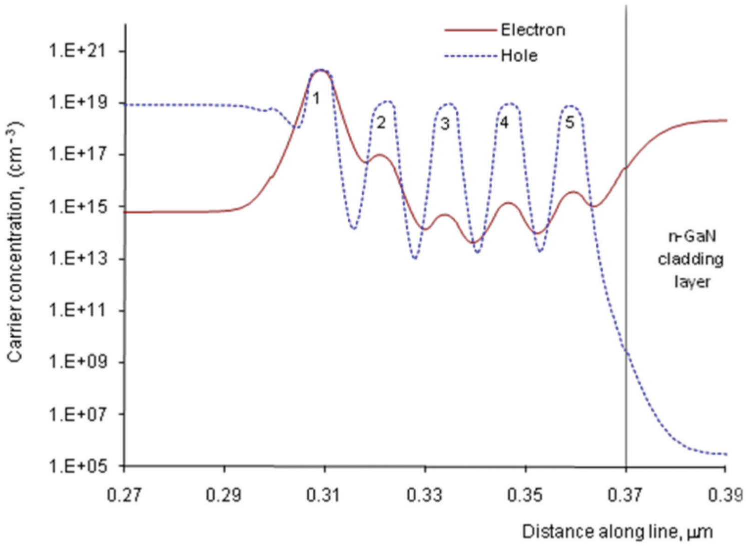

FIGURE 4. (Colour online) The distribution of electron and hole concentration for 5QWs LEDs at applied voltage of 3.5 V. The wells are numbered in the figure

of electrons in the wells for 5QWs LEDs would be improved. This may increase the electrons concentration in the wells and consequently provides more uniformity of the electrons distribution, which would lead to multiple radiative emissions, hence increasing the efficiency of the device. Before we do further investigation on this subject, it is important to find the optimum doping level for the third, fourth, fifth and sixth quantum barriers of 5QWs LEDs. In this work, we varied the doping level of the quantum barriers from zero to 7×10^{19} cm^{-3}.

Figure 5 shows the luminescent power as a function of the input voltage for various n-type doping levels in the selected quantum barriers. It can be seen that the luminescent power increases with increasing doping in the quantum barriers. This is expected as higher doping level of the quantum barriers gives more electrons to supply into the wells, which improves the uniformity of the electrons distribution throughout the wells. On the other hand, further increase of the doping level above 3.0×10^{19} cm^{-3} does not lead to significant improvement of the device due to the reduction in the electron mobility with respect to the electron concentration. At this stage, considerable number of electrons in the wells is also useless considering a limited supply of holes in the valence band as far as the radiative recombination is concerned. In fact, a published experimental work by Ryou et al. (2008) showed that increase in n-type doping in quantum barriers leads to higher barrier height at the valence band, which are consequently blocking the transportation of holes to further wells.

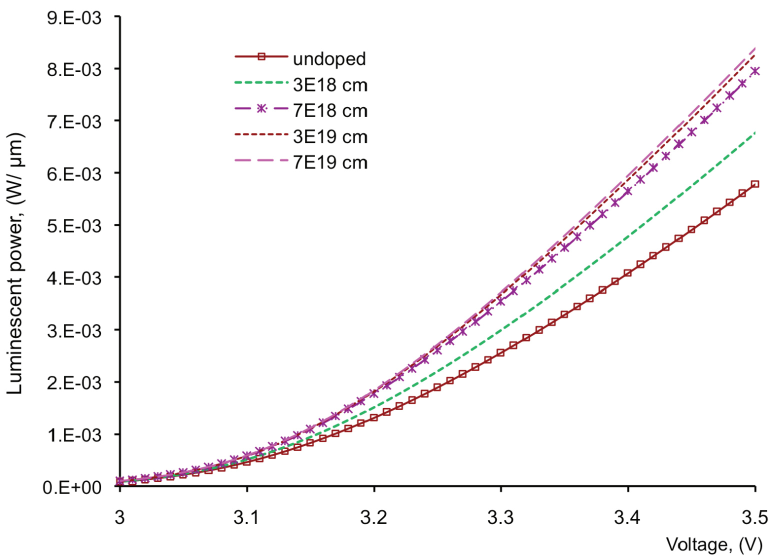

FIGURE 5. (Colour online) The luminescent power versus various doping concentrations in the selected quantum barriers for 5QWs

Figure 6 shows the distribution of carries with the n-doped quantum barriers of 3.0×10^{19} cm^{-3} for 5QWs LEDs. As expected, the holes concentration becomes lower towards n-GaN cladding layer (especially in third, fourth and fifth quantum wells) causing the hole distribution to be less uniform. Meanwhile, Figure 7 shows radiative recombination distribution of 5QWs LEDs with high n-doped (3.0×10^{19} cm^{-3}) in the third, fourth, fifth and sixth quantum barriers. For a comparison, we also include the radiative recombination distribution of the undoped quantum barrier 5QWs LEDs. The n-doped barriers device shows some improvements with peak emission increases by one order of magnitude higher in the first quantum well while two order of magnitudes higher in the second quantum well, with respect to the undoped quantum barrier device. This is consistent to a reported photoluminescence (PL) measurement by Hung et al. (2008) which found that the PL intensity is enhanced when Si-doping is introduced in quantum barriers. It is clearly seen in Figure 7 that the radiative emission is mainly produced in the first quantum well. Note that, radiative recombination is higher in the fourth and fifth quantum well for undoped quantum barrier device. However, the radiative recombination rate is similar for both structures in the third quantum well and it is weak. As been mentioned earlier, the radiative recombination rate is strongly dependent on the number of electrons and holes. Therefore, the decreasing of holes within three last quantum wells is responsible for the weak light emission. From Figures 6 and 7, we suggest that highly doped quantum barrier in 5QWs LEDs is not a preferable design.

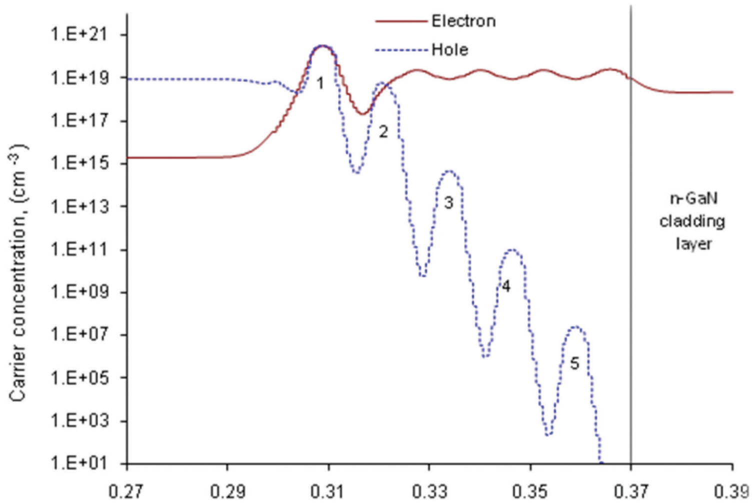

FIGURE 6. (Colour online) The distribution of carrier's concentration for LED with 5QWs with an increased doping of 3.0×1019cm-3. The wells are numbered in the figure

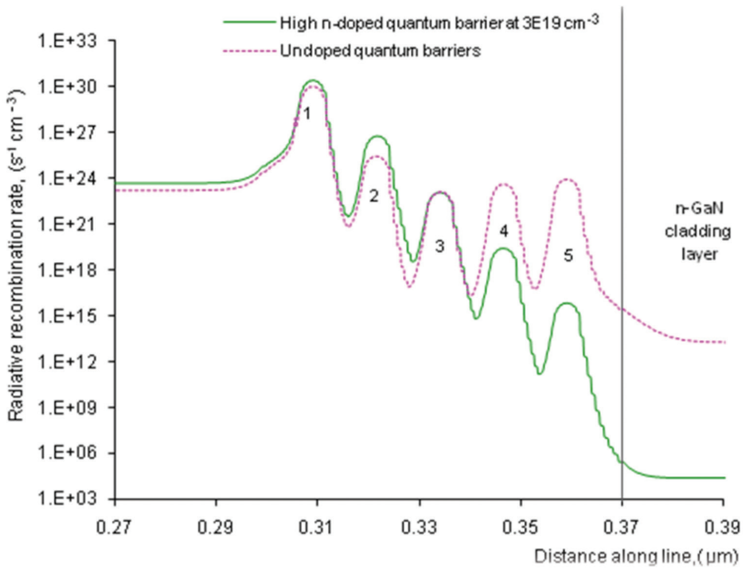

FIGURE 7. (Colour online) The distribution of radiative recombination rate for high n-doped quantum barrier and undoped quantum barrier for 5QWs LEDs. The wells are numbered in the figure

The weak radiative emissions in the fourth and fifth quantum wells show that these wells are not productive. Furthermore, Xia et al. (2012) have found that small number of the quantum wells resulted in low threshold voltage. Therefore, we propose three quantum wells (3QWs) LEDs with the same level of n-type doping at $3.0\times10^{19}cm^{-3}$ in third and fourth quantum barrier. Figure 8 shows radiative recombination distribution of n-doped quantum barrier of a 3QWs LED. Also included is the radiative recombination for undoped quantum barriers of 3QWs, for a comparison. Note that the radiative emissions in the first and second wells for doped quantum barriers are higher than those of undoped quantum barriers. However, in the third well in undoped quantum barrier LEDs structure, the emission is found to be higher than that of doped quantum barriers device. This may due to limited number of holes in the well as the n-type doping in the quantum barriers is increased. In order to achieve a constant multi-spot emission in a MQWs LEDs structure, it is important to have uniform radiative recombination distribution for the entire wells. Therefore, to improve the efficiency of 3QWs device, it might be wise to supply more holes in the third well and hence the third quantum barrier should be doped p-type, instead of n-type. The fourth quantum barrier is maintained n-type with the doping level of $3.0\times10^{19}cm^{-3}$. Figure 9 shows radiative recombination distribution for p-type doped quantum barrier on the third one with the doping level of $3.0\times10^{17}cm^{-3}$ and $3.0\times10^{19}cm^{-3}$, respectively. Also included is undoped quantum barrier and n-doped quantum barrier for comparison.

From the figure, when the third quantum barrier is doped with p-type at higher level; $3.0\times10^{19}cm^{-3}$, the radiative emission becomes the lowest in the second quantum well. On the other hand, the radiative emission in the first and third quantum wells is rather comparable. Such behaviour could be explained by the fact that higher concentration of holes into the third quantum well attracts more electrons and consequently have been confined in the same well. An experimental work by Han et al. (2010) found that p-type doping in the quantum barriers will reduce the barrier height at the valence band. Hence, in this present work, the higher p-type doping level in the third quantum barrier will reduce the barrier height, resulting in higher accumulation of holes in the third well but less in the second well. This implies that the confinement effect of holes in the second well is insignificant. Overall, the structure with p-type doped at $3.0\text{x}10^{17}cm^{-3}$ in third quantum barrier possesses a better homogeneity of radiative recombination rate for the entire quantum wells.

CONCLUSION

Our simulation showed that the efficiency of LEDs reduces as the number of quantum wells increases. It was found that the non-uniformity electrons distribution in the quantum wells is more significant for the device with multiple wells. This problem maybe associated to high mobility and poor confinement of electrons in the wells. As a result, the multiple radiative emissions are not possible. Therefore, we proposed to apply n-type doping in selected quantum barriers, which could help to improve the homogeneity of electrons within the wells even though the holes distribution in the quantum barrier becoming more inhomogeneous. In such structure, the radiative recombination rate increased tremendously and was found to be the highest in the first quantum well. The weak emission in the fourth and fifth quantum well in 5QWs LED suggested that three quantum well LEDs is sufficient to avoid wasted unproductive quantum well. The 3QWs LEDs showed that the radiative emission in n-type doping level in selected quantum barrier is still lower than the

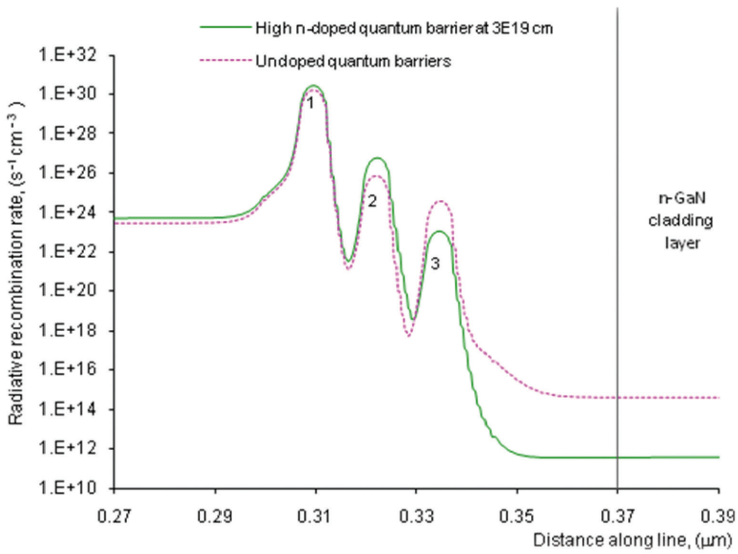

FIGURE 8. (Colour online) The distribution of radiative recombination rate for high n-doped quantum barrier and undoped quantum barrier for the 3QWs LEDs. The wells are numbered in the figure

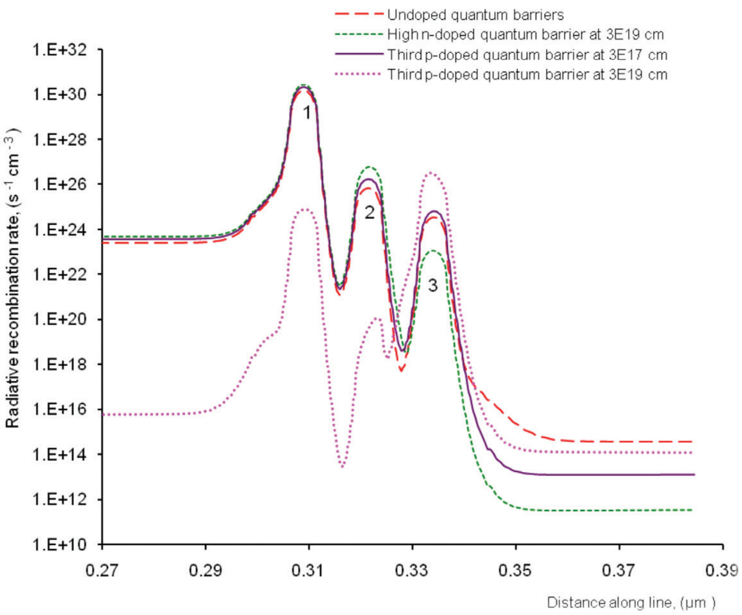

FIGURE 9. (Colour online) The distribution of radiative recombination rate for LEDs structure for various doping in the selected quantum wells for the 3QWs LEDs. The wells are numbered in the figure

structure with undoped quantum barrier due to the lack of hole supply in the third quantum well. With respect to this, we proposed p-type doping in the third quantum barrier. The light emission improved as the p-type doping level increases. Through this simulation work, few types of preferable LEDs design were proposed. One can have a single spot high performance quantum well LED. However, if multiple emission spots are desirable, one can have 5QWs LEDs with undoped quantum barriers sharing high efficient emission in first and second well but wasted in the third, fourth and fifth wells. One could have p-doped third quantum barrier in the 3QWs LED for a more homogeneous emission.

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