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Assessment of various LED structure designs for high-current operation

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Using modelling, we have examined alternative designs of light-emitting diode (LED) structures, aimed at lowering the non-equilibrium carrier concentration and, hence, at suppression of Auger recombination in the active regions of the diodes. Both a multi-quantum-well (MQW) heterostructure and that with a thick single active layer are compared. The MQW structure is found to be ineffective for improvement of the LED internal quantum efficiency (IQE). In contrast, LEDs with a thick single active layers turn out to be quite promising for high-current operation. Detailed simulation provides a guideline for further optimization of the LED heterostructures.

1 Introduction Most of III-nitride LEDs suffer from the efficiency droop typically observed at the current densities greater than ~3-30 A/cm^2. On the basis of both experimental [1] and theoretical [2] studies, Auger recombination has been recently recognized as the principal non-thermal mechanism responsible for the efficiency droop in the LEDs with InGaN quantum well (QW) active layers. To avoid the negative impact of this fundamental mechanism on the device performance, redesigning of conventional LED structures is necessary, aimed at lowering the non-equilibrium carrier concentration in the active region.

At a given current density j, a natural way to lower the carrier concentration in the active region is enlarging of its total thickness d. The most tempting approach implies just increasing the number of QWs in the LED structure, as this does not need any modification of conventional epitaxial procedures used for heterostructure growing. An alternative way based on the use of a thick InGaN active layer seems to be more complicated because of phase separation inherent in bulk InGaN materials [3]. Thus additional efforts may be required to adopt the growth technology for fabrication of the heterostructures with sufficiently thick InGaN active layers. Therefore, the choice of the most promising approach to redesigning of the LED structures should be based on detailed examination of advantages and disadvantages of each of them.

This paper reports on theoretical assessment of different heterostructure designs aimed at improving the high-current LED performance. Both MQW and thick InGaN active regions are considered, keeping unchanged other functional layers in the LED structure. The theoretical predictions are compared with observations available to date.

2 Theory and structure design We consider here a Ga-polar fully strained blue LED structure consisting of a thick n-GaN contact layer ([Si] = 3×10^{18} cm^{-3}), an active region, a 20 nm p-Al$_{0.2}$Ga$_{0.8}$N electron blocking layer ([Mg] = 7×10^{19} cm^{-3}), and a 300 nm p-GaN contact layer ([Mg] = 1×10^{20} cm^{-3}). Two different active region designs are compared. The first one is an MQW active layer comprising of six unintentionally doped 3 nm In$_{0.18}$Ga$_{0.82}$N QWs ([Si] = 5×10^{16} cm^{-3}) separated by 12 nm n-GaN barri-

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ers with the donor concentration varied from 1×10^{17} to 8×10^{18} cm^{-3}. The second type of the active region is a single $In_{0.18}Ga_{0.82}N$ layer ([Si] = 5×10^{16} cm^{-3}), with the thickness varied from 1 to 100 nm.

Simulation of the LED operation has been performed with the SiLENSe 3.42 package [4], implementing a drift-diffusion model of electron and hole transport in the heterostructures and accounting for bimolecular radiative recombination of the carriers, their non-radiative recombination at threading dislocations [5], and Auger recombination. Detailed model description and materials parameters used in the simulation can be found in [2,6].

We consider here LED structures operating at room temperature. Though self-heating of LEDs may be noticeable at high current densities, we ignore this effect in our study, as the device heating is controlled by the chip design, rather than by the choice of a particular heterostructure.
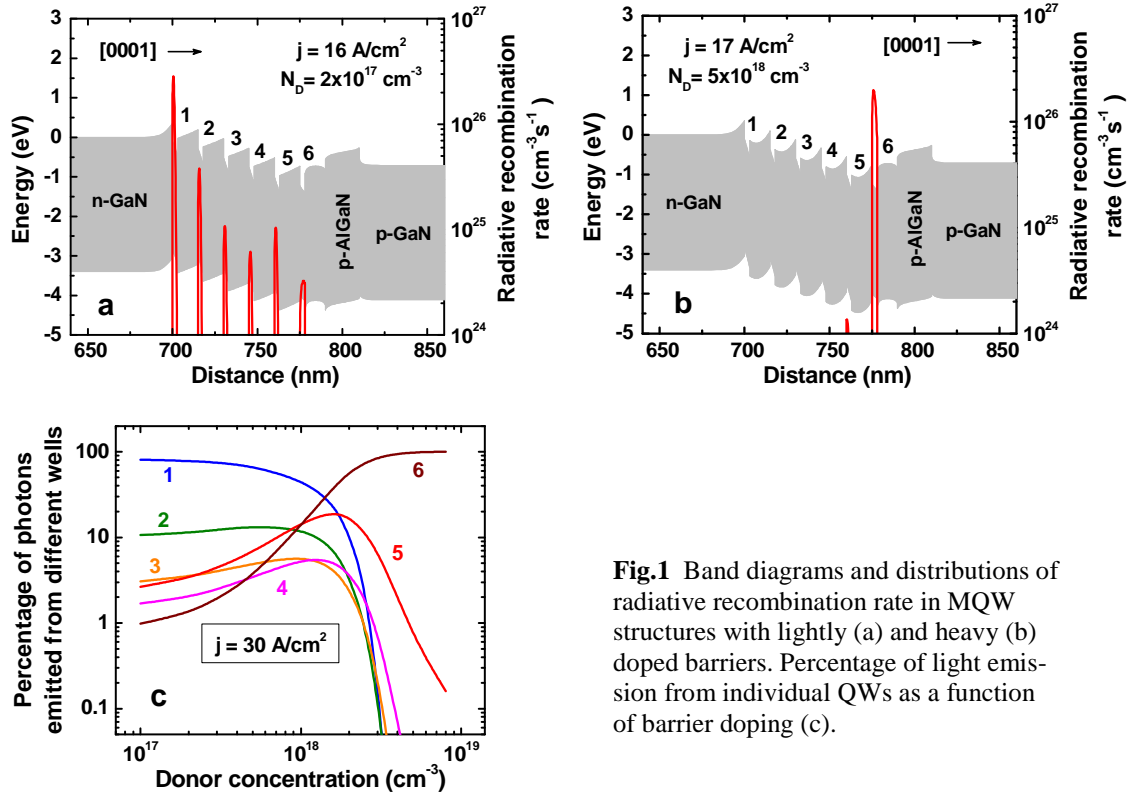
Fig.1 Band diagrams and distributions of radiative recombination rate in MQW structures with lightly (a) and heavy (b) doped barriers. Percentage of light emission from individual QWs as a function of barrier doping (c).

After the band diagram of an LED structure and distributions of electron and hole concentrations in all the layers are computed, the simulator calculates the IQE (η) which is the ratio of the radiative recombination current density to the total current density in the LED structure. This parameter, accounting not only for competition between the radiative and non-radiative recombination channels but also possible carrier leakage, served in our study as a main criterion for the heterostructure performance.

3 Results and discussion Consider, first, the operation of the MQW structure. Figure 1 shows the band diagrams and radiative recombination rates in the LED structure with lightly and heavy doped *n*-GaN barriers. One can see that the recombination rate is non-uniformly distributed among the QWs, which is caused by inhomogeneous electron and hole injection in the individual wells. Other recombination channels, like non-radiative carrier recombination at TDs and Auger recombination, exhibit a similar behaviour. The distribution of the radiative recombination rate in the MQW structure is found to largely depend on the barrier doping. The major rise in the light emission is produced by the QW next to the *n*-GaN contact layer in the structure with lightly doped (Fig.1a) and by the well adjacent to the *p*-AlGaN

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blocking layer in the structure with heavy doped barriers (Fig.1b). The switching between the wells occurs at the donor concentration of ~1.5×10^{18} cm^{-3} (Fig.1c). So, in terms of the carrier injection and recombination, the MQW structure actually operates like a single-quantum-well (SQW) one. Therefore, it is practically impossible to lower the carrier concentration in the active region by only increasing the number of QWs.

Consider now the LED structure with a single active layer. Figure 2a shows IQE of the structure as a function of the active layer thickness and current density. At every thickness, the IQE first rises and then falls down with j. The initial IQE rise is due to the radiative recombination rate increasing faster with the carrier concentration than the rate of non-radiative recombination at TDs. At higher current densities, the contribution of Auger recombination becomes essential, leading to the efficiency droop.

The position of the IQE maximum is found to depend strongly on the active layer thickness. There is a pronounced IQE peak for extremely thin active layers, less than ~2 nm, which occurs at relatively low current densities (Fig.2b). Our simulations predict the electron concentration in such active layer to be much higher than the hole concentration. As a result, the carrier recombination at TDs becomes controlled by the hole migration to the dislocation cores, lowering the non-radiative recombination rate [5]. The simulations are in line with the conclusions made in [7,8] where an increase in IQE was reported for the QW thicknesses between 1 and 2 nm. At the active layer thickness of ~3-5 nm the electron and hole concentrations become nearly equal to each other, and IQE decreases, peaking at ~10-20 A/cm^2. The latter correlates well with numerous measurements of the LED external quantum efficiency (see, for instance, the data compiled in [2]).

Further enlargement of the active layer results in an IQE rise accompanied by a shift of the IQE maximum to higher current densities (Fig.2a). In particular, the IQE maximum is predicted to be at $j \sim 230$ A/cm^2 for the active layer 10 nm thick. Here, IQE becomes even higher than that of LEDs with 3-5 nm QWs (Fig.2b). This result is in excellent quantitative agreement with the data of [9] reporting on characterization of novel double-heterostructure LEDs with 9-13 nm InGaN active regions.
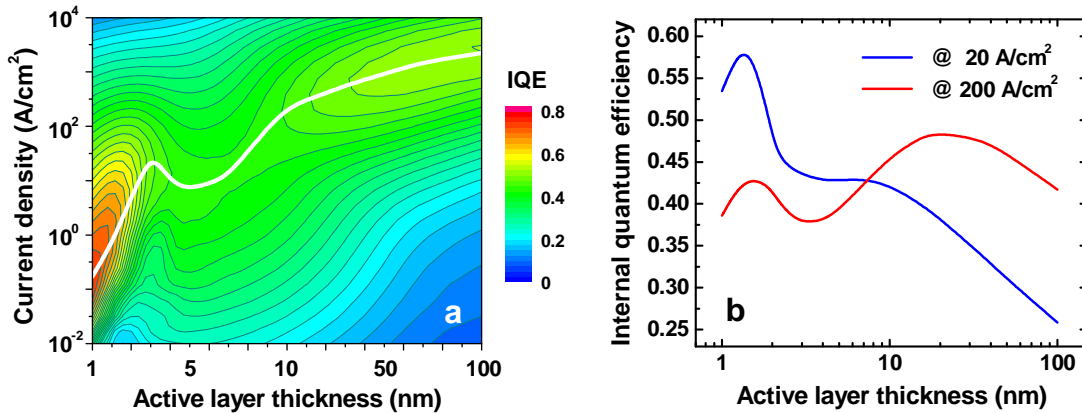
Fig. 2 IQE of blue LED structure with a single active layer as a function of its thickness and current density. White line in (a) indicates location of the IQE maximum.

At the active layer thicknesses larger than 30 nm, the IQE maximum becomes located at ~1-3 kA/cm^2. At such high current densities, the IQE becomes limited not only by Auger recombination but also by the electron leakage into p-layers of the heterostructure.

The quantitative predictions obtained for the active layers thicker than ~20-30 nm should be, however, regarded with some care, as our analysis does not take into account possible strain relaxation in bulk InGaN. Indeed, if the strain is relaxed via misfit dislocation formation at the active layer interfaces, they can additionally contribute to the non-radiative carrier recombination, reducing IQE. On the other hand, the integral radiative recombination in the materials bulk may prevail over the non-radiative carrier re-

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combination at the misfit dislocations in sufficiently thick active layers. That is why, we believe, the possible strain relaxation does not change significantly the qualitative IQE behavior discussed above.

We should also note that the relationship between the active layer thickness d and current density j corresponding to the IQE maximum, which is plotted in Fig.2a by white line, cannot by obtained from the simplified balance equations

$$\frac{j}{qd} = \frac{n}{\tau} + Bn^2 + Cn^3, \quad \eta = \frac{Bn^2}{n/\tau + Bn^2 + Cn^3}, \tag{1}$$

where q is the electron charge, n is the carrier concentration assumed to be nearly the same for electrons and holes, τ is the non-radiative carrier life-time, and B and C are the radiative and Auger recombination constants. Actually, Eqs.(1) gives a linear relationship between j and d, which does not account for separation of electron and hole densities within the active layer due to the Stark effect and the electron leakage in the *p*-region of the heterostructure. In contrast, Fig.2a obtained by full simulation presents a clear guidance for the LED structure optimization: it enables the direct choice of the active layer thickness providing the maximum of IQE at a desirable current density.

4   Summary   We have compared two alternative designs of blue LED structure aimed at suppression of Auger recombination in the active region. An MQW heterostructure is found to be ineffective for this purpose because of inhomogeneous electron and hole injection in individual QWs. In contrast, the use of a thick InGaN single active layer is promising to obtain an IQE maximum at high current densities. This conclusion seems to be valuable not only for LEDs but also for InGaN-based laser diodes where the use of a thick active layer provides additional advantage – a greater optical coupling between the active region and waveguide modes.

Our theoretical results agree well with observations available from [7-9]. The simulations, like those carried out in this study, provide a distinct guideline for further optimization of LED heterostructures aimed at IQE increasing at high-current operation.

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