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Modelling of MQW LED operation

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The operation of multiple-quantum-well (MQW) light emitting diode (LED) heterostructures with selective barrier doping is studied by modelling. The carrier confinement in MQW LEDs and the effects of barrier doping on the emission efficiency and wavelength stability is examined in detail. The simulation predicts the improvement of LED performance by heavy *n*-doping of the barriers between individual quantum wells. The theoretical predictions are compared with available experimental data.

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1 Introduction

The enormous growth of III-nitride-based light emitting diode market in the last years requires a careful optimization of both the fabrication technology and design of these devices. Much effort has been made to improve the material quality [1,2], the efficiency of light extraction from LEDs [3,4], and the contact geometry [4]. However, much less work on the optimization of LED heterostructures has been reported to date. In particular, this concerns the choice between a single-quantum-well (SQW) and a multiple-quantum-well active regions. Despite the reported advantages of using SQW active regions [5], the potentiality of MQW ones, in our opinion, is not yet exhausted and require a more detailed examination.

The modelling reported in this paper is aimed at a better understanding of the operation of MQW LED heterostructures with the focus on the carrier confinement in the active region and the role of selective doping in the barriers separating individual quantum wells. This research was stimulated by the reported improvement of the LED efficiency and wavelength stability due to enhanced barrier doping [4,6].

2 Results and discussion

A blue MQW LED heterostructure similar to those examined in [4,6] has been chosen for the simulation. The Ga-faced structure consists of a GaN:Si contact layer ([Si] = 2×10^{18} cm^{-3}), an MQW active region, an $Al_{0.15}Ga_{0.85}N$:Mg emitter ([Mg] = 1.5×10^{19} cm^{-3}) 60 nm thick, and a GaN:Mg contact layer ([Mg] = 2×10^{19} cm^{-3}). The active region contains four undoped (as assumed) $In_{0.13}Ga_{0.87}N$ quantum wells (QWs) 3 nm thick separated by 12 nm GaN:Si barriers. Each barrier is doped with Si at a concentration varying between 5×10^{17} cm^{-3} and 5×10^{18} cm^{-3}. All the epilayers are considered to be grown coherently on the thick GaN:Si contact layer, i.e. no strain relaxation is assumed to occur in the material.

To simulate the MQW LED operation, we used the SiLENSe package [7] implementing a 1D model based on the Poisson equation for the electric potential and drift-diffusion transport equations for the electron and hole concentrations. Both the radiative recombination of the carriers and their non-radiative

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recombination on threading dislocation cores [8] are considered to predict the internal light emission efficiency, i.e. the ratio of the photon emission rate to the rate of electron-hole pair injection in the LED structure. The Fermi-Dirac statistics is used accounting for high non-equilibrium electron and hole concentrations in the active region. To calculate the light emission spectra, we solve self-consistently the Poisson and Schrödinger equations for the carrier wave functions in each quantum well. A uniform spectral broadening, $\Gamma = 20$ meV, due to the momentum relaxation via electron-electron collisions is taken into account. The complex valence band structure of nitride semiconductors is allowed for within the Luttinger-Kohn approach [9]. All the computations discussed below have been carried out with the threading dislocation density of 10^8 cm^{-2}. This value is an order of magnitude lower than the dislocation density typical of MOCVD-grown heterostructures due to the suppression of dislocation-mediated non-radiative carrier recombination, associated with fluctuations of the In composition in the MQWs [10].

Fig.1 shows the band diagrams and distributions of carrier concentrations in the LED structure with [Si] = 5×10^{18} cm^{-3} in the barriers, computed for two practically important values of current density j. It is seen that in the whole range of current density variation, electrons are uniformly distributed among different QWs. In contrast, holes are injected mainly into the QW adjacent to the *p*-AlGaN emitter at a lower j, while they fill the other QWs at j exceeding 100-200 A/cm^2. The hole distribution among the QWs becomes much more uniform if the lightly doped barriers ([Si] = 5×10^{17} cm^{-3}) are employed in the LED structure. This is due to a lower carrier recombination rate (a higher diffusion length) in the active region directly controlled by the electron concentration.

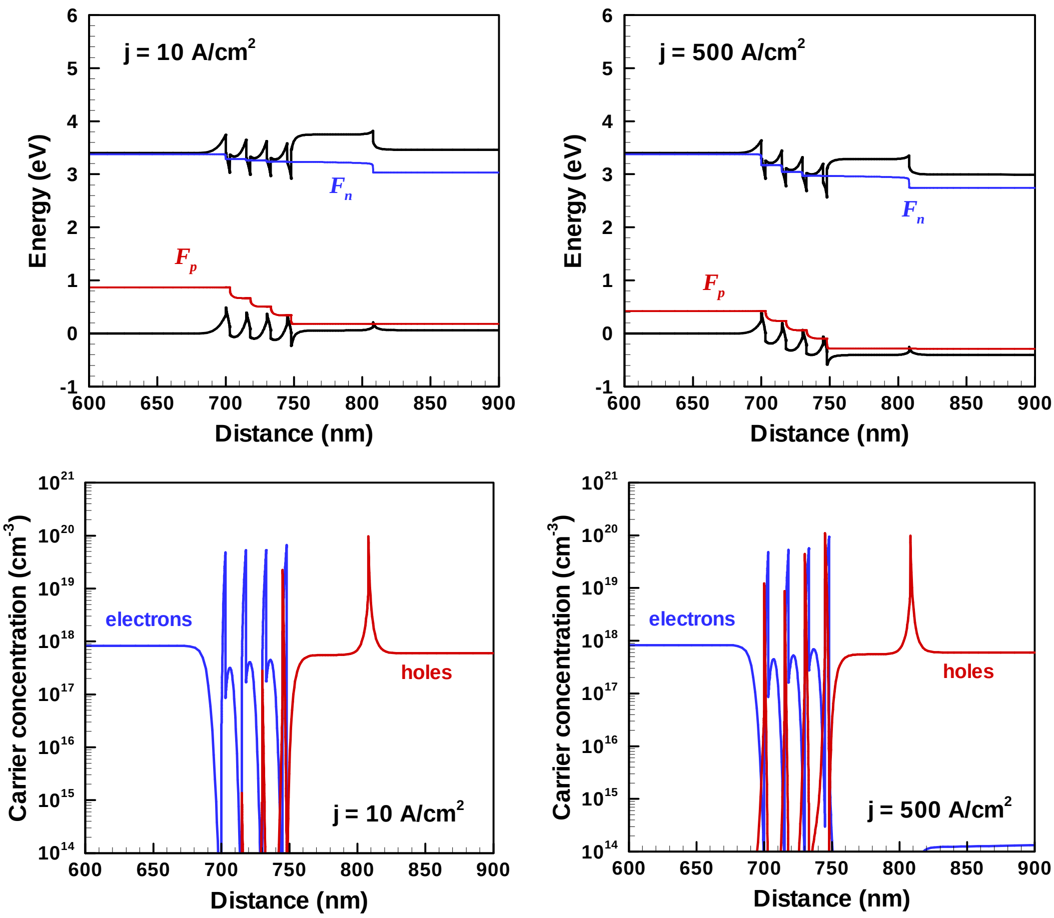

Fig. 1 Band diagrams and distributions of carrier concentrations in MQW LED with [Si] = 5×10^{18} cm^{-3} in the barriers. The quasi-Fermi levels of electrons and holes are denoted as F_n and F_p, respectively.

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The radiative recombination of electrons and holes is found to be localized mainly in the QWs. The non-radiative recombination occurs also in the MQW barriers and *p*-GaN contact layer where mobile electrons can penetrate. The latter effect is caused by an insufficiently high potential barrier in the *p*-AlGaN emitter which fails to confine electrons at high current densities (see Fig.1).

The I-V characteristic of the MQW LED computed for the series resistance of $R_S = 7\ \Omega$ is compared with that measured in the sample b026 in [6] (Fig.2). One can see an excellent agreement between them except for the low-current region where the tunnelling current is believed to dominate, which is not allowed for in the computational model. The comparison shows that the MQW LED operates in the injection-current mode in the practically important range of current density variation, 10-500 A/cm^2.

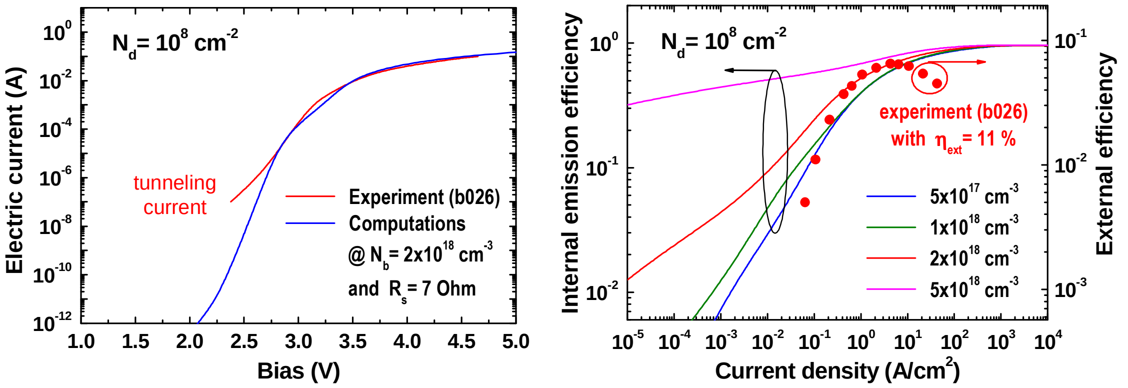

Fig. 2 The I-V characteristic (left) and the internal emission efficiency *versus* the current density (right) computed for various donor concentrations in the barriers. Circles (right) are the external emission efficiency of an LED measured in [6].

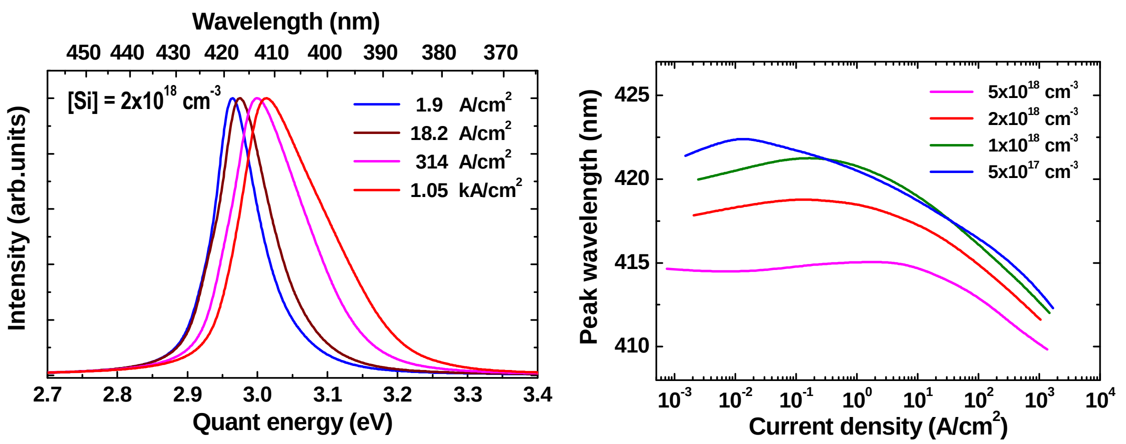

Fig. 3 Emission spectra from the LED structure with [Si] = 2×10^{18} cm^{-3} in the barriers (left) and the peak wavelength as a function of current density computed for various donor concentrations in the barriers (right).

Fig.2 plots the internal emission efficiency as a function of the current density computed for various donor concentrations in the MWQ barriers. For comparison, the external efficiency measured in [6] is also plotted in the figure. One can see that the predicted internal and measured external efficiencies correlate with each other and are even in quantitative agreement, if the efficiency of light extraction from the LED and its collection by the measuring system is assumed to be of ~ 11%. The internal efficiency is found to depend drastically on the donor concentration in the MQW barriers, especially at low currents, which is supported by the data reported in [6].

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Two factors may give rise to the emission efficiency enhancement in a heavily doped LED structure. First, it was shown in [8] that a higher overall electron concentration in the material favours the suppression of non-radiative recombination due to a prolonged carrier capture on threading dislocation cores. Second, in a heavily doped structure, holes are injected mostly into the QW adjacent to the *p*-emitter where the radiative recombination dominates (see Fig.1, left). In contrast, in a lightly doped LED, holes are distributed much more uniformly among the QWs, passing through the barriers where the non-radiative carrier recombination dominates. Suppression of the non-radiative recombination in the barriers due to a non-uniform hole distribution may be an additional factor contributing to the emission efficiency at a higher doping level in the MQW barriers.

Another reason for the use of heavily doped MQW barriers was the observed enhancement of the LED emission wavelength stability [6]. Our simulation confirm that a higher barrier doping results in a better peak wavelength stability at $j \leq 10$ A/cm^2 (Fig.3). At higher current densities, however, a distinct blue shift is predicted for all the structures irrespective of the barrier doping. Typical emission spectra computed for various injection levels are plotted in Fig.3, left. The electroluminescence peak becomes broadened at high current densities, which is due to the contribution of higher electron subbands in the radiative recombination. Both heavy and light holes form a quasi-continuum of states in the quantum wells, which is not resolved in the emission spectra. The predicted peak energy is found to be shifted from the experimental values by ~0.3 eV. This discrepancy may be attributed to either additional doping of the quantum wells with acceptors [11] or poorly known InGaN QW composition. In any case, this uncertainty does not affect the injection properties and the general behavior of the LED structure discussed above.

3 Conclusion

In this paper, we report on the modelling of a MQW LED heterostructure with selectively doped barriers. The device operates in the injection-current mode in the practically important range of current density variation, which is derived from the comparison of the computed and measured I-V characteristics. The simulation predicts an efficient capture of injected holes by the QWs and an insufficient confinement of electrons by the *p*-AlGaN emitter barrier at high current densities j. Heavy MQW barrier doping with donors is found to enhance the internal emission efficiency of the device and to stabilize the emission wavelength at moderate current densities $j \leq 10$ A/cm^2. These predictions agree well with the observations reported in Refs.[4,6]. At higher current densities, the spectra exhibit a distinct blue shift and broadening due to the filling of higher electron subbands.

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