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# Carrier injection and light emission in visible and UV nitride LEDs by modeling

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Polarization effects on carrier injection and light emission are considered by modeling with reference to single-quantum-well blue light emitting diode heterostructures of either Ga- or N-polarity. The model accounts for specific features of nitride semiconductors, spontaneous and piezo-polarization, strong non-radiative recombination on threading dislocation cores, complex valence band structure, etc., and allows detailed analysis of the device operation. The modeling results are compared with available observations.

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## 1 Introduction

Group-III nitrides used for production of visible and ultraviolet (UV) light emitting diodes (LEDs) and laser diodes (LDs) exhibit a number of non-ordinary properties: strong piezoeffect and spontaneous polarization inducing huge built-in electric fields, considerable light emission efficiency at extremely high dislocation density, extremely low efficiency of acceptor activation, etc. All these phenomena complicate intuitive understanding of the mechanisms involved in the device operation and require a careful band-gap and polarity engineering to improve the LED or LD performance. In addition to the common experimental way of the device optimization, numerical modelling is found to be effective for getting a deeper insight into the factors responsible for the LED efficiency and for finding correlations between the device structure and characteristics [1].

In this paper, we report on the modeling study of carrier transport and light emission in nitride-based LEDs. The study is focused on the polarization effects on the injection efficiency, electron confinement, and emission spectra from single-quantum-well (SQW) LED structures of both Ga- and N-polarities. The theoretical predictions are compared with available experimental data.

## 2 Model and results

The 1D model used for simulations is based on the Poisson equation for the electric potential and drift-diffusion transport equations for electron and hole concentrations in an LED structure. Both the radiative recombination of the carriers and their non-radiative recombination on threading dislocation cores [2] are considered as the factors controlling the carrier lifetime. The Fermi-Dirac statistics is used to account for high non-equilibrium electron and hole concentrations in the active region. To calculate light emission spectra, we solve self-consistently the Poisson and Schrödinger equations for the carrier wave functions inside a single or multiple quantum well. The complex valence band structure of nitrides is considered

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within the Luttinger-Kohn approach [3]. The model has been implemented in the SiLENSe 1.0 code [4] used for simulations. In more detail, the model will be described elsewhere.

We consider, as a representative example, a blue SQW LED structure fabricated by S. Nakamura and examined in detail in [5, 6]. The structure consist of a 5 μm n-GaN contact layer, an unintentionally doped (UID) 3.5 nm $In_{0.2}Ga_{0.8}N$ SQW, a 100 nm p-$Al_{0.1}Ga_{0.9}N$ emitter, and a p-GaN contact layer 200 nm thick. The donor ($3\times10^{18}$ $cm^{-3}$) and acceptor ($7\times10^{19}$ $cm^{-3}$) concentrations have been chosen for simulations in accordance with the data of earlier publications by S. Nakamura. In order to understand better the role of polarization effects in the LED operation, we compare the above structure assuming it to be of Ga-polarity with the same structure of N-polarity. Throughout the computations we assume the threading dislocation density in the material, $N_d$ , to be of $10^8$ $cm^{-2}$. This value, being by the order of magnitude lower than the typical dislocation density in MOVPE-grown structures, accounts for suppression of the non-radiative carrier recombination on dislocations due to composition fluctuations in the InGaN SQW.

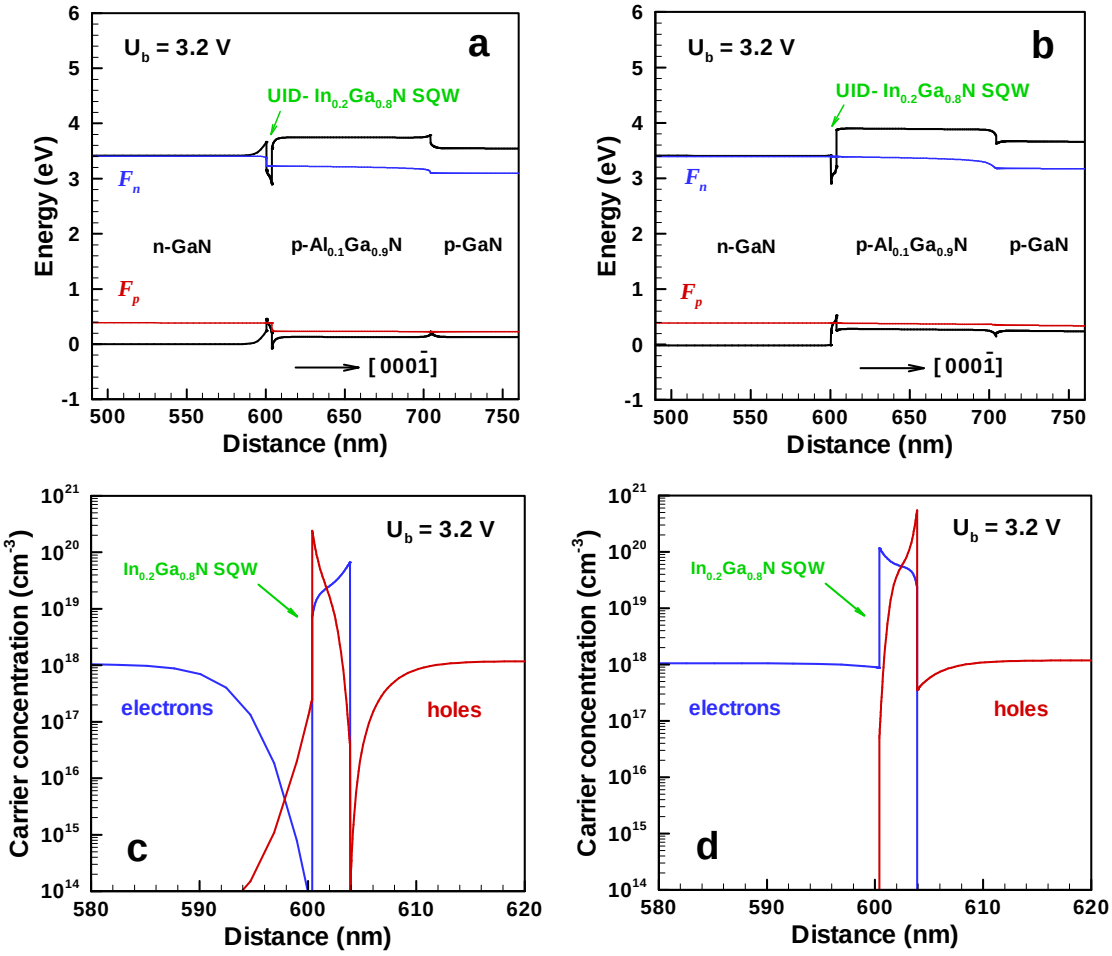


**Fig. 1** Band diagrams and distributions of carrier concentrations in the blue LED structures grown on Ga-faced (a,c) and N-faced (b,d) surfaces. $F_n$ and $F_p$ denote the quasi-Fermi levels of electrons and holes, respectively.

Simulations carried out for the Ga-faced LED structure predict the existence of a potential barrier to electrons, which hinders their injection into the InGaN SQW even at a high forward bias $U_b$ applied to the p-n junction (see Fig.1a). The barrier forms a narrow nearly insulating region next to the bottom SQW interface where the electron quasi-Fermi level and, consequently, the electron concentration drops

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remarkably (Fig.1c). A similar but lower barrier to holes exists near the top SQW interface. Besides, the Ga-faced structure does not provide good electron confinement at high $U_b$ , i.e. electrons can penetrate in the p-AlGaN emitter and holes can penetrate in the n-GaN contact layer where the carries recombine mainly non-radiatively.

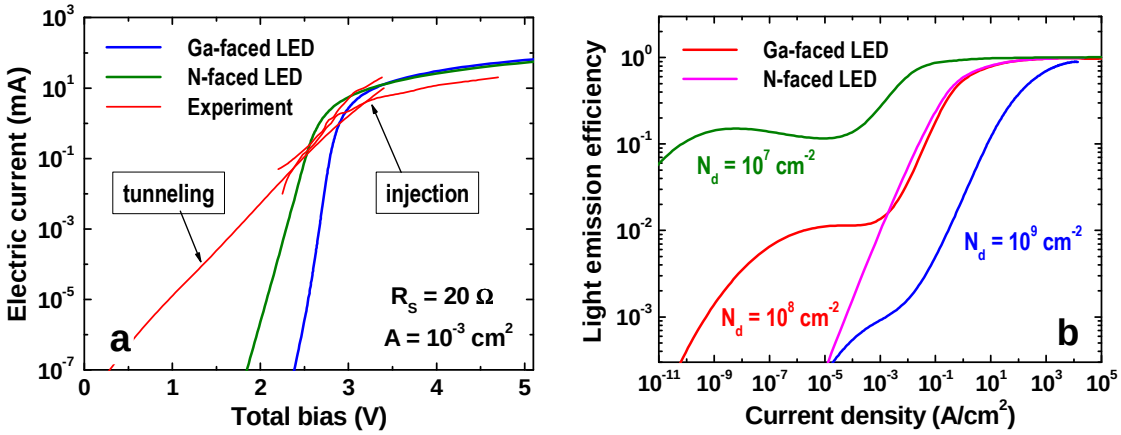


**Fig. 2** Current-voltage (I-V) characteristics of blue LEDs measured on various samples [5, 6] and calculated for the contact area $A = 10^{-3}$ cm$^2$ and serial resistance $R_s = 20$ Ω (a) and the light emission efficiency as a function of current density calculated for different dislocation densities in the Ga-faced structure (b).

In contrast to the Ga-faced LED, the N-faced heterostructure avoids the barriers hindering the carrier injection in the active region, due to the inversion of signs of the polarization charges on the SQW interfaces (Fig.1b,d). Additionally, the electron confinement in the N-faced LED is better than that in the Ga-faced structure – electrons cannot arrive in the p-AlGaN emitter because of a barrier on the top SQW interface while holes are confined by a similar barrier on the bottom interface (Fig.1b). The improved injection efficiency and electron confinement result in a lower turn-on voltage for the N-faced structure compared to the Ga-faced one (Fig.2a).

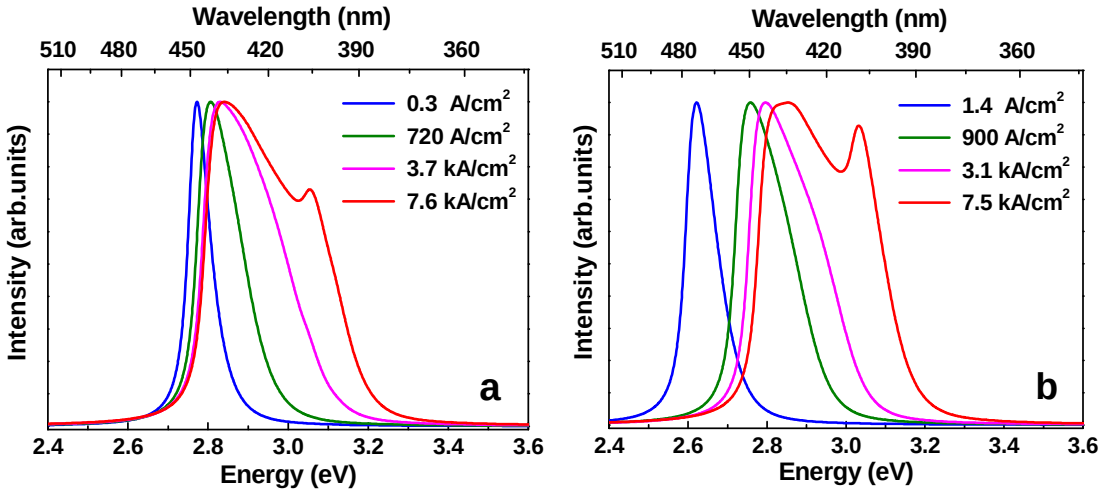


**Fig. 3** Emission spectra of the Ga-faced (a) and N-faced (b) LED structures at various current densities.

In general, the theory predicts adequately the injection-controlled portion of the I-V characteristic of the Ga-faced LED structure (see comparison with the data of [5, 6] in Fig.2a). The tunneling current observed at lower $U_b$ is not allowed for in our computational model but it corresponds to the current

densities much lower than the typical operation density of ~10-100 A/cm$^2$. The internal light emission efficiency, defined as the ratio of the integral radiative recombination rate to the total recombination rate in the structure, is found to depend considerably on both the electric current and threading dislocation density $N_d$ (Fig.2b). The saturation in the emission efficiency at the current density $j \sim 10$ A/cm$^2$ predicted for $N_d = 10^8$ cm$^{-2}$ agrees well with the observations [5, 6]. This justifies the use of the effective value of $N_d$ for the MOVPE-grown LED heterostructures. The variation of the dislocation density results in a drastic shift of the current density corresponding to the emission efficiency saturation. At $j = 20$ A/cm$^2$ corresponding to the typical operation current of 20 mA at the contact area $A = 10^{-3}$ cm$^2$, the internal emission efficiency is equal to ~20% for $N_d = 10^9$ cm$^{-2}$, ~80 % for $N_d = 10^8$ cm$^{-2}$, and ~98% for $N_d = 10^7$ cm$^{-2}$. This clearly demonstrates the importance of the dislocation density reduction to improve an LED efficiency.

The emission spectra of the Ga-faced and N-faced LEDs for various current densities are compared in Fig.3. For Ga-faced structure the predicted peak energy of 2.77-2.80 eV agrees well with the values of 2.65-2.75 eV measured on various samples in [5]. The discrepancy between the theory and experiment is apparently related to deviation of the InGaN SQW composition from that accepted for simulations (this is also confirmed by the scatter of experimental peak energies observed on different samples). It is also seen that the peak energy of the Ga-faced structure varies much more gradually with $j$ than that of the N-faced LED. This is due to the fact that the external electric field applied to the p-n junction of the Ga-faced structure is directed oppositely to the built-in electric field induced in the SQW by the polarization charges. In contrast, in the N-faced structure both external and internal fields have the same direction, which results in a poorer emission wavelength stability upon the bias variation. On the other hand, the shift of the emission wavelength with current predicted for the N-faced structure can be used for tuning of its spectrum in the wide range of 440-480 nm.

## 3 Conclusion

Using numerical modelling, we have studied polarization effects on the carrier injection and light emission in SQW blue LED heterostructures of either Ga- or N-polarity. These structures are found to exhibit quite different carrier injection efficiency and electron confinement in the active region. Due to the interplay between the external and built-in electric fields, the Ga-faced structure provides the emission spectrum much more stable with current than that of the N-faced structure. The light emission efficiency is predicted to strongly depend on the threading dislocation density in the material, which controls the non-radiative recombination rate in the LED. The theoretical results agree well with the available data on I-V characteristics, emission efficiency, and spectra from the Ga-faced LEDs.

Specific features of Ga-faced LED operation discussed in this paper have general character and should exhibit themselves in heterostructures of different design. More complex structures, e.g. those including multiple-quantum-well active region or additional current-blocking layers, can be also effectively analyzed and optimized by modeling.

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