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Effect of localized states on internal quantum efficiency of III-nitride LEDs

Sergey Yu. Karpov[*]

STR Group – Soft-Impact, Ltd., PO Box 83, 27 Engels ave., St. Petersburg 194156, Russia

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[*] Corresponding author: e-mail sergey.karpov@str-soft.com, Phone: +7 (812) 554 45 70, Fax: +7 (812) 326 61 94, Web: http://www.str-soft.com

A model is suggested accounting for effects of localized electron and hole states formed by composition fluctuations in the [illegible] on non-radiative carrier recombination at threading dislocations. The model [illegible] of the abnormal temperature dependence of internal quantum efficiency (IQE) of a green LED structure recently observed at low current densities. The theoretical predictions are in quantitative agreement with experiment in the temperature range between 200 K and 453 K.

1 Introduction The efficiency droop with current has been commonly recognized as the major factor limiting performance of high-power III-nitride LEDs with InGaN active regions. Among a variety of mechanisms suspected to be responsible for the droop, Auger recombination [1–4] and electron overflow/leakage [5–7] are considered as most probable. However, a common opinion on the dominating mechanism is not yet finally formed. Recently, abnormal temperature dependence of IQE of a green LED structure was observed which could not be explained by any simple activation mechanisms [3]. So, not only the IQE droop with current but also its variation with temperature still requires a self-consistent interpretation.

It is well known that composition fluctuations in InGaN quantum wells (QWs) form localized states preventing electrons and holes from recombination at threading dislocations (TDs), thus increasing the IQE of InGaN-based LEDs [8]. This letter demonstrates the effect of localized states on non-radiative carrier recombination to be capable of explaining the data on IQE [3] measured in a wide range of the current density and temperature variation. A simple model accounting for this effect is suggested.

2 Model The localized electrons and holes produce the tails in the density of states (DOS) inside the bandgap of InGaN QW next to the edges of the conduction and valence band, respectively. Assuming an exponential DOS decay in the bandgap, the two-dimensional electron DOS can approximated by the model function [9]

$$g_n(\varepsilon, U_n) = (N_c/kT)\cdot[1+\exp(-\varepsilon/U_n)]^{-1}, \qquad (1)$$

where ε is the electron energy counted from its ground state in the QW ($\varepsilon = 0$), U_n is the parameter characterizing the DOS decay in the bandgap, $N_c = m_n kT/\pi\hbar^2$ is the 2D-effective electron density of states in the QW, k is the Boltzmann constant, T is temperature, m_n is the in-plane effective electron mass, and $\hbar$ is the Planck constant. At $U_n \to 0$ the DOS (1) tends to a conventional step-like function of energy ε.

The sheet electron concentration n in the QW corresponding to the density of states (1) can be found from the analytical expression [9]

$$n = N_c \zeta_n \ln[1+\exp(F_n/\zeta_n kT)], \qquad \zeta_n = 1 + U_n/kT. \qquad (2)$$

Here F_n is the electron quasi-Fermi level. Attributing negative energies ($\varepsilon < 0$) to localized electronic states and positive ones ($\varepsilon > 0$) to delocalized states, one can calculate the concentration of delocalized electrons n_d as follows [10]

$$n_d = \begin{cases} N_c \ln[1+\exp(F_n/kT)], & F_n < 0, \\ n - N_c(\zeta_n - 1)\ln 2, & F_n > 0. \end{cases} \qquad (3)$$

Quite similar equations can be also obtained for holes but with the parameter U_p accounting for the exponential decay of the hole DOS in the bandgap.

To calculate IQE as a function of current density j, the balance equations are used, assuming the electron and hole concentrations in the QW being nearly equal to each other:

$$j = q(R_d + Bn^2 + Cn^3), \qquad \mathrm{IQE} = \frac{Bn^2}{R_d + Bn^2 + Cn^3}, \quad (4)$$

where q is the electron charge, B is the radiative recombination constant, and C is the Auger recombination constant. It is assumed that only delocalized electrons and holes participate in the non-radiative recombination at TDs. Then the rate of the non-radiative recombination can be written in a simplified Shockley–Read form

$$R_d = n_d p_d / (n_d \tau_p + p_d \tau_n). \quad (5)$$

Here p_d is the sheet concentration of delocalized holes calculated by the equations similar to (3), and τ_n and τ_p are the electron and hole life-times estimated within the approach suggested in [11].

3 Results and discussion Figure 1 shows by symbols the data on IQE of a green LED structure reported in [3] for various ambient temperatures. A specific feature of the data is a dramatic IQE improvement observed at low current densities ($j < 0.1$ A/cm^2) while the temperature is lowered. The efficiency droop observed at high current densities ($j > 50$ A/cm^2) is attributed to the contribution of Auger recombination.

The model suggested in Section 2 has been applied to simulate the IQE of a 2.5 nm $In_{0.3}Ga_{0.7}N$ SQW in a wide range of current density and temperature variation. It was assumed that the recombination constant $B(T) = B_0(T_0/T)$ where $B_0 = 7.5 \times 10^{-5}$ cm^2/s and $T_0 = 298$ K. The life-times τ_n and τ_p were calculated by formulae from [11], assuming the TD density to be of 10^9 cm^{-2} and the electron and hole

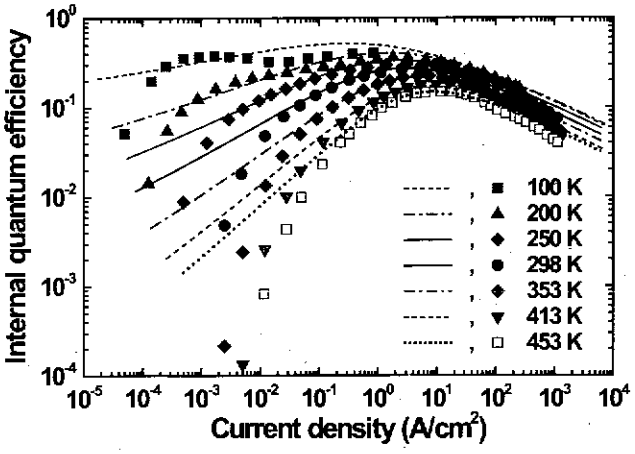

Figure 1 IQE as a function of current density at various ambient temperatures. Symbols are experimental data reported for a green InGaN SQW [3]. Lines are calculations made in this study.

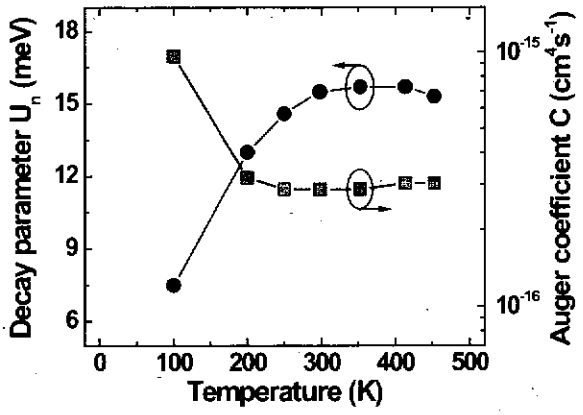

Figure 2 Parameters U_n and C obtained by fitting the model calculations to the data of [3]. The ratio U_n/U_p of about 2 was kept constant in the simulations.

diffusion coefficients in InGaN to be 3.0 and 0.3 cm^2/s, respectively. The ratio U_n/U_p of about 2 was kept constant in the simulations [10]. The effective masses of electrons, $m_n = 0.17m_0$, and holes, $m_p = 1.69m_0$, were used to calculate their effective densities of states (m_0 is the free electron mass).

Two parameters, U_n and C, were fitted to provide the best agreement with the experimental data of [3] for every particular temperature. The results of the IQE calculations are shown in Fig. 1. The values of the parameters obtained by the fitting procedure are summarized in Fig. 2.

One can see from Fig. 1 that the model suggested reproduces well the IQE behaviour in a wide range of the current density (except for very low and very high values of j) and temperature variation. The sharp IQE drop at very low current densities seen in every experimental data set cannot be explained by the recombination processes occurring in the QW, as is suggested by Eqs. (4). It can be rather attributed to additional non-radiative losses related to tunnelling/leakage of electrons and holes along TDs. The discrepancy between the theory and experiment at very high current densities can be explained as follows. Normally IQE of an LED is estimated from the measured external efficiency, assuming the proportionality factor between them, the light extraction efficiency (LEE), to be independent of operation current. The data of [3] were obtained from the LED structures processed by ThinGaN® technology. As we have recently shown [12], LEE of such devices generally decreases with current because of the current crowding near metallic electrodes accompanied by the shading effect on the light extraction. Neglecting the dependence of LEE on current may result in some underestimation of the experimental IQE at very high current densities. Another issue is the decrease of the recombination constant B with the carrier concentration, which is not considered in the above model. Account of this effect would somewhat reduce the theoretical IQE at high current densities.

Consider now the behaviour of fitted parameters U_n and C upon the temperature variation (Fig. 2). Both of

them vary slightly with temperature at $T > 200$ K. The small variation of U_n; from 13.0 meV to 15.7 meV in this temperature range, is the evidence for the fact that exponential decay of electron and hole DOS in the bandgap is a good approximation for the localized states produced in the InGaN QWs. Practically absent dependence of the Auger recombination coefficient C on temperature is an interesting result that should be borne in mind, while considering particular microscopic mechanisms of Auger recombination.

At $T < 200$ K, the fitted parameters U_n and C vary considerably with temperature (see Fig. 2). The main reason for this is dramatic increase in the radiative recombination constant B at low temperatures, as assumed in the suggested model. Actually, the constant B should no longer depend on temperature, if it is low enough, because of the carrier tendency to degeneration. So, the account of the actual dependence of the recombination constant B on temperature is expected to improve the model predictability at $T < 200$ K.

Using the above model, it is possible to compare the contribution of localized states and Auger recombination to IQE of III-nitride LEDs. At a low current density, where the Auger recombination is suppressed, the IQE improvement is controlled by the carrier localization due to InGaN composition fluctuations. According to Eqs. (2) and (3), the fraction of delocalized states is strongly dependent on temperature, which is the reason for abnormal IQE activation observed in [3] at low T. At a high current density, the localized states become saturated, the fraction of delocalized states increases, and IQE becomes controlled by the contribution of Auger processes to the non-radiative carrier recombination. The role of localized states becomes negligible under such operating conditions, resulting in a nearly temperature-independent IQE droop with current.

This study is based on the simplified balance equations considering the recombination processes in the InGaN QW only. This model catches well general behaviour of IQE as a function of current density and temperature. In practice, however, a number of additional factors may become important: non-equivalent electron and hole concentrations and spatial separation of their wave functions in the QW, shift of the ground electron and hole energy levels in the well upon the variation of the bias applied to the LED, non-uniform carrier injection in an MQW structure, etc. Accounting for these factors requires a more elaborated model to use and, perhaps, modification of the recombination and DOS tail parameters compared to those reported in this work.

4 Summary A simple model is suggested to predict IQE of InGaN-based LED structures as a function of current density and temperature. The model accounts for the effect of InGaN composition fluctuation on the rate of non-radiative carrier recombination at TDs via carrier localization. This mechanism is found to be responsible for the observed dramatic IQE improvement at low temperatures and low current densities, thus supporting the guess given in [3] on the essential role of localized states in the InGaN QW under such operation conditions.

At high temperatures and current densities, the role of compositional fluctuations becomes much less important because of dramatic increase of the delocalized electron and hole concentrations in the QW. This results in a temperature-independent IQE droop with current largely controlled by Auger recombination.

In the range of $200 \text{ K} < T < 453$ K, the model provides good quantitative agreement with observations [3] at a practically temperature-independent Auger recombination coefficient and slightly varying decay parameters of electron and hole DOS. Here, the IQE maximum decreases with temperature according to the temperature dependence of the radiative recombination constant.

A strong temperature dependence of the fitted Auger recombination coefficient and decay parameters at $T < 200$ K is the evidence for violation of some model assumptions. The most probable reason for this is a change in the temperature dependence of the radiative recombination coefficient caused by degeneration of non-equilibrium carriers. Accounting for this effect is expected to extend the applicability of the suggested model to lower temperatures.

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