Auger recombination via deep energy levels as a potential cause of efficiency droop in InGaN/GaN LEDs

A A Karpova1,2, D M Samosvat2, G G Zegrya1,2
1 ITMO University, 49 Kronverksky Pr., St. Petersburg, 197101, Russia
2 Ioffe Institute, 26 Politekhnicheskaya St., St. Petersburg, 194021, Russia
va7059va@yandex.ru

Abstract. In the present work a mechanism of nonradiative radiation via deep energy levels is considered for InGaN/GaN LEDs from the first principles. The coefficient and time of such Auger recombination are evaluated numerically and are shown to be enough for causing the efficiency droop in blue and green InGaN/GaN LEDs.

1. Introduction
Semiconductor light emitting diodes (LEDs) of the visible region are known to be one of the most dynamically developing and present-day fields of solid state optoelectronics. Having a constantly growing range of potential applications, nowadays they are used not only for cost-effective and environmentally friendly lightning [1 - 3], but also for high speed wireless communication [4], human physical condition management [1], etc. The special interest is attracted to blue InGaN/GaN LEDs, since the addition of phosphorus to such LEDs allows obtaining white light.

The key problem of InGaN/GaN LEDs operating at high current densities is the efficiency droop, which limits the yield power. Among the various phenomena responsible for this effect one can mention Shockley-Reed-Hall recombination at point and extended defects [5 - 10] and the density-activated defect recombination (DADR) [11], Auger recombination (AR) [12, 13] and close in its nature the process of Auger expulsion [14]. Also there are numerous processes related to the loss of charge carriers from the active region: poor hole injection [15], electron leakage [16], defect-related tunneling to defect states in the barrier region [17], saturation of the available localized states [18], etc.

Despite a significant number of experimental and theoretical works on this topic, to date there is no agreement on what kind of mechanism has a decisive influence on the internal quantum efficiency (IQE) of InGaN/GaN LEDs [19, 20]. Even more, some contradictions between the research results could be revealed.

It is known [3] that lack of lattice-matched substrates causes a high number of point and extended defects in InGaN/GaN systems. Point defects near or in the core of dislocations as well as broken bonds and impurities can induce deep energy levels [8, 21, 22] in III-V alloys. Despite some publications reporting about the negligible role of defects in the efficiency droop [12, 23], some authors are convinced, that effect of defects on efficiency droop is of high importance [6, 8, 10]. Besides Shockley-Reed-Hall recombination, one more nonradiative loss channel could exist in such defect systems, which is defect-assisted AR.
The aim of the present work is to show theoretically that AR via deep energy levels caused by defects or impurities may have an unexpected significant impact on the efficiency droop phenomenon in InGaN/GaN LEDs. Despite the fact that such type of Auger processes has already been studied theoretically \[22, 24\], there are no numerical estimations made exactly for InGaN/GaN systems. There could exist four different processes with electron participation called Ia – Id (figure 1), approximately equal in their effect on the IQE of InGaN/GaN LED. Four similar processes could be presented for holes localized in the active LED region as well.

**Figure 1.** Schemes of electron transitions corresponding to different processes of Auger recombination via deep energy levels.

In the current work a microscopic theory of AR via deep energy levels of Ia type is built with the use of four-band Kane’s model \[25\]. The probability of this process is calculated within the first-order perturbation theory. The rate and the coefficient of such process are derived. Auger coefficient is estimated numerically for InGaN/GaN LED with different In mole fractions.

### 2. Theoretical details

It is known \[26\], that three different mechanisms of AR exist in semiconductor quantum well (QW) structures: a thresholdless, a quasithreshold and a threshold ones. The last mentioned process is related to the transition of the excited particle into the discrete spectrum and could be easily neglected. It is shown \[26\], that the quasithreshold process dominates over the threshold-free process at temperature above 300 K. Thus the consideration of only quasithreshold process is enough to estimate roughly the effect of AR via deep levels.

From now on we would consider a single QW located so that x-axis is its axis of symmetry. To find the rate and the coefficient of studied Auger process the wave functions of carriers are needed. An explicit form of wave functions of carriers localized in QW and expressions determining their boundary conditions, energy spectra and dispersion equations could be found in \[2\]. The wave functions of carriers localized at deep levels might be represented with the use of zero-range potential model \[22\] in the following form:

\[
\psi = C e^{-\kappa r} |s>,
\]

where \(C = (\frac{\kappa}{2\pi})^{1/2}, \kappa = \sqrt{\frac{2m^*E_0}{\hbar}}, m^* – \text{effective electron mass}, E_0 – \text{the carrier binding energy}, |s\) is Bloch functions with angular momentum 0.

The matrix element of this process could be calculated using the Fourier representation:

\[
M = \frac{4\pi e^2}{\kappa} \int \frac{d^3q}{q^2} I_{14}(q) I_{23}(-q),
\]

\[
I_{14}(q) = \int d^3r_1 \psi_1(r_1) \psi_4^*(r_4) \exp(iqr_1),
\]

\[
I_{23}(q) = \int d^3r_2 \psi_2(r_2) \psi_3^*(r_2) \exp(iqr_2),
\]

where \(q = |q_4 - q_4|\) is the momentum transferred in the plane of the QW during the Coulomb interaction, \(e\) is an elementary charge, \(\psi_i(r_i)\) is a wave function of the carrier with index \(i\), \(\epsilon – \text{static dielectric constant of the QW semiconductor. Index i corresponds to the number of carrier: 1 and 2 to electrons localized in the QW, 3 to the hole bound at deep level and 4 to the electron excited into the continuous spectrum.}

The direct substitution of carrier wave functions into equations (3) and (4) allows expressing the overlap integrals \(I_{14}(q)\) and \(I_{23}(q)\) in the present forms:
\[ I_{14}(q) \approx (2\pi)^2 \int_{-\infty}^{+\infty} \psi_1(x) \psi_4(x) \exp(ipx) \, dx \times \delta(q_1 - q_4 + p + q), \]  
(5)

where \(|p|\) and \(|q|\) are transverse and longitudinal transferred momenta, \(\delta(q_1 - q_4 + p + q)\) is Dirac delta function,

\[ I_{23}(q) \approx A_2 C \frac{1}{\kappa_x^2}, \]  
(6)

where \(A_2\) is a normalization constant of the carrier with index 2.

As a result, the matrix element could be represented in a following form

\[ M = \frac{16\pi^4 e^2}{\varepsilon} A_2 C \frac{1}{Q^2} \int_{-\infty}^{+\infty} \psi_1(x) \psi_4(x) \exp(iqx) \, dx. \]  
(7)

It should be noted, that the integral in equation (7) might be equal to zero in case of zero transferred impulse due to orthogonality of corresponding carrier wave functions. To estimate the matrix element in equation (7) it is possible to expand the integrand into series by the transferred impulse in the plane of the QW and obtain:

\[ M = \frac{16\pi^4 e^2}{\varepsilon} \left( a + \frac{x}{\kappa_c} \right)^{-1} \left( \frac{\kappa}{2\pi} \right)^{1/2} \kappa^{-2} k_4^{-2}, \]  
(8)

where \(\kappa_c\) is an \(x\) quasimomentum component of the carrier with index 2 in sub-barrier region, \(k_4\) is a \(x\) quasimomentum component of the carrier with index 4, \(a\) – QW width.

The AR rate is given by:

\[ G = \frac{2\pi}{\hbar} \sum_{k_1,k_2,k_4} |M|^2 f_1 f_2 (1 - f_4) \delta(E_3 + E_4 - E_1 - E_2), \]  
(9)

where \(f_1\) and \(f_2\) are the Fermi distribution functions of the carriers in the initial state, \(f_4\) is the Fermi distribution function of the carrier in the final state, \(E_i\) – energy of the carrier with index \(i\).

The AR coefficient \(C\) is related to the rate \(G\) by the expression:

\[ G = C \left( n_{QW}^{2D} \right)^2 n_i^{2D}. \]  
(10)

where \(n_{QW}^{2D}\) is a 2D electron concentration in QW, \(n_i^{2D}\) is a 2D defect concentration.

The coefficient \(C\) corresponding to the quasithreshold process of AR via deep energy levels could be finally represented in the form

\[ C = 1024\pi^6 \frac{e^4}{\hbar} \delta (a + \frac{x}{\kappa_c})^{-2} \left( \frac{\pi^3 k_4^3}{\kappa} \right)^{-1}, \]  
(11)

where \(E_B = \frac{m_e e^4}{2\varepsilon h^2}\) is the Bohr energy in the region of QW.

3. Results and discussion

We would use the data presented in [8] to evaluate numerically the AR coefficient. According to [8], in InGaAlN/GaN LEDs with \(x = 0.17\) and \(x = 0.21\) emitting at 450 nm and 530 nm the energy levels \(E_c - 1.61\) eV and \(E_c - 1.43\) eV lie near the mid-band gap, where \(E_c\) is the conduction band minimum.

For estimation the following quantities are used: \(m_e = 0.13 m_0\) [27], where \(m_0\) is a free electron mass, \(\varepsilon = 9.7\) [27], \(a = 30\ \text{Å}\) [8], \(\frac{2}{\kappa_c} \ll a, k_4 \approx 8.1 \times 10^9 \lambda^{-0.5}\).

For such InGaN/GaN LEDs the required AR coefficient for 1a process via the abovementioned energy levels are \(C_{blue}^{2D} \approx 4.24 \times 10^{-12} \text{ cm}^4 / s\) and \(C_{green}^{2D} \approx 6.48 \times 10^{-12} \text{ cm}^4 / s\). The 2D and 3D AR coefficients are related as

\[ C_{3D} = C_{2D} a^2. \]  
(12)

It makes possible to obtain \(C_{blue}^{3D} \approx 3.81 \times 10^{-25} \text{ cm}^6 / s\) and \(C_{green}^{3D} \approx 5.83 \times 10^{-25} \text{ cm}^6 / s\).

The values of \(C_{blue}^{3D}\) and \(C_{green}^{3D}\) proportional to \(10^{-25} \text{ cm}^6 / s\) are larger than previously reported experimental and theoretical results for nonradiative coefficient in the framework of ABC-model [19, 20]. Also it can be seen from the estimation, that Auger coefficient increases with the growth of In mole fraction.

Assuming \(n_{QW}^{3D} \approx 10^{18} \text{ cm}^{-3}\) and \(n_i^{3D} \approx 10^{16} \text{ cm}^{-3}\) [8] one can obtain the time \(\tau = \left( C_{QW}^{3D} p^{3D} \right)^{-1}\) of studied AR process in the both InGaN/GaN LEDs: \(\tau_{green} \approx 1.72 \times 10^{-10} \text{ s}\) and \(\tau_{blue} \approx 1.72 \times 10^{-10} \text{ s}\).
2.62 × 10^{-10} \text{s}. Meanwhile the radiative lifetime of carriers in the InGaN/GaN LED emitting at about 470 nm is not less than 2 × 10^{-9} \text{s} [28].

4. Conclusion
In the present work Auger recombination via deep energy levels is considered in blue and green InGaN/GaN LEDs. It is shown, that such process might compete successfully with other already known processes responsible for efficiency droop in InGaN/GaN LEDs and requires the further theoretical investigation.

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