Determination of hole diffusion length in n-GaN

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Abstract. The paper presents the derivation of a model for minority carriers collection based on the reciprocity theorem and its application for determination of hole diffusion length in n-GaN by means of photoluminescence. The estimated hole diffusion lengths at room temperature are 110 nm and 194 nm in the case of low and high excitation, respectively, which could be explained by saturation of non-radiative recombination centers in bulk GaN and at the surface with photogenerated carriers.

1. Introduction

III-nitride optoelectronic devices, like light-emitting diodes and lasers or photodetectors, are of great interest due to their high efficiency and broad spectral range. Carrier transport in such structures is an important issue. Minority carrier diffusion length (usually holes, as even unintentionally doped GaN is n-type with a relatively high electron concentration of $10^{15}$-$10^{17}$ cm$^{-3}$) is one of the key parameters that directly affects the device performance. Different techniques can be used to determine diffusion length, including electron beam induced current [1], photoluminescence [2, 3], cathodoluminescence [3], etc. However, for correct determination of diffusion length, an appropriate processing of experimental data is required.

In this paper, we derive a simple analytical model for minority carrier collection into quantum well (QW) based on the reciprocity theorem and apply it to determine the minority hole diffusion length in n-GaN/InGaN structures from continuous-wave photoluminescence measurements.

2. Experimental details

A set of GaN/InGaN/GaN single quantum well (SQW) structures with different capping layer thickness (i.e. different distance from QW to the surface) was grown by metalorganic chemical vapor deposition on c-face sapphire substrates in our in-house Dragon-125 epitaxial system with a horizontal reactor. Conventional precursors, i.e. trimethylgallium, triethylgallium, trimethylindium and ammonia were used. The growth conditions were exactly the same for all the samples. In order to mitigate the effect of internal spontaneous and piezoelectric polarization fields, GaN layers were doped with [Si]~5*10$^{18}$ cm$^{-3}$ using silane as a precursor. Photoluminescence studies were performed using a continuous wave He-Cd laser (325 nm, ~10 mW) in low and high excitation regimes by changing focused spot diameter from ~5 mm to ~0.5 mm. An AvaSpec-2048 Fiber Optic Spectrometer was used for the spectra measurements.
3. Model derivation

Generally, simulation of charge transport in semiconductors requires self-consistent solving of Poisson and electron- and hole-continuity equations. In simpler cases, when the excess minority carrier density is much smaller than that of the majority one and the electric field is neglected, only diffusion equation for minority carriers can be considered:

\[
D \frac{\partial^2 p(z)}{\partial z^2} - \frac{p(z)}{\tau} + G(z) = 0
\]  

(1)

where \(D\) is diffusion coefficient, \(\tau\) is bulk lifetime, \(G(z)\) is carrier generation profile. However, it also requires using of numerical methods.

A reciprocity theorem formulated and proven by Donolato [4] states that charge collection can be described as a solution of the homogeneous version of equation (1) with appropriate boundary conditions (BCs). Introducing \(P_{QW}(z)\) as “collection probability” instead of \(p(z)\) we get:

\[
D \frac{\partial^2 P_{QW}(z)}{\partial z^2} - \frac{P_{QW}(z)}{\tau} = 0
\]  

(2)

Originally, this model was proposed for charge collection in electron beam induced current (EBIC) analysis. We apply this model to derive an analytical expression for carrier collection into QW.

A general solution of equation (2) is:

\[
P_{QW}(z) = A \cdot e^{\frac{z}{\tau}} + B \cdot e^{\frac{-z}{\tau}}
\]  

(3)

where \(L = \sqrt{D \cdot \tau}\) is diffusion length and coefficients \(A\) and \(B\) should be found from appropriate BCs. Considering QW of zero thickness located at \(z = z_{QW}\) as a perfect collector, the surface at \(z = 0\) and infinite buffer thickness, the BCs are:

\[
\left. \frac{\partial P_{QW}(z)}{\partial z} \right|_{z=0} = \frac{S}{D} \cdot P_{QW}(0) = \frac{S\tau}{L^2} \cdot P_{QW}(0)
\]  

(4a)

\[
P_{QW}(z_{QW}) = 1
\]  

(4b)

\[
P_{QW}(\infty) = 0
\]  

(4c)

where \(S\) is surface recombination velocity. The obtained expression is:

\[
P_{QW}(z) = \begin{cases} 
\frac{\cosh \left( \frac{z}{L} \right) + \frac{S\tau}{L} \sinh \left( \frac{z}{L} \right)}{\cosh \left( \frac{z_{QW}}{L} \right) + \frac{S\tau}{L} \sinh \left( \frac{z_{QW}}{L} \right)}, & \text{for } z \leq z_{QW} \\
\exp \left( -\frac{z - z_{QW}}{L} \right), & \text{for } z \geq z_{QW}
\end{cases}
\]  

(5)

Examples of this curve for different conditions are shown in figure 1.

The intensity of photoluminescence from the QW can be expressed as:

\[
I_{QW} = \eta_{QW} \int_0^\infty G(z)P_{QW}(z)dz \propto \eta_{QW} \int_0^\infty e^{-\alpha z} P_{QW}(z)dz
\]  

(6)
where $\eta$ is a quantum efficiency of QW (portion of radiative recombination acts), $G(z)$ is a photogenerated carriers profile, $\alpha=1.2 \cdot 10^5 \text{ cm}^{-1}$ [5] is the absorption coefficient of GaN at 325 nm.

It is also interesting to find PL intensity not only of QW but of GaN as well. It is not just directly proportional to the integral of $G(z)(1 - P_{QW})$, because both radiative and non-radiative recombinations take place in bulk, but surface recombination is non-radiative one only. It is therefore necessary to determine the probabilities to recombine on surface and in bulk separately. Let us first find the probability $P_S$ to recombine on surface. We start with the same equations as (2) and (3), but with different BCs. The first BC is trivial – the probability to recombine on the surface for the carriers at $z = z_{QW}$ is zero because the probability to get into QW is unity. The second BC is not so obvious. If we used BC similar to (4a), we would get $P_S(z) = 0$ for all $z$. According to Donolato [6], the correct boundary condition for the surface with finite collection velocity is:

$$D \frac{dP_S(z)}{dz} \bigg|_{z=0} = S \cdot P_S(0) - S$$

(7)

and the corresponding solution for the probability to recombine on the surface is:

$$P_S(z) = \begin{cases} 
    \frac{S \tau \left[ \exp\left(-\frac{z}{L}\right) - \exp\left(-\frac{2z_{QW} - z}{L}\right) \right]}{L + S \tau + L \cdot \exp\left(-\frac{2z_{QW}}{L}\right) - S \tau \cdot \exp\left(-\frac{2z_{QW}}{L}\right)}, & \text{for } z \leq z_{QW} \\
    0, & \text{for } z \geq z_{QW}
\end{cases}$$

(8)

Hence, the probability $P_B$ for carriers to recombine in bulk can be expressed as:

$$P_B(z) = 1 - P_S(z) - P_{QW}(z)$$

(9)

and PL intensity of bulk GaN including near-band-edge (NBE) and ‘defect’ yellow band (YB) (see figure 2) emission is:

\[ \text{Intensity} = P_B(z) \]

Figure 1. Examples of the collection probability curves for the cases of zero, non-zero and infinite surface recombination velocity $S$ (solid lines) and small diffusion length (dashed line). The dotted line indicates photogenerated carriers profile.

Figure 2. Normalized PL spectra at low excitation level measured at 5 points over the wafer as shown in the inset. Spectra are shifted vertically for clarity.
\[ I_B = \eta_B \int_0^\infty G(z)P_B(z)dz \propto \eta_B \int_0^\infty e^{-\alpha z}P_B(z)dz \]  \hspace{1cm} (10)

where \( \eta_B \) is a portion of radiative recombination acts.

This model can be easily extended to multiple quantum well (MQW) structures (with appropriate BCs) and/or another excitation type. It should be noted that the model ignores carrier overshoot effect and carrier thermal escape effect, which can be significant for shallow QWs.

4. Results and discussion

Internal polarization fields inside InGaN are strongly concentration-dependent. The change in the magnitude of electric field leads to the change of electron-hole wavefunction overlap, which in turn leads to the change in recombination rates and transition wavelength. Therefore, for the correct comparison between the samples one needs to make sure that the indium content is the same. As one can see from PL spectra in figure 2, the samples demonstrate excellent uniformity both over the individual wafer and between the samples.

Then, integrated intensities of QW and GaN emission (including NBE and YB) were obtained from PL spectra and averaged over 5 points. The results normalized to the intensity of QW of the sample with 10 nm cap are shown in figure 3 as symbols. As one can see, the intensity of QW becomes weaker as the cap thickness is increased in both low and high excitation regimes. However, the intensity drop with cap layer thickness increase is smaller in the case of high excitation. The dependence of the intensity of GaN is more interesting with non-monotonic behavior.

The model contains several parameters, i.e. \( \tau, D, L, S, \eta_{QW} \) and \( \eta_B \) which are not fully independent, and, moreover, the model does not allow to determine all of them. For convenience, we chose \( L = \sqrt{D\tau} \) and \( S\tau \) as fitting model parameters. Parameters \( \eta_{QW} \) and \( \eta_B \) were not used, but the dependencies were normalized to the corresponding intensities of the sample with 10 nm cap layer. Then, the dependences of the intensity of QW versus cap layer thickness were fitted with the model. The obtained dependencies for QW and GaN intensity are shown as solid and dashed lines in figure 3, respectively. As one can see, an excellent agreement for QW intensity was achieved. As for GaN intensity, it agrees “semi-quantitatively” with the experiment, probably, because of non-linear behavior.

**Figure 3.** Integrated PL intensities of QW and GaN versus GaN cap layer thickness for the case of low (a) and high (b) excitation. Symbols are experimental data, averaged over 5 points across each wafer and normalized to the intensity of QW of the structure with 10 nm cap layer; error bars indicate standard deviation. Lines are model fit.
dependence of YB emission intensity on excitation or self-absorption effect. Anyway, the model is able to predict such non-monotonous behavior with a minimum at ~100 nm of cap thickness.

The values of the fitting parameters should be discussed. We obtain $L=110$ nm and $S\tau=201$ nm for the case of low excitation and $L=194$ nm and $S\tau=203$ nm for the case of high one, i.e. the diffusion length almost doubled when the excitation power density was increased by two orders of magnitude while $S\tau$ didn’t change. There could be two situations. In first, $S$ and $\tau$ are independent on excitation density, then the mobility of the minority carriers should increase almost fourfold since $D = \mu \frac{kT}{q}$.

Possible reasons for increase in mobility are decrease of charged impurity scattering rate or switch from unipolar to ambipolar diffusion. However, none of these can increase the mobility (diffusivity) so much [7]. A second, more viable, hypothesis is fourfold increase in non-radiative lifetime $\tau$ in bulk with simultaneous decrease in surface recombination velocity. Both could result from the saturation of non-radiative recombination centers in bulk and at the surface by photogenerated carriers, respectively. The result is in line with [2]. Similar effect of increasing non-radiative lifetime was also reported for iron-, carbon- [8] and magnesium-doped [9] bulk GaN under long-term electron beam irradiation. However, it cannot be excluded that a combination of both effects takes place.

5. Conclusion
In this paper, a model for minority carriers’ collection into quantum well was derived based on the reciprocity theorem. The model was applied to the data of photoluminescence of InGaN/GaN single-quantum well structure to determine a hole diffusion length in n-GaN. The estimated hole diffusion lengths was found to be 110 nm and 194 nm in the case of low and high excitation, respectively, which could be explained by saturation of non-radiative recombination centers in bulk GaN and at the surface with photogenerated carriers.

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