Published in: Appl. Phys. Lett. **81**, No. 23, 4721–4723 (2002)/**DOI** 10.1063/1.1527225

Dislocation Effect on Light Emission Efficiency in Gallium Nitride

Sergey Yu. Karpov[1] and Yuri N. Makarov[2]

[1] Soft-Impact, Ltd., P.O.Box 33, 27 Engels av., St.Petersburg, 194156 Russia
[2] Semiconductor Technology Research, Inc., 1610 Swinton Lane, Richmond VA, 23233, USA

Received 13 May 2002, accepted 16 October 2002

PACS: 78.20-e, 78.66.Fd, 78.20.Bh

We modify the model of non-radiative carrier recombination on threading dislocation cores [Z. Z. Bandić, P. M. Bridger, E. C. Piquette, and T. C. McGill, Solid-State Electronics **44**, 221 (2000)] to estimate quantitatively the light emission efficiency in GaN as a function of the dislocation density and non-equilibrium carrier concentration. The model predictions are in good agreement with available data on the minority carrier diffusion length in GaN. The dislocation density must be reduced, at least, down to ~10^7 cm^{-2} in order to provide a light emission efficiency close to unity. The n-type background doping is found to be favorable for the further efficiency improvement.

Preprint (2002)

Recent progress in the development of nitride-based optoelectronic devices has stimulated much interest in fundamental properties of group-III nitrides, directly related to light emission. Special attention is given to the luminescence of InGaN quantum wells [1,2], the contribution of a piezoelectric field and spontaneous polarization to the emission spectra [3,4], and the Coulomb effect on the radiative recombination rate [5,6]. Recently, non-radiative carrier recombination in nitride compounds became a central point of a number of studies [7,8,9,10,11], primarely with respect to AlGaN/GaN ultra-violet (UV) light emitting diodes (LED) and photodetectors. The correlation between the minority carrier diffusion length and the dislocation density found for GaN [8] supports the idea of dislocations being non-radiative recombination centers. A dramatic increase in the photoluminescence (PL) intensity at a low threading dislocation density in GaN was reported in [10,11]. A similar trend was also observed in InAlGaN LEDs where the dislocation density was reduced to 5×10^7 cm^{-2} by using a special buffer layer heavily doped with silicon [12]. However, there is still a lack of quantitative estimates for the dislocation density acceptable to fabricate high-efficiency optoelectronic devices.

This paper is aimed at understanding the dislocation effect on the light emission efficiency in GaN grown on a lattice-mismatched substrate like sapphire or silicon carbide. We modify the model [8] to get quantitative predictions for the non-radiative recombination rate. Within the modified model, we calculate the emission efficiency as a function of threading dislocation density and non-equilibrium carrier concentration. The latter enables one to predict the dislocation density necessary to get a radiative recombination yield close to unity.

It is known that threading dislocations form in GaN a number of acceptor-like levels with the energy E_D lying within the bandgap [7,13,14]. Hence, the Shockley-Read approach [15] is applicable to non-equilibrium carrier recombination through the dislocation levels. In the case of non-degenerate carriers, the recombination rate on the dislocations, R^{nr}, can be expressed as

$$R^{\mathrm{nr}} = \frac{np - n_i^2}{\tau_p\left(n + n_D\right) + \tau_n\left(p + p_D\right)} \quad . \tag{1}$$

Here, n and p are the electron and hole concentrations, τ_n and τ_p are the lifetimes of electrons and holes, respectively,

$$n_D = N_C \cdot \exp\left(\frac{E_D - E_C}{kT}\right) \quad , \qquad p_D = N_V \cdot \exp\left(\frac{E_V - E_D}{kT}\right) \quad , \tag{2}$$

$n_i = \sqrt{N_C N_V} \cdot \exp(-E_G / 2kT)$ is the intrinsic carrier concentration in the semiconductor, E_C and E_V are the energy levels corresponding to the conduction band bottom and the valence band top, $E_G = E_C - E_V$, N_C and N_V are the electron and hole densities of states in the conduction and valence bands, k is the Boltzmann constant, and T is temperature.

Generally, the non-equilibrium carrier lifetimes τ_n and τ_p are related to the respective generation rates G_n and G_p by the expressions $n\tau_n = G_n$ and $p\tau_p = G_p$. Following [8], we consider the carrier diffusion toward a threading dislocation core, occurring inside a cylindrical volume surrounding the dislocation. The cylinder radius is assumed to be $r_D = (\pi N_D)^{1/2}$, where N_D is the dislocation density. The two-dimensional steady-state diffusion equation for holes is solved with the boundary conditions: (i) $\partial p / \partial r |_{r=r_D} = 0$ and (ii) $D_p \partial p / \partial r |_{r=r_C} = SV_p p$ (similar equations are also valid for electrons). Here, r_C is the dislocation core radius, D_p (D_n) is the hole (electron) diffusivity, and V_p (V_n) is the hole (electron) thermal velocity, S is the fraction of electrically active sites on the dislocation core. In hexagonal (wurtzite) nitrides, the dislocation core radius r_C is equal to the lattice constant a in order of magnitude (see, for instance, the dislocation core configurations discussed in [14]). The value of S may be taken equal to 0.5 for Ga-vacancy or N-vacancy cores but generally it depends on the dislocation type – screw, edge or mixed [11]. Boundary condition (i) allows an individual dislocation to capture the non-equilibrium carriers only from the selected cylindrical volume. Condition (ii) accounts for the fact that the capture rate is limited by the thermal carrier velocity in the material bulk. The solution of the diffusion equations involving the generation terms G_n and G_p with the averaging of the obtained distributions of carrier concentrations over the cylinder cross-section at $r_D >> r_C$ provide the carrier lifetimes

$$\tau_n = \left(4\pi D_n N_D\right)^{-1} \cdot \left[\frac{2D_n}{aV_n S} - \frac{3}{2} - \ln\left(\pi a^2 N_D\right)\right] \quad ,$$
$$\tau_p = \left(4\pi D_p N_D\right)^{-1} \cdot \left[\frac{2D_p}{aV_p S} - \frac{3}{2} - \ln\left(\pi a^2 N_D\right)\right] \quad . \tag{3}$$

The minority carrier diffusion lengths are related to their lifetimes by the conventional expressions $L_{n,p} = \sqrt{D_{n,p}\tau_{n,p}}$.

To estimate the radiative recombination rate R^{rad}, we use an equation valid for non-degenerate carriers: $R^{\mathrm{rad}} = B \cdot \left(np - n_i^2\right)$. Here, $B = 2.4\times10^{-11}$ cm^3/s is the bimolecular recombination rate constant determined experimentally in [16]. Then the light emission efficiency η can be defined as

$$\eta = \frac{R^{\mathrm{rad}}}{R^{\mathrm{rad}} + R^{\mathrm{nr}}} = \frac{B}{B + \left[\tau_p\left(n + n_D\right) + \tau_n\left(p + p_D\right)\right]^{-1}} \tag{4}$$

Here, the carrier concentrations equal $n = n_0 + \Delta n$ and $p = p_0 + \Delta n$, where n_0 and p_0 are the background concentrations controlled by doping the material, and Δn is the non-equilibrium carrier concentration dependent on the excitation type and level.

Published in: Appl. Phys. Lett. **81**, No. 23, 4721–4723 (2002)/**DOI** 10.1063/1.1527225

Fig.1 shows the minority diffusion lengths as a function of the threading dislocation density calculated for the diffusion coefficients $D_n = 2.6$ cm^2/s and $D_p = 0.12$ cm^2/s [8], thermal velocities $V_n = 2.6\times10^7$ cm/s and $V_p = 9.4\times10^6$ cm/s [17], $n_0 = 1.0\times10^{17}$ cm^{-3} , and $S = 0.5$. The dislocation-related energy was taken as $E_D = E_V + 0.4$ eV to correspond to the acceptor-like centers. However, the computation results have proved quite insensitive to E_D variation in a wide range. The experimental data on the diffusion length borrowed from Refs.[8,9] are also plotted in Fig.1 for comparison. It is seen that the calculated electron and hole diffusion lengths are very comparable with each other, in close agreement with observations. The predicted variation in the diffusion length with dislocation density fits well the data of Refs.[8,9].

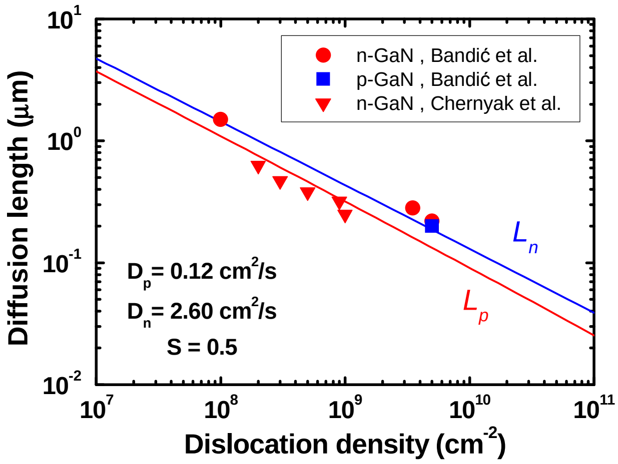

Fig.1. Minority carrier diffusion length as a function of threading dislocation density. Lines are computations, symbols are the data of Refs.[8,9].

The quantitative agreement obtained enables us to use the carrier lifetimes (3) for estimating the light emission efficiency in GaN as a function of threading dislocation density. For this, we have chosen the values $D_n = 15$ cm^2/s and $D_p = 2$ cm^2/s typical for a quality material with the respective electron and hole mobilities of 600 and 80 cm^2/V·s. Plotted in Fig.2 is the light emission efficiency *versus* dislocation density, calculated for various non-equilibrium carrier concentrations Δn . For comparison, we also plot the photoluminescence (PL) intensity as a function of dislocation density, measured in [10,11]. One can see a good qualitative agreement between the theory and experiment, indicating the threading dislocations to be just the factor that controls the light emission efficiency in GaN grown on a mismatched substrate.

Fig.2 demonstrates that the dislocation density must be reduced, at least, down to ~10^7 cm^{-2} in order to provide a light emission efficiency close to unity. To understand the effect of the background doping on the emission efficiency, we have calculated it as a function of non-equilibrium carrier concentration for undoped, n-doped, and p-doped material (the electron and hole background concentration is taken to be 2×10^{17} cm^{-3}). These results are presented in Fig.3. It is seen that the n-type doping is most favorable for getting the maximum efficiency in the wide range of non-equilibrium carrier concentrations. This is due to a lower hole diffusivity in n-GaN, which is the limiting factor for the rate of carrier capture on the dislocation cores.

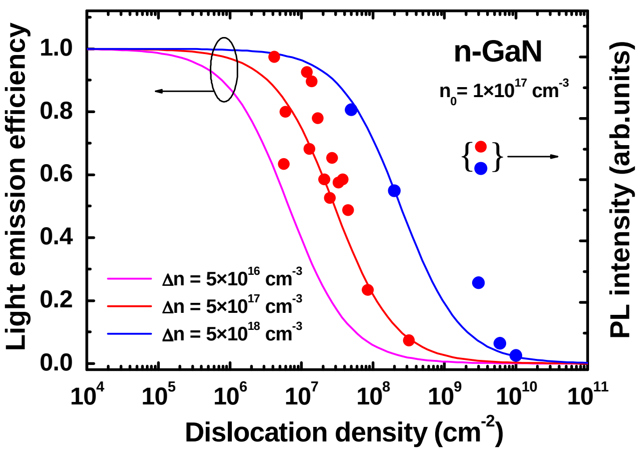

Fig.2. . Light emission efficiency in GaN calculated for different non-equilibrium carrier concentrations (lines, left axis) and the PL intensity (circles, right axis) as a function of dislocation density.

Published in: Appl. Phys. Lett. **81**, No. 23, 4721–4723 (2002)/**DOI** 10.1063/1.1527225

Generally, an increase in the non-equilibrium carrier concentration a higher efficiency via saturation of the non-radiative recombination channel. Nevertheless, the efficiency still remains below ~10% at the dislocation density as high as 10^9 cm^{-2}.

The model suggested also predicts that the material co-doped with n- and p-impurities can provide a higher radiative recombination yield. Indeed, a partial compensation from co-doping lowers considerably the carrier diffusivities. This, in turn, increases the dislocation-mediated carrier lifetimes, which is favorable for the light emission efficiency. An additional benefit may come from the carrier localization away from the dislocations due to the electric potential fluctuations.

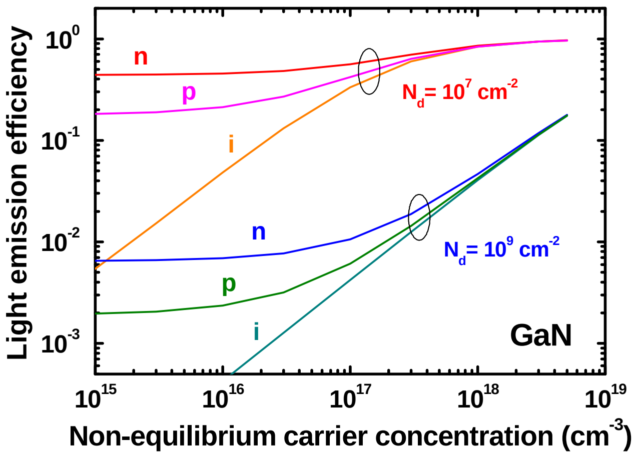

Fig.3. Light emission efficiency *versus* non-equilibrium carrier concentration calculated for n-doped (n), p-doped (p), and undoped (i) GaN. The background concentration of electron and holes in doped material is 2×10^{17} cm^{-3} .

To conclude, a modified model of the carrier recombination on threading dislocation cores has provided estimates of light emission efficiency in GaN grown on a mismatched substrate like sapphire or silicon carbide. The theoretical approach was verified by comparing the predicted minority carrier diffusion lengths with those measured experimentally. A reasonable quantitative agreement with the observations is reached by accounting for the finite capture rate of non-equilibrium carriers on the dislocation cores. The estimates show that the dislocation density must be reduced, at least, to 10^7 cm^{-2} in order to get an emission efficiency close to unity. The efficiency can be remarkably raised by intentional n-type doping of the material.

The above approach can also be applied to other active region materials, like AlGaN, important for UV LEDs and detectors. At low dislocation densities, the contribution of deep-level traps to the non-radiative recombination becomes essential. However, this additional non-radiative channel can be easily accounted for within the model suggested.

References

[1] S. F. Chichibu, H. Marchand, M. S. Minsky, S. Keller, P. T. Fini, J. P. Ibbetson, S. B. Fleischer, J. S. Speck, J. E. Bowers, E. Hu, U. K. Mishra, S. P. DenBaars, T. Deguchi, T. Sota, and S. Nakamura, Appl. Phys. Lett. **74**, 1460 (1999).

[2] C. A. Tran, R. F. Karlicek , Jr., M. Schurman, A. Osinsky, V. Merai, Y. Li, I. Eliashevich, M. G. Brown, J. Nering, I. Ferguson, and R. Stall, J. Cryst. Growth **195**, 397 (1998).

[3] M. Leroux, N. Grandjean, J. Massies, B. Gil, P. Lefebvre, and P. Bigenwald, Phys. Rev. B **60**, 1496 (1999).

[4] S. F. Chichibu, A. C. Abare, M. P. Mack, M. S. Minsky, T. Deguchi, D. Cohen, P. Kozodoy, S. B. Fleischer, S. Keller, J. S. Speck, J. E. Bowers, E. Hu, U. K. Mishra, L. A. Coldren, S. P. DenBaars, K. Wada, T. Sota and S. Nakamura, Mater. Sci. Engineer. B **59**, 298 (1999).

[5] G. B. Ren and P. Blood, Phys. Rev. B **60**, 16675 (1999).

[6] O. Brandt, H.-J. Wünsche, H. Yang, R. Klann, J. R. Müllhäuser, and K. H. Ploog, J. Cryst. Growth. **189/190**, 790 (1998).

[7] J. S. Speck and S. J. Rosner, Physica B **273-274**, 24 (1999).

[8] Z. Z. Bandić, P. M. Bridger, E. C. Piquette, and T. C. McGill, Solid-State Electronics **44**, 221 (2000).

[9] L. Chernyak, A. Osinsky, and A. Schulte, Solid-State Electronics **45**, 1687 (2001).

[10] M. Iwaya, S. Terao, T. Sano, S. Takanami, T. Ukai, R. Nakamura, S. Kamiyama, H. Amano, and I. Akasaki, Phys. Status Solidi A **188**, 117 (2001).

[11] T. Hino, S. Tomiya, T. Miyajima, K. Yanashima, S. Hashimoto, and M. Ikeda, Appl. Phys. Lett. **76**, 3421 (2000).

[12] H. Hirayama, A. Kinoshita, A. Hirata, and Y. Aoyagi, 4th International Symposium on Blue Laser and Light Emitting Diodes, Cordoba (Spain), FrB2, (2002).

[13] A. F. Wright and U. Grossner, Appl. Phys. Lett. **73**, 2751 (1998).

[14] S. M. Lee, M. A. Belkhir, X. Y. Zhu, Y. H. Lee, Y. G. Hwang, and T. Frauenheim, Phys. Lett. B **61**, 16033 (2000).

[15] W. Shockley and W. T. Read, Jr., Phys. Rev. B **87**, 835 (1952).

[16] J. S. Im, A. Moritz, F. Steuber, V. Härle, F. Scholz, and A. Hangleiter, Appl. Phys. Lett. **70**, 631 (1997).

[17] V. Bougrov, M. Levinshtein, S. Rumyantsev, and A. Zubrilov, in *Properties of Advanced Semiconductor Materials: GaN, AlN, InN, BN, SiC, SiGe*, **John Wiley & Sons, Inc.**, New York, Eds. M. E. Levinshtein, S. L. Rumyantsev, M. S. Shur, Chap. 1, p.2, (2001).