Band gap engineering approaches to increase InGaN/GaN LED efficiency

M. Auf der Maur and A. Di Carlo
Dept. of Electronic Engineering
University of Rome "Tor Vergata", Italy
Email: auf.der.maur@ing.uniroma2.it

K. Lorenz
Unidade de Física e Aceleradores
Instituto Tecnologico e Nuclear, Sacavém, Portugal

***Abstract*—Nitride-based LEDs for lighting applications suffer from efficiency issues related especially to the strong polarization fields. In this paper we present a study based on device simulation showing the beneficial impact of different band gap engineering approaches on device performance in particular for green LEDs.**

I. Introduction

The development of highly efficient solid-state lighting (SSL) devices with long lifetime is an important mission, considering that electric lighting in the European Union (EU) accounts for 19% of the total consumed electric power. Nitride-based LEDs have already proven their potential for use in SSL applications [1], [2]. Most commercially available white LEDs are based on a conversion of the light emitted by a blue LED into the yellow part of the visible spectrum by means of a phosphor. This conversion approach suffers from energy losses due to the absorption and reemission process (Stokes losses). Moreover, the emission spectrum and the lifetime of such devices depend mostly on the properties of the phosphor employed.

Higher efficiencies and better control on the emission spectrum can be obtained by using an RGB(Y) approach mixing the light from a red, green and blue LED (and eventually also a yellow one) integrated in a single LED chip. While highly efficient red and blue LEDs are available, green and yellow ones currently show much lower efficiencies. This is known as the "green gap".

The main difficulty for realizing green and yellow LEDs based on the InGaN/GaN material system is the need for very high In contents ($x_{In} \gtrsim 25\%$), leading to highly strained structures and to strong polarization fields. The latter in particular provokes strong quantum confined Stark effect (QCSE) and therefore a decrease in optical matrix elements.

One approach to mitigate the aforementioned problems is to employ band gap engineering techniques by growing structures with compositional grading. Appropriate gradual or step-wise changes in In content in such structures can be used to tune the band edge and strain profiles in order to optimize device performance in particular in terms of internal quantum efficiency (IQE). In addition, strain engineering by compositional grading should also improve crystal quality and In incorporation.

II. Simulation of graded single quantum wells

Using the TiberCAD software [3], [4] we performed a set of simulations of a InGaN/GaN p-i-n single quantum well (QW) structure with different gradings of In content to gain a qualitative insight into the effect of such techniques on wave function overlap and on IQE. The simulations are based on the self-consistent solution of the Poisson and the Schrödinger equations. The latter is formulated in the framework of the k·p theory using the envelope function approximation [5]. We assumed constant quasi Fermi levels for both electrons and holes, thus assuming perfect carrier injection into the QW. Based on the quantum mechanically corrected carrier densities, we calculated the recombination rates using the semiclassical expressions (assuming $n, p \gg n_i$):

$$R_{\mathrm{SRH}} = \frac{np}{\tau_{nr}(n+p)} \quad \text{Shockley-Read-Hall (SRH)} \quad (1)$$

$$R_{\mathrm{rad}} = Bnp \quad \text{radiative} \quad (2)$$

$$R_{\mathrm{Auger}} = C(n+p)np \quad \text{Auger} \quad (3)$$

For our simulations, we assumed $\tau_{nr} = 50$ ns (in the QW), $B = 4 \cdot 10^{-11}$ cm^3/s and $C = 3 \cdot 10^{-31}$ cm^6/s.

In Fig. 1 we show the self-consistent band edges, quasi Fermi levels and ground state energies for a rectangular QW and different grading profiles at a current density of 100 A/cm^2. The IQE has been calculated by $\int R_{\mathrm{rad}} / \int (R_{\mathrm{SRH}} + R_{\mathrm{rad}} + R_{\mathrm{Auger}})$ and is given in Fig. 2. Fig. 3 presents the ground state electron and hole wave functions and the overlap calculated as $\Gamma_{e-h} = \int \psi_e^* \psi_h \, \mathrm{d}V$, whereas in Fig. 4 we report the simulated recombination rates as obtained from (1)–(3).

The simulation results show that considerable improvement in wave function overlap can be obtained by grading the In composition in the QW. Moreover, the overlap seems to increase in presence of a step or peak in In concentration. For the given set of recombination parameters we observe a considerable decrease of Auger recombination with respect to the rectangular QW device, whereas radiative recombination increases due to increased overlap. Consequently, all grading approaches show substantial improvement in IQE.

Interestingly, a higher wave function overlap does not necessarily result in higher IQE. The linearly graded QW for example has approximately the same ground state overlap and the same amount of radiative recombination as the rectangular

978-1-61284-878-5/11/$26.00 ©2011 IEEE

QW. However, Auger recombination is substantially reduced due to a lowering of the peak hole density, leading to a symmetrization between hole and electron ground states.

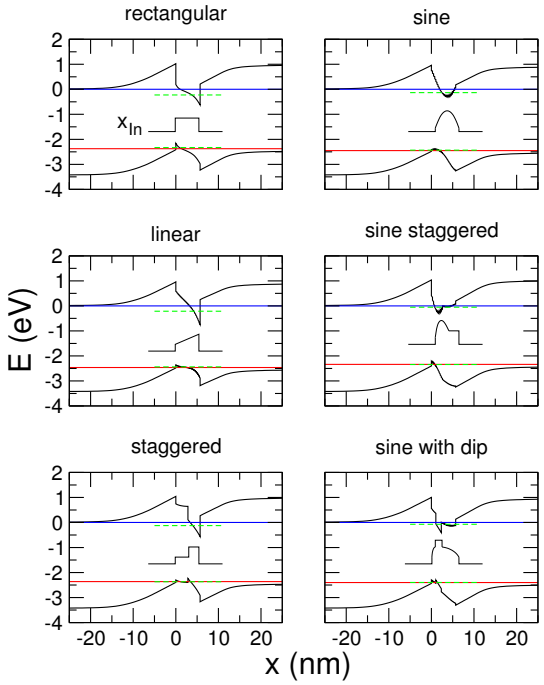

Fig. 1: Band profiles for a single quantum well without grading (rectangular QW) and with different types of compositional grading.

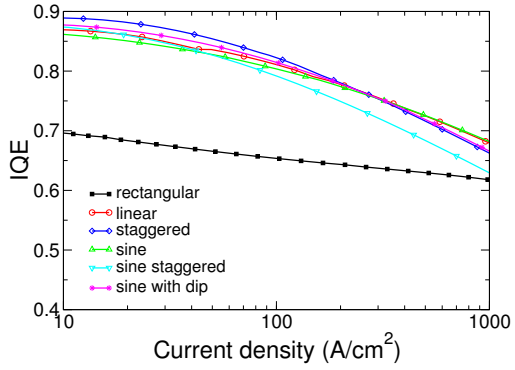

Fig. 2: The internal quantum efficiency (IQE) calculated from the semiclassical recombination rates.

References

[1] M. H. Crawford, "Leds for solid-state lighting: Performance challenges and recent advances," *IEEE J. Sel. Topics in Quantum Electr.*, vol. 15, no. 4, pp. 1028–1040, 2009.

[2] J. Wu, "When group-III nitrides go infrared: New properties and perspectives," *J. Appl. Phys.*, vol. 106, no. 1, 2009.

[3] TiberCAD simulation package, http://www.tibercad.org.

[4] M. Auf der Maur, F. Sacconi, G. Penazzi, G. Romano, M. Povolotskyi, A. Pecchia, and A. Di Carlo, "Concurrent multiscale simulation of electronic devices," *J. Comp. Elec.*, vol. 9, pp. 262 – 268, 2010.

[5] S. L. Chuang and C. Chang, "$\mathbf{k} \cdot \mathbf{p}$ method for strained wurtzite semiconductors," *Physical Review B*, vol. 54, pp. 2491–2504, 1996.

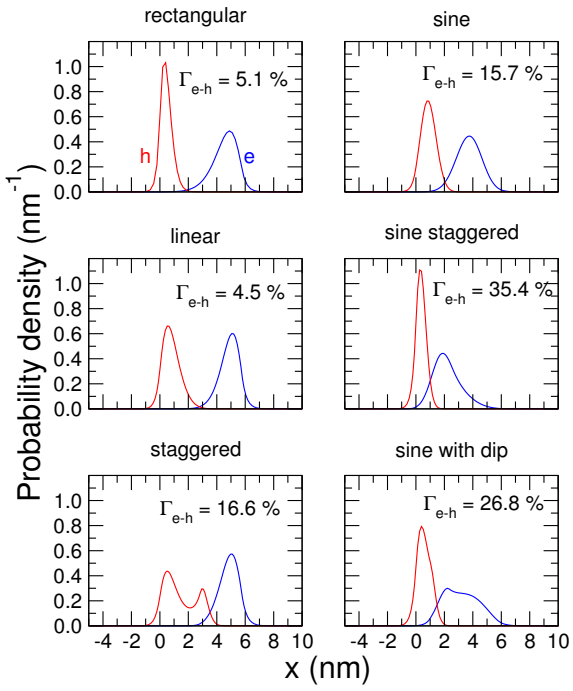

Fig. 3: Electron and hole ground state probability densities. The wave fucntion overlap is indicated for each grading profile.

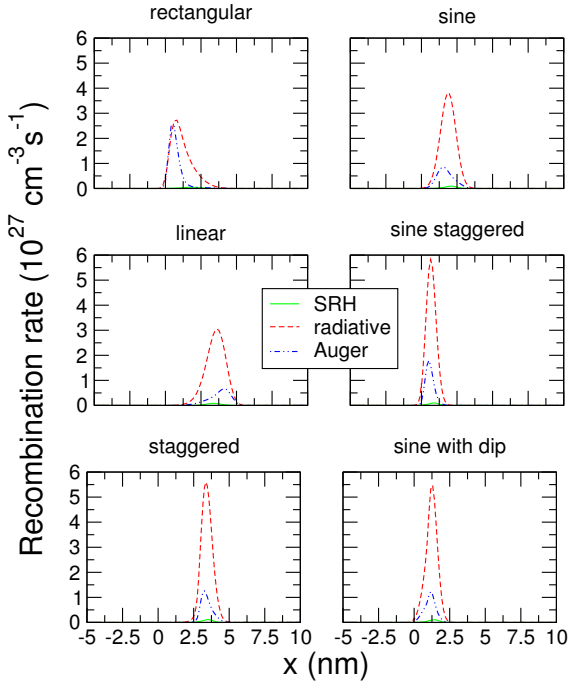

Fig. 4: Semiclassical recombination rates.