Nano-Scale Effects in GaN-based Light-Emitting Diodes

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ABSTRACT

We here investigate the effects of built-in polarization on the properties of non-symmetric InGaN quantum wells. The impact of these nano-scale effects on the performance of blue light emitting diodes is analyzed utilizing advanced numerical simulation.

Keywords: wurtzite semiconductors, GaN, light-emitting diodes, built-in polarization, InGaN quantum well, nano-photonics

1 INTRODUCTION

Breakthrough developments in nitride semiconductor technology have triggered a worldwide surge in research on GaN-based light emitting devices. Blue and green nitride light-emitting diodes (LEDs), for instance, enable more efficient and less costly full-color outdoor displays. Compact ultraviolet AlGaN/GaN light sources are currently under development for applications in solid-state lighting, short-range communication, and bio-chemical detection. GaN-based laser diodes have great potential in a number of applications such as optical data storage and printing.

Light is generated in these devices by spontaneous or stimulated recombination of quantum well electron-hole pairs. However, the nano-scale physics of recombination mechanisms in GaN-based quantum wells is still not fully understood. Polarization, quantum well non-uniformities, and exciton effects may have a major influence [1].

2 POLARIZATION

In c-face nitride materials, both spontaneous and piezoelectric polarization were found to be much stronger than in other III-V compounds [2]. Different alloy compositions show different polarization and net charges remain at the alloy interfaces. For ternary nitride alloys grown on GaN, Fig. 1 gives the net interface charge density as well as the resulting electrostatic field within the alloy. The built-in polarization field significantly affects the properties of quantum wells. The wider the quantum well, the more separated the electrons and holes, and the smaller the optical gain and spontaneous emission. The transition energy is reduced by the built-in field, leading to a red-shift of the emission wavelength. However, with increasing carrier injection into the quantum well, charge screening is expected to reduce polarization field effects.

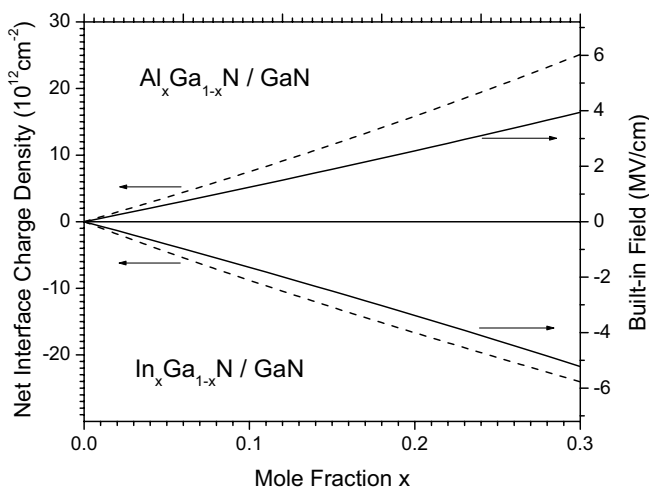

Fig. 1: Density of interface polarization charges (dashed) and resulting electrostatic field (solid) for ternary alloys grown on GaN [2].

3 DEVICE

As a practical example, we here investigate single-quantum-well blue light-emitting diodes as described in [3]. These devices exhibit an output power of 4.8 mW at 20 mA injection current and 3.1 V forward voltage. The low voltage results in a relatively high power efficiency of 7.7% (ratio of light power to electrical power). The external quantum efficiency is as high as 8.7% despite a large dislocation density. Fluctuations of the Indium composition within the InGaN quantum well are assumed to localize carriers in radiative centers and to prevent them from recombining nonradiatively at dislocations [1]. The device was grown by metal organic chemical vapor deposition (MOCVD) on c-face sapphire. Layer sequence and band diagram are shown in

Fig. 2. The 2-nm-thick strained $In_{0.2}Ga_{0.8}N$ quantum well is sandwiched between n-InGaN and p-AlGaN barriers. The p-barrier acts as blocking layer in order to reduce electron leakage from the quantum well into the p-doped regions.

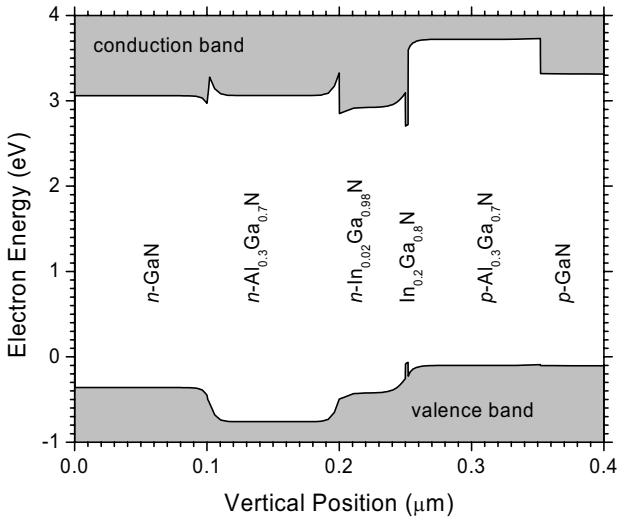

Fig. 2: Energy band diagram of our LED.

4 MODEL

In order to simulate nano-scale effects in the InGaN quantum well and their impact on the device performance, we here employ the simulation software APSYS which self-consistently includes drift and diffusion of electrons and holes, built-in polarization and thermionic emission at hetero-interfaces, as well as spontaneous and defect related recombination of carriers within the quantum well. The polarization charges are considered partially screened by charged interface defects so that only half of them contribute to the built-in polarization field [4]. Schrodinger and Poisson equations are solved iteratively in order to account for the quantum well deformation with changing device bias. Spontaneous emission of photons by electron-hole recombination within the quantum well is calculated using a free-carrier model and assuming non-parabolic valence bands. In the quasi three-dimensional simulation of the LED, current crowding and self-heating effects are taken into account. Further details of the model as well as a discussion of material parameters can be found elsewhere [5].

5 QUANTUM WELL

The effect of the net polarization charges on the quantum well is shown in Fig. 3 including screening by free carriers. Without polarization, the internal electrical field of the pn-junction is positive and the holes accumulate at the p-side of the quantum well. With polarization, the electrical field is strongly negative within the quantum well and the holes accumulate at the n-side. In both cases, the peak of the electron distribution is near the center of the quantum well. Due to the more non-symmetric quantum barriers, there are less confined electrons without polarization. Built-in polarization allows for more quantum levels.

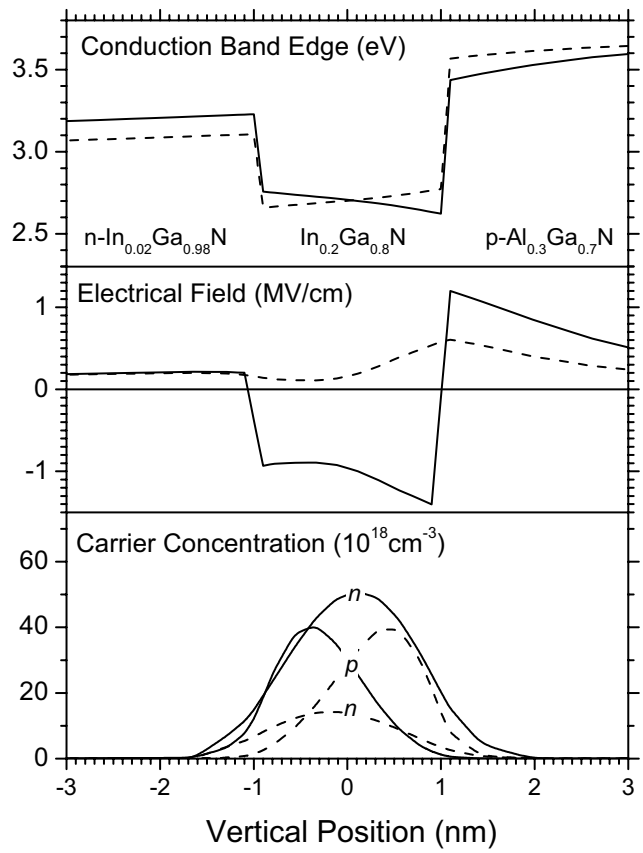

Fig. 3: Conduction band edge, internal electrical field, and carrier profiles with (solid) and without (dashed) built-in polarization for our non-symmetric LED quantum well.

6 EMISSION SPECTRUM

Calculated LED spectra exhibit a significant reduction of the peak emission intensity due to the polarization field (Fig. 4). These spectra represent the radiation from the entire device including current crowding and self-heating. The maximum temperature increase of about 80 K is observed at the edge of the device where the current crowding is strongest. Lorentzian broadening with an intraband scattering time of 0.1 ps gives a full-width at half-maximum (FWHM) of 17 nm for the spectrum without

polarization. Due to the additional confined quantum states, built-in polarization results in a broader line shape with FWHM = 26 nm. This result is close to the measured line broadening of 25 nm [3]. Uniform current injection at room temperature gives smaller FWHM values in both cases [5]. Built-in polarization red-shifts the emission peak by only 3 nm due to the opposite tilt of the quantum well in both cases (cf. Fig. 3).

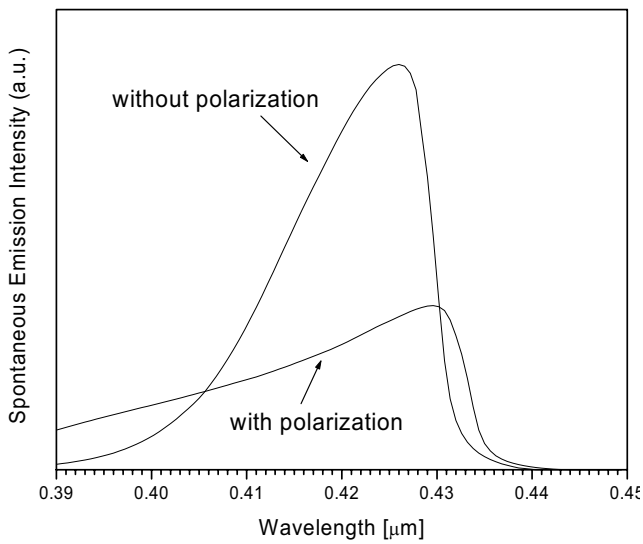

Fig. 4: Emission spectrum calculated with and without polarization charges.

7 LIGHT POWER

The light power generated inside the LED is plotted in Fig. 5 as function of the injection current. It is strongly affected by the non-radiative carrier lifetime τ_{SRH} inside the quantum well. This number is unknown for our device but it is typically considered to be on the order of a few nanoseconds. We therefore show the results for two different lifetimes (solid and dotted curves), illustrating the strong impact of this parameter. With τ_{SRH} = 5ns, the maximum internal quantum efficiency is η_{int} = 48% while τ_{SRH}= 1ns results in η_{int} = 22%. Without built-in polarization, the LED would emit a significantly higher light power with η_{int} = 78% (dashed line in Fig. 5) due to the better overlap of electron and hole wave function within the quantum well (Fig. 3) and the correspondingly higher spontaneous recombination rate (Fig. 4).

The measured light emission is much lower due to inefficient light extraction from the LED. Most of the photons emitted from the quantum well are unable to leave the device due to total internal reflection. For τ_{SRH} = 5ns, the measured external efficiency of 8.7% gives a light extraction efficiency of η_{opt} = 18% for this example device.

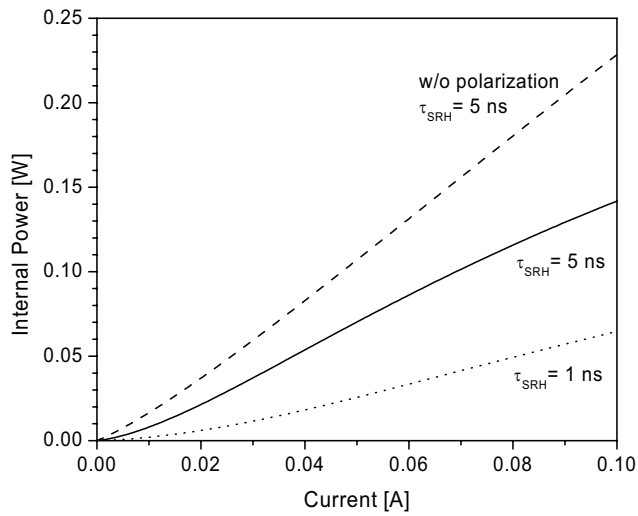

Fig. 5: Calculated internal LED light power vs. injection current for a 300μm x 300μm device (with polarization: solid and dotted lines, without polarization: dashed line, τ_{SRH} gives the non-radiative carrier lifetime within the quantum well).

8 CONCLUSION

Utilizing self-consistent numerical simulation, we were able to demonstrate the strong effect of built-in quantum well polarization on LED characteristics.

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