Polarization-Doped AlGaN Light-Emitting Diode

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Abstract – **The development and application of nitride-based light-emitting diodes is handicapped by the low hole conductivity of Mg-doped layers. Mg-doping becomes increasingly difficult with shorter LED wavelength and higher Al-content of the p-AlGaN layers. As an alternative, polarization-induced hole doping in N-face graded AlGaN was recently demonstrated. Using advanced numerical device simulation, we show that the internal quantum efficiency can be strongly increased and the efficiency droop eliminated by using such graded AlGaN layer instead of the traditional AlGaN electron-blocker layer (EBL).**

I. INTRODUCTION

(Al)GaN-based light-emitting diodes (LEDs) are currently of great interest for applications in lighting, sensing, biotechnology, medical instrumentation and other areas. However, the development of nitride-based LEDs is handicapped by the low electrical conductivity of p-doped material. Heavy Mg doping is required to achieve a sufficient density of free holes, which lowers the hole mobility. P-doping becomes increasingly difficult with shorter LED wavelength and correspondingly higher Aluminium content of the p-AlGaN layers.

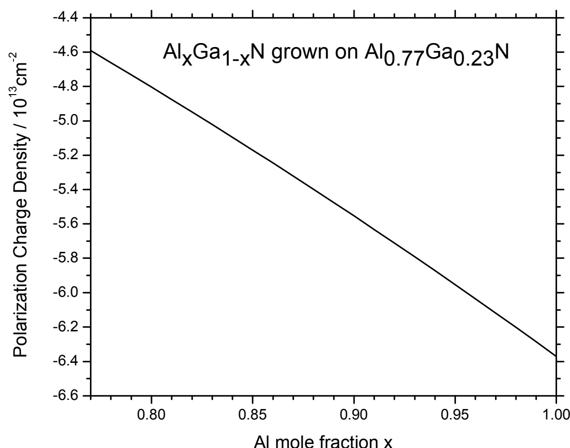

Fig. 1: Two-dimensional (2D) interface polarization charge density of $Al_xGa_{1-x}N$ grown on $Al_{0.77}Ga_{0.23}N$.[1] The bulk charge density of a linearly graded layer is the difference of the values at the end and the start mole fraction, divided by the layer thickness.

As an alternative, polarization-induced hole doping of graded N-face p-AlGaN layers and pn-junctions was recently demonstrated.[2] Significant built-in polarization charges are known to occur at all hetero-interfaces of nitride-based devices. The reason is the high spontaneous and strain-induced polarization in nitride semiconductor materials, which depends on the material composition (Fig. 1). By continuously grading this composition, fixed bulk polarization charges can be generated. In the case of AlGaN, a rising Al mole fraction raises the electron band gap energy. In order to enhance hole injection through the graded AlGaN layer into the active region, the Al mole fraction should therefore be lowest near the active region. However, the typical Ga-face growth process of nitride structures generates a positive polarization charge within such graded AlGaN layer, which does not attract free holes. Thus, N-face growth must be utilized to generate negative bulk charges in the graded AlGaN layer.[3]

This paper investigates the effect of such N-face graded AlGaN layer on the performance of ultra-violet (UV) LEDs. Advanced device simulation software is used as main tool of this investigation.[4]

II. MODELS AND PARAMETERS

The LED simulation self-consistently solves the semiconductor carrier transport equations, coupled to the photon emission from the strained AlGaN quantum wells. Schrödinger and Poisson equations are solved iteratively in order to account for the quantum well deformation with changing device bias (quantum-confined Stark effect). The transport model includes drift and diffusion of electrons and holes, Fermi statistics, built-in polarization and thermionic emission at hetero-interfaces, as well as non-radiative recombination of carriers. The built-in polarization charge density is calculated using the Bernardini model (cf. Fig. 1).[1] The Si donor activation energy is 20meV. The Mg acceptor activation energy varies linearly with the AlGaN composition, it is 170meV for GaN and 470meV for AlN. The acceptor density is often lower than the Mg density and we only consider the acceptor density N_A in the following. Field ionization of acceptors based on the Poole-Frenkel model is included in the simulation but it does not have a significant effect. The carrier mobility strongly depends on composition and doping. The exact value of the mobility is hard to predict, especially for holes. For simplicity, we here employ a constant mobility of 5 cm^2/Vs for holes and 100 cm^2/Vs for electrons. The unstrained room-temperature $Al_xGa_{1-x}N$ energy band gap is calculated using

$$E_g(x) = x\, E_{AlN} + (1-x)\, E_{GaN} - x\,(1-x)\, E_{bow} \qquad (1)$$

with E_{AlN} = 6.28eV, E_{GaN} = 3.42eV, and E_{bow} = 0.7eV. The AlGaN band offset ratio is $\Delta E_c{:}\Delta E_v$ = 50:50.[5]

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Photon extraction from the LED chip and LED self-heating are neglected in this study since we analyze internal mechanisms in pulsed operation. Further details on models and parameters can be found elsewhere.[6]

III. SIMULATION RESULTS

As UV LED example, we investigate a recently published device structure with three 1.5-nm-thick undoped $Al_{0.62}Ga_{0.38}N$ quantum wells (QWs) separated by 6-nm-thick undoped $Al_{0.77}Ga_{0.23}N$ barriers and emitting at 250nm wavelength.[7] The active region is grown on a 2-µm-thick Si-doped $Al_{0.77}Ga_{0.23}N$ buffer layer. Correspondingly, the lattice constant considered in the calculation is a = 3.13 Å for the entire structure. In this Ga-face reference device, the p-side QW is covered by a 25-nm-thick undoped $Al_{0.77}Ga_{0.23}N$ barrier, a 25-nm-thick Mg-doped $Al_{0.95}Ga_{0.05}N$ electron-blocker layer (EBL), and a Mg-doped $Al_{0.77}Ga_{0.23}N$ cladding layer. Figure 2 shows the energy band diagram of the reference structure at $j=170A/cm^2$ current density. Due to the Ga-face growth, the n-side QW interfaces exhibit a negative polarization charge while the p-side QW interface is positively charged, thereby enhancing the escape of electrons from the QW toward the p-side. The electron leakage to the p-side is somewhat hindered by the EBL energy barrier, but this barrier is strongly reduced by positive interface polarization charges (Fig. 2). In the reference simulation, about 60% of the electrons leak across the EBL and prevent the same percentage of holes injected at the p-contact from reaching the active layers. The calculated internal quantum efficiency (IQE) is below 40% and it peaks at $j=20A/cm^2$, in good agreement with the measurement.[7]

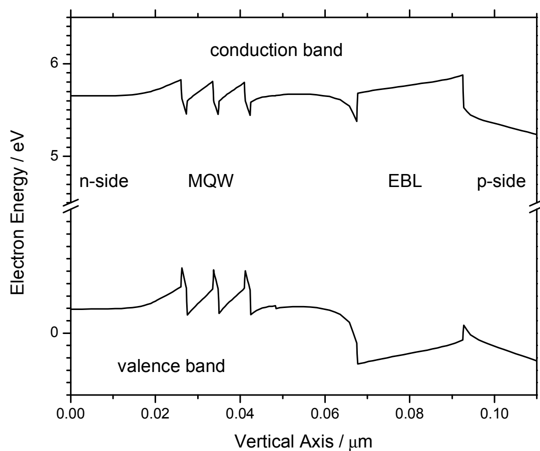

Fig. 2: Energy band diagram of the Ga-face reference LED ($j=170A/cm^2$).

Figure 3 shows the energy band diagram for the same LED structure but grown on an N-face and with the Mg-doped layers replaced by a graded $Al_xGa_{1-x}N$ layer (x=0.77-0.95). The negative bulk polarization charge density of the graded layer is $2.7x10^{18}cm^{-3}$ (cf. Fig. 1) leading to a similarly high density of free holes, even with a much lower acceptor density (Fig. 4). The reversed polarization of the quantum wells seems to block electrons from leaking into the p-side. Compared to the Ga-face reference device, the calculated electron leakage current is strongly reduced, mainly by the increasing energy band gap of the graded layer. The IQE is doubled and the efficiency droop is eliminated. However, the long non-radiative carrier lifetime of 100ns assumed in this simulation is likely to underestimate non-radiative recombination losses, so that the absolute IQE is probably lower in both cases.

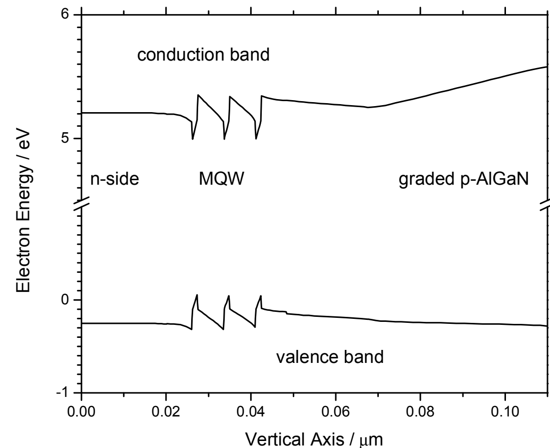

Fig. 3: Energy band diagram of the N-face LED with linearly graded AlGaN layer on the p-side ($j=170A/cm^2$).

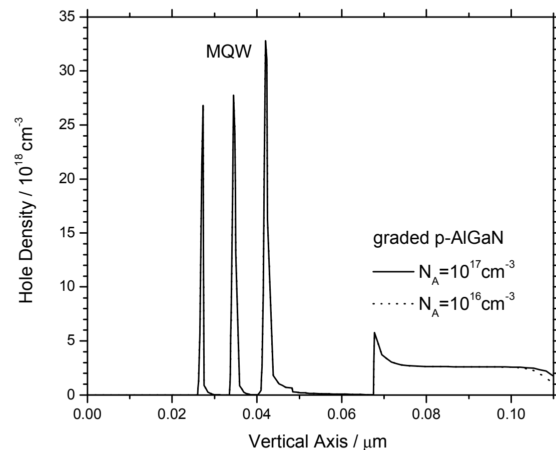

Fig. 4: Hole density profile with different acceptor densities N_A ($j=170A/cm^2$).

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