

# Drift-Diffusion and Ballistic Transport Modeling in III-Nitride Multiple-QW Light Emitting Structures

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**Abstract:** We present the first attempt of charge carrier transport modeling in III-nitride multiple-QW light-emitting diode structures which takes into consideration ballistic overshoot of the device active region. For the purpose of this study, the drift-diffusion based Transport module of our software package has been complemented by a simple model of ballistic carrier transport which proved to be essential for device output characteristics. We demonstrate strong inhomogeneity of the carrier injection into optically active quantum wells of polar and nonpolar III-nitride structures and show that carrier leakage is dominated by ballistic overshoot of the device active region

**Keywords:** Optoelectronics, laser diodes, light-emitting diodes, nitrides, III-V compounds.

## 1. Introduction

Modeling software package developed at Ostendo Technologies for analysis and design of semiconductor light-emitting devices [1-3] includes four basic software blocks or modules addressing, correspondingly, the physics in microscopic active regions, the transport in the diode structure, the optical waveguiding, the thermal management and the database of material parameters as illustrated in Figure 1.

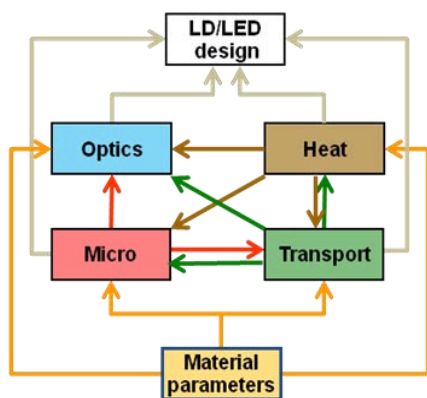
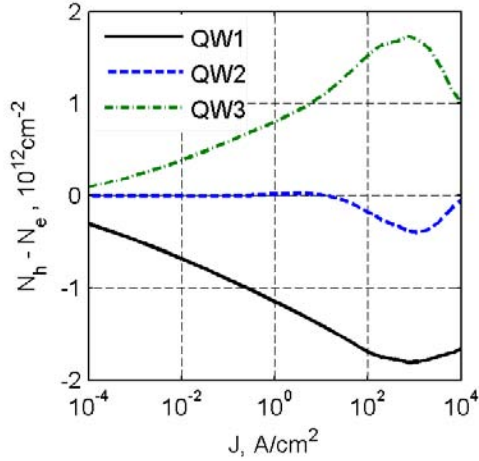


Figure 1. Flowchart of device modeling stages.

In this work we present the further development of our Transport module [3]. The module has been complemented with simple phenomenological description of ballistic overshoot effect assuming constant overshoot velocity and spatially distributed relaxation of quasi-ballistic electrons back into the drift-diffusion subsystem with uniform effective relaxation time. The purpose of the work is to study and understand the main physical reasons underlying the degradation of the external efficiency of III-nitride light emitting structures which impedes the advance of laser diodes (LD) and light emitting diodes (LED) in visible range of optical emission. Ballistic effects in the electron transport were recently suggested as the main source of efficiency degradation in III-nitride LEDs [4]. Our modeling results unambiguously support this suggestion.

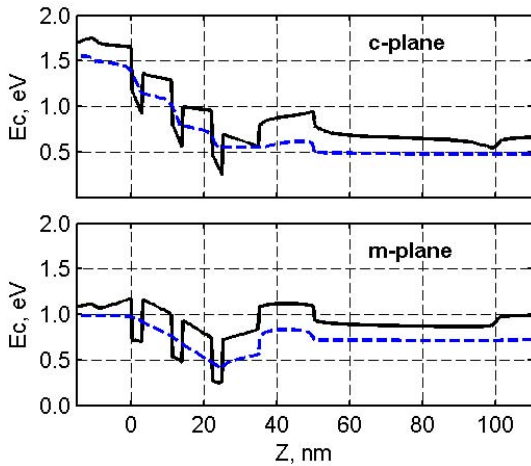
## 2. Electrical inhomogeneity of LD/LED active region

In polar III-nitride heterostructures, polarization-induced interface charges strongly affect electrical homogeneity of the active region, giving rise to high internal potential barriers and excessive potential drop. Nonpolar multiple-QW structures equally suffer from inhomogeneous population of the active QWs and resulting large QW residual charges which support qualitatively the same potential profile as in polar structures [5]. Fig. 2 shows injection dependence of the residual QW concentrations in three-QW nonpolar structure. The model used for calculation and structure parameters are detailed in work [5] and COMSOL presentations [2,3]. Fig. 3 compares conduction band potential profiles in polar (c-plane) and nonpolar (m-plane) structures of the same design with three 3nm QWs in the active region. Opposite charges of extreme n-side QW1 and extreme p-side QW3 in nonpolar structure act in similar way as the built-in interface polarization charges in polar structure. In both types of structures, the highest



**Figure 2.** Residual QW charge concentrations in 3-QW nonpolar diode structure; QWs are numbered starting from the diode n-side.

point of the potential profile is located in the vicinity of the negatively charged QW1 so that the strong built-in electric field in the narrow active region provides the necessary condition for the active region ballistic overshoot.

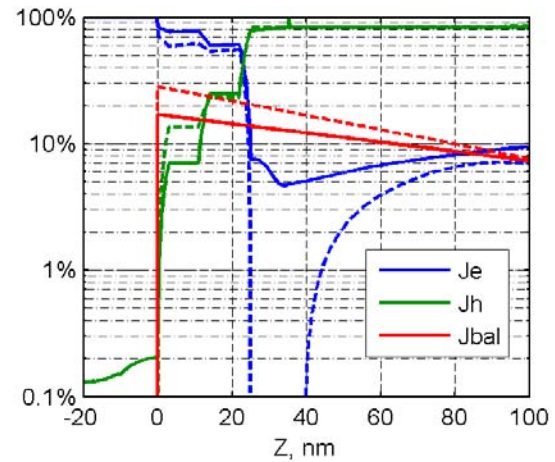


**Figure 3.** Active region electrical inhomogeneity in polar and nonpolar structures at moderate injection level  $1 \text{ kA/cm}^2$ . Dashed lines indicate position of the electron quasi-Fermi level for drift-diffusion carrier subsystem. Point  $Z=100 \text{ nm}$  corresponds to the p-cladding interface position.

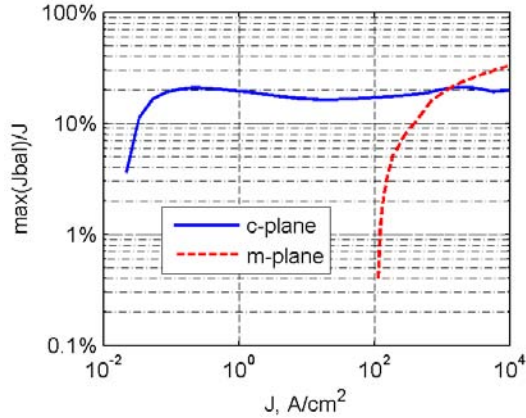
### 3. Active region ballistic overshoot and LD/LED injection characteristics

Our model of ballistic overshoot effect assumes distributed relaxation of quasi-ballistic electrons overflowing the active region back into the drift-diffusion carrier subsystem. Unusual bulge of the quasi-Fermi level in the region of electron blocking layer (EBL) in Fig. 3 reveals the reaction of the drift-diffusion subsystem to the inflow of ballistic carriers. Without ballistic current, quasi-Fermi level always decreases monotonically throughout the structure [3]. Fig 4 shows the spatial distribution of drift-diffusion ( $J_e$ ,  $J_h$ ) and ballistic ( $J_{bal}$ ) current components at total injection of  $10 \text{ kA/cm}^2$ . Transport modeling without ballistic effects would reveal twice as low electronic leakage in polar structure and indiscernible on this plot scale leakage in nonpolar one. This huge difference in polar and nonpolar leakage is completely eliminated by ballistic overflow effect which makes the high-injection leakage in both types of structures comparable; see Fig. 4.

As can be readily seen from Fig. 3, due to the presence of interface polarization charges, potential profile in polar structure is steeper so that the ballistic effects come into play at much lower injection levels.



**Figure 4.** Spatial distribution of injection current components in polar (solid lines) and nonpolar (dashed lines) 3-QW structures of Fig. 2 at high injection level  $10 \text{ kA/cm}^2$ . In structures of both types the electron leakage reaches 10% level at p-cladding interface.



**Figure 5.** Peak value of ballistic current component in polar and nonpolar structures vs. the injection level.

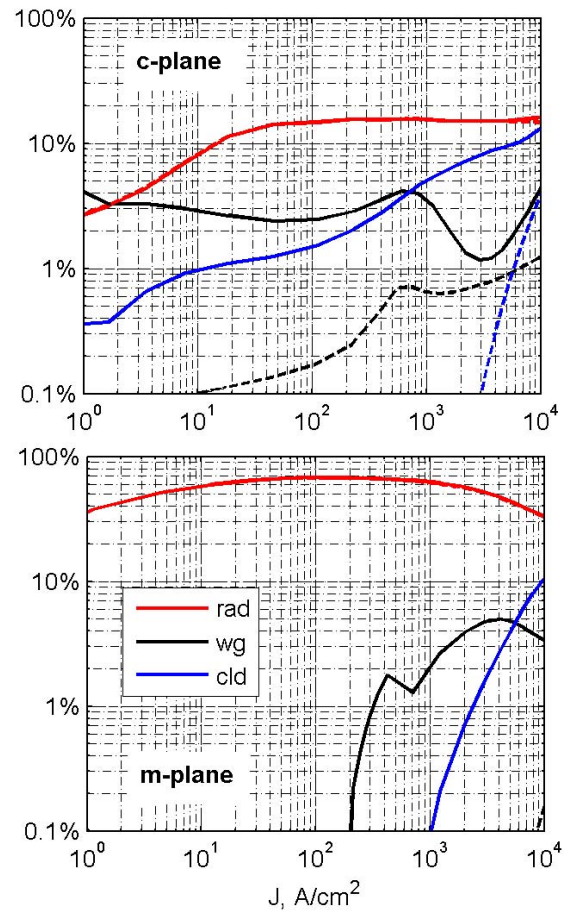
Fig. 5 demonstrates the difference in ballistic characteristics of polar and nonpolar structures at low injection. Since the ballistic current dominates the electron spill-over, this difference naturally explains more stronger efficiency deterioration (efficiency droop) in polar LEDs vs. more stable performance of nonpolar structures observed experimentally [6]. Similarly, the sharp raise of the ballistic component in nonpolar structure at higher injection levels can help understand why, for instance, green laser diodes were implemented practically simultaneously on both polar and nonpolar templates without any substantial advantage of the later.

Fig. 6 compares the injection characteristics in polar and nonpolar structures. P-cladding leakage (cld lines) and waveguide recombination loss (wg lines) are presented as the percentage of the total injection current. In both types of structures, these characteristics are dominated by ballistic overshoot effect though in polar structure (upper panel) noticeable drift-diffusion part is also present, especially at the highest injection levels (dashed curves). In nonpolar structure, EBL is more efficient and drift-diffusion electron leakage is practically nonexistent up to 10 kA/cm<sup>2</sup>.

Electron spill-over due to the active region ballistic overshoot increases the electron concentration in p-waveguide and p-cladding layers. Without ballistic effects, Fermi level position in Fig. 2 is located deeper in band gap of those layers. Dark black curves (wg) in Fig. 5

display the nonradiative recombination losses in the waveguide which are predominantly originated in the p-side waveguide layer next to EBL. Once again, this loss is mostly induced by the ballistic overshoot current; compare solid and dashed curves for polar structure (upper panel) and note a negligible waveguide losses predicted by pure drift-diffusion approximation for nonpolar one (lower panel).

Upper curves (rad) in Fig. 6 present the internal radiative efficiency of active QWs i.e. the ratio of radiative and total QW recombination



**Figure 6.** Electron leakage into p-cladding (cld), waveguide recombination loss (wg) and QW radiative efficiency (rad) in polar and nonpolar structures. Dashed lines indicate waveguide and cladding loss calculated in pure drift-diffusion approximation without ballistic overshoot; for nonpolar structure (lower panel) these curves are located well below the plot scale limits.

currents. QW radiative efficiency remains essentially unchanged with introduction of the ballistic carrier subsystem into transport description which means that QW populations in our structures were unaffected by the active region ballistic overshoot.

#### 4. Conclusions

COMSOL Multiphysics make possible creating flexible and yet comprehensive physical models facilitating the design of the most complicated optoelectronic devices. In this work we provide a brief description of full-scale modeling of the injection efficiency of III-nitride based multi-QW polar and nonpolar light-emitting structures. Our updated Transport module takes into account both drift-diffusion and ballistic current components. In this first simulation we show that due to inherently high electrical inhomogeneity of III-nitride MQW structures the active region ballistic overshoot effect is one of the major factors limiting the injection characteristics of III-nitride light emitting devices.

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