Subthreshold characteristics of GaN-based LEDs: trap-assisted tunneling and coupled defects

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Subthreshold characteristics of GaN-based LEDs: trap-assisted tunneling and coupled defects

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***Abstract*—The presence of defects in GaN-based LEDs is frequently associated with the efficiency droop. It is therefore interesting to study the sub-threshold diode current, where non-radiative recombination effects appear more evident. In this work, we reproduce the high ideality factors observed in the I-V characteristics of GaN-based LEDs by means of a quantum-corrected drift-diffusion model based on the solution of the Schrödinger equation. Our results indicate that, in highly defective structures, the anomalous characteristics cannot be entirely attributed to trap-assisted tunneling as previously assumed. We conclude that the unexpectedly large ideality factors observed in GaN-based LEDs can be explained by extending the conventional theory of SRH theory of isolated recombination centers to the case of coupled defects.**

***Index Terms*—GaN-based LEDs, trap-assisted tunneling, coupled defect-level recombination.**

I. Introduction

GaN-based LEDs have emerged as the most popular technology for high efficiency solid-state lighting. One of the most significant and long-lasting challenges facing high-power GaN-based LEDs is the efficiency droop, *i.e.,* the decline of the quantum efficiency with increasing current and temperature [1], [2]. As droop has been correlated with the presence of defects, understanding and modeling these nonradiative recombination channels is crucial for the optimization of the device performance. The impact of defects appears more prominent in the subthreshold regime, below the optical turn-on of the diode, where ideality factors larger than two are typically observed. Such deviations from ideal I-V characteristics are considered the fingerprint of trap-assisted tunneling (TAT). TAT is usually described within the conventional Shockley-Read-Hall (SRH) theory by means of field-enhanced lifetimes within the drift-diffusion (DD) formalism [3]. While this approach may successfully reproduce experimental results, the somewhat arbitrary fitting of the model parameters, *e.g.*, the tunneling mass, raises the question whether the agreement with experiments is obtained by capturing the correct physics or simply by overfitting. In this work, by using a DD model complemented with a rigorous description of the local density of states (LDOS), we show that in some structures, the large ideality factors cannot be entirely attributed to TAT. Moreover, the possibility of interactions between defects cannot be neglected when their distance is comparable to the tunneling path length. Inspired by previous work on silicon solar cells, we extend the conventional single-level SRH formalism to include transitions between trap levels [4]. Our results show that the inclusion of a deep donor-acceptor-pair (DAP) recombination process reproduces the experimental results with a limited set of fitting parameters, namely the SRH lifetimes of the defects and their coupling rate.

II. Model

Quantum corrections can be introduced in DD models by means of different techniques: the density gradient approximation [5], the landscape localization formalism [6] or the Poisson-Schrödinger approach [7]. All these methods share the same idea of finding an effective potential to correct the band diagram. The resulting effective band diagram appears as a smoothed version of the original one, with the effective potential raising the dips of the band edges to describe quantization effects and lowering the barriers to account for tunneling. In this work, we find the quantum potential from the LDOS of the nanostructure computed from the solution of Schrödinger equation [7]. Nonequilibrium Green's function (NEGF) calculations show that TAT can be reproduced within a DD framework by replacing the classical charge in the conventional Shockley-Read-Hall theory with the correct quantum charge [8]. However, even in the presence of strong band bending, such field-enhanced SRH recombination cannot explain ideality factors greater than six. Therefore, we extend the conventional SRH theory of isolated defects to consider coupled defects. We assume two interacting levels, the upper level mainly exchanging charges with the conduction band, while the lower level is mainly coupled with the valence band, *i.e.*, a donor-acceptor pair. If the recombination rate is limited by the coupling rate, an intrinsic saturation effect occurs, leading to a significant increase of the ideality factor. Solving the rate equations in this case yields the recombination rate [9]:

$$R = R_{12} - \sqrt{R_{12}^2 - \frac{np - n_i^2}{\tau_{n1}\tau_{p2}(1-\epsilon)}}, \qquad (1)$$

with

$$R_{12} = \frac{(n+n_1)(p+p_2)}{2r_{12}\tau_{n1}\tau_{p2}(1-\epsilon)} + \frac{\tau_{n1}(p+p_1)+\tau_{p2}(n+n_2)}{2\tau_{n1}\tau_{p2}(1-\epsilon)}, \qquad (2)$$

where r_{12} is the coupling rate between the levels, $\epsilon = \exp\left(-|E_{\mathrm{trap},2} - E_{\mathrm{trap},1}|/V_{\mathrm{T}}\right)$, $E_{\mathrm{trap},1,2}$ are the trap energy levels measured with respect to the intrinsic Fermi level, and

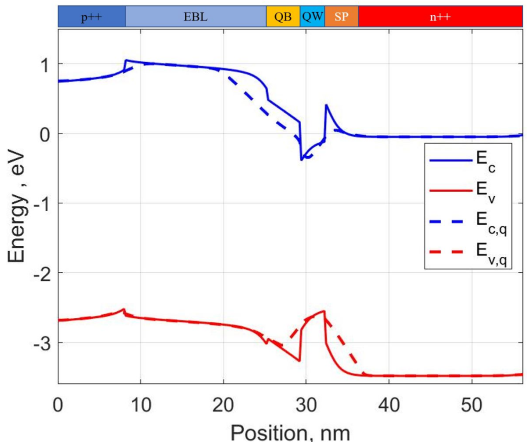

Fig. 1. Band diagram of the LED under study computed at 2.6 V without (solid lines) and with (dashed lines) quantum corrections.

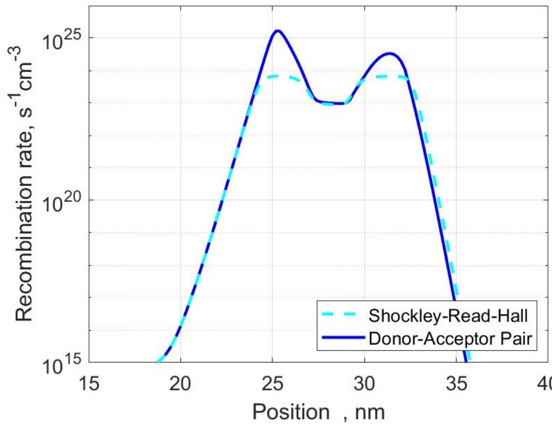

Fig. 2. Trap-assisted recombination rates computed at 2.6 V with the single-level SRH and DAP models. For comparison, in both models, the trap levels are assumed near midgap with the same lifetime of 10^{-12} s for both electrons and holes. The inter-level recombination in the DAP model has been selected as $r_{12} = 7 \times 10^{23}\ \mathrm{s}^{-1}\ \mathrm{cm}^{-3}$.

$\tau_{\mathrm{n}1,2}$, $\tau_{\mathrm{p}1,2}$ are the electron and hole lifetimes, which depend on the capture cross section and density of the defects.

III. Results

The structure under study is a single-quantum-well LED, indicated as device B1 in [10]. Fig. 1 shows the band diagram of the structure at 2.6 V. Notice that in the active region, the effective band edges $E_{\mathrm{c,q}}$, $E_{\mathrm{v,q}}$ (dashed lines) are significantly below E_{c}, E_{v} (solid lines), indicating the presence of tail states, which may partecipate in the tunneling process. This effect is more prominent in the conduction band than in the valence band due to the lower electron effective mass. Fig. 2 reports a magnification, in the active region, of the recombination rates computed at 2.6 V with the conventional SRH and the DAP model. Two recombination peaks can be noticed, one at the EBL/QB interface and one at the spacer/QW interface. These are the regions where TAT is more effective since there are more tail states available for tunnelling. The two models behave very similarly when the recombination rates are lower than r_{12} (the isolated defects are described by the same parameters of the coupled defects). However, once the recombination rate reaches approximately $7 \times 10^{23}\,\mathrm{s}^{-1}\mathrm{cm}^{-3}$, the DAP recombination rate saturates. This is due to the recombination channel being limited by the inter-level coupling rate r_{12}, which does not allow the recombination to grow further leading to the saturation of the current. Finally, Fig. 3 compares the I-V characteristics of the device computed with the single-level SRH recombination rate and the DAP model. At low voltages, both curves exhibit the same behaviour, with ideality factors around six. However, at higher voltages, where the recombination rate reaches r_{12}, notable differences arise. The current density computed with the single-level SRH model continues to increase uniformly until radiative recombination dominates around 2.5 V. In contrast, the current obtained with the DAP model exhibits slower growth after 2 V due to recombination channel saturation, resulting in an increased ideality factor in agreement with experiments.

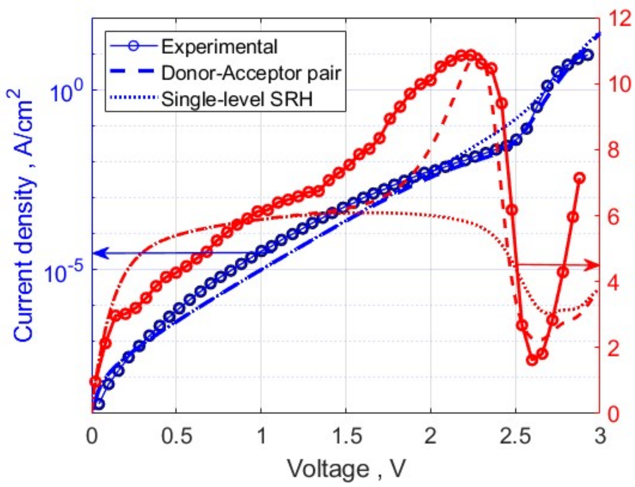

Fig. 3. I-V characteristics (blue curves, left axis) and ideality factors (red curves, right axis) computed with the single-level SRH (dotted line) and DAP (dashed line) model. Experimental results (circles) are from [10].

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