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Impact of random alloy fluctuations on the carrier distribution in multi-color (In,Ga)N/GaN quantum well systems

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The efficiency of (In,Ga)N-based light emitting diodes (LEDs) is limited by the failure of holes to evenly distribute across the (In,Ga)N/GaN multi-quantum well stack which forms the active region. To tackle this problem, it is important to understand carrier transport in these alloys. In this work, we study the impact that random alloy fluctuations have on the distribution of electrons and holes in such devices. To do so, an atomistic tight-binding model is employed to account for alloy fluctuations on a microscopic level and the resulting tight-binding energy landscape forms input to a quantum corrected drift-diffusion model. Here, quantum corrections are introduced via localization landscape theory. Similar to experimental studies in the literature, we have focused on a multi-quantum well system where two of the three wells have the same In content while the third well differs in In content. By changing the order of wells in this ‘multi-color’ quantum well structure and looking at the relative radiative recombination rates of the different emitted wavelengths, we (i) gain insight into the distribution of carriers in such a system and (ii) can compare our findings to trends observed in experiment. We focus on three factors and evaluate the impact that each have on carrier distribution: an electron blocking layer, quantum corrections and random alloy fluctuations. We find that the electron blocking layer is of secondary importance. However, in order to recover experimentally observed features – namely that the *p*-side quantum well dominates the light emission – both quantum corrections *and* random alloy fluctuations should be considered. The widely assumed homogeneous virtual crystal approximation fails to capture the characteristic light emission distribution across a multi-quantum well stack.

I. INTRODUCTION

At the heart of modern light emitting diodes (LEDs) operating in the blue to violet spectral region are (In,Ga)N/GaN multi-quantum well (MQW) systems [1]. While the efficiency of these LEDs is and can be high, pushing the emission to longer visible wavelengths (with higher InN content), or to ultra-violet wavelengths (with (Al,Ga)N alloys) provides technological challenges [2, 3]. In general, understanding the carrier distribution can help to guide maximizing the efficiency in an LED, since ideally the carriers shall be distributed evenly across the entire MQW region so that all QWs will contribute to emission [4]. However, previous experimental studies on carrier distribution in (In,Ga)N/GaN MQW systems have indicated that mainly the well closest to the *p*-doped contact side contributes to the light emission process [4–7]. These samples were specifically designed to gain insight into the carrier distribution inside the active region of an LED. Overall, this has been attributed to a sequential filling of the QWs, resulting in a high hole density only in the *p*-side QW. To establish accurate carrier transport models the trends found in the experimental studies of Refs. [4–7] need to be predicted, without introducing extra free parameters to simulation models.

Widely used 1-D simulation methods employing a Schrödinger-Poisson-drift-diffusion approach – the

workhorse of many commercial software packages – fail to predict the poor hole distribution across an (In,Ga)N MQW region [8]. Previous theoretical studies have reproduced the experimentally observed behaviour, however this required (i) treating bound carriers in a quantum mechanical picture, (ii) softening of the QW barrier interface to account for tunneling effects, (iii) distinguishing between continuum and bound carriers in the carrier transport model (multi-population model), and (iv) allowing for scattering between the different populations [8]. But, the impact of alloy disorder is basically neglected in this advanced but also complex carrier transport model.

Alloy disorder impacts different materials in different manners. For example, dilute nitride alloys like Ga(As,N) result in a modification of the conduction band, as the nitrogen introduces states above the conduction band edge of GaAs. This leads to hybridization with the conduction band edge, and leads to an unusual band evolution with nitrogen content [9]. Similarly, disorder in (Ga,In)P impacts primarily the conduction band edge [10–12]. On the other hand, disorder in III-N materials such as (In,Ga)N results in a modification of states in the *valence band* [13, 14]. This results in carrier localization, particularly for holes, in (In,Ga)N alloys.

Experimental and theoretical studies on the electronic [15–17] and optical [18, 19] properties of (In,Ga)N systems have already revealed that these properties are

significantly impacted by alloy fluctuation induced carrier localization effects. However, the impact of alloy disorder on the carrier transport has only been targeted recently [20–25]. Here, studies are ranging from fully atomistic quantum mechanical approaches [20] up to modified continuum-based models [21–25]. Previously in the literature, transport through a disordered alloy has been addressed with a continuum approach by creating a random distribution of atoms, and averaging over a volume to get a “local” alloy content [23, 25]. This was then used to determine fluctuating conduction and valence band confining energies. In this case, there is uncertainty in the band edge energies which will depend on (i) the volume over which the alloy is averaged, and (ii) the parameters used to calculate local strain and polarization.

To avoid these uncertainties while still accounting for alloy fluctuations in transport calculations, we have recently developed a three-dimensional (3-D) multiscale simulation framework that connects atomistic tight-binding theory with a modified, quantum corrected drift-diffusion (DD) solver. The tight-binding model has been extensively benchmarked against both *ab initio* theory and experiments. A comparison between the continuum- and atomistic-based approaches would provide useful insight into the effectiveness of the continuum model. However, the uncertainties mentioned above make such a comparison extremely challenging. Therefore, we limit ourselves here to starting from an atomistic setting which has been suitably benchmarked.

The framework has been employed to investigate unipolar carrier transport and it was found that alloy fluctuations result in an increase in carrier transport of electrons (in an *n-i-n* system) [21], but decreases transport in the case of holes (in a *p-i-p* systems) [22]. As the impact of alloy disorder is different for electron and hole species, one can infer that this may also impact carrier distribution in bi-polar devices. In the present work we apply this scheme for the first time to investigate the active region of (In,Ga)N-based MQW LED structures (thus *p-i-n* systems), and target a system which allows us to directly study the problem of carrier distribution across MQW systems.

In this paper we show that when employing our quantum corrected 3-D simulation framework that accounts for random alloy fluctuations, the experimentally observed trends are captured (namely that light emission occurs mainly from the *p*-side QW) without introducing for instance a multi-population scheme. This highlights that our developed solver presents an ideal starting point for future device design studies.

To highlight clearly the impact that 3-D random alloy fluctuations have on the carrier distribution in the active region of an (In,Ga)N-based LED, we use as a reference point a virtual crystal approximation (VCA) which effectively can be described by a 1-D model. This allows us to identify 3-D alloy fluctuations as a key mechanism for explaining experimental results.

Our studies show, and when using the same input pa-

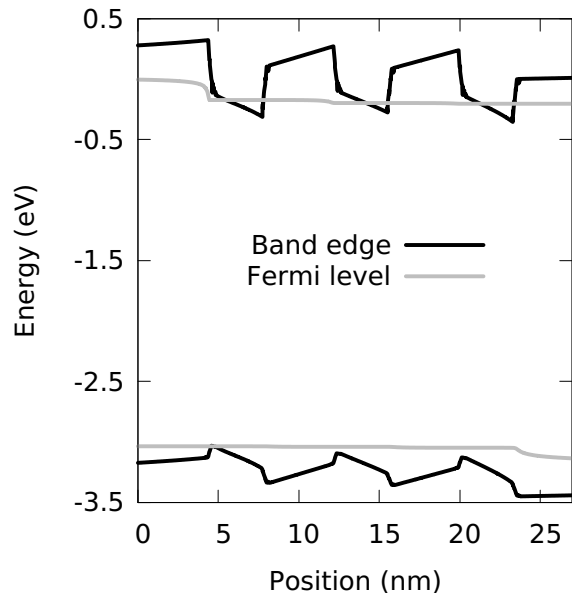


FIG. 1. Conduction and valence band edges (black) along with the quasi-Fermi energies for electrons and holes (grey) in an (In,Ga)N/GaN multi-quantum well system described in virtual crystal approximation. The band edge profile and the quasi Fermi levels are shown at a current density of 50 A/cm^2 . The leftmost (In,Ga)N quantum well contains 12.5% indium while the other two (In,Ga)N wells (centre and right) contain 10% indium. The *n*- (*p*-)doped region is to the left (right) of the quantum wells (see Fig. 2).

rameter set, only the model accounting for random alloy fluctuations produces trends that are consistent with the experimental data. The widely employed VCA yields results that are in contradiction with the experimental data, namely that radiative recombination stems mainly from the well *furthest away* from the *p*-side. Overall, this highlights (i) that alloy fluctuations are essential to achieve an accurate description of the carrier transport and (ii) have to be taken into account when theoretically guiding the design of energy efficient III-N light emitters.

The paper is organized as follows: in Section II we outline the model structure used for calculations and briefly summarise some of the literature experimental data from Ref. [5]. The theoretical framework which we use is summarized in Section III. Our results are discussed in Section IV. Finally Section V presents our conclusions.

II. MODEL MQW STRUCTURES AND LITERATURE EXPERIMENTAL FINDINGS

To investigate the carrier distribution in (In,Ga)N/GaN MQW systems we proceed similar to experimental studies in the literature [5, 7] and target MQW systems where one of the wells in the MQW stack has a slightly higher In content compared to the remaining wells. In our case, we study MQW systems with

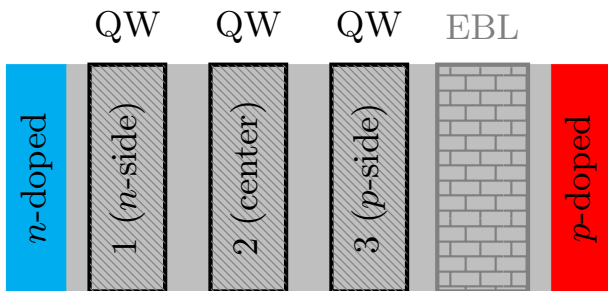


FIG. 2. Schematic illustration of multi-quantum well system. The n -doped region is shown in blue, the p -doped is in red and undoped regions are in grey. The quantum wells (QWs) are numbered starting from the n -side. The electron blocking layer (EBL) is positioned on the p -side, between the QWs and the n -doped region – this is absent in some of the simulations.

three (In,Ga)N/GaN wells. Here two are $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ (“shallow”) wells and one is an $\text{In}_{0.125}\text{Ga}_{0.875}\text{N}$ (“deep”) QW. These QWs are 3 nm wide and separated by 5 nm GaN barriers. The band edge profile of such a system along the transport (c -) direction, using a VCA, is shown in Fig. 1 at a current density of 50 A/cm² across the c -plane.

In the following, we investigate the carrier transport properties in two settings: (i) on an atomistic level accounting for random alloy fluctuations and (ii) in the frame of a VCA thus neglecting alloy fluctuations. In the latter VCA case (ii), at a given z -position (along the c -direction), there is no variation in material properties within the growth plane (c -plane). This assumption is also made in the widely used 1-D transport simulations on (In,Ga)N MQWs.

To study the carrier distribution in MQW systems using the simulation settings (i) and (ii), we follow again the experimental approach e.g. presented in Ref. [5] and the deep QW is moved from the n -side (position 1 (n -side) in Fig. 2) to the p -side (position 3 (p -side) in Fig. 2). In the case of the random alloy structures, the same microscopic configuration is kept for each well and only the ordering is changed.

For each of these systems the ratio of radiative recombination from the shallow wells to the deep well is calculated using:

$$\varrho = \frac{\mathcal{R}_{\Omega_S}^{RAD}}{\mathcal{R}_{\Omega_D}^{RAD}} \quad (1)$$

where

$$\mathcal{R}_{\Omega_i}^{RAD} = \int_{\Omega_i} R^{RAD}(\mathbf{r})dV, \quad (2)$$

is the total radiative recombination from the region Ω_i . Here, Ω_D is the region containing the deep QW, Ω_S is the region containing the shallow wells (as there are two shallow QWs this is the union of the two shallow QW regions). Since we are studying a system with three QWs,

an even distribution of carriers across the MQWs would result in a ratio of $\varrho = 2$. A small (large) value of ϱ means emission is dominated by the deep (shallow) wells. Previous experimental work on a similar system by Galler *et al.* [5] found that ϱ was small (i.e. emission is dominated by the deep QW) *only when the deep well was closest to the p -doped side of the MQW system* (thus position 3 (p -side) in Fig.2). The authors conclude that holes are responsible for this behavior, and argue that they are mainly found in the p -side QW and not in wells further away from the p -side. As a consequence, the overall emission from the (In,Ga)N/GaN MQW system is dominated by the emission from this well closest to the p -doped region. In line with Ref. [5], we calculate ϱ at a current density of 50 A/cm², which allows us to compare the here predicted trends with the trends found in the experimental studies. The theoretical framework employed to gain insight into ϱ is discussed in the following section.

III. THEORETICAL FRAMEWORK

In this section, we introduce the underlying (microscopic) theory of our multiscale simulations. We start in Section III A with the electronic structure model, an atomistic tight-binding (TB) model, and discuss the drift-diffusion approach in Section III B. Since all these ingredients have been discussed in detail in Refs. [21, 22], we here give only a brief summary.

A. Tight-binding energy landscape

We model the electronic structure of the above described (In,Ga)N MQW systems on an atomistic level with a nearest-neighbour, sp^3 TB model [26]. Here, local strain and polarization effects are included using a valence force field model and local polarization theory, respectively [27].

To connect the TB model to a DD solver we proceed as follows. Firstly, the TB model is used to extract a potential energy landscape describing the MQW region of the device using an atomistic framework. To do so, at each atomic site in the three dimensional (3-D) supercell, a local TB Hamiltonian is constructed from the full TB Hamiltonian [16]; A similar approach was used to extract local band edge profiles by Schliwa *et al.* while studying strain effects in quantum dots [28]. Subsequently, only the local TB Hamiltonian is diagonalized, yielding the local confining conduction and valence band edge energy at each lattice site. These local confining band edge energies include now already effects arising from alloy fluctuations and connected fluctuations in strain and built-in polarization field. The obtained 3-D confining energy landscape, after employing a Gaussian softening, forms the basis for our DD calculations.

In previous studies we have investigated and discussed in detail the influence of the Gaussian softening on trans-

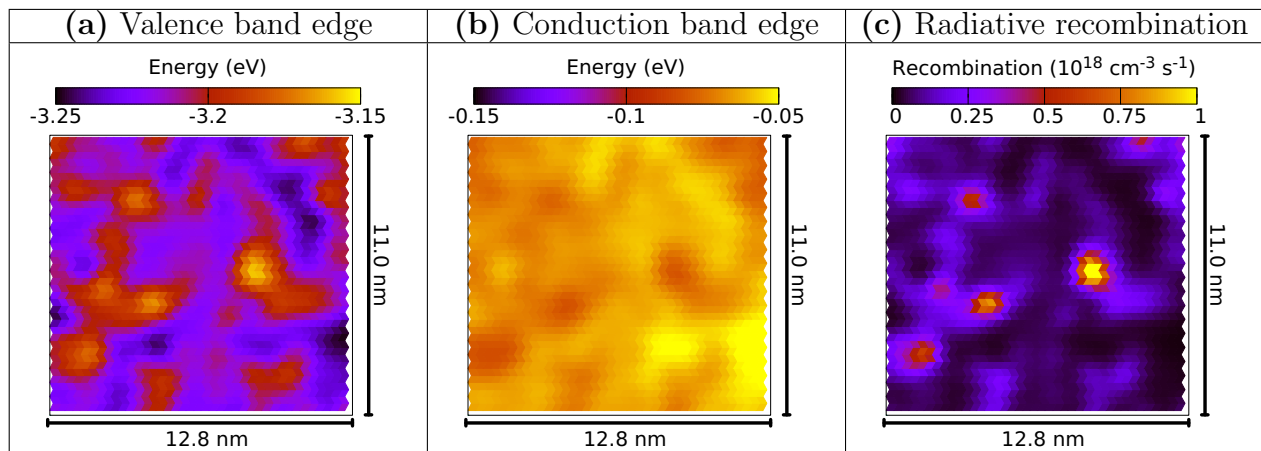


FIG. 3. Profile of (a) valence band edge energy, (b) conduction band edge energy, and (c) radiative recombination rate in the growth plane (c -plane) of an $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ quantum well; the current density is 50 A/cm^2 in all depicted figures. The slice displayed is the through the center well. The data are shown in all cases on a linear scale.

port calculations for electrons and holes [21, 22]. Here, we choose a Gaussian broadening on the order of the GaN lattice constant, $\sigma_{c,v} = a^{\text{GaN}} = 0.3189 \text{ nm}$, in all calculations. This value is large enough to average over a number of neighboring sites, while also small enough to retain fluctuations in the energy landscape.

B. Device simulation

A conduction and valence band at a single atomic site itself is not physically meaningful, as the electron and hole wave functions will extend over a volume. Instead, we have calculated the *local confinement potential energy* which can be used to study single particle states via, for example, solving the Schrödinger equation in the effective mass approximation. This accounts for quantum corrections, and is often coupled with the DD equations (which will be discussed below) to include quantum effects in a transport calculation.

Such a Schrödinger-Poisson solver is widely available in commercial software packages. However, in these packages it is largely restricted to 1-D simulations, since the extension to a 3-D system is computationally basically unfeasible. Instead of solving the large eigenvalue problem connected to evaluating the Schrödinger equation, we have implemented quantum corrections via localization landscape theory (LLT) [29]. Below, using 1-D quantum corrected DD calculations, we will show that this numerically more efficient LLT approach gives results similar to a fully self-consistent Schrödinger-Poisson solver.

From LLT we extract an effective confining potential for the conduction and valence band edge starting from the TB energy landscape.

An example of the resulting quantum corrected energy landscape is given in Fig. 3 (a) and (b). Here, in-plane band edge profiles for a single atomic plane through an $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ QW, after LLT has been applied, are shown.

As Fig. 3 (a) reveals, the fluctuations in the valence band edge energy due to alloy fluctuations are of the order of 100 meV. In combination with the high effective hole mass, these fluctuations are large enough to give rise to strong carrier localization effects as seen in other studies already [26, 30, 31]. We therefore expect that, especially for holes, the inclusion of random alloy fluctuations in the simulation will impact the carrier distribution. Consequently recombination rates are also expected to be noticeably influenced.

The variation in the conduction band edge energy is significantly smaller (order of 30 meV), as can be seen in Figure 3 (b). Since the effective electron mass is much lower in comparison with the holes, electron wave functions are less strongly perturbed by alloy fluctuations. As discussed above, this is in line with previous observations of localization in III-N alloys.

The impact that these fluctuations in the band edge energies have on the radiative recombination is also seen in Fig. 3 (c); the radiative recombination is calculated with `ddfermi` as will be described in section III B. The correlation between the valence band edge maxima and regions of high radiative recombination can be clearly identified; similar spatial profiles can be seen for non-radiative (Auger) recombination (not shown).

In order to highlight the impact of random alloy fluctuations on carrier transport and the distribution of carriers across a MQW system, we compare our atomistic calculations with the outcome of a VCA. In the latter case a homogeneous effective crystal is constructed where material properties are chosen to be interpolated properties of the binaries InN and GaN within the QW region. Here a linear, composition weighted interpolation scheme is employed. A bandgap bowing of -2.0 eV is used, consistent with the underlying atomistic TB model [27]. The VCA description, without any Gaussian broadening, is similar to commercially available packages. However, and in contrast to commercial software packages, quantum cor-

rections via LLT can also be taken into account in our VCA simulations, following the approach used for the random alloy case.

The devices are simulated in the frame of a (quantum corrected) DD model. This is run on a 3-D mesh which is built from the underlying TB mesh. The mesh construction is discussed in Appendix A. The DD builds on the van Roosbroeck system of equations [32]:

$$-\nabla \cdot (\varepsilon_s(\mathbf{r})\nabla\psi(\mathbf{r})) = q(p(\mathbf{r}) - n(\mathbf{r}) + C(\mathbf{r})) , \quad (3a)$$

$$\nabla \cdot \mathbf{j}_n(\mathbf{r}) = qR(\mathbf{r}) , \quad (3b)$$

$$\nabla \cdot \mathbf{j}_p(\mathbf{r}) = -qR(\mathbf{r}) , \quad (3c)$$

$$\mathbf{j}_n(\mathbf{r}) = -q\mu_n n(\mathbf{r})\nabla\varphi_n(\mathbf{r}) , \quad (3d)$$

$$\mathbf{j}_p(\mathbf{r}) = -q\mu_p p(\mathbf{r})\nabla\varphi_p(\mathbf{r}) . \quad (3e)$$

In the above equations, q is the elementary charge, $\varepsilon_s(\mathbf{r}) = \varepsilon_0\varepsilon_r(\mathbf{r})$ is the dielectric permittivity, $\psi(\mathbf{r})$ is the device electrostatic potential, $p(\mathbf{r})$ and $n(\mathbf{r})$ are the hole and electron densities, $C(\mathbf{r}) = N_D^+(\mathbf{r}) - N_A^+(\mathbf{r})$ is the net activated dopant density, $\mathbf{j}_n(\mathbf{r})$, $\mathbf{j}_p(\mathbf{r})$, $\varphi_n(\mathbf{r})$ and $\varphi_p(\mathbf{r})$ are the electron and hole current densities and the respective quasi-Fermi potentials. The total recombination rate is denoted by R .

The carrier densities are related to the band edge energies, $E_c^{dd}(\mathbf{r})$ and $E_v^{dd}(\mathbf{r})$, and quasi-Fermi potentials, $\varphi_n(\mathbf{r})$ and $\varphi_p(\mathbf{r})$, via the state equations [33]

$$n(\mathbf{r}) = N_c \mathcal{F} \left(\frac{q(\psi(\mathbf{r}) - \varphi_n(\mathbf{r})) - E_c^{dd}(\mathbf{r})}{k_B T} \right) , \quad (4a)$$

$$p(\mathbf{r}) = N_v \mathcal{F} \left(\frac{E_v^{dd}(\mathbf{r}) - q(\psi(\mathbf{r}) - \varphi_p(\mathbf{r}))}{k_B T} \right) . \quad (4b)$$

Here, N_c and N_v are the effective density of states for the conduction and valence band, respectively.

For the function \mathcal{F} , we use Fermi-Dirac statistics, and k_B is the Boltzmann constant. A temperature of $T = 300$ K has been used in all calculations. It is to note that the valence band, $E_v^{dd}(\mathbf{r})$, and conduction band edge energy, $E_c^{dd}(\mathbf{r})$, can be described either by a VCA, a VCA including quantum corrections via LLT, or an atomistic random alloy calculation including LLT-based quantum corrections.

Both the effective landscape extracted from LLT and the effective density of states will depend on the choice of effective mass, $m_{e,h}^*$. This will impact the transport properties calculated in the DD model. As already discussed, previous studies compared directly the TB electronic structure with a single band model, allowing us

Parameter		Value in each region		
Name	Units	<i>p</i> -GaN	<i>i</i> -InGaN	<i>n</i> -GaN
Doping	cm ⁻³	5 × 10 ¹⁸	1 × 10 ¹⁶	5 × 10 ¹⁸
μ_h	† cm ² /Vs	5	10	23
μ_e	† cm ² /Vs	32	300	200
m_h^*	† m_0	1.87	1.84	1.87
m_e^*	† m_0	0.20	0.18	0.20

TABLE I. Material parameters used in the different regions of the simulation supercell. Parameters denoted with † are taken from [25].

to calibrate our model. While studying transport we assume isotropic effective masses for electrons and holes; the mass in each simulation cell region is shown in Table I, using masses from Ref. [25]. Future studies can investigate the importance of anisotropic masses, in particular how this influences the localization landscape derived from LLT.

The recombination rates in equations (3b) and (3c) will depend on the overlap of electron and hole wave functions. This could be calculated in theory using the wave functions determined by solving the Schrödinger equation. As we have already stressed, this is basically unfeasible in a 3-D system where alloy fluctuations are considered. The solution to LLT could be used to approximate the wave function overlaps, as in Ref. [29, 34]. Instead, we make the often-used approximation of using the overlap of the *densities*: The total recombination rate in Eqs. (3b) and (3c), R , is calculated using the ABC model [35, 36]. Here, R is the sum of (defect related) Shockley-Read-Hall, R^{SRH} , radiative, R^{RAD} and (non-radiative) Auger recombination rate, R^{AUG} . An outline of the formalism and choice of parameters for the ABC model is found in Appendix B, and Table II.

The numerical approximation of the van Roosbroeck system is implemented (in 3-D) in `ddfermi` [37]. We employ the finite volume method (FVM) and the current is discretized using the SEDAN (excess chemical potential) approach [38–40], which yields a thermodynamically consistent flux approximation in the sense of Ref. [33]. The importance of using a thermodynamically consistent flux approximation was shown in [41].

IV. RESULTS

In this section we present the results of our study on the carrier distribution in the above described (In,Ga)N/GaN MQW systems. First we consider a VCA in Section IV A, where the impact of alloy fluctuations are neglected. This is studied (i) without and (ii) with the inclusion of quantum corrections. In Section IV B, as second step, the impact of alloy fluctuations is studied, including quantum corrections.

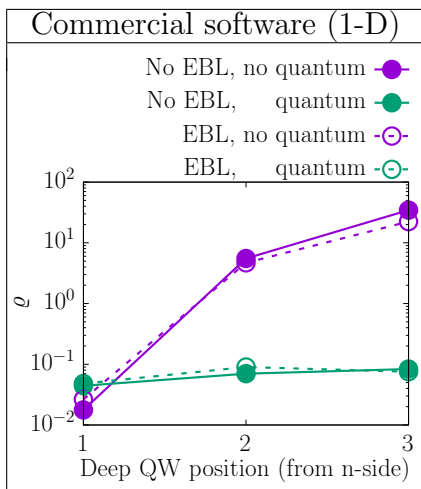


FIG. 4. Ratio of radiative recombination ρ , Eq. (1), from the shallow wells ($\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$) to recombination from the deep well ($\text{In}_{0.125}\text{Ga}_{0.875}\text{N}$) calculated as a function of the position of the deep well in the multi-quantum well stack. Here ρ is evaluated using `nextnano` excluding (purple) and including (green) quantum corrections via a self-consistent Schrödinger-Poisson-drift diffusion solver; results are shown when excluding (solid, filled circles) and including (dotted, open circles) an $\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}$ blocking layer.

A. Carrier transport in (In,Ga)N-based LEDs assuming homogeneous virtual crystals

To examine the impact of random alloy fluctuations on the carrier distribution in an (In,Ga)N/GaN MQW stack, we start with a ‘standard’ 1-D simulation approach neglecting random alloy fluctuations as a reference. In a first step, we study the system using the commercial software `nextnano` [42] and focus on the impact that including an electron blocking layer (EBL) has on results. This is then compared to results implementing `ddfermi`. We utilize the same parameter set in both `nextnano` and `ddfermi` simulations, allowing for a direct comparison between the results. In `nextnano` a self-consistent Schrödinger-Poisson-DD calculation is performed where a $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian is used to calculate eigenstates across the full simulation domain. When including quantum corrections in `ddfermi`, LLT is used, which is based on a 1-band effective mass model. So following the `ddfermi` set-up, in `nextnano` we employ also a 1-band model for the calculation of the electron and hole densities in Section IV A 1. After making a comparison between `nextnano` and `ddfermi` we analyse the impact of an electron blocking layer in Section IV A 2. This also allows us to benchmark our LLT-DD approach against commercially available Schrödinger-Poisson-DD calculations.

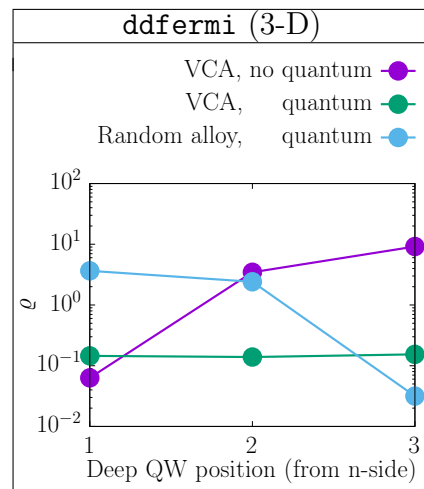


FIG. 5. Ratio of radiative recombination ρ , Eq. (1), from the shallow wells ($\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$) to recombination from the deep well ($\text{In}_{0.125}\text{Ga}_{0.875}\text{N}$) calculated as a function of the position of the deep well in the multi-quantum well stack. Here ρ is evaluated using `ddfermi` excluding (purple), including (green) quantum corrections via localization landscape theory (LLT) using a virtual crystal approximation (VCA) and a random alloy calculation including LLT-based quantum corrections (blue); these calculations neglect the AlGaIn blocking layer.

1. `nextnano` simulation without EBL

The calculated radiative recombination ratio ρ , Eq. (1), for the systems outlined in Section II at 50 A/cm^2 is shown in Fig. 4. Turning first to the data without quantum corrections (purple, solid), we find that in the case of the employed VCA continuum-based description, ρ is small when the deep QW is at the n-side (position 1 (n-side) Fig. 2) and larger when the deep well is at the p-side (position 3 (p-side) Fig. 2). Thus, the 1-D model predicts the opposite trend when compared to experiment [5].

Even when quantum corrections are included via a self-consistent Schrödinger-Poisson-DD method, the results for ρ excluding alloy fluctuations do not reflect the results seen in experiment: Overall, Fig. 4 (green, solid) reveals that when including quantum corrections in the VCA calculations, the position of the deep QW has little impact on the ratio of the relative radiative recombination, ρ . These results will be studied in more detail in Section IV A 3.

2. Impact of EBL on `nextnano` simulations

To study how the presence of an EBL affects the ratio of radiative recombination ρ , Eq. (1), the systems outlined in Section II are simulated with and without a 20 nm $\text{Al}_{0.15}\text{Ga}_{0.85}\text{N}$ EBL using `nextnano`. The EBL is separated from the p-side QW (position 3 (p-side) in

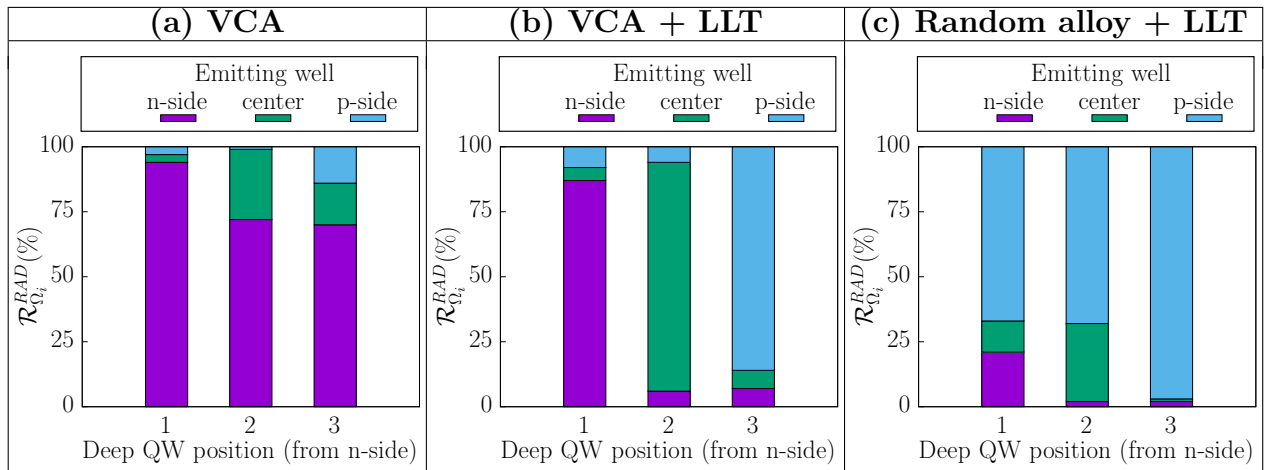


FIG. 6. Contribution of each quantum well (n -side; centre; p -side) in the (In,Ga)N multi-quantum well system to the total radiative recombination $\mathcal{R}_{\Omega_i}^{RAD}$ for $i \in \{n\text{-side}, \text{center}, p\text{-side}\}$ as a percentage of the total radiative recombination from all 3 quantum wells for (a) virtual crystal approximation (VCA), (b) virtual crystal approximation with quantum corrections included via localization landscape theory (VCA + LLT) and (c) a random alloy calculation including localization landscape theory based quantum corrections (Random alloy + LLT). That data are shown as a function of the position of the deep quantum well (x -axis). Each bar contains the percentage recombination from the n -side quantum well (purple), the center quantum well (green) and the p -side quantum well (blue). Labelling is consistent with that introduced in Fig. 2.

Fig. 2) by a 10 nm GaN barrier. Similar settings for an (Al,Ga)N EBL have been used in previous studies [25]. The nextnano calculated ratio of radiative recombination ρ , when varying the position of the deep QW in the MQW stack, are depicted in Fig. 4 excluding (open circles) and including (closed circles) the EBL.

The inclusion of an EBL does not have a significant impact on the ratio of recombination for both the calculation excluding (purple) and including (green) quantum corrections. As such, this feature of an LED is of secondary importance for the aims of this work.

In general the EBL needs to be treated as a random alloy. Previous studies of (Al,Ga)N barriers in uni-polar device settings have found that the impact of these barriers is lower than what is expected from a 1-D simulation for both electrons [43] and holes [44]. Thus given that our VCA calculations show that the presence of the EBL is of secondary importance for our study, we expect a similar conclusion when treating the EBL with alloy fluctuations. Therefore, it is unlikely that the EBL impacts the here presented result, however this question may be targeted in future studies.

3. *ddfermi* simulations

Utilizing commercial software in 1-D failed to reproduce the experimentally observed trends. One key element missing from this simulation is the presence of alloy disorder. As such, we next simulate the structures in *ddfermi* at a current density of 50 A/cm² using a VCA, VCA with quantum corrections via LLT and a 3-D random alloy system including quantum corrections via LLT.

We note that the biases required to simulate a current density of 50 A/cm² (≈ 3.1 V–3.2 V) are slightly higher than observed experimentally [45]. The DD model contains a number of free parameters, such as the electron and hole mobilities. In future, the model could be benchmarked against experimental results in order to get good agreement between the I-V curves, while also including alloy-induced carrier localization effects.

The calculated radiative recombination ratio ρ calculated with *ddfermi* is shown in Fig. 5. Again, as in the nextnano calculations, the data without quantum corrections (purple) shows the *opposite* trend to that observed in experiments. This is illustrated further in Fig. 6 (a), which displays the contribution (in percent) to the radiative recombination rate from each QW (colors) in the MQW stack. The data are shown as a function of position of the deep QW in the MQW system. This confirms that it is always the QW which is closest to the n -doped side (position 1) that dominates the recombination process; the n -side QW contributes $\approx 95\%$ when the deep QW is at position 1, $\approx 70\%$ when the deep QW is at position 2 or 3. Again, we stress that this is the *opposite* trend to the experimental findings in Ref. [5].

To shed more light on this result, the upper row in Figure 7 depicts the average hole (black, solid), electron (black, dashed) and radiative recombination (red) rate along the c -axis when the deep QW (In_{0.125}Ga_{0.875}N well) is (a) closest to the n -side (position 1), (b) in the centre of the MQW stack (position 2) and (c) closest to the p -side (position 3). Focusing on the VCA data, Figs. 7 (i) (a-c), we see the cause of the dominant recombination from the n -side QW: the hole density is always high in this region, independent of which well is closest to the n -side. In particular, the p -side QW fails to cap-

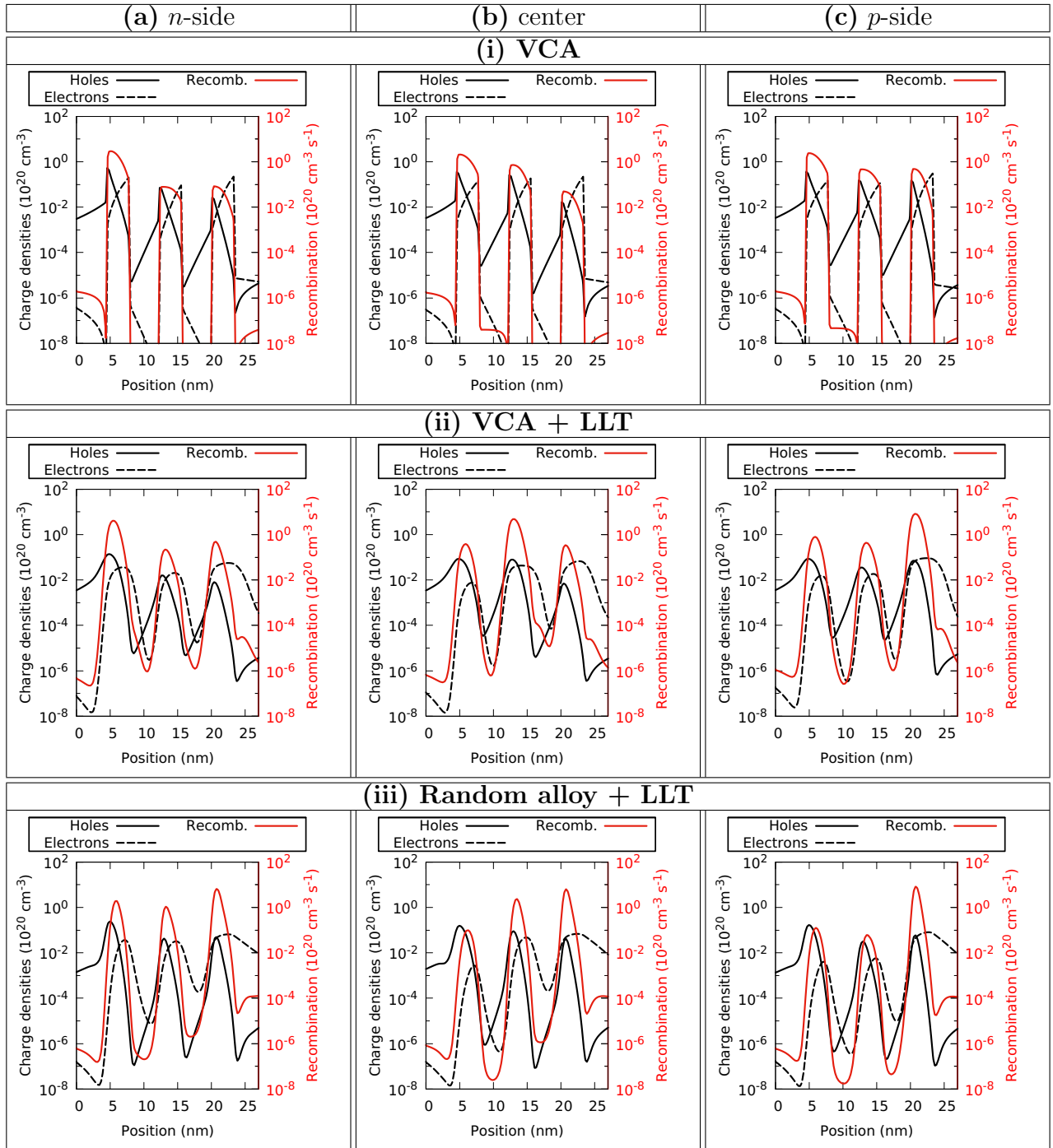


FIG. 7. Hole density (black, solid), electron density (black, dashed), and radiative recombination rate (red, solid) averaged over each atomic plane along the transport direction. Results from calculations building on (i) a virtual crystal approximation (top), (ii) a virtual crystal including quantum corrections via localization landscape theory (LLT) (center) and a (iii) random alloy description including LLT-based quantum corrections (bottom); the deep well is located at (a) the n -side (left), (b) the center (middle) and (c) the p -side (right). The data are shown on a log scale.

ture holes effectively and consistently has the lowest hole density. We note that a similar behavior is also found in the nextnano calculations discussed in Section IV A 1.

We saw in Section IV A 1 that including using a VCA with quantum corrections via a self-consistent

Schrödinger-Poisson-DD calculation does not reflect the result seen in the experiment. Similarly with `ddfermi`, including quantum corrections via LLT does not reproduce the observed experimental trends for ρ . Figure 5 (green) reveals that when including quantum cor-

rections in the VCA calculations, the position of the deep QW has little impact on the ratio of the relative radiative recombination, ρ . This is similar to results obtained in Fig. 4 using `nextnano`. As results between `nextnano` and `ddfermi` without quantum corrections and with corrections from Schrödinger equation (`nextnano`) or LLT (`ddfermi`), this indicates that *LLT can provide a good, numerically efficient approximation of the Schrödinger equation in DD simulations.*

From Fig. 6 (b) one can also gain more insight into this behavior and how quantum corrections impact the carrier distribution in the MQW stack. In the *absence* of quantum corrections but utilizing a VCA, Fig. 6 (a), the well closest to the *n*-side dominates the relative radiative recombination ratio ρ independent of the position of the deep well in MQW systems. When *including* quantum corrections this situation is now changed: the deep QW is now the dominant emitter independent of its position in the MQW stack, see Fig. 6 (c).

This behavior becomes clear when analyzing the electron and hole densities as a function of the position of the deep well in the (In,Ga)N/GaN MQWs, as shown in Fig. 7 (ii). Looking at the electron densities first, we find that electrons preferentially occupy the well closest to the *p*-side. This effect is enhanced when the deep QW is closest to the *p*-side (cf. Fig. 7 (ii) (c)). In our previous study on uni-polar electron transport [21], we have already seen that including quantum corrections leads to a softening of the potential barrier at the QW barrier interfaces. This in turn can lead to an increased electron current at a fixed bias point, when compared to a VCA system without LLT treatment, and thus the electrons can more easily ‘overshoot’ the wells in the MQW system. As a consequence, a lower electron density in the well closest to the *n*-side is observed.

Turning to the hole density, the situation is different. Here, we find that holes preferentially populate the well closest to the *n*-side. Only when the deep QW is closest to the *p*-side, the hole density in this well is noticeably increased. However, when comparing the distribution of holes in the MQW as a function of the position of deep well in absence (Fig. 7 (i)) and presence (Fig. 7 (ii)) of quantum corrections, the results are not very different. This indicates that quantum corrections, at least when employing a VCA, are of secondary importance for the hole distribution. This finding is consistent with our previous results on uni-polar hole transport [22], where we have discussed that due to the high effective hole mass and the small valence band offset, quantum corrections have a smaller impact on the hole transport when compared to electrons. As a consequence, the distribution of holes follows a similar pattern to that of the VCA where quantum corrections are neglected.

Finally, when looking at the ratio of radiative recombination ρ , it is important to note that this quantity is not only determined by having both large electron and hole densities in the same well but also by their spatial overlap. As one can infer from Fig. 7 (ii) (a-c), the largest

radiative recombination rate is always observed in the deepest well. This indicates also that the spatial overlap of electron and hole densities largest in the deep QW regardless of its position across the MQW system. We stress again that even when including quantum corrections in the VCA calculations, the resulting trend in ρ is not reflecting the trend observed in experimental studies [5].

B. Impact of a random alloy fluctuations on the carrier transport in (In,Ga)N/GaN MQWs

In the last step, we move away from the VCA description of the system and include, in addition to quantum corrections, also random alloy fluctuations in the calculations. Figure 5 (blue) shows that, and this time in line with the experimental results by Galler *et. al* [5], the deep QW only contributes significantly to the radiative recombination when it is *closest to the p-side* (position 3). In fact, when including random alloy fluctuations in the calculations, the well closest to the *p*-side always has the largest contribution to total radiative recombination, as can be seen in Fig. 6 (c).

To understand this behavior, Fig. 7 (iii) depicts the electron and hole densities in the different wells as a function of the position of the deep well in the MQW systems. Looking at the electron density first, in comparison to the VCA calculations both including and excluding quantum corrections, random alloy fluctuations lead to a reduction in electron density at the *n*-side QW. As discussed above and previously, quantum corrections can lead to increased electron transport, and including alloy fluctuations adds further to this effect due to the softening of the barrier at the well interfaces [21]. As a consequence, the electrons can more easily ‘overshoot’ the wells in the MQWs, which can also be seen in the increased electron density beyond the *p*-side QW when alloy fluctuations and quantum corrections are included. However, in comparison to the VCA result including quantum corrections, the electron density in the *p*-side well is only slightly affected by alloy fluctuations.

In contrast, hole densities in the *p*-side QW are more dramatically changed by alloy fluctuations. As Figs. 7 (ii) and 7 (iii) show, in comparison to the VCA description, alloy fluctuations lead to an increase in the hole density in the *p-side QW* (position 3) even when the deep QW is closest to the *n*-side (position 1) or in the centre (position 2) of the MQW system. While the smoothing of the well barrier interface can increase hole transport, as in the case of electrons, there are now also alloy disorder induced localization effects to contend with. As discussed in our previous work, these localization effects are *detrimental* to hole transport [22] and result in an increased hole density in the *p*-side QW. As a consequence, the well closest to the *p*-side dominates radiative recombination, regardless of the position of the deep well.

We note that there is still a reasonable hole density

present in the n -side QW (Fig. 7 (iii) (a-c)). In general, the distribution of carriers will also depend on the GaN barrier width and a 5 nm barrier is narrow enough to allow for some hole transport across the MQW [7]; a similar dependence of hole transmission on the barrier width has been seen in previous non-equilibrium Green's function studies [20]. Thus we expect that increasing the barrier width will mainly lead to a reduction of the hole density in the well furthest away from the p -side, but should to a lesser extent affect the hole density in the well closest to the p -side. Therefore, even for a larger barrier width than the here considered 5 nm, we expect that the recombination will still be dominated by the p -side QW.

The framework we have presented is capable of reproducing results observed in experiments of similar studies. As such, we can now simulate LED structures while targeting the question of higher efficiency. Our results have shown that alloy fluctuations lead to holes getting more easily trapped in the p -side QW. Therefore, increasing the number of quantum wells in an MQW stack may not lead to increased device performance: even though the active volume is increased there is a lack of free holes to contribute to recombination. On the other hand, due to the strong polarization field in III-N c -plane QWs decreasing the electron-hole overlap, increasing the well width may not lead to an increase in efficiency either. We have seen above that changing the well composition can impact the carrier distribution across a MQW stack. This may provide an avenue for investigation to see if this can be used to increase efficiency. The model employed here can be used to guide such experiments, as well as investigating the impact of various barrier or well widths and compositions.

The framework is also transferable to other material systems, where alloy disorder plays an important role. For example, (Al,Ga)N/(Al,Ga)N quantum well systems emitting in the UV part of the spectrum can be targeted, where disorder occurs in both the well and the barrier – in such systems, one would expect that carrier transport and recombination will be impacted also by alloy disorder.

V. CONCLUSIONS

In this work we applied a 3-D quantum corrected multiscale simulation framework to gain insight into the impact of random alloy fluctuations on the electron and hole distribution across the active region of an (In,Ga)N/GaN LED. To study the spatial distribution of carriers we have followed literature experimental studies [5] and analyzed the radiative recombination ratio in a multi-quantum well system, where one of the wells in the system has a higher indium content (deeper well) and its position is varied within the stack. Our benchmarking with commercial software reveals that a “standard” VCA-Schrödinger-Poisson-drift-diffusion is replicated well with the VCA-LLT-Poisson-drift-diffusion approach, allowing for more

efficient calculations.

Equipped with this model our analysis reveals that including (random) alloy fluctuations in the calculations is vital for reproducing trends seen in experiment. More specifically, when using the widely employed virtual crystal approximation (VCA), the hole density in the well closest to the p -doped region of the device is reduced compared to our atomistic random alloy calculation – the reduction is strongest (\approx order of magnitude) when the deep well is not also located at the p -side.

As a consequence, and in contrast to the experiment, in VCA the well closest to the p -side contributes very little to the radiative recombination process, an effect that can be reduced by accounting for quantum corrections. While this leads to enhanced radiative recombination from the well closest to the p -side, at least when this well is the deep well, it still does not reflect the trends observed in the experimental studies. However, when including random alloy fluctuations and quantum corrections in our 3-D simulation framework, these effects lead to an increase in the hole density in the well closest to the p -side. This is due to carrier localization, which traps holes in the p -side quantum well. Consequently, this well dominates the radiative recombination process in line with the experimental data. We note that in addition to quantum corrections and alloy fluctuations no further ingredients are required (e.g. multi-population model) to explain the experimentally observed trends. Therefore, our calculations highlight that alloy fluctuations are a key ingredient in simulations guiding the design of III-N based devices. Thus, the here developed model presents an ideal starting point for future calculations.

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Appendix A: Mesh generation

The generation of the energy landscape to be used in the active region, e.g. the (In,Ga)N/GaN MQW system, was outlined in Section III A. Now, a full device mesh including the n - and p -doped regions needs to be constructed on which the DD equations are solved. To achieve this we proceed as follows and divide the device mesh into two regions: an atomistic and a macroscopic one. The atomistic region is used to describe the MQW region and has as many grid points as atoms in the sys-

tem. These points contain information about the conduction and valence band edge energies calculated from TB, as discussed above.

In order to capture the effects of carrier localization in the calculations, the in-plane dimensions of our 3-D simulation cell should be larger than the localization length of the holes, given that electrons are less strongly affected by alloy fluctuations [17]. In our atomistic calculations we use a system with in-plane dimensions of $12.8 \times 11.0 \text{ nm}^2$. This is large enough to see the effects of hole localization as the in-plane hole localization length for $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ QWs is of the order of 1 nm [46]. The in-plane dimensions can be seen in Fig. 3 (a) and (b) where the in-plane valence and conduction band edges of an $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ QW are shown. In case of the VCA, given that there are no variations in material properties (band edge energies) within the growth plane (c -plane), a much smaller in-plane area is sufficient ($1.3 \times 1.1 \text{ nm}^2$), which reduces the numerical effort.

LLT is solved on this (finite element) mesh using a finite element method (FEM). The DD calculations are carried out employing a Voronoi finite volume method (FVM) [33]. Therefore, the generated FEM mesh must be transferred to an appropriate FVM mesh. Every point from the FEM mesh is included on the FVM mesh, as well as extra points required to produce a boundary-conforming Delaunay tetrahedral mesh; conduction and valence band data are then interpolated onto these additional nodes. This mesh is then embedded within a macroscopic device mesh which contains information about the p - and n -doped regions. In our atomistic transport studies here, we focus on systems without an (Al,Ga)N electron blocking layer (EBL). In principle, an atomistic mesh resolution would be required for the EBL, given the alloy fluctuations in (Al,Ga)N. However, and as we have discussed in Section IV A 2 of the main text, an (Al,Ga)N EBL is of secondary importance for the questions targeted in the present study and so we exclude this from our simulation cell. Therefore, outside active MQW region of the system, pure GaN is assumed. Thus, the conduction and valence band edge values are position independent (except for changes due an applied bias). The absence of strongly fluctuating band edges in the macroscopic mesh region allows us to use a sparse mesh and scale the simulation to a full device. The mesh is created using `TetGen` [47] and the interpolation is handled via `WIAS-pdelib` [48]. More details on the mesh generation can be found in Ref. [21].

Appendix B: Recombination

As discussed in the main text, recombination is considered using the ABC model. In this case the SRH rate

is obtained from:

$$R^{SRH}(\mathbf{r}) = \frac{r(n,p)}{\tau_p(n(\mathbf{r}) + n_i(\mathbf{r})) + \tau_n(p(\mathbf{r}) + n_i(\mathbf{r}))}, \quad (\text{B1})$$

the radiative part via

$$R^{RAD}(\mathbf{r}) = B_0 r(n,p), \quad (\text{B2})$$

and the Auger rate is calculated as

$$R^{AUG}(\mathbf{r}) = (C_n n(\mathbf{r}) + C_p p(\mathbf{r})) r(n,p). \quad (\text{B3})$$

In Eqs. (B1) to (B3)

$$r(n,p) = n(\mathbf{r})p(\mathbf{r}) - n_i^2(\mathbf{r})$$

and

$$n_i^2(\mathbf{r}) = n(\mathbf{r})p(\mathbf{r}) \exp\left(\frac{q\varphi_n - q\varphi_p}{k_B T}\right).$$

The above equations require further input, namely the radiative recombination coefficient B_0 , the Auger recombination coefficients C_p and C_n as well as the SRH lifetimes τ_p and τ_n . All these parameters will in principle carry a composition dependence [49–51]. Furthermore, B_0 , C_p and C_n will also be carrier density dependent [18, 52, 53]. We follow here the widely made assumption that these coefficients are constant across the InGa_{0.9}N MQW region [23, 25]. In the following we take a weighted average of parameters calculated in Ref. [49] for an electron and hole density of $3.8 \times 10^{18} \text{ cm}^{-3}$, which is a good approximation for the average carrier densities in the QWs at a current density of 50 A/cm^2 . As our active region consists of two $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ QWs and one $\text{In}_{0.125}\text{Ga}_{0.875}\text{N}$ QW we evaluate the different recombination coefficients as follows:

$$R_i^{\text{eff}} = \frac{2 \times (R_i^{10\%}) + 0.5 \times (R_i^{15\%} + R_i^{10\%})}{3}. \quad (\text{B4})$$

Here, $R_i^x \in \{B_0^x, C_n^x, C_p^x\}$ ($x \in [0.1, 0.15]$) are the radiative recombination, electron-electron-hole and hole-hole-electron Auger recombination coefficients, respectively. As there are no values for an $\text{In}_{0.125}\text{Ga}_{0.875}\text{N}$ QW in Ref. [49], a linear average of the coefficients in $\text{In}_{0.1}\text{Ga}_{0.9}\text{N}$ and $\text{In}_{0.15}\text{Ga}_{0.85}\text{N}$ wells has been used. A summary of the material parameters employed in all simulations is given in Table II.

Parameter		Value in each region		
Name	Units	p -GaN	i -InGaN	n -GaN
τ_p	† s	10	1×10^{-7}	7×10^{-10}
τ_n	† s	6×10^{-10}	1×10^{-7}	10
B_0	‡ cm^3/s	2.8×10^{-11}	2.8×10^{-11}	2.8×10^{-11}
C_p	‡ cm^6/s	5.7×10^{-30}	5.7×10^{-30}	5.7×10^{-30}
C_n	‡ cm^6/s	1×10^{-31}	1×10^{-31}	1×10^{-31}

TABLE II. Material parameters used in the different regions of the simulation supercell. Parameters denoted with † are taken from [25]; parameters denoted with ‡ are derived from [49] as described in the main text.

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