Random alloy fluctuations and structural inhomogeneities in c-plane In$_x$Ga$_{1-x}$N quantum wells: theory of ground and excited electron and hole states.

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We present a detailed theoretical analysis of the electronic structure of c-plane InGaN/GaN quantum wells with indium contents varying between 10% and 25%. The electronic structure of the quantum wells is treated by means of an atomistic tight-binding model, accounting for variations in strain and built-in field due to random alloy fluctuations. Our analysis reveals strong localisation effects in the hole states. These effects are found not only in the ground states, but also the excited states. We conclude that localisation effects persist to of order 100 meV into the valence band, for as little as 10% indium in the quantum well, giving rise to a significant density of localised states. We find, from an examination of the modulus overlap of the wave functions, that the hole states can be divided into three regimes of localisation. Our results also show that localisation effects due to random alloy fluctuations are far less pronounced for electron states. However, the combination of electrostatic built-in field, alloy fluctuations and structural inhomogeneities, such as well-width fluctuations, can nevertheless lead to significant localisation effects in the electron states, especially at higher indium contents. Overall, our results are indicative of individually localised electron and hole states, consistent with the experimentally proposed explanation of time-dependent photoluminescence results in c-plane InGaN/GaN QWs.

I. INTRODUCTION

Nitride semiconductors have attracted considerable interest for a variety of different applications, ranging from photovoltaic cells up to optoelectronic devices such as light-emitting devices (LEDs). For instance, the cornerstone of modern LEDs operating in the blue to green spectral region are InGaN/GaN quantum wells (QWs) grown along the crystallographic c axis. The success of these devices is remarkable given the extremely high defect densities (> 10$^8$ cm$^{-2}$) in InGaN/GaN materials, which mainly originate from the large lattice mismatch between GaN and the underlying substrate, sapphire (16%). The widely accepted explanation for the defect-insensitive efficiency of InGaN-based devices is that carrier localisation effects introduced by alloy fluctuations prevent diffusion to non-radiative recombination centres. Using positron annihilation measurements, Chichibu et al. demonstrated the presence of such carrier localisation effects in nitride-based alloys. In addition to these measurements, photoluminescence (PL) spectroscopy studies by different groups also gave clear indications that the optical properties of c-plane InGaN/GaN QWs are significantly affected by localisation phenomena. For example, temperature dependent PL measurements have shown that the PL peak energy follows an “S-shaped” temperature dependence. This particular form of the shift of the PL peak position is attributed to the redistribution of carriers between different localised states. Furthermore, time-dependent PL measurements revealed non-exponential decay transients and that the decay times extracted from the curves vary across the PL curve. Morel et al. proposed as an explanation for this that the radiative recombination process in c-plane InGaN/GaN QWs is dominated by individually localised carriers. The varying spatial separations of these separately localised carriers, both in the c-plane and perpendicular to it, lead to variations in the radiative recombination time. Using this assumption, Morel et al. were able to obtain a good agreement between theoretical predictions and the experimental data.

Even though, as discussed above, there is considerable experimental evidence for the importance and presence of localisation effects due to alloy fluctuations, it is only recently that these effects have been considered in theoretical studies. The applied theoretical frameworks range from modified continuum-based descriptions up to fully atomistic models. These studies have focused mainly on ground state properties, which are important to understand and explain experimental studies at low temperature; however, in order to understand the results of experiments conducted at ambient temperature, as well as the transport properties of the system, many excited states must be considered. Already the “S-shaped” temperature dependence of the PL peak position indicates that excited states exhibit localisation features. These localised states modify the form of the density of states in such a way that there is a smooth tail of states at the low energy end of the density of states in a QW structure. Because of this, these states are often referred to as “tail states.”

In this paper we address the impact of random alloy fluctuations on the localisation features of both ground and excited states in c-plane InGaN/GaN QW systems. To cover the experimentally relevant indium composition ranges, we analyse InGaN/GaN QWs with indium
contents of 10%, 15% and 25%. Furthermore, since experimental studies highlight also that structural inhomogeneities, such as well width fluctuations, impact the electronic and optical properties of nitride-based heterostructures significantly we include these effects also in our atomistic analysis. Our theoretical framework is based on an atomistic $sp^3$ tight-binding (TB) model, which includes effects such as strain and polarisation field variations due to the considered random alloy fluctuations.

Our calculations reveal that random alloy fluctuations lead to strong hole wave function localisation effects in both ground and excited states. We find here that over an energy range of order 100 meV a significant density of localised valence states is expected. The presented data also indicates that these localised states significantly affect the probability for transferring carriers from one site/state to another. When studying whether or not the hole wave functions overlap with each other, three different regimes become apparent. The first corresponds to “strongly localised states” with almost no spatial overlap with all other states considered. The second and third regimes consist of what we refer to as “semi-localised states” and “delocalised states”, respectively, where the spatial overlap is significantly increased with respect to the “strongly localised” states. Our data also shows that the number of states, and therefore the energy range, constituting each of these regimes, depends on the indium content of the system in question.

While our calculations reveal that random alloy fluctuations lead to very strong hole wave function localisation effects, the situation is different for the electron states. Compared with the hole states, the alloy fluctuations lead to much less pronounced electron wave function perturbations. The primary sources of the localisation of electron states are the electrostatic built-in field and well width fluctuations present in $c$-plane InGaN/GaN heterostructures. Also for the excited electron states, localisation effects are strongly reduced compared with the holes.

The combination of macroscopic built-in field, random alloy and well width fluctuations leads to a spatial separation of electron and hole wave functions both in the $c$ plane and perpendicular to it. In standard continuum-based models, InGaN/GaN QWs are treated as ideal one-dimensional systems, which can be described by averaged material parameters. These approaches can account only for the spatial separation of electron and hole wave functions along the growth direction due to the presence of the built-in field. Thus, in contrast to the here applied fully atomistic three-dimensional approach, in-plane spatial separations are not captured. Our results indicate that electrons and holes are individually localised and that the wave function overlap should therefore also depend on the relative in-plane position of the carriers. Thus, the here obtained findings are consistent with the “pseudo 2-D donor-acceptor pair system” proposed by Morel et al. to explain time-dependent PL results of $c$-plane InGaN/GaN QWs.

The manuscript is organised as follows. In Sec. we introduce the components of our theoretical framework. In Sec. we discuss the QW model system under consideration and the input from available experimental structural data. The results of our calculations are presented in Sec. before addressing ground state properties in Sec. before turning to the excited states in Sec. We relate our theoretical data to experimental findings in Sec. before summarising our work in Sec.

II. THEORETICAL FRAMEWORK

In this section we briefly introduce the atomistic theoretical framework used to study the electronic structure of $c$-plane InGaN/GaN QWs with varying indium content. Our approach can be divided into three main components. First, the large lattice mismatch between InN and GaN (approx. 11%) gives rise to a strain field in InGaN/GaN heterostructures. To treat this strain field on an atomistic level, and thus account for random alloy fluctuations on a microscopic level, we employ a valence-force-field (VFF) model based on that introduced by Martin. Our VFF includes electrostatic effects explicitly and reproduces important real-wurtzite system attributes such as non-ideal $c/a$ ratios and internal parameters $u$. We have implemented this model in the software package LAMMPS. More details are given in Ref.

Second, the strong intrinsic electrostatic built-in fields in nitride heterostructures have to be included to achieve a realistic description of the electronic structure of $c$-plane InGaN/GaN QWs. In wurtzite III-N materials the lack of inversion symmetry leads to a non-vanishing sum of electric dipole moments and thus to a macroscopic electric polariation. This polarisation has two contributions, one of which is strain independent, known as the spontaneous polarisation, and the other of which is the strain dependent piezoelectric polarisation. In addition to the macroscopic polarisation, random alloy fluctuations lead also to local polarisation variations. Recently, we have developed a local polarisation theory capable of accounting for both the macroscopic and local intrinsic polarisation. Our theory receives input for its material parameters from density functional theory (DFT) within the Heyd-Scuseria-Ernzerhof (HSE) screened exchange hybrid functional scheme. The starting point for this approach is to split the wurtzite polarisation vector, made up of spontaneous and piezoelectric contributions, into macroscopic and microscopic terms. The macroscopic term is the so called clamped-ion contribution where ions are not allowed to move and this part is related to the piezoelectric coefficients $e_{ij}^0$. The local contribution involves the deformation of the nearest neighbor environment around the atom under consideration. With this we can define a dipole moment for each tetrahedron over the entire cell. From this we can calculate the corresponding
polarisation (dipole moment/Volume). The last step is now to calculate the resulting built-in potential. Usually this is done by solving Poisson’s equation. However, since we are dealing with an atomic grid this becomes difficult. To circumvent this problem we make use of the multipole expansion of a distribution of electric charges, with which we can calculate the electrostatic potential at position \( r \) due to the presence of a point dipole at \( r' \). In doing so we avoid numerical problems arising from solving Possion’s equation by, for instance, a finite difference method on an irregular wurtzite crystal. Consequently, we find that the situation the macroscopic component of the built-in potential, which is effectively the potential one would expect in a capacitor, is modified in the QW by local fluctuations sitting on top of the potential slope in this region. The details of the local polarisation and point dipole method are described in Ref. 28 in more detail. Note that we are here interested only in the intrinsic properties of InGaN/GaN QWs, thus we do not include the effects of any externally applied bias, as one would have in an LED structure.

Thirdly, to determine the effects of alloy, strain and built-in potential fluctuations on the electronic structure of InGaN/GaN QWs, we use an atomistic, nearest neighbor \( sp^3 \) TB model. Before treating the InGaN alloy we start from the binary materials InN and GaN. The required TB parameters are determined by fitting the TB bulk band structures of InN and GaN to those calculated using HSE hybrid-functional DFT. Due to the minimal basis used in \( sp^3 \) TB, the description of the conduction band at the L- and M-valleys is less accurate. However, from our HSE-DFT calculations we find that, for the nitrides, there is a very large energetic separation between the conduction band minimum at the \( \Gamma \)-point and the \( M \) and \( L \) valleys. Because of this, the evolution of the energy gap is dominated by the band structure around \( k = 0 \); thus because the TB model used here captures well the valence band and the conduction band at \( \Gamma \), it is particularly suitable for treating nitride semiconductors.

Equipped with this knowledge about the binary materials, we can then treat the InGaN alloy on a microscopic level. To this end, at each atomic site, the TB parameters are set according to the bulk values of their constituent atoms. For the cation sites (Ga,In), there is no ambiguity in assigning the on-site and nearest neighbor TB matrix elements, since these always have nitrogen atoms as their nearest neighbors. However, the nearest neighbor environment of the anions (N) will vary depending on the local indium distribution. To treat this effect, different approaches have been used in the literature. One ansatz is to start already at the bulk band structure level and use the same on-site TB matrix elements for N in InN and GaN. In doing so the ambiguity for the N-atom on-site energies in an InGaN alloy is removed. However, by assuming the same N-atom on-site energies in InN and GaN, one basically fixes the band offset between InN and GaN. Such an approach limits the transferability of the TB parameters to other systems. Given these arguments, we apply here another widely used approach to treat the on-site energies of a common atom species in an alloy. The assignment here is performed using weighted averages for the on-site energies, where the weights are determined by the number of nearest neighbor In or Ga atoms. This is a widely used and benchmarked approach to treat alloys in an atomistic TB framework.\(^{15,30,32}\) The band offset is included by shifting the InN on-site TB parameters by the valence band offset \( \Delta E_{\text{VB}} = 0.62 \text{ eV} \). The value for \( \Delta E_{\text{VB}} \) is taken from HSE-DFT calculations.\(^{43}\) Strain and built-in potential effects are included in the description as on-site corrections to the TB Hamiltonian. The procedure is detailed in Ref. 28. This framework has already been successfully applied to other wurtzite III-N alloys, such as AlGaN and AlInN.\(^{34,35}\) And similar approaches have been used also to effectively describe other alloy systems, such as GaBiAs/GaAs QWs.\(^{36}\)

Having discussed the theoretical framework, we introduce the model \( c \)-plane InGaN/GaN QW systems in the next section.

### III. INGAN QW SYSTEM

Here we introduce the QW systems to which we apply our theoretical framework. The QW structures being studied are similar in indium contents to QWs studied experimentally in Ref. 37. To model \( c \)-plane \( \text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN} \) QWs we use \( \approx 82,000 \) atom supercells (equivalent to a system size of \( \approx 10 \text{ nm} \times 9 \text{ nm} \times 10 \text{ nm} \)) with periodic boundary conditions. The QW in these supercells is around 3.5 nm wide. These supercell dimensions have been chosen such that the experimentally reported carrier localisation lengths of 1.1–3.1 nm\(^{37}\) can be accommodated within the cell without spurious coupling to periodic replicas. Following Refs. 28–41, we assume that InGaN is a random alloy and distribute indium atoms at the cation sites of the active region with a probability given by the nominal indium content of the configuration in question. In doing so we do not assume any preferential orientation or correlation of indium atoms.

To examine the impact of the microscopic indium configuration on the electronic structure, we consider twenty different random atomic configurations for each composition studied. These configurations are generated for nominal indium contents of 10%, 15% and 25%, which cover the experimentally relevant range of indium contents.\(^{37}\) It should be noted that we are interested here in general trends rather than a detailed statistical analysis of the results. Such an analysis would require significantly more random configurations. However, for our purposes, to shed light on trends and basic properties of the InGaN/GaN QWs with varying indium content, including effects of random alloy fluctuations, a sample of twenty different configurations per alloy content is sufficient.

In Refs. 37 and 42 well-width fluctuations were observed at the upper interface [GaN on InGaN] of \( c \)-plane
A. Ground state properties

A first quantitative measure for the impact of alloy fluctuations on the electronic structure of c-plane InGaN/GaN QW systems is given by the variation in ground state transition energies about their configurational average. In Fig. 1 the energy of the ground state transition, $E_g$, is plotted against the configuration number, $n$, for each nominal indium concentration [10%, 15% and 25%]. For each case the average transition energy is indicated by a dashed line. The values obtained for the 10% (black square), 15% (open blue circle) and 25% (solid red circle) indium systems are 2.871 eV, 2.533 eV and 1.964 eV, respectively. As expected, the transition energy shifts to lower energies with increasing indium content. Apparent from Fig. 1 is the significant spread in transition energies about their averages across all indium contents. This demonstrates that random alloy effects are important for as little as 10% indium in the well. The fluctuations in $E_g$ are also consistent with the large PL linewidths observed experimentally. The here calculated average transition energies will be compared to experimental PL peak energies reported in the literature.

To investigate the origin of the variance of the transition energies, we look now to the variation of the corresponding electron and hole ground state energies about their respective averages. In Fig. 2 the electron ground state energies, $E_{GS}$ [Fig. 2 (a)], and hole ground state energies, $E_{GS}^h$ [Fig. 2 (b)], are plotted as a function of the configuration number, $n$. The average ground state energies are again indicated as dashed lines. The data are shown for the different indium contents $x$. The average hole ground state energy increases with increasing indium content since the valence band offset increases. For 10% $[x = 0.1$, black square], 15% $[x = 0.15$, blue circle] and 25% $[x = 0.25$, red solid circle] indium the average energies are 334 meV, 489 meV and 785 meV, respectively [cf. Fig. 2 (b)]. The zero of energy is taken as the valence band edge of the unstrained bulk GaN. However, due to the macroscopic built-in potential and random alloy fluctuations, the valence and conduction band edges will vary with position across the QW structure, with the calculated hole energies then including a contribution from these factors. For the comparison with the experiment only the transition energies are relevant, which are independent of the choice of the zero of energy. The average ground state energies of the electrons likewise decrease with increasing indium content, since the conduction band offset is increased [cf. Fig. 2 (a)]. The average electron ground state energies are 3.205 eV, 3.022 eV and 2.763 eV for 10%, 15% and 25% indium, respectively. On comparison of the variations in Fig. 2 (a) and (b), in general, it is evident that the hole ground state energy, $E_{GS}^h$, is very sensitive to the configuration number, $n$. This further indicates that the alloy microstructure plays an important role for the valence band states. More specifically, from Fig. 2 we find that the $E_{GS}^h$...
FIG. 2. (Color online) (a), Electron ground state energy, $E_{GS}^e$, and (b), hole ground state energy, $E_{GS}^h$, in an In$_x$Ga$_{1-x}$N/GaN QW as function of the different random microscopic configurations, $n$. The indium content $x$ in the well is $x = 0.10$ (10%, black square), $x = 0.15$ (15%, blue circle) and $x = 0.25$ (25%, red solid circle). The average ground state energies are indicated by dashed lines.

The electron ground state energies, $E_{GS}^e$, vary between $\sim \pm 100$ meV around their average energies whilst the electron ground state energies, $E_{GS}^h$, vary at most from the average by $\sim \pm 50$ meV. However, for the electron ground states, the large value of $\pm 50$ meV arises mainly from the 15% indium case while for 10% and 25% indium we find only $\sim \pm 10$ meV and $\sim \pm 20$ meV, respectively. Furthermore, for the 15% indium case, the spread in the electron ground state energies about their average energy is comparable with the spread in the energies of the hole states.

To shed more light on the results shown in Fig. 2 (a) and (b), Figs. 3, 4 and 5 show isosurfaces of the electron (red) and hole (green) ground state charge densities for selected configurations in the case of 10%, 25% and 15% indium in the QW, respectively. The “Side View” for each of these cases is a view perpendicular to the c-axis, while the “Top View” is a view looking down the c-axis. The light and dark isosurfaces correspond to 10% and 50% of the respective maximum charge density values. The selected configurations correspond to situations with positive and negative deviations from the average ground state energy plus one configuration that is close to the average value.

We analyse in a first step configurations $n = 9, 13$ and 20 of the 10% indium case. The corresponding charge densities are displayed in Fig. 3. In general we find that the electron and hole wave functions are spatially separated along the c-axis due to the presence of the electrostatic built-in field. Looking at configurations 9 and 20, we see from the electron charge densities that they are almost spread across the entire c-plane in the QW region. However, a closer inspection also reveals that the ground state electron wave functions are affected by the presence of the random alloy fluctuations. This is evinced by the lower probability densities in certain parts of the QW region. For configurations 9 and 20 we find also that the assumed well width fluctuation is of secondary importance. A different behaviour in our calculations is observed when looking at configuration 13, where the charge density is localised very strongly in the well-width fluctuation. This particularity of the ground state wave function, confined in the well-width fluctuation, is also reflected in the energy value, which shows the largest absolute deviation from the average [cf. Fig. 2 (a)]. However, we stress here again that we have assumed only a particular type of well-width fluctuation. We will discuss the importance of the well-width fluctuation in more detail below.

For the hole ground states the situation is different. Looking at the charge densities (green isosurfaces) in Fig. 3, much stronger localisation effects are visible for all configurations. The “strength” and spatial position of the localisation changes greatly from configuration to configuration. This behaviour reflects the sensitivity of the hole ground state energies to a particular microscopic configuration, as seen in Fig. 2 (b). In general this sensitivity to the alloy microstructure can be attributed to the larger effective mass of the holes when compared to the electrons, and their associated tendency to be localised at In-N-In chains, as shown by DFT calculations. It is important to note that the observed hole localisation features both in-plane as well as along the c-axis are vastly different from a standard continuum-based description. When looking at configuration 13, the hole wave function localises near the bottom QW/barrier interface. This situation might be expected from a continuum-based description. However, a fully continuum-based description would not account for the clearly visible in-plane localisation effect, since in such an approach InGaN/GaN QWs are usually treated
as one dimensional systems. For configurations 9 and 20, the wave functions are localised in regions clearly above the bottom QW interface. This would also not be expected from a continuum description. This strong localisation experienced by the holes validates the aforementioned conclusion that random alloy fluctuations significantly impact the system properties for as little as 10% indium in the QW. The results shown in Fig. 3 also indicate that the wave function overlap between electron and hole ground states is not only affected by the spatial separation along the growth direction but also by the spatial separation in the c-plane. We will come back to this observation in Sec. V where we discuss the observed results with respect to experimental data.

Before turning to the 15% indium case, we focus on the 25% indium results, shown in Fig. 4, in the next step. When looking at the electron charge densities (red) of the here displayed configurations 4, 13 and 15, it is evident that the electron wave functions are all localised by the well-width fluctuation. This results from the increased built-in field in the 25% indium case when compared with the 10% indium case [cf. Fig. 3]. Since the well-width fluctuation introduces an extra in-plane/lateral confinement for the electron wave functions, one could expect larger variations in the corresponding electron ground state energies when compared with the 10% indium system, where the considered well-width fluctuations are only of secondary importance. This is because different microscopic configurations of the indium atoms in the well-width fluctuation will lead to different effective confining regions for the electrons. For instance, a concentration of indium in the centre of the well width fluctuation (configuration 13) can lead to a ground state with a very different energy from that of a configuration where the indium is concentrated near the barrier material (configuration 15); the state near the barrier is effectively confined in a smaller region and will have its energy increased by the effects of the barrier. This picture of small changes in indium content leading to large changes in confinement and energy is consistent with the data shown in Fig. 2 (a), and discussed above. Turning to the hole ground states, we find a similar behaviour.
as in the 10% indium case with strong localisation features for each configuration. In configurations 13 and 15 the hole wave function is localised close to the bottom QW interface, while the hole ground state wave function in configuration 4 is localised two monolayers above the lower QW interface. Due to the increased built-in field in the 25% indium case one would expect that the hole wave functions are localised near the bottom interface. In this sense, with the hole wave function not being localised near the bottom QW interface, one could expect that configuration 4 represents an extreme case. This is confirmed in the large deviation of its ground state energy from the average ground state energy, as displayed in Fig. 2 (b). When looking at the “Top View” of the electron and hole ground state charge densities, we find that electron and hole wave functions are separately localised due to the built-in field, random alloy fluctuations and well width fluctuations. Again, the wave function overlap between electrons and holes is not only affected by the spatial separation along the growth direction but also in the c-plane. When looking, for instance, at the charge densities of the electron and hole wave functions from configuration 15, we find that electron and hole wave functions are localised at similar in-plane positions. This is in contrast to configuration 4 and 13, where we are left with a clear spatial separation also in the c-plane. Again, we will come back to the importance of these properties in Sec. V.

We now turn to the 15% indium case. Here we have selected configurations 3, 4 and 8. The corresponding electron and hole ground state charge densities are displayed in Fig. 5. As discussed above, the variation in the hole ground state energies [cf. Fig. 2(b)] is comparable to the variations observed in the 10% and 25% indium case, respectively. The isosurfaces of the hole charge densities (green) displayed in Fig. 5 show also a similar behaviour as in the 10% and 25% indium systems. However, in comparison with the 10% or 25% indium case, the electron ground state energies in the 15% indium system show much larger variations [cf. Fig. 2(a)]. When looking at the isosurfaces of the electron charge densities (red) for configurations 3, 4 and 8, the origin of this behaviour becomes clear. In terms of the importance of the well-width fluctuation, the 15% indium case represents an intermediate situation. For example, in the case of configuration 8, the electron wave function is mainly localised inside
FIG. 5. (Color online) Isosurface plots of the electron (red), $|\psi_e|^2$, and hole (green), $|\psi_h|^2$, ground state charge densities in the In$_{0.15}$Ga$_{0.85}$N/GaN QW. The light (dark) isosurface corresponds to 10% (50%) of the maximum charge density. The results are shown perpendicular (“Side View”) and parallel (“Top View”) to the c-axis for three different random microscopic configurations (Config 3, Config 4, Config 8).

The well width fluctuation, while configuration 4 shows still significant charge density contributions outside the well-width fluctuation. From this one could expect that the energies of these different configurations are very different, and indeed this is confirmed by Fig 2 (a). In summary, the presence of the well-width fluctuation in combination with the built-in field explains the initially surprising result of the stronger variation in the electron ground state energies for the 15% indium case in our calculations.

Overall, even though we have considered here only one particular type of well-width fluctuation, our results clearly demonstrate that their presence can contribute significantly to variations in both transition energies and localisation effects. It should also be mentioned that our results for electrons are consistent with the work by Watson-Parris et al. [10,19], who studied the impact of well-width fluctuations on the electronic structure of InGaN QWs in the framework of a modified effective mass approach. In the study by Watson-Parris et al. [10,19], disk-shaped well-width fluctuations with diameters ranging from 5 nm to 20 nm have been studied. The influence of these fluctuations on the electron wave function localisation characteristics has been analysed for c-plane InGaN/GaN QWs with indium contents between 5% and 25%. At 10% indium content, the results with and without well-width fluctuations are similar in terms of the electron ground state localisation length. Only a slight decrease in the localisation length is observed when the well-width fluctuations are included, indicating that well-width fluctuations for lower indium contents are of secondary importance, consistently with our results [cf. Fig. 3]. Watson-Parris et al. [10,19] showed also that at 25% indium, well width fluctuations lead to a significant reduction of the electron ground state localisation length, when compared to a calculation without well width fluctuations. This corroborates our earlier mentioned conclusion that the importance of well width fluctuations in localising the electron wave functions will depend on the indium content. Therefore, even though we have assumed only one particular type of well-width fluctuation, our presented results provide a first indication of the importance of well-width fluctuations on the electronic structure of c-plane InGaN/GaN QWs with different indium contents.

So far our discussion of localisation effects has been...
Electrons

| (a) 10% | (b) 15% | (c) 25% |
|---------|---------|---------|
| ![Graph](image1.png) | ![Graph](image2.png) | ![Graph](image3.png) |

Holes

| (d) 10% | (e) 15% | (f) 25% |
|---------|---------|---------|
| ![Graph](image4.png) | ![Graph](image5.png) | ![Graph](image6.png) |

FIG. 6. Electron and hole ground state normalised inverse participation ratios (IPR) plotted as a function of the ground state energies of each of the 20 microscopically different configurations, for nominal indium contents of 10%, 15% and 25%. The IPRs are normalised to that of the 10% electron ground state with the highest IPR, which is Config 13 (cf. Fig. 5).

Based on inspecting the charge densities of the electron and hole ground state wave functions. To study localisation effects now on a more quantitative basis we use the metric of the inverse participation ratio (IPR). This provides a more objective measure of localisation and also allows the examination and comparison of the localisation characteristics of many states at once. The participation ratio was first introduced by Bell to assess the localisation properties of atomic vibrations. In this context it gave insights into the fraction of the total number of atoms in the system which participate effectively in the vibrations of a particular normal mode. The IPR is the inverse of this quantity, and is commonly used as a measure of localisation in TB models. In our TB formalism, a carrier wave function, \( \psi \), is given by:

\[
\psi = \sum_i \sum_{\alpha} a_{i\alpha} \phi_{i\alpha},
\]

where the index \( i \) runs over the \( N \) lattice sites, and the index \( \alpha \) denotes the different orbitals in our \( sp^3 \) TB basis at each site. The term \( a_{i\alpha} \) represents the amplitude of the wave function, \( \psi \), constructed with the basis \( \phi_{i\alpha} \), at the site \( i \). On the basis of Eq. the IPR may be defined as:

\[
\text{IPR} = \frac{\sum_{i=1}^{N} \left( \sum_{\alpha} |a_{i\alpha}|^2 \right)^2}{\left( \sum_{i=1}^{N} \sum_{\alpha} |a_{i\alpha}|^2 \right)^2}.
\]

For a completely localised state, which will be expressible in terms of orbitals at only one atomic site, the IPR will be one; for a completely delocalised state, which is comprised of a linear combination of equal parts of orbitals at all atomic sites, the IPR will be \( N^{-1} \); and for a state which is intermediate between localised and delocalised, the IPR varies continuously between one and \( N^{-1} \).

In the following we have normalised the calculated IPR values to the IPR value of the electron ground state with the largest IPR value (1.529x10^{-4}) in the 10% indium case, which is configuration 13, shown in Fig. 3 (b). Therefore, the normalised IPR values, IPR, can exceed values of one and can be interpreted as giving the extent to which the state under consideration is more or
less localised than the electron ground state of configuration 13 shown in Fig. 3. Normalising the IPR values in this way gives a more intuitive and visual picture of the localisation properties of the state in question.

The ground state electron and hole IPR values are shown as a function of their respective energies in Fig. 6. Figure 6(a), (b) and (c) correspond to the electron ground states in the 10%, 15% and 25% indium content systems, respectively. The data for the holes is depicted in Fig. 6(d), (e) and (f). Figure 6 confirms that the hole states are, in general, far more localised than the electron states. More specifically, we find hole states which are up to 350 times more localised than the electron ground state to which they are normalised, and never less than 5 times more localised. Furthermore, Fig. 6 reveals that the IPR values of the hole states significantly vary between different configurations, highlighting again that the hole ground states are very sensitive to the microscopic alloy structure.

To discuss the results in more detail, we start with the IPR values of the electron ground states [Fig. 6(a), (b), and (c)]. When comparing the electron IPR values for the different indium contents, we find that in general the IPR values increase with increasing indium content. Since the macroscopic strain increases with increasing indium content, the piezoelectric built-in field increases as well. Thus, with increasing indium content an increasing confinement (along the c-axis) for the electron ground state can be expected. Additionally, with increasing indium content, the considered well-width fluctuation becomes increasingly important and adds an extra in-plane confinement. This is consistent with the trends observed across Fig. 6(a-c) for the electron IPR values. However, when looking at the holes [Fig. 6(d), (e), and (f)], we see that this trend is not as clearly visible as in the electron case. This arises from several factors. In particular, the 10% indium content [cf. Fig. 6(d)], we have three exceptionally strongly localised states. Their IPR values are of the order of, or even exceed, the maximum values of the 15% [Fig. 6(e)] and 25% [Fig. 6(f)] indium case. Therefore, to treat these exceptional states accurately, a larger number of configurations would have to be considered to perform more reliable statistical averages. However, this is beyond the scope of the present study. Here we are mainly interested in identifying general trends and to gain first insights into the effects of random alloy fluctuations on the electronic structure of c-plane InGaN/GaN QWs with varying indium contents.

Based on the results presented, the argument of an increased built-in field with increased indium content, used to explain the trends in the electron ground states, cannot be directly applied to the hole states. The reason for this is that the hole states show not only a strong localisation along the growth direction, it is also evident from Figs. 6(d), and (e) that the hole localisation has a very strong in-plane localisation component. This component is not greatly affected by the presence of the macroscopic built-in field along the growth direction. Thus the localisation behaviour of the hole states is less dominated by the macroscopic built-in field and governed more by fluctuations in the local indium environment. Consistent with this, we find very large changes in the IPR values of the ground state hole wave functions between different configurations at nominally the same indium content, even though the macroscopic built-in field should be very similar for a fixed indium content. Further to this, we note a tendency for localisation (IPR) to increase as the holes become more strongly confined, with a general rise from left to right in each of Fig. 6(d), (e), and (f); nevertheless, the fluctuations in the IPR values are about as large as the trend itself.

So far we have focused our attention on localisation effects in ground state properties. This provides key information for experiments performed at low temperatures. However, when the optical properties of c-plane InGaN/GaN QWs are studied experimentally at ambient temperature, or when InGaN based devices are operating at room temperature, excited states become relevant. Thus a knowledge of the localisation characteristics of excited electron and hole states is also important for understanding c-plane InGaN QWs. This is the focus of the next section.

B. Excited states

After studying the ground state localisation properties by means of the IPR values, here we apply the same metric to the excited states. We start by investigating, in Fig. 7 selected configurations for 10%, 15% and 25% indium before looking at results averaged over the 20 different random configurations, considered for each composition. The benefit of studying selected configurations first is that we can then display the results both as a function of the energy and the state number. This is not possible for the averaged data where the data is best displayed as a function of the state number. This stems from the fact that the ground state energies fluctuate significantly between different configurations [cf. Fig. 6]. The configurations selected here have a ground state IPR value which is close to the average IPR of all the ground states of that indium content, for electrons and holes. Figure 7 shows the IPR values for the first 60 electron and hole states as a function of the energy, measured with respect to the corresponding ground state energy. We take the absolute value of this energy difference so that with increasing energy the states move deeper into the valence or conduction band. The state numbers are given on the second x-axis at the top of each figure. Figure 7 reveals a greater energy range covered by the first 60 electron states than by the 60 hole states. This is due to the larger hole effective mass in comparison with the electron effective mass. This results in a smaller spacing between two sequential hole states than for electrons and
FIG. 7. Normalised electron (top row) and hole (bottom row) inverse participation ratios (IPR) plotted against the state energy as measured from the conduction or valence band edge. The results are given for particular representative configurations with indium contents of 10%, 15% and 25% (see text for selection criteria). The IPRs are normalised with respect to the IPR of the most localised 10% electron ground state, which is configuration 13.

Looking at the electron states first, we note that in general the IPR values for the first few excited states increase with increasing indium content [Fig. 7(a), (b) and (c)]. We attribute this effect to the increasing piezoelectric built-in field with increasing indium content. A similar trend is also observed for the hole states [Fig. 7(d), (e) and (f)]. For instance, the IPR values of the first 5 hole states increase with increasing indium content. Thus, one can expect that for the holes, the energy depth into the valence band to which there are still localised states found, increases with increasing indium content. This is consistent with the experimentally observed increase of the PL width, stokes shift, and absorption edge broadening with indium content. The localised states in this energy range are sometimes referred to as “tail states” due to the manner in which they modify the form of the density of states; the localised states appear as a

consequently 60 hole states cover a smaller energy range than 60 electron states.

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Electrons

| State number | IPR | (E_s - E_{cbe}) meV |
|--------------|-----|---------------------|
| 5            | 2   | 0                   |
| 10           | 1.5 | 100                 |
| 20           | 1   | 200                 |
| 45           | 0.5 | 400                 |
| 50           | 0.5 | 500                 |

Holes

| State number | IPR | (E_s - E_{vbe}) meV |
|--------------|-----|---------------------|
| 2            | 2   | 0                   |
| 10           | 1.5 | 100                 |
| 25           | 1   | 200                 |
| 35           | 0.5 | 300                 |
| 40           | 0.5 | 400                 |
| 50           | 0.5 | 500                 |

\[
\text{IPR} = \frac{\langle |\Psi|^2 \rangle}{\langle |\Psi|^2 \rangle^2}
\]
properties of these systems at elevated temperatures.

So far we have focused our attention only on selected configurations. To illustrate the generality of the observed behaviour in the excited states, Fig. 8 displays the IPR values for the first 60 (a) electron and (b) hole states averaged over the 20 different configurations. These averaged normalised IPR values are denoted by $\text{IPR}_{\text{AVG}}$. The results are shown for 10% (dashed green line), 15% (red solid line), and 25% (dashed-crossed blue line) indium. Overall it is evident that the hole states show much stronger localisation effects [higher IPR values] when compared with the electrons. Figure 8 also corroborates the earlier observed trend that with increasing indium content there is an increased persistence of localisation effects into the valence and conduction bands.

In an infinite system, the energy beyond which there are no more localised states can be expected at a definite energy, $E_{\text{mob}}$, referred to as the mobility edge. However, even when using periodic boundary conditions, one is left with a system of finite size. While each of these systems represents a portion of the real QW, there remain finite-size effects that would not be present in the real, laterally infinite, QW. For example, even though the highest valence state generally has a very high IPR value in our finite-sized supercells, the most weakly bound of these states may be resonant with delocalised QW states in the infinite system. We refer to such states of our finite systems as “quasi-localised” states. These states should be excluded in estimations of the energy range of localisation. Taking this into consideration, we can nevertheless combine the results obtained for the ground and excited states in order to gain a first estimate of the energy range of localised states which exist in the valence band before the onset of delocalisation. We refer first to Fig. 6 where it is evident that the ground state energies for the holes vary by at least 100 meV across different random indium configurations. We further note from Fig. 6 that all of these hole states have very high IPR values and can thus be considered strongly localised in comparison with the electrons. Taking a conservative measure for the localisation depth and keeping in mind the ”quasi-localisation” effect described above, we consider only the four energetically highest valence states for each indium concentration studied to estimate the depth of localisation in the valence band. This gives us approximately an energy spread of 50-60 meV.

Turning now to the excited state data, we see, from the selected configurations studied in Fig. 7 that, for instance, in the 10% indium case strong localisation effects ($\text{IPR}_{\text{AVG}} > 10$) extend for at least an energy range of 40 to 50 meV below the hole ground state. With increasing indium content this range further extends [cf. Figs. 7(e) and (f)]. That these are not atypical behaviours in our ensemble is supported by reference to Fig. 8. Hence, combining the conservative estimate for the energy range of localised states inferred from our ground state data and the insights from the excited state studies, we estimate that already in case of 10% indium a total spread of localised states amounts to $\approx 100$ meV. Thus, we expect an energy range of at least 100 meV over which there will be a significant density of localised valence states in c-plane InGaN/GaN QWs with indium contents at above or equal to 10%.

Even though we cannot determine the density of localised states exactly, we can still analyse how the wave function overlap between carriers in different states is af-
FIG. 9. Modulus wave function overlaps, $\sigma_{\text{nm}}$, of the first 40 states for electrons and holes in particular configurations of In$_x$Ga$_{1-x}$N/GaN QWs with indium contents of 10% ($x=0.1$), 15% ($x=0.15$), and 25% ($x=0.25$). The magnitude of the modulus overlap between state $n$ and $m$ is indicated by the color of the point $(n,m)$ on the plot.

Electrons

(a) 10%

(b) 15%

(c) 25%

Holes

(d) 10%

(e) 15%

(f) 25%

Table of values for $\sigma_{\text{nm}}$

| $\sigma_{\text{nm}}$ | $\sigma_{\text{nm}}$ | $\sigma_{\text{nm}}$ |
|---------------------|---------------------|---------------------|
| $\sigma_{\text{nm}}$ | $\sigma_{\text{nm}}$ | $\sigma_{\text{nm}}$ |

value for many states $\psi_m$ will then have a widely spread out wave function. Conversely, if a state $\psi_j$ has a small $\sigma_{jm}$ for many other states, $\psi_m$, it means that the wave function $\psi_j$ is localised in a particular spatial region of the QW. Note that we are dealing here with the modulus overlap; our definition for the overlap does not take into account the parity of the respective wave functions. Our metric simply indicates the extent to which the densities of the involved carriers are spatially coincident.

Figure 9 (a),(b), and (c) show, for the same configurations chosen in Fig. 7, the modulus overlaps, $\sigma_{\text{nm}}$, of each electron state with every other electron state. The data for the hole states are displayed in Fig. 9 (d),(e) and (f). We have considered the first 40 electron and hole states. The left column, (a) and (d), contains the...
results for 10% indium, the middle column, (b) and (d), the data for the 15% indium case while the right column, (c) and (f), depicts the situation for the QW with 25% indium.

We begin our analysis by focusing on the modulus hole wave function overlap $\sigma_{nm}^h$ [Fig. 9 (d), (e) and (f)]. In the 25% case, (f), there are three distinct regimes in $\sigma_{nm}^h$ visible. Over the first five states a dark region of very poor overlap [small $\sigma_{nm}^h$ value] is visible. This indicates a region of strongly localised states, with the hole localisation length well below the supercell size (10 nm) considered here. This is consistent with the very high IPR values shown in Fig. 6. After the first five states, from state 6 to 10, we find a region of “semi-localised” states, with $\sigma_{nm}^h$ values around 0.3 to 0.7. Beyond these states we find an area in the $\sigma_{nm}^h$ plot that has values between 0.7 and 1. We classify these states as “delocalised states”. Looking at the 15% indium case [Fig. 9 (e)] we find again these three regions but with the “delocalised” region being much larger, and both the “semi-localised” and “localised” region being greatly reduced. For the 10% indium case it is very hard to discern a region which could be described as “strongly localised” in the same sense as for 25% indium, but there is still clearly visible a “semi-localised” region. Consistent with our discussion of Figs. 7 and 8, it can be concluded that for the holes the location of the “mobility edge” depends on the indium content.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig10}
\caption{Planar integrated probability densities of electrons, $P_i^e(z_m)$, [(a),(b) and (c)] and holes, $P_i^h(z_m)$, [(d),(e) and (f)] in c-plane InGaN quantum wells with indium contents of 10%, 15% and 25%, for the first 40 states. The index $i$ refers to the state number, and the index $m$ refers to the layer of the quantum well. The boundaries of the quantum well active region are indicated by blue dashed lines on the figure. To emphasise the different colour scales, a different colour scheme has been used for electrons and holes.}
\end{figure}
Looking at the electron states, in the upper row of Fig. 9, the minimum values of $\sigma_{nm}^e$, are much larger [$\sigma_{nm}^e \approx 0.4$] when compared to the holes [$\sigma_{nm}^h \approx 0.05$]. We attribute this to the fact that the electron states, as discussed in Sec. [V A], are less perturbed by the alloy fluctuations. The light and dark overlap “bands” of the figure correspond to the overlaps between states localised inside the QW and states which start to spread into the GaN barrier material. When looking at the positions (state numbers) of the dark regions with low $\sigma_{nm}^e$ values, we find that these regions in general move to higher state numbers with increasing indium content. The different positions (state numbers) of these “bands” for the different indium contents can be imputed to changes in the conduction band confinement potential. Please note that with increasing indium content, the electron wave functions also begin to become localised by the well-width fluctuations, which then also affects $\sigma_{nm}^e$.

To support these arguments and to further clarify the features seen in the $\sigma_{nm}^e$ values, we now present the planar integrated probability density, $P_i$, of each state $\psi_i$:

$$P_i(z_m) = \sum_{k,l} |\psi_i(x_k,y_l,z_m)|^2,$$

where $x_k$ and $y_l$ are the in-plane (c-plane) indices and $z_m$ denotes the layer index along the c axis. The quantity $P_i(z_m)$ gives the probability that the electron or hole state $i$ be found in the layer specified by the index $z_m$. This allows us to shed light on the localisation characteristic of the different states along the c axis.

Figure 10 shows $P_i(z_m)$ plotted for the first 40 elec-
FIG. 12. Modulus wave function overlaps of the 40 electron and hole states, in In$_x$Ga$_{1-x}$N/GaN quantum well systems averaged over 20 different microscopic configurations. The averaged overlaps are denoted by $\bar{\sigma}_{eh}^{nm}$. The data are shown for three different indium contents, 10%, 15% and 25%.

tron [upper row] and hole states [lower row] for 10%, 15% and 25% indium [left to right in Fig. 10]. In each figure, the horizontal axis denotes the state number and $P_i(z_m)$ is given on the vertical axis. Thus the point (1,2) will give the probability that the electron/hole described by the first eigenstate be found in the second layer of the supercell. As a guide to the eye we indicate the QW boundaries as (blue) dashed lines. Figure 10 confirms that much of the structure observed in the $\sigma_{nm}^{eh}$ values displayed in Figs. 9 (a-c), arises from variations in overlap with increasing height, $z_m$, in the QW. Conversely, Fig. 10 indicates that for the holes it is primarily the in-plane separation and in-plane variation in overlap, rather than the separation in $z_m$, that leads to the structure observed in $\sigma_{nm}^{eh}$ shown in Figs. 9 (d-f).

So far we have focused our discussion on selected configurations to illustrate trends in the localisation characteristics of ground and excited states. In order to demonstrate the generality of these results we have calculated the modulus wave function overlap averaged over all configurations for each of the indium contents considered here. This is denoted by $\bar{\sigma}_{nm}^{eh}$ for electrons, and $\bar{\sigma}_{nm}^{eh}$ for holes. The $\bar{\sigma}_{nm}^{eh}$ results are displayed in Fig. 11 which shows that $\bar{\sigma}_{nm}^{eh}$ reflects the trends observed in the selected configurations [cf. Fig. 9]. Notably, the overlap structure in the electrons is preserved. For the holes the different regimes of localisation are again apparent across the different indium contents, especially the increasing width of the “strong-localisation” region with increasing indium content.

To gain further insight into the impact of random alloy fluctuations and varying indium content on the electronic and optical properties of c-plane InGaN/GaN QWs, we analyse in a next step the modulus overlap, $\sigma_{nm}^{eh}$, of the first 40 electron and hole wave functions. The results are shown in Fig. 12. The data give first indications of how the emission efficiency of the QWs are affected by changes in the indium content. Our results reveal that with increasing indium content the electron and hole modulus wave function overlap decreases. This effect can be attributed primarily to the increasing strain-dependent macroscopic piezoelectric polarization field in the QW. Consequently, one observes a stronger spatial separation of the electron and hole wave functions along the c-axis. However, the increasing in-plane localisation introduced by well width and alloy fluctuations, which also increase with increasing indium content (from 10% to 25%), as shown earlier, will also contribute to an increasing reduction in overlap. This finding is consistent with previous experimental studies on InGaN/GaN QWs, wherein the internal quantum efficiency decreases rapidly with increasing indium content for long emission wavelengths. However, our data indicates also that when looking at $\sigma_{nm}^{eh}$ for a fixed indium content, the modulus overlap is state number dependent and increases in general with increasing state number. For instance, when looking at the electron ground state, $n = 1$, in the in 10% In case, we find a low $\sigma_{nm}^{eh}$ value for hole states with $m < 5$, while the value is clearly larger when $m > 35$. This indicates a more efficient radiative recombination rate for transitions involving the electron ground states and excited hole states. We attribute this behavior to the effect observed in Fig. 11 wherein regions of “delocalised hole states” are found.
TABLE I. Comparison between calculated average ground state transition energies (Calc) and experimental PL peak energies (Exp) obtained at low temperatures ($T = 6 K$) in In$_x$Ga$_{1-x}$N/GaN c-plane QWs. The QW well width is denoted by $L$ and the transition energies/PL peak position energies are given by $E_g$.

|       | $x$ | $L$ (nm) | $E_g$ (eV) |
|-------|-----|----------|------------|
| Exp   | 0.25| 3.3      | 2.162      |
| Calc  | 0.25| 3.5      | 1.964      |
| Exp   | 0.15| 2.9      | 2.707      |
| Calc  | 0.15| 3.5      | 2.533      |
| Exp   | 0.12| 2.7      | 2.994      |
| Calc  | 0.10| 3.5      | 2.871      |

V. COMPARISON WITH EXPERIMENTAL DATA

In a first step of our theory-experiment correlation we analyse the calculated average ground state transition energies and compare them with measured PL peak energies from the literature. The data are summarised in Table I. The here considered indium contents $x$ are very close to the experimental values; however, we have kept the well width $L$ constant, while in the experiment this quantity varies between the different samples. Nevertheless, the reported theoretical data is in good agreement with the experimental values, and given that our well width in general is larger than the experimental value, we slightly underestimate the PL peak energies.

Our theoretical findings on the nature of the localisation in these systems also support several experimental studies and their proposed explanations. For instance, the experimentally observed shift in the PL peak position with temperature, usually referred to as the “S-shape” dependence, is normally attributed to the existence of localised carriers in c-plane InGaN/GaN QWs. Based on our data we can conclude that localisation effects play not only a significant role in ground but also in excited hole states. This is even the case in c-plane InGaN/GaN QWs with as little as 10% indium. From our data we expect an energy range of order 100 meV over which there will be a significant density of localised valence states in c-plane InGaN/GaN QWs. This is consistent with the minimum energy ranges which can be inferred from the blue shift due to thermal redistribution amongst localised states in temperature dependent PL and electroluminescence (EL) experiments, which ranges from 55 - 200 meV.

VI. CONCLUSION

In summary, we have presented a detailed analysis of the electronic structure of c-plane In$_x$Ga$_{1-x}$N/GaN QWs with indium contents of $x = 0.1$, 0.15 and 0.25, covering the experimentally relevant range. To perform this analysis we have used a fully atomistic description, including local alloy, strain and built-in field variations arising from random alloy fluctuations. In addition to going beyond the usually applied continuum-based description for these systems, we give insight into not only ground state properties but also excited state properties.

From our analysis we conclude that for as little as 10% indium in the QW, the valence band structure is strongly affected by localisation effects. Our results indicate that well width fluctuations could lead to electron wave function localisation effects in addition to localisation effects introduced by random alloy fluctuations. These observations hold not only for ground states but also for excited states. From an initial estimate of our data, we conclude that even at 10% indium in the well, we are left with an energy range of order 100 meV into the valence band that should be dominated by strongly localised states. Our data also indicate that this energy range increases with increasing indium content. Experimental data, such as the “S-shape” dependence of the PL peak position with temperature gives clear experimental evidence of the presence of such (excited) localised states. Our theoretical findings are therefore consistent with experimental
observations.

Moreover, by looking at (modulus) wave function overlaps between the first 40 hole or electron states, we gained initial insights into the probability of transferring carriers from one site/state to another. Our investigations indicated different regimes ranging from strongly “localised states” up to “delocalised states”. While the localised states have very little overlap with all other states, the delocalised states reveal a high overlap with most of the other considered states. These features are relevant for experimental studies at ambient temperature and transport properties. In particular, the strong wave function localisation should affect the hole transport in c-plane InGaN-based multi-QW LEDs significantly. The observed localisation effects will impact both the vertical transport along the c-axis through the different QWs, and also the lateral transport and thus how the carriers spread within the growth plane of the QW. Thus, these localisation features are relevant in general for InGaN-based devices operating at room temperature and above. The obtained data will now form the basis for more detailed transport and in general device-related calculations.

Finally, our theoretical study showed that built-in field, random alloy and well width fluctuations lead to the situation of independently localised electron and hole wave functions in c-plane InGaN/GaN QWs. This holds for as little as 10% indium in the QW. This finding is consistent with the “pseudo 2-D donor-acceptor pair” model proposed by Morel et al.13 to explain time resolved PL measurements of c-plane InGaN/GaN QWs.

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