

Impact of carrier-density screening on Urbach-tail energies and optical polarization in (Al,Ga)N quantum well systems

Robert Finn^{1,*}, Michael O'Donovan², Thomas Koprucki², and Stefan Schulz^{1,3}

¹*Tyndall National Institute, University College Cork, Cork T12 R5CP, Ireland*

²*Weierstrass Institute (WIAS), Mohrenstr. 39, 10117 Berlin, Germany*

³*School of Physics, University College Cork, Cork T12 YN60, Ireland*



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Aluminum gallium nitride [(Al,Ga)N] presents an ideal platform for designing ultraviolet (UV) light emitters across the entire UV spectral range. However, in the deep-UV spectral range (<280 nm) these emitters exhibit very low quantum efficiencies, which in part is linked to the light-polarization characteristics of (Al,Ga)N quantum wells (QWs). In this study, we provide insight into the degree of optical polarization of (Al,Ga)N QW systems operating across the UV-C spectral range by means of an atomistic multiband electronic structure model. Our model not only captures the difference in valence-band ordering in AlN and GaN but it also accounts for alloy-disorder-induced band-mixing effects originating from random alloy fluctuations in (Al,Ga)N QWs. The latter aspect is often not captured in widely employed continuum-based models. The impact of alloy disorder on the electronic structure is studied in terms of Urbach-tail energies, which reflect the broadening of the valence-band density of states due to carrier-localization effects. We find that especially in wider wells, Urbach-tail energies are reduced with increasing carrier densities in the well, highlighting that alloy-disorder-induced carrier-localization effects in (Al,Ga)N QWs are also tightly linked to electrostatic built-in fields. Our calculations show that for QWs designed to emit at the longer-wavelength end of the UV-C spectrum, carrier density and well width are of secondary importance for their light-emission properties, meaning that one observes mainly transverse electrical polarization. However, for (Al,Ga)N QWs with high Al contents, we find that both well width and carrier density will impact the degree of optical polarization. Our calculations suggest that wider wells will increase the degree of optical polarization and may therefore be an option to improve the light-extraction efficiency in deep-UV light emitters.

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I. INTRODUCTION

The semiconductor alloy aluminum gallium nitride [(Al,Ga)N] has gained significant attention in the past decade as the direct band gap of this semiconductor alloy can in principle span the entire UV range [UV-A (315–400 nm), UV-B (280–315 nm), and UV-C (200–280 nm)]. Applications that require efficient UV light sources, e.g., light-emitting diodes (LEDs) or lasers, operating over this wide spectral window include water purification, sterilization, plant lighting, sensing, etc. [1]. (Al,Ga)N-based UV light-emitting devices come with significant advantages over widely employed low- and medium-pressure

mercury lamps, as they (i) provide flexible and tunable wavelengths, (ii) do not require toxic mercury, (iii) show no warm-up time, and (iv) exhibit extremely long lifetimes [1,2]. However, when compared to indium gallium nitride [(In,Ga)N], which is used in light emitters operating in the visible spectral range, current UV-light-emitting devices utilizing (Al,Ga)N alloys still exhibit poor external quantum efficiencies, especially in the deep-UV range (<280 nm). Multiple factors contribute to the low efficiency of, e.g., (Al,Ga)N LEDs, which include high threading dislocations and point-defect densities, poor radiative recombination rates, and low light-extraction efficiencies (LEEs) [1]. The latter two aspects in particular are tightly linked to fundamental properties of (Al,Ga)N alloys and heterostructures. First, the thermodynamically stable phase of (Al,Ga)N alloys is the wurtzite crystal structure [1,3] and its lack of inversion symmetry results in a spontaneous polarization field along the wurtzite c axis. In a nitride heterostructure, e.g., an $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_y\text{Ga}_{1-y}\text{N}$ quantum well (QW), which lies at the heart of UV LEDs, discontinuities

*Contact author: robert.finn@tyndall.ie

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in spontaneous polarization lead to strong electrostatic built-in fields [1,4,5]. In addition, the lattice mismatch between $\text{Al}_x\text{Ga}_{1-x}\text{N}$ and $\text{Al}_y\text{Ga}_{1-y}\text{N}$ gives rise to a strain-induced piezoelectric polarization field [6]. These electrostatic built-in fields result in a spatial separation of electron and hole wave functions in a QW, affecting and reducing the radiative recombination rate [7]. Moreover, the LEE is impacted by the valence-band ordering in an (Al,Ga)N heterostructure. In general, while in both GaN and AlN the conduction-band minimum and the valence-band maximum are at the Γ -point, the valence-band structure of AlN is different from that of its GaN counterpart [8–13]. More specifically, the valence-band edge (VBE) in AlN is formed by a band of Γ_7 symmetry with p_z orbital character. The radiative recombination process involving this band and the conduction band at the Γ -point results in light that is mainly of transverse-magnetic (TM) polarization, where the electric field, $\mathbf{E}$, is orientated parallel to the c axis. In GaN the VBE is of Γ_9 character [12,13]; in this case, the emitted light is mainly transverse-electric (TE) polarized, with $\mathbf{E}$ orientated perpendicular to the c axis. For transverse-magnetic fields (TM, $\mathbf{E} \parallel \mathbf{c}$) the transmission pattern is in the c plane (the growth plane). As a consequence, the extraction through the (0001) surface for TM-polarized light is much smaller when compared to transverse electric (TE, $\mathbf{E} \perp \mathbf{c}$), where the emission pattern is both in and out of the c plane [14–16]. As LED structures are in general surface emitting, the TM-polarized light emission is detrimental for the LEE and thus the efficiency of the device [16–21]. The Al content in the well, but also quantum confinement and strain effects, affect the crossover from TE to (purely) TM polarization in (Al,Ga)N-based LEDs. In addition to these factors, experimental and theoretical studies already give indications that alloy-disorder-induced carrier-localization effects significantly impact the optical properties of (Al,Ga)N QWs [22–25]. Carrier localization can, e.g., manifest through a broad photoluminescence (PL) linewidth or broad absorption spectra, where the latter is often described in terms of Urbach-tail energies [26–28].

The impact of alloy disorder on the degree of optical polarization (DOP), usually defined as the ratio of TE- to TM-polarized emission [10,29], is largely unexplored in theoretical studies of (Al,Ga)N QWs, as it presents a significant challenge for several reasons. First, standard and widely available one-dimensional (1D) multiband $\mathbf{k} \cdot \mathbf{p}$ simulations of (Al,Ga)N QWs and heterostructures describe the alloy by averaged material parameters; local fluctuations in the alloy content are neglected [30,31]. Second, modified continuum-based models, which allow for local fluctuations in alloy content in a three-dimensional (3D) simulation, have recently been employed to describe the impact of alloy disorder on the electronic and optical properties of (In,Ga)N QWs; such studies are in general based on single-band effective-mass models [32–34].

These single-band models cannot intrinsically capture alloy-disorder-induced valence-band mixing effects and would have to be extended to modified 3D multiband $\mathbf{k} \cdot \mathbf{p}$ models. However, studies using these more sophisticated continuum-based models are sparse for (Al,Ga)N systems. A recent study employing such an advanced treatment also relies on a combination of single-band effective-mass approximation and localization-landscape theory to obtain the carrier-confinement energy landscape underlying a 3D multiband $\mathbf{k} \cdot \mathbf{p}$ model [17]. Third, to treat carrier-localization effects, atomistic calculations are in principle an ideal starting point. However, to do so, large (in-plane and out-of-plane) supercells are required to capture both disorder in the growth plane but also barrier materials. First-principles approaches, such as density-functional theory (DFT), can provide the required microscopic insight into the electronic structure of III-N materials and alloys. For “conventional” DFT implementations, however, large supercells present a significant, basically unfeasible, computational challenge [35,36].

In recent years, empirical tight-binding models (ETBMs) have demonstrated that they can capture carrier-localization effects accurately on an atomistic level while at the same time allowing for the treatment of very large supercells [35]. We have developed ETBMs to describe the electronic structure of (Al,Ga)N bulk and QW systems [24, 37]. Here, we employ this atomistic multiband model to gain insight into Urbach-tail energies and the DOP of (Al,Ga)N-based QWs. In (Al,Ga)N heterostructures, theoretical studies on Urbach-tail energies are sparse and the connected broadening of the density of states is most often treated as a free adjustable parameter in, e.g., $\mathbf{k} \cdot \mathbf{p}$ calculations of optical gain [25,28]. Moreover, the broadening of the density of states can also impact the DOP, an aspect usually not considered in previous theoretical studies. Given that alloy composition and quantum confinement on a macroscopic level will play an important role for the electronic structure of (Al,Ga)N wells in general, we investigate QWs with two distinctly different alloy compositions ($\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ and $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$) and of varied well widths ($L_w = 1.3$ nm, 2.3 nm, and 3.3 nm). $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ wells often form the active region of UV-C emitters operating at the longer-wavelength end of the UV-C spectrum [28,38]. Based on experimental [38] and theoretical ($\mathbf{k} \cdot \mathbf{p}$) [28,39,40] literature data, these emitters are expected to mainly emit TE-polarized light. On the other hand, $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QWs have been chosen to investigate a system emitting (i) in the deep-UV range and (ii) mainly TM-polarized light; similar Al contents are reported in the literature for deep-UV emitters, both experimentally [41–43] and theoretically ($\mathbf{k} \cdot \mathbf{p}$ models) [28,39,40,43]. It should be noted that we have kept each system fixed at the same 15% Al composition contrast between well and barrier. Thus, our analysis should allow

for a comparative investigation between emitters operating in two distinct UV-C wavelength ranges. We note that in previous studies, to keep the emission wavelengths fixed [17,44,45], well width and Al content have often been changed simultaneously. In that case, strain and polarization fields as well as quantum confinement change, making it difficult to disentangle the impact of all these factors on, e.g., the DOP. Therefore, our studies allow for focusing on the different effects separately. Moreover, our investigations also target varying carrier densities in the well, in order to gain insight into experimental relevant settings.

Our atomistic multiband investigations reveal that carrier confinement, especially for narrower wells, e.g., $L_w = 1.3$ nm, is much weaker in the high-Al-content system $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ when compared to the $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ QW structures. While this effect may be beneficial for carrier transport in multi-QW structures operating in the deep-UV spectral region, the connected carrier leakage may also lead to an increase in defect-related recombination.

When studying the DOP of the QW systems considered, we find that wider wells lead to a higher DOP value, which in general is desired for good LEEs for UV LEDs. However, in $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ wells, this finding is of secondary importance, as the light emitted for all well widths and carrier densities studied is already predominantly of TE polarization. For the higher-Al-content structure, the $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ wells, the situation is more subtle. While the DOP increases with increasing well width, it is in general still TM polarized. We observe that the shift toward TE polarization with increasing well width is stronger in the lower-carrier-density regime, e.g., $n = 1 \times 10^{18} \text{ cm}^{-3}$. Nevertheless, even for a high carrier density of $n = 1 \times 10^{20} \text{ cm}^{-3}$, an $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QW of width $L_w = 3.3$ nm still exhibits a slightly higher DOP when compared to the same system with a width of $L_w = 1.3$ nm. This again highlights the potential benefit of wider wells in terms of improving and tailoring the LEE in deep-UV (Al,Ga)N-based emitters.

The paper is organized as follows. In Sec. II, we discuss the theoretical background of our studies, while in Sec. III we present our results. Finally, a summary and our conclusions are given in Sec. IV.

II. THEORETICAL BACKGROUND

In Sec. II A, we provide an overview of differences in the valence-band structure of AlN and GaN systems, which are important for understanding the DOP in (Al,Ga)N-based QWs. The electronic structure model underlying our investigations of the density of states (DOS) and the DOP is outlined in Sec. II B; the (Al,Ga)N QWs studied in this work are discussed in Sec. II C.

A. Valence-band structure of AlN and GaN

The DOP in (Al,Ga)N alloys is tightly linked to the symmetry properties of the valence bands involved in the optical transitions between conduction and valence bands. Given the direct-band-gap nature of both wurtzite GaN and AlN, the symmetry of the three valence bands energetically closest to the band edge at the Γ -point plays an important role for the DOP; lower-lying valence states are energetically far away from the VBE at Γ . In general, the symmetry of the energetically highest-lying three valence bands can be described by p_x -, p_y -, and p_z -like orbitals or respective linear combinations [3]. Crystal-field splitting and spin-orbit coupling (SOC) lift the degeneracy between these bands, which are sometimes termed as A , B , and C valence bands [29,46,47]. However, the ordering of these bands depends on several factors. For instance, the crystal-field splitting energy, Δ_{cr} , in AlN is of *opposite* sign to Δ_{cr} in GaN or InN. In the literature, Δ_{cr} values can vary [48,49] but for AlN, $\Delta_{\text{cr}}^{\text{AlN}} \approx -200$ meV, whereas for GaN, $\Delta_{\text{cr}}^{\text{GaN}} \approx 30$ meV. The sign of Δ_{cr} determines which valence band forms the VBE, as the SOC energy is usually small, particularly when compared to other III–V material systems [50].

The polarization state of the light emitted via the radiative recombination process involving the conduction-band edge (CBE) and the VBE is determined by the symmetry (orbital character) of the VBE state at the Γ -point. Due to the negative $\Delta_{\text{cr}}^{\text{AlN}}$ value in AlN, the VBE is formed by the so-called C band, which is of Γ_7 symmetry [12,13]; this band is sometimes also called the crystal-field split-off hole (CH) band. Energetically below the C band are the A and B bands, which are mainly split by the small SOC energy in nitrides (approximately 10–20 meV) [50]. The A band is of Γ_9 [12,13] symmetry and is often labeled as the heavy-hole (HH) band; the B band, or light-hole (LH) band, has Γ_7 symmetry. In terms of the basis states forming these bands, the upper Γ_7 band exhibits mainly p_z -like character, while both Γ_9 and Γ_7 are mainly p_x - and p_y -like in character [10]. For GaN, due to the positive crystal-field splitting energy, the valence-band order is reversed: the VBE is the A band, while the B and C bands are energetically below the VBE [12,13,29,48]. Given the difference in the orbital character/symmetry of the VBE, light emitted from AlN is TM polarized because the p_z orbitals forming the VBE are orientated along the growth direction and $\mathbf{E} \parallel \mathbf{c}$. Since the VBE in GaN is formed by p_x - and p_y -like basis states, the light-emission pattern is more involved. In this case, where $\mathbf{E} \perp \mathbf{c}$, it leads to emission perpendicular to but also within the growth plane [14]. However, in general, the emission pattern for GaN (or low-Al-content systems) is denoted as TE polarized [8–10,16,17,29] and regarded as emission mainly along the c axis of the underlying wurtzite crystal, at least compared to emission of pure TM-polarized light. We follow this widely used definition here. As standard

UV (Al,Ga)N LEDs are top- and bottom-surface emitting and are grown along the wurtzite c axis, TE-polarized light emission is desired to achieve a high LEE of the device [10,16–18].

The above highlights that the valence-band ordering in (Al,Ga)N-based QWs plays an important role when designing UV LEDs, especially in the deep UV, where high Al contents in the active region are required. However, in addition to the Al content, further factors impact the valence-band ordering in $\text{Al}_x\text{Ga}_{1-x}\text{N}/\text{Al}_y\text{Ga}_{1-y}\text{N}$ wells. These factors include contributions from strain [17], quantum confinement, and built-in polarization fields [10].

In Fig. 1, we give a schematic illustration of how strain, confinement, and built-in fields affect the valence-band ordering in an (Al,Ga)N system. A high Al content is assumed in Fig. 1, so that the VBE is given by the C band (p_z -like band) and the band ordering is illustrated in the absence of strain, confinement, and built-in polarization-field effects. The evolution of Δ_{cr} with Al content determines the energetic separation of the bands in a strain-free bulk (Al,Ga)N system. In our previous work [37], we have found a nonlinear behavior of Δ_{cr} with Al content, in good agreement with experimental studies. The impact of in-plane biaxial compressive strain on the band structure, as, e.g., found in a QW structure, is illustrated in Fig. 1(b). With respect to the unstrained case, the A and B bands are shifted to higher energies, while the C band shifts to lower energy. Depending on the strain and Al content in the well, this may already lead to a crossover of the C

and A/B bands, but in any case a reduced energy separation between the C band (p_z -like states) and A and B bands (mainly p_x - and p_y -like states) is expected. Again it should be noted that the magnitude of $\Delta_{\text{cr}}(x)$ in the alloy will play an important role for the energetic separation of the bands. The reduced energetic separation between the different bands can thus lead to band-mixing effects (e.g., mixing of p_x -, p_y -, and p_z -like states), which affects the DOP.

In Fig. 1(c), we visualize the impact of quantum confinement along the c axis on the band separation. This type of confinement further reduces the energetic separation of the three bands in our example. This stems from the fact that the effective hole mass of the C band along the confinement or growth direction is lower when compared to the A and B bands; e.g., in AlN, $m_{\parallel}^{h,C} = 0.25m_0$ and $m_{\parallel}^{h,A} = 3.125m_0$ [48], where $m_{\parallel}^h$ denotes hole effective mass (calculated far from the Gamma point) parallel to the c axis. Therefore, to tailor the valence-band ordering and thus the light-polarization characteristics, one may adjust the QW width to modify and control the quantum confinement. However, this may also be achieved by changing the contrast in Al composition between well and barrier, since this will modify the valence-band offset.

A further factor that affects the confinement in a III-N well is the built-in polarization field. This field spatially separates electron and hole wave functions by localizing them at opposite interfaces of the well. Thus, the hole wave function may be confined to a length smaller than the well width L_w ; this “additional” confinement can further influence the valence-band ordering, as schematically indicated in Fig. 1(d). Several factors impact the strength of this field, including the composition difference between QW and barriers and the overall strain in the well and barrier. However, with an increasing carrier density in the QW, the polarization field may be screened so that this polarization-field-induced confinement effect is reduced. This means that the valence-band ordering in an (Al,Ga)N QW system can also be carrier-density dependent.

The above is based on the assumption that in an (Al,Ga)N QW, all these different contributions can be described on a macroscopic level, i.e., that local features of the alloy microstructure are of secondary importance. Our recent calculations [24], but also experimental data [22,51], indicate that alloy disorder can give rise to carrier-localization effects in (Al,Ga)N QWs. Such localization effects can be driven by local strain, confinement, and polarization-field fluctuations and, e.g., lead to a broadening of the density of states, introducing an Urbach tail. The importance of these microscopic features for the DOP are not well understood and require a 3D multiband electronic structure model to capture alloy-disorder-induced valence-band mixing effects in (Al,Ga)N QWs. A recent 3D $\mathbf{k} \cdot \mathbf{p}$ study [17] has focused primarily on the impact of

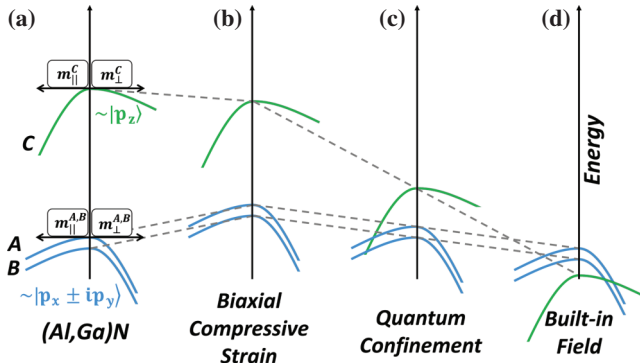


FIG. 1. A schematic illustration of the valence-band order for high-aluminum-content-containing (Al,Ga)N systems when (a) unstrained, (b) under biaxial compressive strain, (c) in the presence of quantum confinement, and (d) with intrinsic built-in fields. The heavy-hole, light-hole, and crystal-field split-off bands are denoted as the A , B , and C bands, respectively. Note that our schematic is to highlight general trends. Quantum confinement will break the translation invariance, e.g., along the wurtzite c axis, and a band structure cannot be defined along this direction. The above should, however, indicate how quantized energy levels that are constructed from, e.g., $|p_z\rangle$ -like basis states are affected by confinement effects.

substrate strain on the DOP, while Urbach-tail energies and how the broadening of the density of states changes with Al content, well width, or carrier density are not reported. Given the importance of the density of states for the DOP in (Al,Ga)N systems, we target Urbach-tail energies and the DOP in the framework of an atomistic multiband electronic structure model that captures both macroscopic and microscopic contributions. The theoretical framework used is outlined below.

B. Empirical tight-binding model

As already mentioned in the previous section, alloy disorder can influence the electronic and optical properties of (Al,Ga)N QWs significantly. To address the impact of alloy disorder on the electronic structure and ultimately the DOP on an atomistic level, we employ a nearest-neighbor multiband sp^3 ETBM. The details of the model have been presented in our previous work in detail on bulk and QW systems [24,37]. The main ingredients involve a valence-force-field model to determine relaxed atomic positions in an (Al,Ga)N QW. To account for polarization-field effects stemming from, e.g., (local) strain fields, we have developed a local-polarization-potential method. This method has been benchmarked against DFT-based Berry-phase calculations. The tight-binding parameters required for the sp^3 ETBM have been treated as parameters and determined by fitting the ETBM electronic band structure to hybrid functional DFT band structures. To model alloys with this approach, the ETBM hopping-matrix elements are set according to nearest-neighbor anion-cation species; for the on-site energies of Ga and Al atoms the respective bulk values are used. In case of N atoms, weighted averages of the on-site bulk values in AlN and GaN are employed; the weighted averages are determined by the number of Ga and Al atoms as nearest neighbors of a N atom; this is a widely used approximation in ETBMs [52–54]. A valence-band offset of 0.9 eV for AlN/GaN is assumed, which lies within the range of reported values of 0.85–1.15 eV [55,56]. To account for strain effects, a local strain tensor is calculated and via a Pikus-Bir approach included as a site-diagonal correction in the ETBM Hamiltonian [57]. The required deformation potentials are again taken from hybrid functional DFT studies. Finally, the (local) built-in polarization potentials are included as an on-site diagonal correction to the Hamiltonian. Overall, our ETBM has been benchmarked against experimental data, showing a good agreement in terms of the energy gap of bulk $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys as a function of the Al composition x [37]. Moreover, good agreement between ETBM and experiment have been found for the optical-polarization switching in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ bulk alloys [37]. Based on these previous studies, our established ETBM presents an ideal starting point to investigate the impact of alloy disorder on the DOP in (Al,Ga)N QW systems.

C. Model quantum well system, density of states, and degree of optical polarization

Overall, our aim is to study the impact of alloy disorder on the electronic and optical properties or, more specifically the DOP, of (Al,Ga)N-based QWs operating in different wavelength windows. In general, the emission wavelength of such structures is mainly tailored by adjusting the Al content and well width. As discussed above, both factors will impact the valence-band ordering and thus the DOP. We focus on two systems in the following, targeting the upper UV-C range (approximately 280 nm) and deep-UV-C emitters (approximately 230 nm) to gain insight into similarities, but also differences, in these wavelength ranges.

The first QW system investigated is an $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}$ well with an $\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ barrier. Such structures are often considered in the literature to realize emitters in the upper UV-C range [28,38]. Literature data show that these systems exhibit TE-polarized light emission [28,38–40,43]. To also study the impact of alloy disorder on electronic and optical properties of (Al,Ga)N-based emitters in the deep-UV-C range, we investigate $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$ QWs with $\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ barriers. For such structures, literature results find TM-polarized light emission due to the high Al content in the well [10,39,40,43].

We note that while the Al content in the well and the barrier is different for the two structures, the Al content *contrast* between the barrier and the well is kept constant in our studies. Furthermore, the Al content in the underlying substrate plays a role for the strain state in the QW-barrier system and thus the DOP [17], particularly for systems with a high Al content in the active region [22,23,40]. Here, we assume that the wells and barriers are strained to a pure AlN substrate.

To investigate the impact of the well width, L_w , on the DOP, we consider, for both systems, three different well widths, namely, $L_w = 1.3$ nm, 2.3 nm, and 3.3 nm. The electronic structure of the (Al,Ga)N well systems with the different well widths discussed above is modeled with our atomistic ETBM on supercells with dimensions of approximately $10 \times 9 \times 10$ nm³ (81 920 atoms).

To gain insight into the DOP, it is important to note that in an “ideal” QW structure, i.e., in the absence of carrier-localization effects, the valence sub-band structure also plays an important role. At elevated temperatures or carrier densities, carriers may not only populate the topmost valence sub-band but also energetically lower-lying bands, which in (Al,Ga)N wells may exhibit different orbital and as such different light-polarization characteristics. Thus, in general, an orbital resolved DOS can provide important insight into the DOP and how it changes with, e.g., well width or Al content. However, in the presence of alloy-disorder-induced carrier-localization effects, defining valence sub-bands is in general not possible, since

the in-plane wave vector is no longer a good quantum number. Moreover, carrier-localization effects lead to a broadening of the DOS, usually characterized by a so-called Urbach tail and a corresponding Urbach-tail energy. Thus, it is useful to study changes in the Urbach-tail energies for (Al,Ga)N QW systems before turning to the DOP. While we focus in the following on the Urbach-tail energies, we also note that alloy disorder can lead to changes in the band structure further away from the band edges. Prominent examples where these effects become important include alloy-disorder-induced carrier scattering [58] or Auger-Meitner recombination processes [59,60].

We focus on Urbach-tail energies for the valence band, as (i) our previous studies have shown that alloy-disorder effects impact hole states more significantly than electron states and (ii) the DOP is tightly linked to the orbital character of the valence (hole) states. In order to do so, we calculate the hole density of states (h-DOS) employing the atomistic ETBM introduced above. However, further factors need to be considered when discussing Urbach-tail energies. As already mentioned above, the intrinsic electrostatic built-in field in an (Al,Ga)N QW is screened with increasing carrier density in the well. As a consequence, the electronic structure of a well is also changed and, as such, impacts the Urbach tails and the DOP. In order to account for the polarization-field screening effect, a self-consistent Schrödinger-Poisson calculation is required. However, performing a self-consistent ETBM-Poisson calculation on our large atomistic 3D supercell for different well widths and (Al,Ga)N QW systems as well as varying carrier densities is numerically prohibitive. Instead, we employ the method established in Ref. [59], in which the screening potential at a given carrier density in the well is determined by a self-consistent 1D Schrödinger-Poisson calculation, which is then included in the full atomistic ETBM. Diagonalizing the “screened” ETBM Hamiltonian accounts for changes in the electronic structure due to built-in field screening effects, while still accounting for the impact of alloy disorder. Our recent studies on (In,Ga)N QW systems have shown that the method outlined produces results in good agreement with experiment in terms of, e.g., carrier densities at which screening of the built-in field becomes significant or the onset of the efficiency droop [59]. Therefore, we adopt this same approach here for (Al,Ga)N QW systems.

To cover carrier densities relevant to the efficiency droop in III-N LEDs ($n \approx 10^{19} \text{ cm}^{-3}$) [23,60–62] and thus to be able to provide insight into trends in the Urbach-tail energy and the DOP in this regime, we study carrier densities between $n = 1 \times 10^{18} \text{ cm}^{-3}$ and $n = 1 \times 10^{20} \text{ cm}^{-3}$. While at typical LED operating conditions, carrier densities of the order of $n = 1 \times 10^{20} \text{ cm}^{-3}$ are not found, in optical-excitation studies, such high carrier densities can be realized [23,61] and are considered in theoretical studies of, e.g., Auger-Meitner recombination processes. Thus,

the carrier-density regime beyond $n \approx 1 \times 10^{19} \text{ cm}^{-3}$ is important for III-N-based light emitters.

Having described how the electronic structure is obtained when accounting for carrier-density screening effects, the DOS and Urbach-tail energies are determined as follows. Given the finite supercell size, a sufficiently large number of (i) alloy microstructures and (ii) calculated single-particle states need to be considered to be able to resolve the Urbach-tail energies. Looking first at the number of single-particle states, the hole energies from all configurations are collated and grouped into energy bins for each (Al,Ga)N QW system and carrier density. The size of these energy bins can now be adjusted to avoid empty bins and to reduce the number of required alloy configurations explicitly calculated. However, at the same time the bin size cannot be too large, as otherwise the Urbach-tail energies are “washed out.” We find that for the chosen supercell size, 150 alloy configurations and 150 states per alloy configuration strike a balance between accuracy and computational effort, and also to accommodate the high carrier densities discussed above. The bin sizes have been adjusted for each system, since the quantum confinement and thus the electronic structure is affected by changes in the well width and carrier-density-dependent screening effects.

Taking the $L_w = 3.3 \text{ nm Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ QW as an example, in Fig. 2 we demonstrate how Urbach-tail energies, E_U , for the holes are determined. In general, the VBE of unstrained AlN is used as the zero of energy. Strain and polarization fields will shift energies with respect to the unstrained AlN VBE. Moreover, instead of looking at the h-DOS itself, we take the derivative of

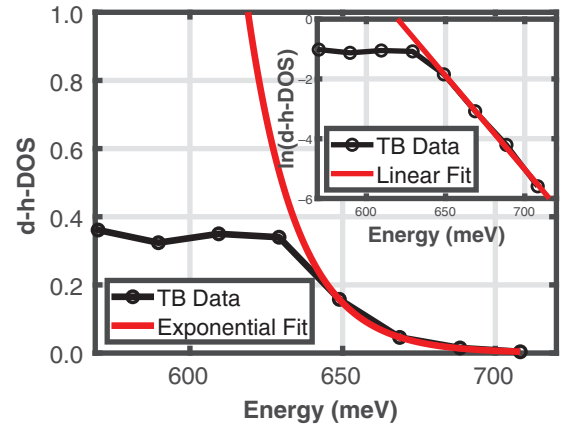


FIG. 2. The derivative of the hole density of states (d-h-DOS) calculated for the $L_w = 3.3 \text{ nm Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ QW at low carrier densities, i.e., in the absence of built-in field screening effects. Tight-binding (TB) data (black circles) and the exponential fit to the Urbach tail (red line) are given. The inset shows the natural logarithm of the TB d-h-DOS data fitted with a linear function.

h-DOS (d-h-DOS) with respect to energy, ε , numerically. The reason for this is that the modification to the DOS due to alloy disorder, the Urbach tail, can be described by an exponential tail, $\propto \exp(-(\varepsilon/E_u))$; in the “standard” DOS for an ideal QW (parabolic band), the h-DOS would exhibit a piecewise constant dependence on energy. Taking the derivative of h-DOS with respect to energy ε , one can identify the Urbach-tail region in the d-h-DOS, which is again $\propto \exp(-(\varepsilon/E_u))$. Thus, this allows us to extract E_u from the ETBM data. The exponential tail in d-h-DOS is clearly visible in Fig. 2. The inset figure displays the natural logarithm of the data, which reflects the expected straight line. From the slope of the line of best fit, E_u is extracted. This method is employed below to determine E_u for the considered QW systems at different carrier densities.

III. RESULTS

In this section, we discuss the Urbach-tail energies and DOPs of (Al,Ga)N QW systems. Special attention is paid to the impact of (i) Al content, (ii) well width, and (iii) carrier density on the results. In Sec. III A, we start with the lower-Al-content system, namely, $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ QWs, before turning to the higher-Al-content structure, $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$, in Sec. III B.

A. $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ quantum well systems

In Sec. III A 1, we analyze the Urbach-tail energies of $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ QWs of different widths. In Sec. III A 2, the DOP is studied.

1. Urbach tails

Following the procedure outlined in Sec. II C, in Fig. 3 we display the extracted Urbach-tail energies, E_u , for $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ QWs of different widths L_w as a function of the carrier density, n , in the well. In the low-carrier-density regime, $n = 1 \times 10^{18} \text{ cm}^{-3}$, the Urbach-tail energy increases with increasing L_w . This finding indicates that with increasing well width, hole-localization effects increase. It is also revealed in Fig. 3 that at least for the $L_w = 2.3 \text{ nm}$ and $L_w = 3.3 \text{ nm}$ systems, the Urbach-tail energy E_u decreases with increasing carrier density. E_u changes by approximately 3 meV in both systems when increasing the carrier density from $n = 1 \times 10^{18}$ to $n = 1 \times 10^{20}$, which corresponds to a reduction of approximately 20% in E_u and indicates that alloy-disorder-induced carrier localization is amplified by the built-in field. This conclusion is further supported by the data from the $L_w = 1.3 \text{ nm}$ system, in which the potential drop across the QW is smaller when compared to the wider well system. For the narrower well width, E_u is approximately constant and may even slightly exceed the

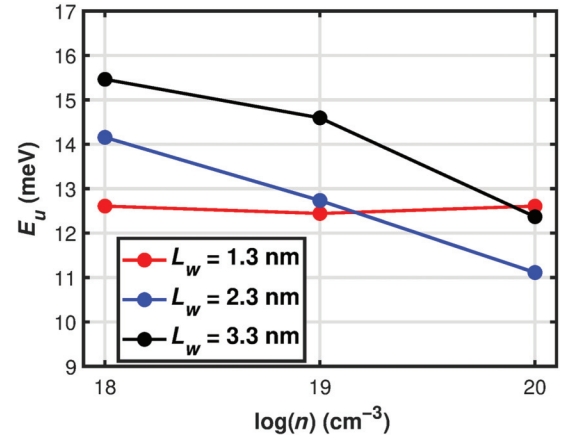


FIG. 3. The Urbach-tail energy, E_u , for $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ QWs of width $L_w = 1.3 \text{ nm}$ (red), $L_w = 2.3 \text{ nm}$ (blue), and $L_w = 3.3 \text{ nm}$ (black) as a function of carrier density n .

Urbach-tail energies of the systems with $L_w = 2.3 \text{ nm}$ and $L_w = 3.3 \text{ nm}$ at high carrier densities.

To gain further insight into the interplay of carrier-localization effects and the built-in field, we discuss in the following the planar integrated probability density [63],

$$P_m(k) = \sum_{ij} \sum_{\alpha} |c_{ijk}^{\alpha,m}|^2, \quad (1)$$

which builds on the ETBM wave function ψ_m , expressed as

$$\psi_m = \sum_{ijk} \sum_{\alpha} c_{ijk}^{\alpha,m} \phi_{ijk}^{\alpha}. \quad (2)$$

The spatial x , y , and z coordinates of the $N = 81\,920$ lattice sites in the supercell are labeled above by i , j , and k , respectively. The sp^3 ETBM basis states are denoted by ϕ_{ijk}^{α} , with $\alpha \in \{s, p_x, p_y, p_z\}$, and $c_{ijk}^{\alpha,m}$ being the expansion coefficients at each of the lattice sites for the single-particle hole state m . The expansion coefficients for a given state m are obtained by diagonalizing the ETBM Hamiltonian.

The quantity $P_m(k)$ gives the probability that the hole state ψ_m is found in the layer specified by k along the c axis of the system. In Figs. 4(a)–4(f), $P_m(k)$ is displayed for an arbitrarily chosen configuration for the three well widths considered. The data are plotted for low ($n = 1 \times 10^{18} \text{ cm}^{-3}$) and high ($n = 1 \times 10^{20} \text{ cm}^{-3}$) carrier-density values; the color bar is kept fixed for easier comparison between the different systems and thus to gain a first insight into the question of how screening of the built-in field changes carrier-localization effects in wells with different well widths and carrier densities. The maximum of the color bar is determined by the maximum $P_m(k)$ value found in the $L_w = 3.3 \text{ nm}$

$\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QW system at a carrier density of $n = 1 \times 10^{18} \text{ cm}^{-3}$, which is discussed in Sec. III B.

In general, Figs. 4(a)–4(f) highlight that carrier-confinement effects along the c axis arise from (i) the polarization field and (ii) the well width. However, information about in-plane localization effects is also encoded in $P_m(k)$: for a wave function that is delocalized in the c plane and along the growth direction, $P_m(k)$ will not exhibit strong variations. Therefore, the absence of large variations in $P_m(k)$ for a given state is indicative of the absence of strong carrier-localization effects both due to built-in field and alloy disorder, in the growth plane and along the c axis.

For the low carrier density of $n = 1 \times 10^{18} \text{ cm}^{-3}$, Figs. 4(a)–4(c) reveal the expected behavior, namely, that the built-in polarization field confines the hole charge density to the lower QW-barrier interface. In Figs. 4(a)–4(c), we also show that the impact of the built-in polarization field is less pronounced in the $L_w = 1.3 \text{ nm}$ QW system [Fig. 4(a)], as the potential drop is much smaller

in this system when, e.g., compared to $L_w = 3.3 \text{ nm}$. In the $L_w = 2.3 \text{ nm}$ [Fig. 4(b)] and $L_w = 3.3 \text{ nm}$ [Fig. 4(c)] QWs, the hole wave functions are clearly confined to much shorter lengths along the c axis than the quantum confinement introduced by the respective QW width (indicated by dashed lines). The confinement lengths here may even be below or close to 1.3 nm .

Therefore, at low carrier densities, the hole wave function for the $L_w = 2.3 \text{ nm}$ and $L_w = 3.3 \text{ nm}$ QW experiences strong confining potentials, which are driven by the large potential drop present in these systems. In the $L_w = 1.3 \text{ nm}$ well, the quantum confinement due to the well width plays a larger role. Due to the strong confinement regime in all three cases, local fluctuations in Ga content can then lead to carrier-localization effects, given the lower band gap of GaN, when compared to AlN and the high effective hole masses in general [24].

With increasing carrier density in the well, the built-in field is screened. In Figs. 4(d)–4(f), we display $P_m(k)$ at the higher carrier density of $n = 1 \times 10^{20} \text{ cm}^{-3}$. The screening effect is of secondary importance for the

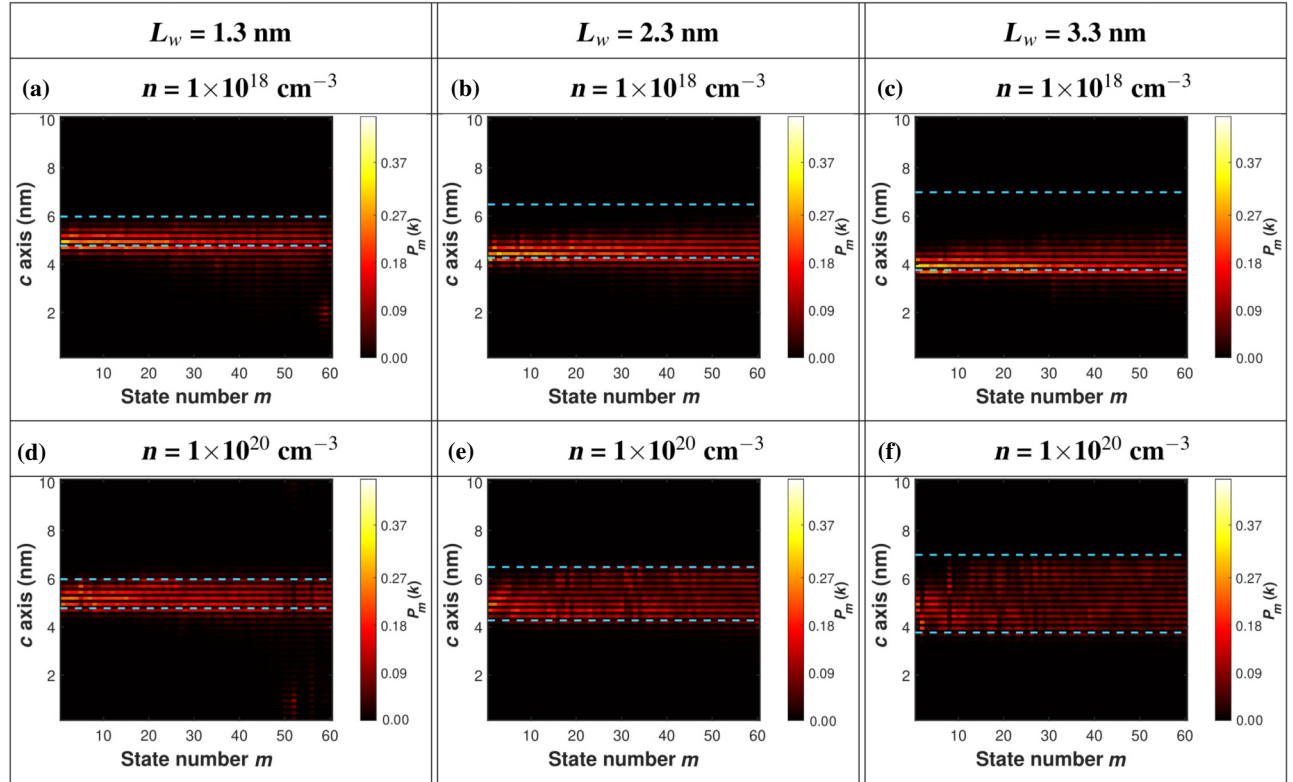


FIG. 4. The planar integrated probability densities of holes, $P_m(k)$, for an arbitrarily chosen alloy configuration of $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ QWs of width (a),(d) $L_w = 1.3 \text{ nm}$, (b),(e) $L_w = 2.3 \text{ nm}$, and (c),(f) $L_w = 3.3 \text{ nm}$. The data are displayed at carrier densities of (a)–(c) $n = 1 \times 10^{18} \text{ cm}^{-3}$ and (d)–(f) $n = 1 \times 10^{20} \text{ cm}^{-3}$, for 60 hole states. Index m refers to the single-particle hole state number, with $m = 1$ being the ground state, while k refers to the layer in the supercell along the wurtzite c axis. The QW boundaries are indicated by the dashed light blue lines. The color bar is kept the same between the different figures and is determined by the maximum $P_m(k)$ value found in the $L_w = 3.3 \text{ nm}$ $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QW system at a carrier density of $n = 1 \times 10^{18} \text{ cm}^{-3}$, discussed in Sec. III B.

$L_w = 1.3$ nm system, as quantum confinement is to a large extent introduced by the well width and not the built-in potential. This is contrasted with the $L_w = 2.3$ nm and $L_w = 3.3$ nm wells, where the screening of the built-in field with increasing carrier density noticeably impacts carrier localization. Although there are a few energy states with a high probability of being found in certain planes, overall the charge densities tend to become more delocalized along the c axis within the QW region. As already discussed above, the absence of strong variations in $P_m(k)$ values also indicates the absence of strong in-plane carrier-localization effects. The reduction in carrier-localization effects with increasing carrier density explains the approximately 20% reduction in Urbach-tail energies shown in Fig. 3 for the wider wells. Our findings thus show that alloy-disorder-induced carrier-localization effects in wider (Al,Ga)N QWs are noticeably enhanced by polarization fields. With increasing carrier density these localization effects are strongly reduced with increasing built-in field screening effects because carrier confinement is mainly driven by the well width rather than polarization fields. However, in narrower wells this is not the case, as the potential drop is small, and even in the higher-carrier-density regime, the quantum confinement is determined to a larger extent by the narrow well width. Thus, in narrower wells, carrier localization may still be prevalent but here driven by alloy disorder rather than the polarization field.

2. Degree of optical polarization

To calculate the DOP, we follow previous work [24] and focus on the orbital character of the occupied hole/valence states as a function of the carrier density for a fixed temperature of $T = 300$ K. We assume that electron states are predominantly s -like in character, which is confirmed by our ETBM calculations. Thus, it is sufficient to focus on the valence-band structure. To do so, we define the DOP, ρ , as follows:

$$\rho = \frac{\sum_{\tilde{N}=1}^{150} \sum_i f(E_{i,\tilde{N}}, T) (I_x^{i,\tilde{N}} + I_y^{i,\tilde{N}} - I_z^{i,\tilde{N}})}{\sum_{\tilde{N}=1}^{150} \sum_i f(E_{i,\tilde{N}}, T) (I_x^{i,\tilde{N}} + I_y^{i,\tilde{N}} + I_z^{i,\tilde{N}})}. \quad (3)$$

Here, $\tilde{N}$ denotes the alloy configuration; $I_\alpha^{i,\tilde{N}}$ is the p_x ($\alpha = x$), p_y ($\alpha = y$), or p_z ($\alpha = z$) orbital contribution in the i th QW state with energy $E_{i,\tilde{N}}$; and $f(E_{i,\tilde{N}}, T)$ denotes the Fermi function at temperature T , where the (quasi) Fermi level is defined with respect to the band-edge energies and determined by the carrier density in the system. Using Eq. (3), we define that $\rho = 1$ corresponds to TE-polarized light emission from the well at a given carrier density at $T = 300$ K, while $\rho = -1$ indicates TM-polarized emission. The above approach allows us to gain insight into the

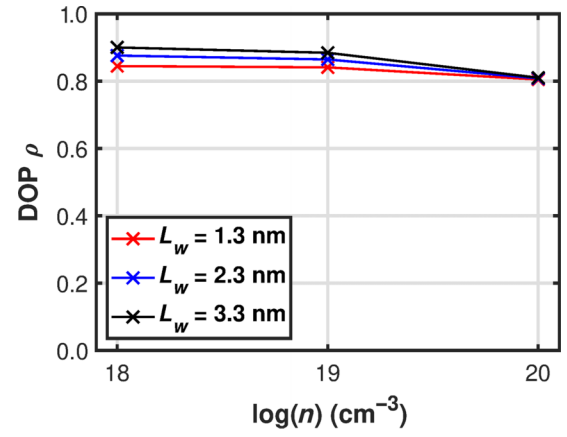


FIG. 5. The averaged degree of optical polarization, DOP ρ , over 150 configurations at a temperature of 300 K for $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ QWs of width $L_w = 1.3$ nm (red), $L_w = 2.3$ nm (blue), and $L_w = 3.3$ nm (black) as a function of the carrier density n .

light-polarization properties in general. It does not provide insight into the relative strength of TM- to TE-polarized transition, i.e., it does not provide a full emission spectrum. The above can be understood as a necessary condition for TE- or TM-polarized light emission: in the absence of, e.g., a p_x/p_y -like orbital character in a hole state, TE-polarized light emission is absent. The definition of TE- and TM-polarized light emission builds on the widely used simplified description discussed in Sec. II A. Future studies may target polarization-resolved emission spectra [64] but to shed light onto how built-in polarization fields, alloy disorder, and well width affect the DOP, Eq. (3) provides a good starting point for such an investigation.

In Fig. 5, we display the DOP for the different well widths considered, revealing that the emission of the $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}$ QW system studied is strongly TE polarized and that the well width and carrier density only slightly affect the DOP. These findings are in line with experimental and theoretical data from the literature [28,38–40,43]. Looking at the data displayed in Fig. 5 in more detail, one observes that with increasing well width L_w the DOP increases slightly, especially when considering a low carrier density $n = 1 \times 10^{18} \text{ cm}^{-3}$. Moreover, and independent of L_w , we find that with increasing carrier density, the DOP decreases slightly. We attribute these effects to changes in the electrostatic polarization field. As discussed in the previous section, the larger potential drop in the wider wells leads to stronger wave-function-localization effects at the lower QW-barrier interface (cf. Fig. 4). Given that p_z -like basis states exhibit a lower effective mass along the c axis (see the discussion in Sec. II A), one expects that states with a large p_z -orbital contribution are pushed to lower energies and thus do not contribute significantly to the DOP. This explains why the DOP increases

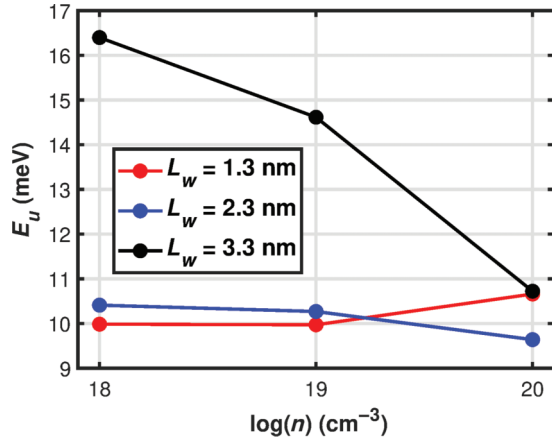


FIG. 6. The Urbach-tail energies, E_u , for $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QWs of width $L_w = 1.3$ nm (red), $L_w = 2.3$ nm (blue), and $L_w = 3.3$ nm (black) as a function of carrier density n .

slightly with increasing well width. However, with increasing carrier density, the polarization field is screened and so are carrier-localization effects, especially for wider wells. Thus, states with a higher p_z -orbital contribution may be found energetically closer to the VBE. Based on Eq. (3), if states with higher p_z -orbital character are being populated, the DOP reduces, thus explaining the slight decrease in the DOP with increasing carrier density.

Overall, our calculations show that the DOP in $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ QWs is largely determined by macroscopic effects such as strain and polarization-field effects. As we will see in the following, this is not necessarily the case at higher Al contents in the well and barrier.

B. $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ quantum well system

Having discussed Urbach-tail energies and DOP for the lower Al content wells in the previous section, we now turn to investigating these quantities for the higher-Al-content structures with $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$. As highlighted in Sec. II C, such a system would be considered when targeting emitters in the deep-UV spectral range and where competition between TE and TM polarization is important for the LEE. We start again, in Sec. III B 1, with Urbach-tail energies, before turning to the DOP in Sec. III B 2.

1. Urbach tails

In Fig. 6, we depict the Urbach-tail energies for $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QWs of $L_w = 1.3$ nm, $L_w = 2.3$ nm, and $L_w = 3.3$ nm, as a function of the carrier density n .

For the $L_w = 3.3$ nm QW system, E_u decreases with increasing carrier density. In contrast, E_u exhibits a much weaker carrier-density dependence in the $L_w = 1.3$ nm and

$L_w = 2.3$ nm wells; also, the E_u values for $L_w = 1.3$ nm and $L_w = 2.3$ nm systems are (much) smaller in magnitude when compared to the $L_w = 3.3$ nm $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$ QW or equivalent $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}$ wells (cf. Fig. 3). Furthermore, in Fig. 6 we show that the Urbach-tail energies in the $L_w = 1.3$ nm and $L_w = 2.3$ nm wells behave differently with increasing n : while E_u increases slightly with increasing n for $L_w = 1.3$ nm, for $L_w = 2.3$ nm, E_u decreases slightly.

To shed more light onto these findings, in Fig. 7 we depict the planar integrated hole probability densities $P_m(k)$ for the $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$ QWs considered. Looking at the $L_w = 3.3$ nm QW system first, we find a behavior similar to that of the $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}$ wells discussed in Sec. III A. In the low-carrier-density regime of $n = 1 \times 10^{18} \text{ cm}^{-3}$, the built-in potential leads to a strong localization of the hole wave functions at the QW-barrier interface [cf. Fig. 7(c)]. When the carrier density reaches $n = 1 \times 10^{20} \text{ cm}^{-3}$, the built-in field is screened and carrier-localization effects are reduced [cf. Fig. 7(f)]. In the high-carrier-density regime, there are only a few extremely high $P_m(k)$ values, thus indicating that alloy-disorder-induced carrier-localization effects are weaker in this regime. Overall, these findings explain the reduction in E_u with increasing n .

Turning to the $L_w = 1.3$ nm QW and comparing $P_m(k)$ for $n = 1 \times 10^{18} \text{ cm}^{-3}$ [cf. Fig. 7(a)] and $n = 1 \times 10^{20} \text{ cm}^{-3}$ [cf. Fig. 7(d)], one observes that carrier localization is very different for these systems, especially for the states near the VBE and thus close to the ground state, $m = 1$. While in the high-carrier-density regime, $n = 1 \times 10^{20} \text{ cm}^{-3}$, the hole charge densities are localized *inside* the well, for the low-carrier-density case, $n = 1 \times 10^{18} \text{ cm}^{-3}$, the charge density spreads more into the barrier material. This indicates a weaker carrier confinement in the $n = 1 \times 10^{18} \text{ cm}^{-3}$ case when compared to $n = 1 \times 10^{20} \text{ cm}^{-3}$. This means that screening the built-in field results in improved carrier confinement for the narrow well. The stronger confinement in the well leads to a slight increase in the Urbach-tail energy E_u when the carrier density increases to $n = 1 \times 10^{20} \text{ cm}^{-3}$.

The $L_w = 2.3$ nm QW system behaves similarly to the $L_w = 1.3$ nm structure in the low-carrier-density regime of $n = 1 \times 10^{18} \text{ cm}^{-3}$, which means that the hole wave functions also leak into the barrier material. Thus the Urbach-tail energies at $n = 1 \times 10^{18} \text{ cm}^{-3}$ for $L_w = 1.3$ nm and $L_w = 2.3$ nm are expected to be similar in magnitude, consistent with Fig. 6. When screening the polarization field by increasing the carrier density in the well to $n = 1 \times 10^{20} \text{ cm}^{-3}$ [cf. Fig. 7(e)], the hole wave functions start to localize inside the well again. However, in comparison to the $L_w = 1.3$ nm system, the potential drop is larger in the $L_w = 2.3$ nm QW system and, as such, screening of the built-in field becomes more important. At the highest carrier density, the wave functions are now mainly

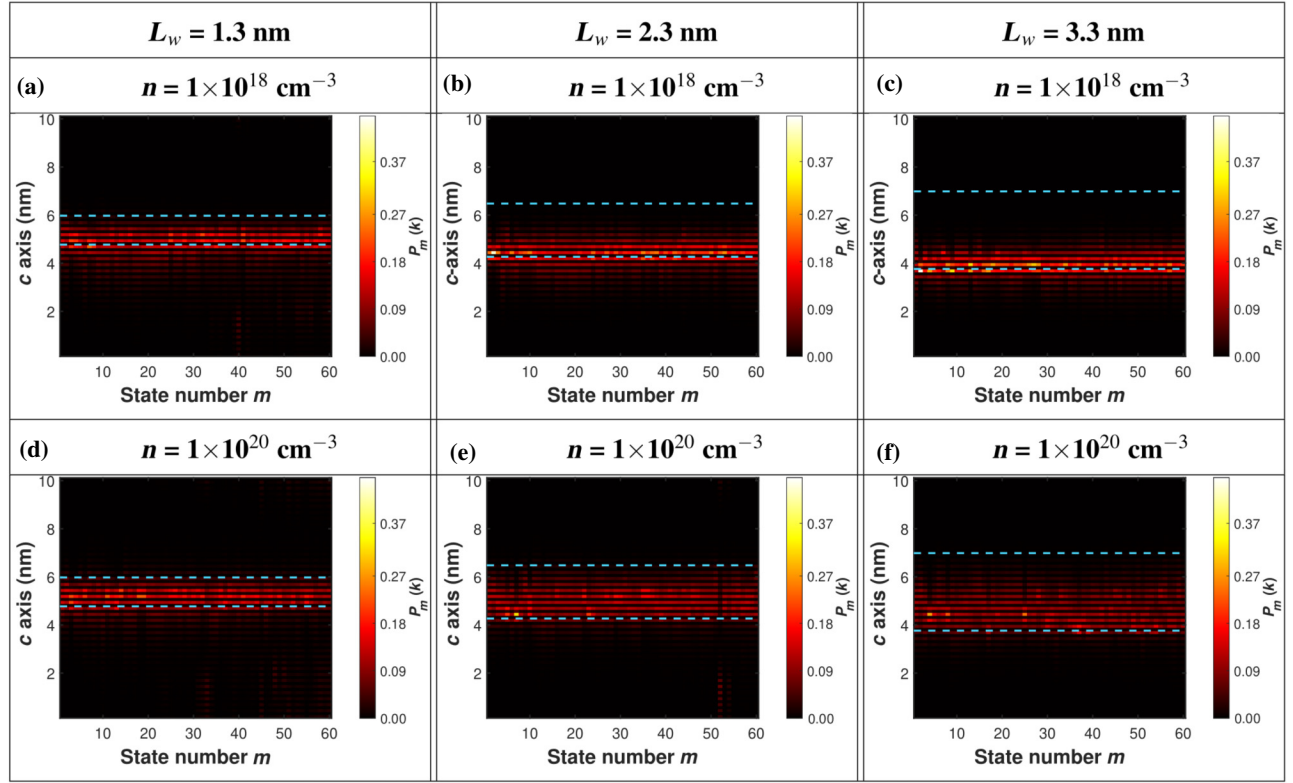


FIG. 7. The planar integrated probability densities of holes, $P_m(k)$, for an arbitrarily chosen configuration of $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QWs of width (a),(d) $L_w = 1.3$ nm, (b),(e) $L_w = 2.3$ nm, and (c),(f) $L_w = 3.3$ nm. The data are displayed at carrier densities of (a)–(c) $n = 1 \times 10^{18} \text{ cm}^{-3}$ and (d)–(f) $n = 1 \times 10^{20} \text{ cm}^{-3}$, for 60 states. Index m refers to the single-particle hole state number, with $m = 1$ being the ground state, while k refers to the layer in the supercell along the wurtzite c axis. The QW boundaries are indicated by the dashed light blue lines. $P_m(k)$ has been plotted to the maximum $P_m(k)$ value found in the $L_w = 3.3$ nm $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QW system at a carrier density of $n = 1 \times 10^{18} \text{ cm}^{-3}$.

confined by the well width, as the potential drop is strongly reduced due to built-in field screening effects. Therefore, one may expect to see a reduction in the Urbach-tail energies in the $L_w = 2.3$ nm system $n = 1 \times 10^{20} \text{ cm}^{-3}$ when compared to the $L_w = 1.3$ nm system [cf. Fig. 6], due to the hole wave function extending along a greater well width and not sampling alloy disorder of only a few monolayers as in the case of the strong built-in field at low carrier densities. In general, a reduction of the Urbach-tail energy can be attributed to a delocalization of the hole wave functions. This is supported by Fig. 7 in the sense that (i) the wave functions spread over a larger region of the QW with increasing n and (ii) large $P_m(k)$ values on only a few layers k are absent.

To further highlight changes in the carrier confinement and its impact on wave-function-localization effects, which is more difficult to quantify from visually inspecting Figs. 4 and 7 due to the unified color bar and given that these figures are based on one configuration only, in Fig. 8 we show the probability of finding the hole charge density inside the QW, $|\Psi_h^{\text{avg}}|^2$, as a function of the energy E_i^{avg} . Each energy state m is averaged over

all 150 configurations and the energy is shifted to the average ground-state energy E_1^{avg} for each QW system. Here, a higher energy means further away from the VBE. For comparison, in Figs. 8(a)–8(c) we display $|\Psi_h^{\text{avg}}|^2$ for $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}$ wells, while in Figs. 8(d)–8(f) we depict the data for the $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$ wells, at carrier densities of $n = 1 \times 10^{18} \text{ cm}^{-3}$ and $n = 1 \times 10^{20} \text{ cm}^{-3}$. Each energy level has been color coded to visualize the average orbital character. It is revealed in Fig. 8 that with increasing carrier density, the wave-function confinement inside the QW is increased due to screening of the polarization field. However, we also note that even though the Al contrast between well and barrier is the same in $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ and $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ systems, the confinement is in general weaker in the high-Al-content system (cf. Fig. 8). We attribute this effect to the combination of two factors. First, in the high-Al-content regime, QW states have a higher p_z orbital contribution. Second, p_z -like basis states or bands have a low effective mass along the wurtzite c axis (cf. Fig. 1). Thus, confinement effects and changes in confinement due to carrier-density screening will more strongly impact the electronic structure of

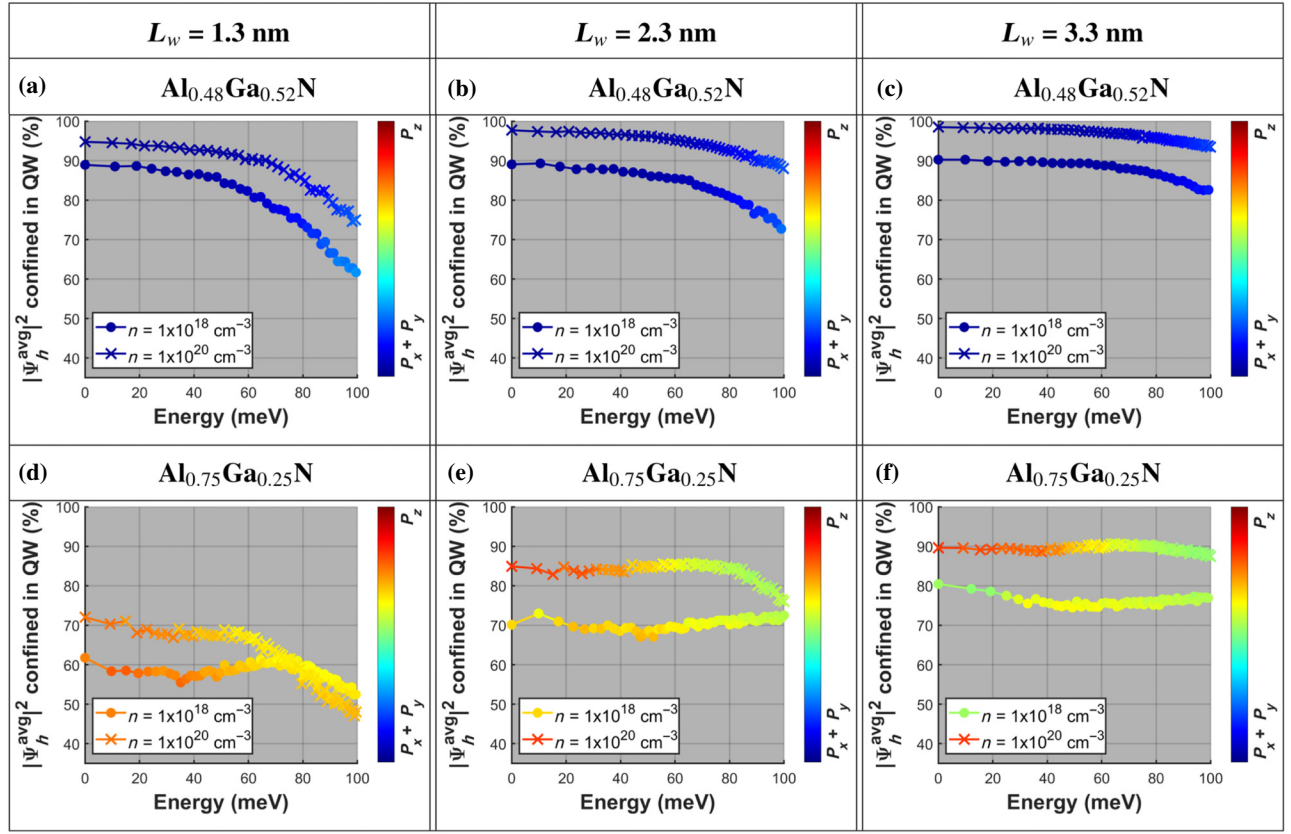


FIG. 8. The average probability of hole charge density, $|\psi_h^{\text{avg}}|^2$, confined inside the (Al,Ga)N QWs as a function of energy. The data are averaged over the 150 configurations. The average state energy is plotted with respect to the averaged ground-state energy of each QW system. (a)–(c) The $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ QWs for (a) $L_w = 1.3$ nm, (b) $L_w = 2.3$ nm, and (c) $L_w = 3.3$ nm. (d)–(f) The $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QWs for (d) $L_w = 1.3$ nm, (e) $L_w = 2.3$ nm, and (f) $L_w = 3.3$ nm. For each QW system, $|\psi_h^{\text{avg}}|^2$ is plotted for two carrier densities: $n = 1 \times 10^{18} \text{ cm}^{-3}$ (circles) and $n = 1 \times 10^{20} \text{ cm}^{-3}$ (crosses). The color coding gives the averaged orbital contribution of each energy level (red, p_z ; blue, $p_x + p_y$).

the QW. Moreover, hole wave functions with a high p_z -orbital character will be leaking into the barrier. Therefore, all this contributes to the reduced carrier confinement seen in Fig. 8. Narrow QWs with high Al contents are widely used in deep-UV LEDs [39,42]. These structures often suffer from low EQEs. Our calculations provide a possible reason for this behavior: if the wave functions are weakly confined, recombination at defects may be more likely, due to a higher probability of the hole charge densities at a defect site, assuming a delocalized electron wave function. Thus our findings suggest that using wider wells for (Al,Ga)N-based deep-UV LEDs can be beneficial for the device performance. As expected from our discussion in Sec. II A, in Fig. 8 we also confirm that the orbital character of the hole states is sensitive to QW width and carrier density. Thus, the DOP will also be impacted by these factors. It should be noted that while in Fig. 8 we display the average orbital character for each state, the population of the different states with carriers is not accounted for in this plot. In the following section, we discuss the impact of well width and carrier density on the

DOP in $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QWs for different carrier densities in more detail. Thus, we account for both the orbital character, as shown in Fig. 8, and population of the different states when evaluating the DOP.

2. Degree of optical polarization

Before turning to the DOP in $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QWs, we briefly revisit the $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}$ wells. The color coding in Figs. 8(a)–8(c) reveals that in the $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}$ QWs, the hole states in an energy range of 100 meV below the VBE are predominantly p_x - and p_y -like in orbital character. Building on our definition for the DOP ρ [Eq. (3)], this confirms the earlier finding that independent of well width or carrier density, light emitted from the $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}$ QWs will be predominantly TE polarized.

Turning, in a second step, to the $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}$ systems [Figs. 8(d)–8(f)], one finds a more complex behavior. First, one observes that the orbital character of the states varies with energy. Independent of the well width or carrier density, states near the VBE are a mixture of p_x -, p_y -, and p_z -like orbitals, in contrast to the $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}$ wells.

Looking at the low carrier density of $n = 1 \times 10^{18} \text{ cm}^{-3}$ results for the three different wells, it is indicated in Figs. 8(d)–8(f) that with increasing well width, the p_z -orbital contribution in the states energetically closest to VBE, i.e., the zero of energy, is reduced. This is indicative of an increasing DOP with increasing well width at low carrier densities. One may expect the opposite behavior, given that the quantum confinement due to the increasing well width is reduced and that the states with predominantly p_z orbital character may shift to energies closer to the VBE; this expectation is based on the fact that p_z -like states exhibit a lower effective mass along the c axis. However, with increasing well width, the potential drop across the well also increases and thus increases the carrier confinement at the well-barrier interface. This is also reflected in the increase of $|\Psi_h^{\text{avg}}|^2$ with increasing well width at the fixed carrier density of $n = 1 \times 10^{18} \text{ cm}^{-3}$. Therefore, due to the lower effective mass of p_z -like states along the c -axis growth direction, stronger confinement arising from the built-in potential will shift p_z -like states energetically away from the VBE.

With increasing carrier density, the built-in field is screened and the confinement effect introduced by this field is reduced. Consequently, at a high carrier density of $n = 1 \times 10^{20} \text{ cm}^{-3}$, the p_z orbital character near the VBE increases with increasing well width L_w , as revealed in Figs. 8(d)–8(f). Thus, at high carrier densities, the DOP is expected to decrease with increasing well width L_w .

Equipped with this insight, we use Eq. (3) to study the DOP in the $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QWs as a function of the carrier density at a fixed temperature of $T = 300 \text{ K}$. The calculated DOP values are shown in Fig. 9. The data indicate that the emission is indeed noticeably TM polarized for this high-Al-content system, which is in contrast to the $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ wells investigated in Sec. III A but in line with similar experimental observations in the literature [43].

Looking at the DOP as a function of the carrier density n for a fixed well width, in Fig. 9 we show that for the narrow well width of $L_w = 1.3 \text{ nm}$, the DOP increases with increasing carrier density. We attribute this to the effect that at low carrier densities, the hole wave functions are much weaker bound in the $L_w = 1.3 \text{ nm}$ QW system when compared to the high-carrier-density regime, which is supported by the data in Fig. 8. In the wider wells, e.g., $L_w = 2.3 \text{ nm}$ and $L_w = 3.3 \text{ nm}$, the DOP decreases with increasing carrier density. The observed behavior stems from changes in the confining potential discussed above, originating from the screening of the built-in field with increasing carrier density. Also, given that these screening effects are more pronounced in the wider well, the DOP changes with increasing carrier density n more strongly in the $L_w = 3.3 \text{ nm}$ system when compared to $L_w = 2.3 \text{ nm}$. However, even at high carrier densities of $n = 1 \times 10^{20} \text{ cm}^{-3}$, a slightly larger DOP is observed in

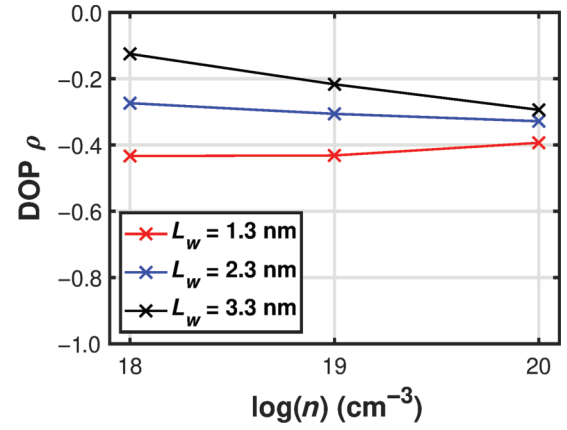


FIG. 9. The averaged degree of optical polarization, DOP ρ , over 150 configurations at a temperature of 300 K for $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QWs of width $L_w = 1.3 \text{ nm}$ (red), $L_w = 2.3 \text{ nm}$ (blue), and $L_w = 3.3 \text{ nm}$ (black) as a function of the carrier density n .

the $L_w = 3.3 \text{ nm}$ system when compared to $L_w = 2.3 \text{ nm}$ and especially $L_w = 1.3 \text{ nm}$. At lower carrier densities, this difference is even larger and favors the wider wells even more for a higher DOP value.

While narrow wells, e.g., $L_w = 1 \text{ nm}$ or $L_w = 1.5 \text{ nm}$, are often employed in deep-UV light sources [39,42], our analysis indicates that wider wells can be beneficial for these emitters for several reasons. First, as shown above, in the higher-Al-content regime, carrier confinement in narrow wells can be poor. While this may be an advantage for carrier transport in multi-QW systems, these systems can also be prone to defect-related recombination processes. Second, wider wells are promising candidates in order to lower the steady-state carrier density inside the well, which may lead to a reduction in, e.g., Auger-Meitner-related recombination processes [65]. Based on our DOP calculations, wider wells with lower carrier densities will also lead to a higher DOP value when compared to the same carrier density in a narrower well. However, it should also be noted that, in general, it is expected that the radiative recombination rate is reduced in wider wells compared to narrower wells due to the quantum confined Stark effect. In addition to this, growing wider wells can also lead to material-science-specific challenges, including strain relaxation and the formation of extended defects [66]. The latter aspect will also affect radiative recombination efficiencies [67]. However, recent experimental investigations have focused on well widths that are much larger than the range studied here, thus targeting high-quality wide well systems for UV LEDs [10,44]. Further studies are now required to analyze the competition between radiative and nonradiative recombination and the DOP in deep-UV light emitters, utilizing wider wells.

IV. SUMMARY AND CONCLUSIONS

In this work, we have analyzed the DOP in (Al,Ga)N QWs operating in the UV-C spectral range by means of an atomistic multiband electronic structure model. Our model accounts for alloy-disorder-induced band-mixing effects, which are often neglected in widely available continuum-based simulation frameworks. In our study, special attention has been paid to the impact of (i) Al content, (ii) carrier density, and (iii) well width on Urbach-tail energies and the DOP.

We have considered two (Al,Ga)N-based QW systems, which differ in the Al content in the well and barrier. However, for a consistent comparison, the Al contrast between well and barrier is kept constant in our investigations. The considered QW systems, $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ and $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ wells, are representative of structures found in the literature to achieve light emission in the deep-UV-C spectral range, $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$, and the longer-wavelength end of the UV-C window, $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$. Even though the contrast in Al content is kept constant between these two systems, our calculations show that carrier confinement, especially for narrower wells, e.g., $L_w = 1.3$ nm, is much weaker in the high-Al-content system. This effect may be beneficial for carrier transport in deep-UV light emitters with high Al content; however, it can lead also to the situation in which these emitters are more prone to defect-related recombination, since the wave functions can spread significantly into the barrier material.

In terms of the DOP, our calculations show that, in general, wider wells lead to a higher DOP value. In the lower-Al-content system, $\text{Al}_{0.48}\text{Ga}_{0.52}\text{N}/\text{Al}_{0.63}\text{Ga}_{0.37}\text{N}$ wells, this observation is of secondary importance, as the light is predominantly TE polarized, which can enable a high LEE. This finding of predominantly TE-polarized emission is independent of the well widths and carrier densities studied. The situation is more complicated in the higher-Al-content $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QW system. In general, with increasing well width, the DOP increases, so that emission is tending toward TE polarization. We observe in our study that this effect is more pronounced at lower carrier densities, e.g., $n = 1 \times 10^{18} \text{ cm}^{-3}$. However, even at high carrier densities of $n = 1 \times 10^{20} \text{ cm}^{-3}$, an $\text{Al}_{0.75}\text{Ga}_{0.25}\text{N}/\text{Al}_{0.90}\text{Ga}_{0.10}\text{N}$ QW of width $L_w = 3.3$ nm still exhibits a slightly higher DOP when compared to the same system with a width of $L_w = 1.3$ nm.

Overall, for (Al,Ga)N-based light emitters operating in the deep-UV spectral range, our calculations indicate that, in terms of carrier-confinement and light-polarization characteristics, wider wells are advantageous. However, it should also be noted that there are several challenges in using wider wells for UV light emitters. This includes, e.g., difficulties in growing high-quality low-defect-density wide QW systems. Moreover, the wider well width can

also lead to a reduction in the radiative recombination rate. These factors can offset the benefits of wider wells in terms of stronger carrier confinement in the well and an increased DOP. Therefore, future studies may target a detailed analysis of balancing these competing factors as a function of the well width in deep-UV light emitters to improve their efficiencies.

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DATA AVAILABILITY

The data that support the findings of this study are openly available at Ref. [68].

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