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Polarization matching design of InGaN-based semi-polar quantum wells—A case study of (11\(\bar{2}\)2) orientation
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Polarization matching design of InGaN-based semi-polar quantum wells—A case study of (1122) orientation

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We present a theoretical study of the polarization engineering in semi-polar III-nitrides heterostructures. As a case study, we investigate the influence of GaN, AlGaN, and AlInN barrier material on the performance of semi-polar (1122) InGaN-based quantum wells (QWs) for blue (450 nm) and yellow (560 nm) emission. We show that the magnitude of the total built-in electric field across the QW can be controlled by the barrier material. Our results indicate that AlInN is a promising candidate to achieve (i) reduced wavelength shifts with increasing currents and (ii) strongly increased electron-hole wave function overlap, important for reduced optical recombination times. © 2014 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4864478]

In recent years, III-nitrides, such as InN, GaN, AlN and their respective alloys, have attracted considerable interest since their direct band gaps span, in principle, over the whole visible spectral range. This makes them ideal candidates for optoelectronic devices, such as light emitting diodes (LEDs) and laser diodes (LDs).1 In particular, InGaN-based quantum wells (QWs) grown on c-plane GaN received much attention. However, a main drawback in realizing high performance devices based on c-plane nitride heterostructures is the inherent electrostatic built-in fields giving rise to a spatial separation of electron and hole wave functions in the active region.2 Consequently, the radiative recombination rate is significantly decreased. Moreover, due to the screening of the built-in fields, c-plane nitride-based optoelectronic devices show a large emission wavelength shift for typical operating currents.3–5 This shift is larger for LEDs emitting in green and yellow spectral regimes.

Several different approaches have been discussed in the literature to diminish the detrimental effect of these built-in fields. When using conventional c-plane substrates, the growth of quantum dots instead of QWs6,7 or polarization matching between QW and barrier material8,9 has been suggested and used. In addition, the growth on non- and semi-polar substrate orientations was applied to eliminate or reduce the electrostatic built-in fields.10–13 For example, as shown by Zhao et al.,14,15 the reduction of the electric field inside the active region can be more effective for particular semi-polar crystallographic orientations. Zhao et al. investigated structures grown on (2121) and (202T) planes and showed that LEDs with superior emission characteristic can be achieved using the (202T) orientation. It is important to note, that the built-in electric field, the optimal growth conditions, and the In incorporation differs for each semi-polar plane.

In this paper, we show that the QW emission can be optimized for a chosen semi-polar orientation. We utilize polarization matching between the QW and the barrier to reduce the built-in field in LEDs designed for operation in blue (450 nm) and yellow (560 nm) spectral regimes. More specifically, we investigate the semi-polar (1122) orientation, known for a very high indium incorporation,16 and design InGaN-based LED structures with GaN, AlGaN, and AlInN barrier layers. We show that AlInN is a promising barrier material candidate to be used in high performance LEDs. The designed InGaN/AlInN structures show large carrier wave function overlap and improved color stability, i.e., reduced wavelength shift with increasing currents. In addition, the composition of the active region as well as the barrier can be tuned to further improve the device performance at a given current density. Although shown for a particular semi-polar orientation, the method of polarization matching presented here can be used in general for any growth plane.

Our calculations use the commercial SiLENSe package17 based on a one-dimensional drift-diffusion model and including specific features of the nitride materials, e.g., strong electrostatic built-in fields arising from spontaneous and piezoelectric polarization. To take the effect of strain on the band edges into account, we first perform our own strain dependent k · p calculations and derive strain dependent band offsets. A similar approach including strain effects has recently been used by Zhao et al.14,15 In addition, it has been highlighted by different groups that the band gap bowing parameter in InGaN18,19 and even more pronounced in AlInN20,21 shows a strong composition dependence. To account for this, we include in the model composition dependent band gap bowing parameters obtained from atomistic tight-binding supercell calculations, which show a very good agreement over the whole composition range with experimental data on InGaN19 and AlInN21 alloys.

We use as a model structure a 3 nm thick InGaN single QW sandwiched between 10 nm thick barriers and p- and n-doped GaN layers as shown schematically in Fig. 1. We focus on GaN, AlGaN, and AllnN as the barrier material. Although AllnN with 18% In is lattice matched to c-plane GaN, it is not fully lattice matched to the semi-polar (1122) orientation. For an accurate modelling and design of the active region of an LED structure, strain effects are of central importance, given the large lattice mismatch between the well and the barrier material. However, when assuming AlInN barrier layers which are almost lattice matched to the
underlying GaN, strain effects are of secondary importance. For the sake of a simplified discussion, we neglect the impact of the strain on the band edges in the AlInN barrier layer region and account for their composition dependent bowing only. Given that we focus on AlInN with 20% In, in comparison to the active region, this approximation should be well justified. The composition of the AlGaN barrier with 10% of Al was chosen to match the band gap of the studied AlInN layer which is 3.53 eV at room temperature. Since the band gap of the reference GaN is around 100 meV smaller, both AlInN and AlGaN barriers should provide slightly stronger confinement of carriers inside the QW. We start the discussion with the analysis of the built-in electric fields across the QW with three different barrier materials.

It is well known that semi-polar QWs still exhibit electrostatic built-in fields, arising from orientation dependent spontaneous and piezoelectric polarization.\(^{22}\) The total built-in potential \(\varphi_{\text{tot}}\) across the QW is given by\(^{9}\)

\[
\varphi_{\text{tot}}(z) = \varphi_{\text{sp}}(z) + \varphi_{\text{pz}}(z) = \left\{ \frac{(P_{\text{sp}}^{\text{QW}} - P_{\text{sp}}^{\text{QW}}) + P_{\text{pz}}^{\text{QW}}}{2\varepsilon_0 e_{\text{QW}}} \right\} \left( |z| - \frac{h}{2} \right),
\]

where \(P_{\text{sp}}^{\text{QW}}\) and \(P_{\text{sp}}^{\text{QW}}\) are the spontaneous polarization of, respectively, the QW and the barrier, \(P_{\text{pz}}^{\text{QW}}\) is the piezoelectric polarization of the QW, and \(h\) is the QW thickness with interfaces at \(z = -h/2\) and \(z = h/2\). \(\varepsilon_0 e_{\text{QW}}\) is the QW dielectric constant, and \(\varepsilon_0\) is the vacuum permittivity. The drop of built-in electric potential \(\Delta\varphi_{\text{tot}}\) across the QW defines the strength of the spatial separation of electrons and holes and, thus, the efficiency of optical recombination. In consequence, small and large \(\Delta\varphi_{\text{tot}}\) corresponds to, respectively, high and low electron-hole wave function overlap \(\langle \psi_e | \psi_h \rangle^2\). Both spontaneous and piezoelectric contributions can effectively reduce \(\Delta\varphi_{\text{tot}}\), provided \(\varphi_{\text{sp}}\) and \(\varphi_{\text{pz}}\) are of opposite signs and comparable in magnitude. The quantities \(\varphi_{\text{sp}}, \varphi_{\text{pz}}\), and \(\varphi_{\text{tot}}\) across an \(\text{In}_{0.17}\text{Ga}_{0.83}\text{N}\) QW for GaN, AlGaN, and AlInN barrier materials in the semi-polar (1122) orientation are shown in Fig. 2. In the InGaN/GaN case, \(\varphi_{\text{tot}}\) is dominated by the piezoelectric polarization potential \(\varphi_{\text{pz}}\). However, a small amount of Al in the barrier layer results in a much stronger \(\varphi_{\text{sp}}\) which is of opposite sign to \(\varphi_{\text{pz}}\) (see Fig. 2(b)). This increase of \(\varphi_{\text{sp}}\) is due to the fact that the spontaneous polarization in AlN is roughly two times larger than in GaN.\(^{19}\) Although the \(\varphi_{\text{sp}}\) contribution is much smaller than the piezoelectric part for the studied composition, further optimization of the AlGaN layer will reduce \(\Delta\varphi_{\text{tot}}\) and improve the wave function overlap inside the active region.

In comparison to systems with GaN and AlGaN barriers, for the InGaN/AlInN structure, \(\Delta\varphi_{\text{tot}}\) is of opposite sign as shown in Fig. 2(c). Here, \(\varphi_{\text{sp}}\) is roughly twice as large as \(\varphi_{\text{pz}}\) due to a much higher AlN content. The important implication is that \(\Delta\varphi_{\text{tot}}\) across the QW with the AlInN barrier layer can be substantially reduced and be eliminated by using an InGaN QWs with higher In content. For this case, the piezoelectric contribution will increase, therefore \(\varphi_{\text{sp}}\) and \(\varphi_{\text{pz}}\) will cancel each other by polarization matching. In Fig. 3, we present \(\Delta\varphi_{\text{tot}}\) along the growth direction for the studied barriers as a function of the In content in the QW. Due to the small spontaneous polarization in the case of GaN and AlGaN, \(\Delta\varphi_{\text{tot}} < 0\) for all InGaN QWs compositions. The situation for InGaN/AlInN is more complicated. For InGaN QWs with \(\sim 29\%\) In, the system is polarization matched (\(\Delta\varphi_{\text{tot}} = 0\)). After taking the external potential of the p-n junction and the applied bias into account, our simulations indicate that at 10 A/cm\(^2\) the optimal QW composition for which \(\Delta\varphi_{\text{tot}} = 0\) corresponds to 23% In. Any variation from

![FIG. 1. Schematic illustration of a modelled LED structure.](image)

![FIG. 2. Spontaneous, piezoelectric, and total built-in potential across the \(\text{In}_{0.17}\text{Ga}_{0.83}\text{N}\) QW along the growth direction for structures with (a) GaN, (b) Al\(_{0.1}\)Ga\(_{0.9}\)N, and (c) Al\(_{0.3}\)In\(_{0.7}\)N barriers.](image)
this composition results in a non-zero drop of the potential across the active region and an increased spatial separation of the charge carriers in the QW. As a result, for the QW with In < 23%, $|\Delta \varphi_{\text{tot}}|$ decreases with an increasing InN content. Therefore, a larger wave function overlap, and a more efficient LED is expected for a QW with a higher In content. On the other hand, for the QW with In > 23%, $|\Delta \varphi_{\text{tot}}|$ increases and thus $|\langle \psi_{e} | \psi_{h} \rangle|^2$ decreases with an increasing In content similar to designs with GaN and AlGaN barriers.

We next focus our discussion on the simulation of LEDs containing the three different barrier materials. First, we consider an LED designed for blue emission at 450 nm corresponding to an InGaN QW with 17% In. Here, we focus on the emission characteristic and the carrier wave function overlap. A detailed analysis of the internal quantum efficiency droop phenomena widely discussed in the literature is beyond the scope of the present study. Figure 4(a) displays the simulated electroluminescence (EL) emission wavelength as a function of the current density and for structures with different barrier materials (GaN, AlGaN, and AlInN). Using GaN and AlGaN as barrier layers results in a large shift of the emitted light from 455 nm at 1 A/cm$^2$ to 435 nm at 1000 A/cm$^2$. The structure containing AlInN, on the other hand, behaves significantly different. The shift of the emitted light is much smaller and is less than 10 nm in the presented current range. The overall emission wavelength is, however, lower and is 440 nm at 10 A/cm$^2$. In order to compensate for this blue shift, the In content of the QW was raised from 17% to 20%. As it can be seen, the emission wavelength shift is not increased and is still smaller than that of structures with GaN and AlGaN barriers. In addition to the strongly reduced wavelength shift in the LED structure with an AlInN barrier, we find also that $|\langle \psi_{e} | \psi_{h} \rangle|^2$ is strongly increased compared to systems with GaN and AlGaN barri-

![FIG. 3. Drop of total built-in electric potential within the QW along the growth direction for structures with GaN, AlGaN, and AlInN barrier layers as a function of InGaN composition.](image)

![FIG. 4. In$_{0.17}$Ga$_{0.83}$N-based LED designed for blue emission (450 nm): Simulated EL emission wavelength (a) and squared electron-hole wave function overlap (b) for structures containing GaN, AlGaN, and AlInN barriers.](image)
AlGaN barriers show a shift of more than 30 nm in the same range of currents. Due to the large $\phi_{pe}$ and thus an increased $|\Delta \phi_{lev}|$ across the QW, $\left|\langle \psi_e | \psi_h \rangle \right|^2$ is reduced for all cases as shown in Fig. 6(b) in comparison to Fig. 4(b). Despite this fact, however, the wave function overlap for the InGaN/AlInN structure is still nearly three times larger than for structures containing GaN and AlGaN barriers. Values in the range of 10%–25% are calculated for structures with GaN and AlGaN barriers, whereas LEDs containing AlInN show values of 45%–60%. These results indicate that AlInN is a promising barrier material to be used in high performance yellow LED structures.

In summary, we studied semi-polar (1122) InGaN-based LEDs for blue (450 nm) and yellow (560 nm) emission using GaN, AlGaN, and AlInN as barrier materials. In comparison to GaN and AlGaN, structures with AlInN show a good color stability and higher electron-hole wave function overlaps. Wavelength shifts lower than 10 and 20 nm and the wave function overlap higher than 90% and 40% were calculated for emission at 450 and 560 nm, respectively. Although a large built-in electric potential drop is expected for QWs with GaN and AlGaN barriers under applied bias, it is not necessarily the case for the system containing AlInN. Here, a large spontaneous polarization of the barrier material counteracts the piezoelectric polarization and the external electric potential. As a result, the total built-in electric field inside the QW can be controlled by composition engineering of the AlInN barrier and the InGaN active region. Finally, we show that the polarization matching method used for c-plane III-nitrides can be optimized for any growth orientation.

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