Effect of strain and barrier composition on the polarization of light emission from AlGaN/AlN quantum wells

J. E. Northrup, C. L. Chua, Z. Yang, T. Wunderer, M. Kneissl et al.

Citation: Appl. Phys. Lett. 100, 021101 (2012); doi: 10.1063/1.3675451

View online: http://dx.doi.org/10.1063/1.3675451

View Table of Contents: http://apl.aip.org/resource/1/APPLAB/v100/i2

Published by the American Institute of Physics.

Related Articles

Enhanced life time and suppressed efficiency roll-off in phosphorescent organic light-emitting diodes with multiple quantum well structures
AIP Advances 2, 012117 (2012)

Metal-assisted electroless fabrication of nanoporous p-GaN for increasing the light extraction efficiency of light emitting diodes
AIP Advances 2, 012109 (2012)

Work-function-tuned multilayer graphene as current spreading electrode in blue light-emitting diodes

Spectroscopic study of white organic light-emitting devices with various thicknesses of emissive layer

Barrierless hole injection through sub-bandgap occupied states in organic light emitting diodes using substoichiometric MoOx anode interfacial layer

Additional information on Appl. Phys. Lett.

Journal Homepage: http://apl.aip.org/

Journal Information: http://apl.aip.org/about/about_the_journal

Top downloads: http://apl.aip.org/features/most_downloaded

Information for Authors: http://apl.aip.org/authors
Effect of strain and barrier composition on the polarization of light emission from AlGaN/AlN quantum wells

J. E. Northrup, C. L. Chua, Z. Yang, T. Wunderer, M. Kneissl, N. M. Johnson, and T. Kolbe

1Palo Alto Research Center, 3333 Coyote Hill Road, Palo Alto California 94304, USA
2Institute of Solid State Physics, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

(Received 7 October 2011; accepted 14 December 2011; published online 9 January 2012)

For AlGaN-based multi-quantum-well light emitters grown on c-plane substrates there is a tendency for the polarization of the emitted light to switch from transverse electric (TE) polarization to transverse magnetic (TM) polarization as the wavelength decreases. This transition depends on various factors that include the strain in the quantum well. Experimental results are presented that illustrate the phenomenon for nitride light emitting diodes (LEDs) grown on sapphire and on bulk AlN. Model calculations are presented which quantify the dependence of the TE/TM switch on the quantum well strain and the Al composition in the barriers surrounding the well. © 2012 American Institute of Physics. [doi:10.1063/1.3675451]

The AlGaN alloy system is employed to construct light emitting diodes (LEDs) and lasers operating in the deep ultraviolet (UV). An extreme example of such is the p-n junction LED in AlN that emits light at a wavelength of 210 nm. For AlGaN-based light emitters grown on c-plane substrates, several studies indicate that the polarization of the emitted light switches from transverse electric (TE) polarization to transverse magnetic (TM) polarization as the wavelength decreases. This phenomenon is illustrated in Figure 1 where we plot measured polarization for light emitting devices as a function of the wavelength. A crossover from TE to TM polarization at short wavelengths is an issue for light extraction from top or bottom emitting UV LEDs grown on the c-plane because light that propagates along the c-axis must have TE polarization. It is, therefore, desirable to engineer the active region so that TE polarization is achieved. In this paper, we demonstrate experimentally that the polarization of the light can be controlled by engineering the strain state of the active region. In addition, we present model calculations which quantify the dependence of the polarization on strain and quantum confinement of the holes in the active region.

To illustrate the effect of strain on the polarization of light emitted from AlGaN LEDs grown on c-plane we grew identical LEDs on either sapphire or bulk AlN. The growth and characterization of pseudomorphic AlGaN heterostructures on AlN substrates is described elsewhere. In each case, the light emission occurred at about 253 nm. Small differences in the wavelength arise from substrate dependent variations in the Al composition in the active zones, from variations in the quantum well widths, and from the change in the strain state. For example, our model shows that a change in quantum well strain by 1% can shift the wavelength by ~6 nm. The integrated in-plane-emitted TE and TM polarized electroluminescence light intensities, denoted by $I_{TE}$ and $I_{TM}$, were measured for each device with the setup described in Ref. 3. When these LEDs were fabricated in material grown on sapphire, the polarization was predominantly TM, but when the same device structure was grown on bulk AlN, the polarization was strongly TE. For three devices grown on sapphire (devices 2, 3, and 4 in Fig. 1), we find $P = (I_{TE} - I_{TM}) / (I_{TE} + I_{TM})$ to be negative, indicative of TM polarization. The small variations in $P$ ($AP = 0.2$) arise from different template preparation, e.g., slight differences in template composition and strain due to unintentional variations in growth processes. For an identical device grown on bulk AlN (device 1 in Fig. 1), we find a dramatic difference: $P > 0.75$. Below, we present model calculations to show that this large increase in polarization is due to the change in the strain state of the quantum wells.

The polarization of light emitted from an AlGaN quantum well laser or LED depends on the character of the lowest energy hole excitation in the quantum well (QW). If the lowest energy excitation is a heavy hole, then TE polarization is obtained. If the lowest energy excitation is a split-off hole, the

![FIG. 1. (Color online) Degree of polarization of emission from LEDs fabricated on sapphire or AlN substrates. For the devices grown on sapphire, TE polarization is obtained at wavelengths greater than ~310 nm and TM polarization is obtained for wavelengths less than ~310 nm. Device 1, in the upper left hand corner, was grown on AlN and emits highly polarized TE light at 253 nm. The quantum wells in devices 2, 3, and 4 are identical in design to device 1 but are grown on sapphire. The long dashed line is intended to illustrate the trend for LEDs grown on sapphire.](image-url)
polarization is TM. The character of the lowest energy hole state in the QW depends on the Al composition and changes from heavy-hole to split-off-hole at a certain Al composition \( x_s \). When the Al composition in the QW exceeds \( x_s \), the polarization of the emitted light switches from TE to TM.

Calculations of the quantum well state energies were performed with a \( k \cdot p \) band structure model appropriate for strained wurtzite AlGaN as discussed by Chuang and Chang. The purpose of the calculations is to determine the dependence of \( x_s \) on the strain in the QW and the Al composition in the AlGaN barrier surrounding the quantum well. For most of the calculations we employ a single QW of width 3 nm, as this is typical for LEDs. We include partially screened spontaneous and piezoelectric polarization fields in the model. The band structure parameters entering the model have been discussed in the literature. These parameters are listed in Table I.

To determine the strain in the active region, we assume that the well and barriers have been grown pseudomorphically on a substrate such as bulk AlN or \( Al_yGa_{1-y}N \). The Al composition \( y \) of the thick substrate fixes the in-plane lattice constant of each material in the structure. Variation of the parameter \( y \) is a convenient means to explore computationally a range of different active region strain states. The Al composition of the barrier is denoted \( x_{\text{bar}} \), and the Al composition of the well is denoted as \( x_{\text{well}} \). The in-plane lattice constants of the well and barrier are assumed to be the same as the substrate, and the strains in the well and barriers are obtained by employing Vegard’s law to determine the lattice constant of relaxed AlGaN.

We have calculated the energies of the QW states for selected combinations of \( y, x_{\text{well}}, \) and \( x_{\text{bar}} \). The energies of the hole states are obtained by solving the coupled effective mass equations at the \( \Gamma \) point \((k_x=k_y=0)\) of the two-dimensional Brillouin zone

\[
-\partial_z(k_{13}(z) \partial_z(g_1(n,z))) + V_{hh}(z) g_1(n,z) = e(n)g_1(n,z),
\]

(1a)

\[
-\partial_z(k_{13}(z) \partial_z(g_2(n,z))) + V_{lh}(z) g_2(n,z) + \Delta(z) g_3(n,z) = e(n)g_2(n,z),
\]

(1b)

\[
-\partial_z(k_{13}(z) \partial_z(g_3(n,z))) + V_{ch}(z) g_3(n,z) + \Delta(z) g_2(n,z) = e(n)g_3(n,z).
\]

(1c)

The effective mass terms \( k_{13}(z) \) and \( k_{1}(z) \) are determined by the parameters \( A_1 \) and \( A_3 \) and depend on the alloy composition. The potential terms \( V_{lh}(z) \), \( V_{lh}(z) \), \( V_{ch}(z) \), and \( \Delta(z) \) depend on the elastic constants, deformation potentials, and the spin-orbit and crystal field splitting. Values for these band structure parameters are listed in Table I for GaN and AlN. Linear interpolation is employed to obtain these parameters for AlGaN alloys. The piezoelectric and spontaneous polarization fields in the quantum well are determined as discussed by Bernardini for each set of \((y, x_{\text{bar}}, x_{\text{well}})\).

The total polarization field \( E_0 \) is reduced by a factor \( S \) between 0.6 and 0.3 (\( E = SE_0 \)) corresponding roughly to a free carrier density between 1 and \( 2 \times 10^{19}/cm^3 \). Energies are calculated for the three lowest energy hole excitations: \( n = 1, 2, 3 \). Examination of the envelope functions \( g_1, g_2, \) and \( g_3 \) allows us to determine the character of the hole states. TE polarized emission results when the lowest energy hole excitation is dominated by \( g_1 \), and TM polarized emission results when the lowest energy state is dominated by \( g_3 \). Typically, we perform a series of calculations employing different values of \( x_{\text{well}} \) for fixed \( y \) and \( x_{\text{bar}} \). From these calculations, we may determine \( x_s(y,x_{\text{bar}}) \).

The two envelope functions shown in Fig. 2 correspond to a heavy-hole state and a split-off hole state. These functions were obtained for \( y = 1 \) and \( x_{\text{bar}} = 1 \). The state on the left was obtained for \( x_{\text{well}} < x_s \) and is dominated by \( g_1 \), while the state on the right was obtained for \( x_{\text{well}} > x_s \) and is dominated by \( g_3 \). Due to the smaller effective mass of the split-off holes, the envelope function for the split-off hole state is less localized than that for the heavy-hole state. The split-off

![FIG. 2. (Color online) (a) Plots on the left correspond a heavy-hole state (dominated by g1) and TE polarization. (b) Plots on the right correspond to a split-off hole state (dominated by g3) and TM polarization. x_{bar} = 1 and y = 1 in both cases. The normalized envelope function for the split-off hole state shown on the right is less localized than that for the heavy-hole state on the left. The quantum well width is 3 nm. Dashed lines represent energy levels of the n = 1 state in both plots.](image-url)
hole energy is, therefore, more sensitive to the barrier potential than the heavy-hole state, and that is why changing the Al barrier composition can affect the relative energies of these two hole states.

Table II shows the dependence of \( x_s \) on the Al composition in the barrier. In this set of calculations, the quantum well thickness was fixed at 3 nm, and the layers are assumed to be grown pseudomorphically on AlN \((y = 1.0)\). The barrier composition is varied from \( x_{\text{bar}} = 0.7 \) to \( x_{\text{bar}} = 1.0 \). The critical Al composition for switching \( x_s \) increases as the barrier composition increases. By increasing \( x_{\text{bar}} \) from 0.7 to 1.0 one can extend the wavelength range for which TE polarization is obtained by about 15 nm. This dependence on \( x_{\text{bar}} \) arises because for a given \( x_{\text{well}} \) a larger barrier composition leads to greater degree of confinement of the wave-functions within the well. Since the effective mass for the states with \( p_z \)-character \((g3)\) is less than the mass of the states with \( p_x \) and \( p_y \) character \((g1 \text{ and } g2)\), the hole states with \( g3 \) character are more sensitive to confinement. The energies of states with \( g3 \) character are pushed to relatively higher values by the quantum confinement and this favors occupation of the heavy-hole state giving rise to TE polarization. For \( x_{\text{bar}} = 1.0 \), the model indicates that TE polarization may be obtained for values of \( x_{\text{well}} \) up to about 0.75 corresponding to a wavelength of around 230 nm. To examine the effect of the quantum well width on \( x_s \), we considered the system with \( y = 1.0 \) and \( x_{\text{bar}} = 0.7 \). This set of structural parameters is relevant for lasers grown on bulk AlN substrates and designed to lase near 250 nm. We determined \( x_s \) for well widths ranging between 2 nm and 5 nm and found variations in \( x_s \) of less than 0.01 for well widths in this range.

Achieving TE polarization at short wavelengths requires that the AlGaN in the quantum well be compressively strained. This can be achieved via pseudomorphic growth on bulk AlN where the in-plane lattice constant \( a_{\text{QW}} \) of the AlGaN quantum well remains equal to that of bulk AlN. If relaxation occurs, so that \( a_{\text{QW}} \) becomes larger than that of bulk AlN, the onset of TM polarization shifts to lower values of \( x_{\text{well}} \) and longer wavelengths. This effect is quantified in Fig. 3, where we plot the minimum wavelength at which TE polarization can be achieved \( (\lambda_{\text{min}} \text{ (TE)}) \) as a function of the relaxation of the in-plane AlGaN lattice constant in the well. As \( a_{\text{QW}} - a_{\text{bulk-AlN}} \) becomes larger, \( \lambda_{\text{min}} \text{ (TE)} \) increases. \( \lambda_{\text{min}} \text{ (TE)} \) also depends on the Al composition of the barrier.

**TABLE II.** This table indicates the dependence of \( x_s \) on \( x_{\text{bar}} \) for \( y = 1 \), and for screening of polarization fields \( S = 0.3 \) or \( S = 0.6 \). The width of the QW is 3 nm in all cases. As \( x_{\text{bar}} \) increases the quantum confinement in the well increases and this pushes \( x_s \) to larger values. The values of \( x_s \) are seen to be weakly dependent on the degree of screening of the polarization fields.

<table>
<thead>
<tr>
<th>( x_{\text{bar}} )</th>
<th>( x_s )</th>
<th>( \lambda_{\text{(nm)}} )</th>
<th>( y )</th>
<th>( S )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.7</td>
<td>0.65</td>
<td>245</td>
<td>1</td>
<td>0.3</td>
</tr>
<tr>
<td>0.8</td>
<td>0.685</td>
<td>240</td>
<td>1</td>
<td>0.3</td>
</tr>
<tr>
<td>0.9</td>
<td>0.72</td>
<td>235</td>
<td>1</td>
<td>0.3</td>
</tr>
<tr>
<td>1.0</td>
<td>0.755</td>
<td>230</td>
<td>1</td>
<td>0.3</td>
</tr>
<tr>
<td>0.7</td>
<td>0.64</td>
<td>246</td>
<td>1</td>
<td>0.6</td>
</tr>
<tr>
<td>0.8</td>
<td>0.67</td>
<td>242</td>
<td>1</td>
<td>0.6</td>
</tr>
<tr>
<td>0.9</td>
<td>0.71</td>
<td>236</td>
<td>1</td>
<td>0.6</td>
</tr>
<tr>
<td>1.0</td>
<td>0.755</td>
<td>230</td>
<td>1</td>
<td>0.6</td>
</tr>
</tbody>
</table>

**FIG. 3.** We plot the minimum wavelength at which TE polarization can be achieved \( (\lambda_{\text{min}} \text{ (TE)}) \) as a function of the relaxation of the in-plane AlGaN lattice constant in the well. As \( a_{\text{QW}} - a_{\text{bulk-AlN}} \) becomes larger \( \lambda_{\text{min}} \text{ (TE)} \) increases. \( \lambda_{\text{min}} \text{ (TE)} \) depends on the Al composition of the barrier with larger values of \( x_{\text{bar}} \) allowing shorter wavelength light to exhibit TE polarization. The straight lines are guides to the eye.

**FIG. 4.** This plot indicates the strain \( \varepsilon \) required to achieve TE polarization at prescribed wavelengths. In all cases, the 3 nm well is embedded in AlGaN barrier material having \( x_{\text{bar}} = 0.7 \). If light emission with TE polarization at \( \sim 250 \) nm is desired, then \( \varepsilon \) should be less (more compressive) than \( -0.0037 \). For a QW composed of Al\(_{0.5}\)Ga\(_{0.5}\)N (which will emit light at approximately 268 nm) that is grown pseudomorphically on bulk AlN, the strain in the QW is \( \varepsilon = -0.0125 \). TE polarization of the \( \sim 268 \) nm light emission is therefore expected in such a structure. Figure 4 illustrates and quantifies the general point: as the strain increases and this pushes \( x_{\text{well}} \) to larger values. The values of \( x_s \) are seen to be weakly dependent on the degree of screening of the polarization fields.
in the quantum well becomes more compressive, it becomes possible to achieve TE polarization at shorter wavelengths.

Devices 1-4 shown in Figure 1 have $x_{\text{bar}} \sim 0.7$ and emit at 253 nm. According to computational results presented in Fig. 3, the polarization will switch from TE to TM depending on the strain in the quantum well. For an active region that is pseudomorphic to bulk AlN, $a_{\text{QW}} - a_{\text{bulk-AlN}} = 0$, and the expected polarization is TE, in agreement with the measurement for device 1. For devices 2-4 grown on sapphire, we expect polarization to be TE, in agreement with the measurement for device 1. For devices 2-4 grown on sapphire, we propose that the strain state of the active regions corresponds to $a_{\text{QW}} - a_{\text{bulk-AlN}} > 0.01 \text{ Å}$. In these devices, the compressive strain in the active region is less than that required for TE polarization.

Wunderer et al. reported optically pumped lasing at 267 nm in a pseudomorphic AlGaN layer grown on a bulk AlN c-plane substrate. The QW was 267 nm in a pseudomorphic AlGaN layer grown on a bulk AlN c-plane substrate. TE polarization.

Fig. 3, the polarization will switch from TE to TM depending on the strain in the quantum well. For an active region that is pseudomorphic to bulk AlN (y = 0.76), then the quantum well will be less (compressively) strained ($\varepsilon = -0.0058$). For $y = 0.9$ and $x_{\text{bar}} = 0.76$, we find the crossover from TE to TM occurs at $x_{\text{well}} = 0.625$, so light emission for a composition of 0.67 will again be TM polarized. In either case, our model is consistent with TM polarization as reported by Kawanishi.

In summary, we report model calculations which quantify the dependence of polarization of light emission on Al barrier composition and strain for AlGaN light emitting devices. The results show that both factors are important in controlling the polarization. The results are in agreement with experiments for optically pumped lasers (267 nm) and LEDs (253 nm) grown pseudomorphically on bulk AlN.

This work was supported by the Defense Advanced Research Projects Agency CMUVT Program under U.S. Army Cooperative Agreement No. W911NF-10-02-0102.