

Valence band engineering and light emission polarization in deep UV LEDs

Boxiu Cai, Wenjie Chen, Ronghua Wang and Debdeep Jena
Dept. of Electrical Engineering, University of Notre Dame, Notre Dame, IN 46556

Abstract—This work started from the valence band structures of unstrained wurtzite AlGaIn alloys by $k \cdot p$ theory, and presented on the light emission polarization from the conduction band to the valence bands based on the momentum-matrix element. When the Al fraction x is larger than 0.25, especially in the deep ultra-violet (DUV) LED active layers ($x > 0.80$), the edge emission is dominant; otherwise, the surface emission is favorable. The emission polarization can be switched due to the quantum well confinement because of different energy offsets at the zone center.

1. Introduction

Wide band-gap semiconductors, especially AlGaIn material system with the high Al composition, has received considerable attention for deep UV (DUV) light emitting diodes (LEDs) [1, 2]. 210nm DUV LED has already been achieved using AlN as the intrinsic layer, though the external quantum efficiency is quite low [3]. However, it has been pointed out that, both theoretically and experimentally, as the Al composition increases, c-axis polarization becomes the dominant component in the emission light, which means more light emits from the edge [2, 4-5]. To explain this phenomenon, people have calculated the band structure of wurtzite semiconductors using $k \cdot p$ theory, and from there, the momentum of optical transition has also been calculated [6, 7]. It has also been pointed out that with the quantum well confinement the light polarization can be changed, so the surface emission is possible even at high Al composition [8].

In this work, we have calculated the valence band structure of unstrained AlGaIn at different Al composition, and also the corresponding emission light polarization. We found that the polarization changes at a particular Al composition. Then we have investigated the influence of quantum well confinement on the valence band structure of AlGaIn.

2. Valence Band Engineering of Unstrained AlGaIn

Given the periodic Bloch function $u_{nk}(r)$ of electrons in wurtzite III-Nitrides, k.p theory gives the Schrodinger equation as

$$Hu_{nk}(r) = (H_0 + \frac{\hbar^2 k^2}{2m_0} + \frac{\hbar}{m_0} k \cdot p + H_{so})u_{nk}(r), \quad (1)$$

in which

$$H_0 = \frac{p^2}{2m_0} + V(r), \quad (2)$$

and H_{so} is the spin-orbit interaction.

The set of basis functions near the zone center and 6*6 Hamiltonian matrix are given in Ref. [6] are as follows:

$$u_1 = |-\frac{(X+iY)}{\sqrt{2}} \uparrow\rangle, u_2 = |\frac{(X-iY)}{\sqrt{2}} \uparrow\rangle, u_3 = |Z \uparrow\rangle, \\ u_4 = |\frac{X-iY}{\sqrt{2}} \downarrow\rangle, u_5 = |-\frac{X+iY}{\sqrt{2}} \downarrow\rangle, u_6 = |Z \downarrow\rangle \quad (3)$$

and

$$H = \begin{bmatrix} F & -K^* & -H^* & 0 & 0 & 0 \\ -K & G & H & 0 & 0 & \Delta \\ -H & H^* & \lambda & 0 & \Delta & 0 \\ 0 & 0 & 0 & F & -K & H \\ 0 & 0 & \Delta & -K^* & G & -H^* \\ 0 & \Delta & 0 & H^* & -H & \lambda \end{bmatrix}$$

in which

$$F = \Delta_1 + \Delta_2 + \lambda + \theta,$$

$$G = \Delta_1 - \Delta_2 + \lambda + \theta$$

$$\begin{aligned}
\lambda &= \frac{\hbar^2}{2m_0} [A_1 k_z^2 + A_2 (k_x^2 + k_y^2)], \\
\theta &= \frac{\hbar^2}{2m_0} (A_3 k_z^2 + A_4 k_t^2), \\
K &= \frac{\hbar^2}{2m_0} A_5 (k_x + ik_y)^2, \\
H &= \frac{\hbar^2}{2m_0} A_6 k_z (k_x + ik_y), \\
\Delta &= \sqrt{2}\Delta_3, \\
k_t &= \sqrt{k_x^2 + k_y^2},
\end{aligned} \tag{4}$$

and A_i is the Luttinger parameter, Δ_1 equals the crystal-field split energy Δ_{cr} , Δ_2 and Δ_3 equal to one third of the spin-orbit split energy Δ_{so} . Then the eigen values of the energy are given as:

$$\begin{aligned}
E_1 &= F, \\
E_2 &= \frac{G + \lambda}{2} + \sqrt{\left(\frac{G - \lambda}{2}\right)^2 + \Delta^2}, \\
E_3 &= \frac{G + \lambda}{2} - \sqrt{\left(\frac{G - \lambda}{2}\right)^2 + \Delta^2}.
\end{aligned} \tag{5}$$

Plotting these eigen values as a function of the wave vector \mathbf{k} , along k_x and k_z directions respectively, we can obtain the valence band structures for different Al fraction AlGa_N, which depends on A_i and Δ_i parameters. The A_i parameters for GaN and AlN are taken from Ref. [9], Δ_1 from Ref. [4] (38 meV for GaN and -219 meV for AlN), and Δ_2 also from Ref. [9] (17 meV for GaN and 19 meV for AlN). Generally speaking, if $\Delta_1 > \Delta_2 > 0$ (GaN), the three valence bands from top to bottom are heavy-hole (HH), light-hole (LH), and crystal-field split-off hole (CH), corresponding to E_1 , E_2 and E_3 , respectively; while when $\Delta_1 < 0$ (AlN), the valence bands from top to bottom are CH, HH and LH, corresponding to E_2 , E_1 and E_3 , respectively. For AlGa_N alloys, linear interpolation was applied for Δ_2 and A_i parameters between GaN and AlN. Based on the photoluminescence (PL) results in Ref. [4], that $\Delta_1 = 0$ when the Al fraction $x = 0.25$, a bowing parameter b was added in the Δ_1 interpolation as $\Delta_1(\text{AlGa}_N) = x\Delta_1(\text{AlN}) + (1-x)\Delta_1(\text{GaN}) + bx(1-x)$, where $b = 0.14$ eV. Given these parameters, the valence band dispersions for unstrained GaN, AlGa_N ($x = 0.25$) and AlN wurtzite crystal were plotted in Fig. 1.

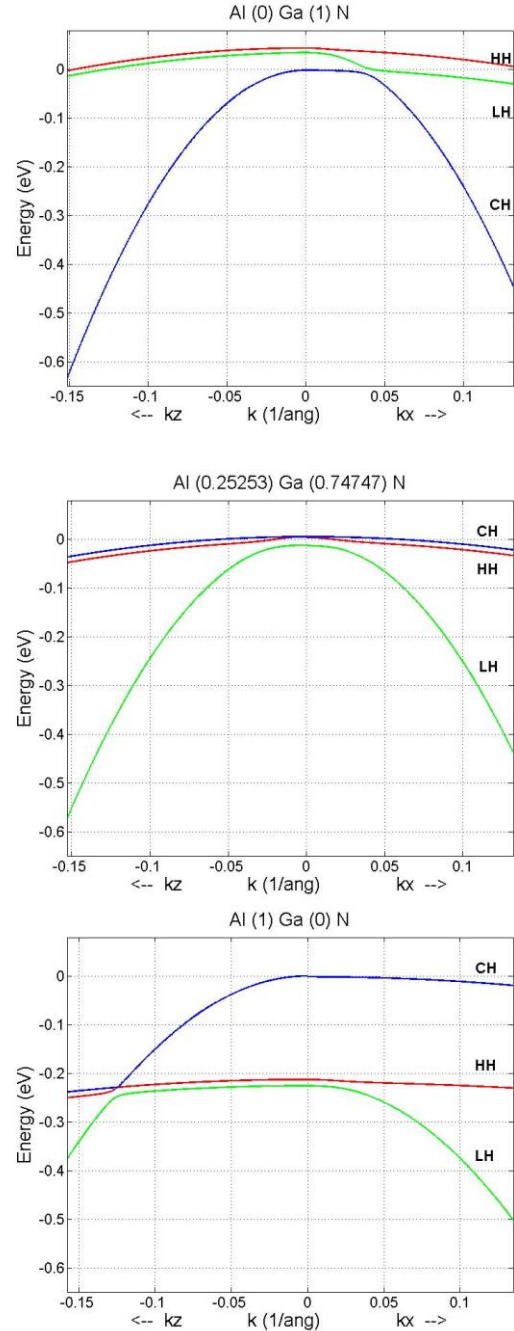


Fig. 1 Valence band dispersions for unstrained GaN, AlGa_N ($x = 0.25$) and AlN wurtzite crystal.

3. Light Emission Polarization in AlGa_N

The transition between conduction band and valence band depends on the symmetry properties of the zone center wave functions. The conduction band wave function has a S-like symmetry, including all X, Y and Z components; HH band just has X and Y components; for LH band, X and

Y are the dominant components; while for CH band, Z is dominant [7]. Kane's model [10] defined the inter-band momentum-matrix elements as

$$\left\langle S \left| \frac{\hbar}{i} \frac{\partial}{\partial z} \right| Z \right\rangle = \frac{m_0}{\hbar} P_{\parallel},$$

$$\left\langle S \left| \frac{\hbar}{i} \frac{\partial}{\partial z} \right| X \right\rangle = \left\langle S \left| \frac{\hbar}{i} \frac{\partial}{\partial z} \right| Y \right\rangle = \frac{m_0}{\hbar} P_{\perp}, \quad (6)$$

where

$$P_{\parallel}^2 = \frac{\hbar^2}{2m_0} \left(\frac{m_0}{m_e^z} - 1 \right) \frac{(E_g + \Delta_1 + \Delta_2)(E_g + 2\Delta_2) - 2\Delta_3^2}{E_g + 2\Delta_2},$$

$$P_{\perp}^2 = \frac{\hbar^2}{2m_0} \left(\frac{m_0}{m_e^t} - 1 \right) \frac{E_g [(E_g + \Delta_1 + \Delta_2)(E_g + 2\Delta_2) - 2\Delta_3^2]}{(E_g + \Delta_1 + \Delta_2)(E_g + \Delta_2) - \Delta_3^2}. \quad (7)$$

From (7), the C-HH transition will only give surface emission ($\hat{e} \perp c$), i.e. TE polarized, and C-LH transition will favor surface emission as well, while C-CH transition will favor edge emission ($\hat{e} \parallel c$), i.e. TM polarized. Table I gives the momentum matrix element $|\langle S | \hat{e} \cdot p | V \rangle|^2$ for TE and TM polarizations in unstrained AlGaN ($x > 0.25$) [6]. Fig. 2 shows the emission intensity between the conduction band and three valence bands of AlGaN with different Al fractions. For AlN bulk crystal, $P=0.998$, same as the calculation results in Ref. [2, 11], which means almost all the light emission is from the edge.

Table I Inter-band momentum-matrix elements (I) for TE and TM polarization, in which $E_i = \frac{2m_0}{\hbar^2} P_i^2$,

$$a = \frac{E_2}{\sqrt{E_2^2 + 2\Delta_3^2}} \text{ and } b = \frac{\sqrt{2}\Delta_3}{\sqrt{E_2^2 + 2\Delta_3^2}}.$$

Valence energy	$\hat{e} \parallel c$	$\hat{e} \perp c$
E_2 (E_{CH})	$b^2 \left(\frac{m_0}{2} E_{\parallel} \right)$	$a^2 \left(\frac{m_0}{4} E_{\perp} \right)$
E_1 (E_{HH})	0	$\frac{m_0}{4} E_{\perp}$
E_3 (E_{LH})	$a^2 \left(\frac{m_0}{2} E_{\parallel} \right)$	$b^2 \left(\frac{m_0}{4} E_{\perp} \right)$

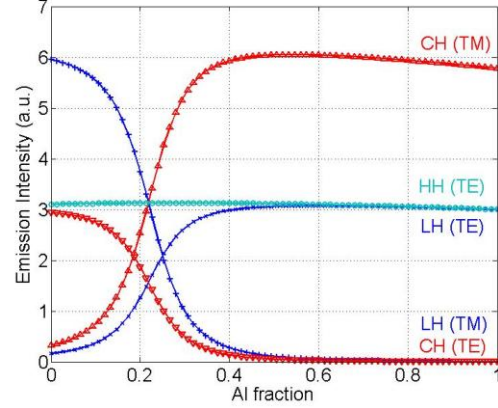


Fig. 2 Plot of the momentum-matrix elements as the emission intensity via different Al fractions.

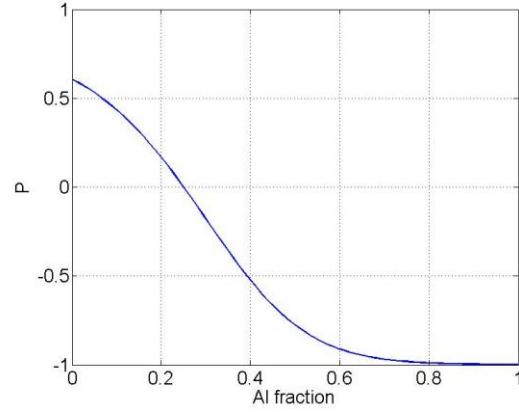


Fig. 3 The degree of polarization versus Al fraction.

Considering all three C-CH, C-HH, C-LH transitions, the TM/TE polarized emission intensity I_i can be written as

$$I_i = I_{i-CH} + I_{i-HH} e^{(E_{HH} - E_{CH})/kT} + I_{i-LH} e^{(E_{LH} - E_{CH})/kT}.$$

The degree of polarization, defining as $P = (I_{\perp} - I_{\parallel}) / (I_{\perp} + I_{\parallel})$, versus Al fraction x is shown in Fig. 3, which matches the experimental results in Ref [4] very well. It is shown that the emission of AlGaN with high Al fraction favors TM polarization, i.e. edge emission. When $x > 0.80$, the edge emission will be dominant. This is helpful to increase the external efficiency in DUV LEDs with AlGaN ($x > 0.80$) quantum wells.

4. Polarization Switch in Quantum Confined AlGaN

Different from the bulk material, the energy of electrons in the quantum well is free along x and y

directions, but quantized along the growth direction (c axis), with the particular vector $k_z = \frac{\pi}{W}$, in which W is the quantum well width. For AlGaN ($x > 0.25$), the top valence band is CH without quantum confinement, but it can be switched to HH with quantum confinement, in the case that $E_{HH} - \Delta_{HH} > E_{CH} - \Delta_{CH}$, where Δ_{CH} and Δ_{HH} are the band offsets due to the quantum confinement. Here, the infinite quantum well model was used to calculate the band offsets, which was reasonable since the calculated results always gave a deep ground state in the well. With varying quantum well width W , the second derivative of the $E - k_z$ dispersion curve at $k_z = \frac{\pi}{W}$ was taken to obtain the hole effective mass of each band. Once the HH band is on top of CH band, the dominant polarization will be switched from TM to TE. The new energy level difference between E_{ch} and E_{hh} after quantum confinement was plotted in Fig. 4 as a function the well width for AlGaN ($x=0.81$). The curve has a fluctuation near $W=3.3$ nm, due to the methodology used to extract the effective mass at $k_z = \frac{\pi}{W}$, which needs further check. This result, different from the quantum well confinement calculation in Ref. [8], indicates that when the well width is in the range of 3.3-4.3 nm the emission polarization switch will occur.

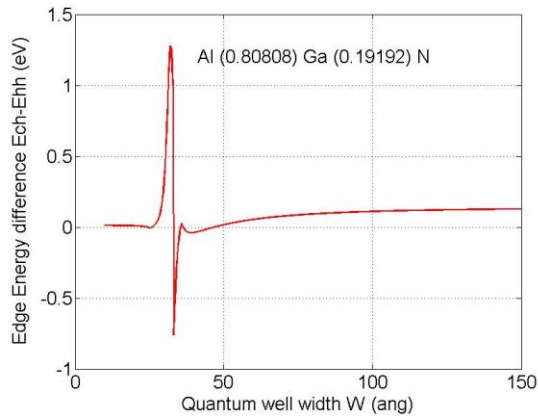


Fig. 4. Light emission polarization switch in unstrained AlGaN ($x=0.81$) due to quantum confinement.

5. Conclusions

Based on Kane's model, the band structures of unstrained AlGaN were calculated using $k \cdot p$ theory. The valence band splits into HH, LH and CH bands due to the crystal-field and spin-orbit interaction. The momentum-matrix determines the emission intensity and the polarization from the conduction band to each valence band. When the Al fraction is larger than 0.25, the edge emission is dominant; otherwise, the surface emission is favorable. With the quantum well confinement, the emission polarization can be switched from edge to surface emission due to different energy offsets among three valence bands with various effective mass.

References

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