Effects of Giant Optical Anisotropy in R-plane GaN/AlGaN Quantum Wells by Valence Band Mixing

Chun-Nan Chen, Kao-Feng Yarn, and Win-Jet Luo
Department of Electronic Engineering, Far East University
Hsin-Shih, Tainan 744, Taiwan

Jih-Chen Chiang, Ikai Lo, Wan-Tsang Wang, Ming-Hong Gau, and Hsiu-Fen Kao
Department of Physics and Center for Nanoscience and Nanotechnology
National Sun Yat-Sen University, Kaohsiung, Taiwan

Meng-En Lee
Department of Physics, National Kaohsiung Normal University
Kaohsiung Country, Taiwan

Wei-Ching Chuang
Department of Electro-Optics Engineering, National Formosa University, Yulin, Taiwan

Wen-Chung Chang and Tsung-Chan Cheng
Department of Electronic Engineering, Southern Taiwan University of Technology, Tainan, Taiwan

Abstract — Investigation of optical anisotropy spectra in the R-plane (i.e., the [10¯12]-oriented layer plane) of GaN/Al_{0.2}Ga_{0.8}N quantum wells with different widths is studied. The optical matrix elements in the wurtzite quantum wells are calculated using the k·p finite difference scheme. The calculations show that the valence band mixing effect produces giant in-plane optical anisotropy in [10¯12]-oriented GaN/Al_{0.2}Ga_{0.8}N quantum wells with a narrow width. The nature of the in-plane optical anisotropy is found to be dependent on the well width. Specifically, it is found that the anisotropy changes from x'-polarization to y'-polarization as the well width increases.

DOI: 10.2529/PIERS060801054904

1. INTRODUCTION

GaN-based semiconductors have received increasing attention in the past decade as a result of their unique properties and potential applications in the electronics and optoelectronics fields. [1–5] Recent advances in crystal growth techniques now enable the fabrication of high-quality |||-nitride based semiconductor heterostructures on substrates with orientations other than the conventional [0001] direction. [6, 7] The optical and electronic properties of such semiconductor heterostructures are quite different from those of semiconductor crystals grown on conventionally orientated substrates. For example, Rau, et al. [8] and Sun, et al. [9] identified the existence of giant in-plane optical anisotropy (over 90%) in non-polar |||-nitride based wurtzite quantum wells, while Sharma, et al. [10] observed weaker optical anisotropy (∼32%) in semi-polar |||-nitride based wurtzite quantum wells. This study employs an arbitrarily-oriented [hkil] Hamiltonian potential matrix to conduct a comprehensive investigation into in-plane optical anisotropy in semi-polar wurtzite quantum wells. The optical anisotropy spectrum is calculated for semi-polar [1012]-oriented GaN/Al_{0.2}Ga_{0.8}N quantum wells of different widths. It is shown that the valence band mixing (VBM) effect results in giant optical anisotropy in thin [1012]-oriented GaN/Al_{0.2}Ga_{0.8}N quantum wells. The physical origin of the giant in-plane optical anisotropy (over 90%) observed in non-polar quantum wells is discussed elsewhere, and is therefore not considered here. The current optical transition calculations are based on the formalism introduced by Lew Yan Voon and Ram-Mohan [11] and are solved using the k·p finite difference scheme. [12, 13] In the calculations, the directions of the x-, y- and z-axes are assumed to lie along the [1010], [1210] and [0001] directions, respectively. Furthermore, the three unit vectors in the prime coordinates (x', y', z') are given by y' = ̂y, z' = ̂z cos θ + ̂x sin θ and x' = ̂x cos θ − ̂z sin θ, respectively, where θ is the polar angle and ̂z' is the growth direction. Note that the polar angles θ = 0°, 43.2° and 90° correspond to the z' = [0001], [1012] and [1010] growth directions, respectively.
2. RESULTS AND DISCUSSION

Figure 1(a) shows the GaN valence band structures along the [1010]- and [1012]-directions without taking the spin-orbit interaction into consideration (i.e., $\Delta_2 = \Delta_3 = 0$). In this figure, the growth direction is chosen to be [1012], and hence in the prime coordinate system $(x', y', z')$, $z' = [1012]$ and $k_{z'}/[1012]$. It is observed that the valence bands along the [1010] direction are pure $|Y\rangle$- (labeled $Y$), pure $|Z\rangle$- (labeled $Z$) and pure $|X\rangle$- (labeled $X$) states, respectively. These pure states arises because the off-diagonal terms (i.e., $N_1k_xk_y$, $N_2k_xk_z$ and $N_3k_yk_z$) in the $3 \times 3$ valence band Hamiltonian given in Eq. (26) of Ref. [14] are all equal to zero in the [1010] direction. [14] However, in the [1012] direction, the off-diagonal term, i.e., $N_2k_xk_z$, is not equal to zero, and hence mixing occurs between the $|X\rangle$- and $|Z\rangle$-bands. Prior to mixing, as shown by the dashed lines with open squared symbol, the $|X\rangle$-band (labeled $X$) and the $|Z\rangle$-band (labeled $Z$) have a lower energy than the $|Y\rangle$-band (labeled $Y$). However, after mixing (please refer to the solid lines), the upper $X$-$Z$ mixing band (labeled $X'X'Z'$) has a higher energy than the $|Y\rangle$-band (labeled $Y'$) when the wave vector $k_z$ is greater than $\sim 0.07(1/\A)\) because the coupling term, i.e., $N_2k_xk_z$, increases rapidly with increasing $k_z$. In this figure, the upper (lower) $X$-$Z$ mixing band is labeled as $X'X'Z'(Z'X'Z')$ because it is not only an $|X\rangle$- (or $|Z\rangle$-like) $X$-$Z$ mixing band, but also an $|X'\rangle$- (or $|Z'\rangle$-like) $X'Z'$-mixing band. Additionally, the $|Y\rangle$-band is labeled as $Y'$ because the $|Y'\rangle$- and $|Y'\rangle$-bands are identical. Clearly, the $X$-$Z$ valence band mixing leads to a crossover of the $Y'$- and $X'XZ$ bands in the [1012] direction. The dashed lines in Fig. 1(b) show the GaN valence band structures along the [1010]- and [1012]-directions when the spin-orbital interaction is taken into consideration (i.e., $\Delta_2 = \Delta_3 \neq 0$). Here for convenience, the valence bands are labeled (from top to bottom) as the heavy-hole (HH) band, the light-hole (LH) band, and the crystal-field (CH) band, respectively. It is seen that strong mixing between the $Y'$- and $X'XZ$- bands near their crossing point causes the HH (LH) band along the [1012]-direction to change from a $|Y\rangle$- (or $|X\rangle$-like) state to an $|X'\rangle$- (or $|Y'\rangle$-like) state as the wave vector $k$ increases. Additionally, it is also seen that the $X'$-like HH and $Y'$-like LH bands are widely separated when $k_z$ is larger than $\sim 0.1(1/\A)\). In this study, these phenomena are referred to as the valence band mixing (VBM) effect. As discussed later, the VBM effect implies that strong in-plane $x'$-polarization anisotropy exists in a [1012]-oriented unstrained quantum well with a narrow well width ($L$) (e.g., $L < 30\A$).

![Figure 1: (a) Valence band structures of [1012]-oriented GaN crystal for $\Delta_2 = \Delta_3 = 0$ (solid lines). In comparison with the solid lines, the dashed lines with open squared symbols show the valence band structures when the coupling between the $|X\rangle$- and $|Z\rangle$-states is not included (i.e., assuming $N_2k_xk_z = 0$), (b) Valence band structures of [1012]-oriented GaN crystal for $\Delta_2 = \Delta_3 \neq 0$ (dashed lines) and $\Delta_2 = \Delta_3 = 0$ (solid lines).](image-url)
like asymmetric ($|X'^{A}|$)-like state, and the CH1 band is a strongly $|Z'|$-like symmetric ($|Z'^{S}|$)-like state. Meanwhile, in the $k_x'$ direction, the $\Gamma$-point effective mass of the HH2 band is negative and the $\Gamma$-point effective mass of the HH1 band is lighter than that of the LH1 band. As a result, strong 2-band mixings of ($X'^{S}$, $Y'^{S}$) and ($X'^{S}$, $X'^{A}$) occur near $k_x = 0.03(1/\AA)$ and 0.07(1/Å), respectively. Consequently, as $k_{y'}$ increases, the HH1 band changes from an ($X'^{S}$)-like state to a ($Z'^{S}$)-like state, while the LH1 band transits from a ($Z'^{S}$)-like state, through an $X'^{S}$-state, to an ($X'^{A}$)-like state. In the present study, this phenomenon is referred to as the quantum-well valence-band mixing (QWVBM) effect. Similarly, the QWVBM effect leads to 2-band mixing of ($X'^{A}$, $Y'^{S}$) near $k_{y'} = 0.07(1/\AA)$. As $k_{y'}$ increases, the LH1 band therefore changes from a ($Y'^{S}$)-like state to an ($X'^{A}$)-like state.

However, it is observed that the HH1 band remains in an ($X'^{S}$)-like state. This indicates that the weak $X'^{S}$-$Y'^{S}$ mixing causes the photo-luminescence generated by the C1-HH1 ($C1$-LH1) subband to be strongly polarized along the $\Gamma$-point valence band (VB) band (y'-axis). Certainly, the $X'^{S}$-$Y'^{S}$ mixing becomes weaker as the energy separation between the HH1 and LH1 bands increases. In a thin $[10\bar{1}2]$-oriented wurtzite GaN unstrained quantum well ($L < 30\AA$), the VBM$_{X'}$ effect results in a large energy difference between the $|X'^{S}|$-like HH1 band and the $|Y'^{S}|$-like LH1 band near the zone center, and this implies the presence of strong in-plane $x'$-polarization anisotropy. In Fig. 3, as $k_{x'}$ increases toward the 2-band ($X'^{S}$, $Y'^{S}$) mixing region ($k_{x'} \approx 0.03(1/\AA)$), the QWVBM ($X'^{S}$-$Y'^{S}$ mixing) effect causes $|M_{x'}|^2_{C1-HH1}$ and $|M_{y'}|^2_{C1-LH1}$ to fall rapidly to zero and $|M_{y'}|^2_{C1-HH1}$ to increase to its maximum value. Similarly, the QWVBM effect causes $|M_{y'}|^2_{C1-LH1}$ to vanish for $k_{x'} > 0.07(1/\AA)$ and to assume a single-peak structure with a peak near $k_{x'} = 0.03(1/\AA)$.

Figure 4 shows the in-plane optical anisotropies at the zone center (i.e., $\rho(k_{x'} = k_{y'} = 0)$) of the $z'$-oriented GaN/A$_{0.2}$Ga$_{0.8}$N quantum wells. Note that the in-plane optical anisotropy, $\rho$, is

![Figure 2: In-plane (i.e., x'-y' plane) valence subband structure of [1012]-oriented GaN/A$_{0.2}$Ga$_{0.8}$N quantum well with 15Å well width.](image1)

![Figure 3: Squared optical matrix elements of in-plane (i.e., x'-y' plane) optical transitions for [1012]-oriented GaN/A$_{0.2}$Ga$_{0.8}$N quantum well with 15Å well width.](image2)
defined as

\[ \rho = \frac{|M_x|^2 - |M_y'|^2}{|M_x|^2 + |M_y'|^2} \]

It can be seen that the largest optical anisotropy \((y'-\text{polarization})\) occurs in the [10\(\overline{1}0\)]-oriented quantum wells, while subsidiary anisotropy \((x'-\text{polarization})\) appears in the thin [10\(\overline{1}2\)]-oriented quantum wells \((L < 30\ang)\). The strong anisotropy in the thin [10\(\overline{1}2\)]-oriented quantum wells is \(y'\)-polarized and is caused by the crystal field effect (which will be discussed elsewhere). Most interestingly, in the [10\(\overline{1}2\)]-oriented quantum wells, it is observed that as the well width increases and reaches a critical value of \(L_C\) \((L_C \approx 30\ang)\), the in-plane anisotropy changes from \(x'\)-polarization to \(y'\)-polarization. Again, this phenomenon is caused by the VBM effect (i.e., the HH band shown in Fig. 1 changes from a \(|X'\rangle\)-like state to a \(|Y'\rangle\)-like state as the wave vector \(k_{z'}\) decreases). The critical value, \(L_C\), decreases (increases) with increasing compressive (tensile) strain since compressive (tensile) strain enlarges (reduces) the crystal field split energy and therefore weakens (enhances) the coupling between the \(|X\rangle\) and \(|Z\rangle\) bands (refer to Fig. 1). Clearly, when the compressive (tensile) strain is sufficiently high, only \(y'\)-polarization \((x'\)-polarization\) anisotropy exists. Finally, in-plane optical anisotropy is not found in the [0001]-oriented quantum wells because this particular quantum well belongs to the \(D_{6h}\) high-symmetry point group. The results presented in this study are in good agreement with the experimental findings reported in the literature. For example, Rau, et al. [8] and Sun, et al. [9] identified the presence of giant in-plane optical anisotropy (over 90\%) in non-polar \(||\) nitride based wurtzite quantum wells, while Sharma et al. [10] observed weaker optical anisotropy (~32\%) in semi-polar \(||\) nitride based wurtzite quantum wells.

3. CONCLUSION

In conclusion, this study has calculated the optical transition of GaN/Al\(_{0.2}\)GaN quantum wells of different well widths using the \(k\cdot p\) finite difference scheme. The results have shown that giant in-plane optical anisotropy exists in the R-plane (i.e., [10\(\overline{1}2\)]-oriented layer plane) of GaN/Al\(_{0.2}\)GaN quantum wells with a narrow width as a result of the valence band mixing effect. The anisotropy in [10\(\overline{1}2\)]-oriented quantum wells is width dependent, i.e., the in-plane anisotropy changes from \(x'\)-polarization to \(y'\)-polarization as the well width increases. The results presented in this study are in good agreement with the experimental findings reported in the literature and
provide valuable guidelines for the design of polarization stabilization devices based on polarization control or selectivity.

REFERENCES