

Characteristics of Polarized Light Emission in a -Plane GaN-Based Multiple Quantum Wells

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Abstract—In this paper, we investigated polarized light emission properties on a series of a -plane GaN/AlGaIn multiple quantum wells grown on r -plane sapphire substrates with various well widths by using the polarization-dependent photoluminescence measurement. To clarify reasons of polarization properties in light emission, we applied the 6×6 $k \cdot p$ model to simulate the E - K dispersion relationship and wave functions to obtain optical transitions of different polarized emissions. According to our results, the sub-bands of $|Y\rangle$ -like states are raised toward the top of the valence sub-band level with increasing the well width. And the optical matrix element of y -polarized light emission will dominate the optical transition, leading to the increase of degree of polarization in the thicker well.

Index Terms— a -Plane, GaN, GaN/AlGaIn multiple quantum wells, nonpolar, polarization.

I. INTRODUCTION

RECENTLY, GaN-based semiconductor materials with the wurtzite (WZ) crystal structure have been popular due to their versatile applications in UV to visible light emitting diodes, laser diodes, solar-blind photo-detectors and power electronics. The GaN/AlGaIn quantum wells (QWs) grown on the c -plane sapphire has found unique application in deep ultraviolet optoelectronic devices useful for curing, purification and bio-sensing [1, 2]. However, due to the quantum confined Stark effect (QCSE) aroused from the large spontaneous and piezoelectric polarization fields along the c -direction, the band structure in the c -plane GaN/AlGaIn MQWs tilting in a triangular shape would cause the electron wave functions separate from the hole wave functions spatially in the well thus decreasing the optical transition efficiency [3], increasing the radiative lifetime and red-shifting the emission peak. Growth of nonpolar crystal orientations such as a -plane (11 $\bar{2}$ 0) [4, 5] and m -plane (1 $\bar{1}$ 00) [6] have been proposed to eliminate the pronounced QCSE [7]. Recently, a -plane GaN/AlGaIn MQWs have demonstrated enhanced recombination efficiency due to the lack of built-in polarization field and the emission energy

Manuscript received December 20, 2011; revised February 22, 2012; accepted March 12, 2012. Date of current version May 8, 2012. This work was supported in part by the Ministry of Education Aim for the Top University Program and the National Science Council in Taiwan under Contract NSC 99-2221-E-009-035-MY3.

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Digital Object Identifier 10.1109/JQE.2012.2191140

peaks show weaker well-width dependence in comparison to the c -plane GaN/AlGaIn MQWs [8]. Due to the asymmetry of the WZ GaN crystal and inherited anisotropic biaxial strains, the original wave functions of $|X+iY\rangle$ and $|X-iY\rangle$ states were separated into $|Y\rangle$ -like state and $|Z\rangle$ -like state in the nonpolar a -plane orientation [9–11]. The nonpolar structure has also exhibited optical polarization anisotropy with respect to the in-plane direction which is unlike the case in the c -plane WZ crystal structure emitting the symmetrically in-plane optical polarization [12]. Furthermore, the band structures of a -plane InGaIn/GaN MQWs with different quantum well widths have been solved by the 6×6 $k \cdot p$ method and simulation results have been applied to explain the experimental results in the nonpolar structures and to study the polarization of light emission properties [9, 13].

In this study, we used the photoluminescence (PL) measurement to investigate the emission properties on a series of a -plane GaN/AlGaIn MQWs with various well thicknesses grown by metal-organic chemical vapor deposition (MOCVD). The optical polarization properties were analyzed according to the polarization dependent PL measurement. This analysis can be used to determine the degree of polarization (DOP) of the emission. Then, the 6×6 $k \cdot p$ method was constructed for the a -plane GaN/AlGaIn MQWs structures to simulate the optical emission properties by calculating the dispersion relationships of the energy level and the corresponding wave functions. The issues of valence-band states mixing and polarized emissions were also discussed.

II. EXPERIMENT AND THEORETICAL MODELING

The structures of MQW samples containing five a -plane GaN/Al_{0.17}Ga_{0.83}N QWs were grown on a 1.5 μm -thick unintentionally doped GaN buffer layer on r -plane sapphire substrates by a low pressure rotating disc MOCVD system. While fixing the thickness of Al_{0.17}Ga_{0.83}N barriers to be 10 nm, the thickness of GaN wells varied from 1.5 nm to 7.33 nm in five different samples. The Al composition x of Al _{x} Ga_{1- x} N barriers and the thickness of QW and barrier were characterized by the X-ray measurement. For PL measurements, the samples were pumped at room temperature by a 266 nm pulse laser with an excitation power of 5 mW, generated by a frequency tripled mode-locked Ti: sapphire laser (Mira 900). An ultraviolet linear polarizer was placed in front of a monochromator (Triax 550) with a photomultiplier tube (PMT) for ultraviolet-visible range to obtain linearly polarized PL spectra. In the case of polarization dependent

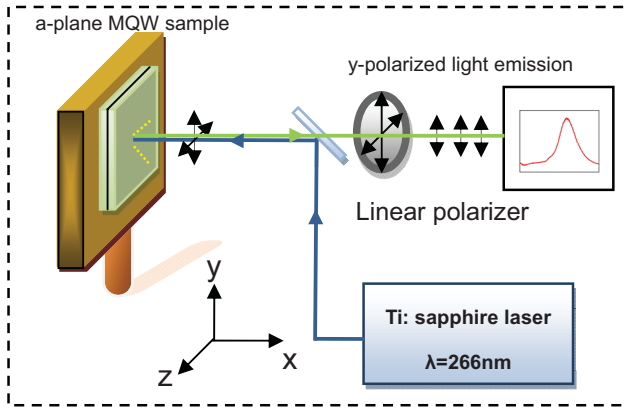


Fig. 1. Schematic of an *a*-plane GaN/AlGaIn MQW sample and the polarization dependent PL measurement setup. Z axis is along the *c* crystal orientation.

PL measurement, a polarizer angle of 0 degree designated the electric field of the emission light parallel to the *c* crystal direction ($E \parallel c$) and a polarizer angle of 90 degree designated the electric field of the emission light parallel to the *m* crystal direction ($E \perp c$). The degree of polarization was defined as $DOP = (I_{E \perp c} - I_{E \parallel c}) / (I_{E \perp c} + I_{E \parallel c})$, where $I_{E \perp c}$ and $I_{E \parallel c}$ were the PL integrated intensity values with the electric fields of light emissions parallel to the *c* and *m* crystal directions, respectively. Fig. 1 shows the sample structure and the polarization dependent PL measurement setup.

Moreover, we have constructed a theoretical model to investigate the relationship between the polarized spontaneous emission spectra and each valence band state of *a*-plane GaN/AlGaIn QWs structure. The *k*·*p* approximation was applied here to derive the perturbed Hamiltonians [14]. We then use the *k*·*p* Hamiltonians and the parameters of (Al)GaN materials following the values reported in Table I (Ref. [15]) to calculate the band structures in the *a*-plane GaN/AlGaIn QW. The differential operators in Hamiltonians can be solved by using the finite-difference method [16]. The piezoelectric and spontaneous polarization fields have been included in the calculation. In addition, the amount of strain in GaN/AlGaIn has been considered. Thus, we can obtain the conduction and valence subband energy levels (E_n^c , E_m^v) and the corresponding wave functions (φ_n^c , φ_m^v) by solving the effective-mass and 6×6 *k*·*p* Hamiltonian equations. The polarized light emission can be separated from the polarization-dependent optical matrix element [13], $|\hat{a} \cdot \vec{M}|^2 = |\langle \varphi_n^c | \hat{a} \cdot \vec{P}_a | \varphi_m^v \rangle|^2$, where \hat{a} is the light polarization direction. After obtaining optical matrix elements, the spontaneous emission spectrum [10] r_{sp} ($\text{cm}^{-2}\text{s}^{-1}\text{eV}^{-1}$) can be figured out as followed,

$$r_{sp}(E) = \frac{e^2 n_r E}{m_0 \epsilon_0 c^3 \eta^2} \sum_{nm} \int \frac{2}{(2\pi)^2} dk_y dk_z |\hat{a} \cdot \vec{M}|^2 \cdot \frac{1}{\sigma \sqrt{2\pi}} \cdot \exp \left[\frac{-(E_n^c - E_m^v - E)^2}{2\sigma^2} \right] \cdot f_e \left[E_n^c(\vec{k}) \right] f_h \left[E_m^v(\vec{k}) \right].$$

Here σ is the inhomogeneous broadening factor, f_e and f_h are the Fermi-Dirac occupation factors, n_r is the refractive index and *z* is along the *c* crystal orientation.

TABLE I
MATERIAL PARAMETERS OF WURTZITE NITRIDE
BINARY ALLOYS

Parameters	GaN	AlN
a (Å) at T = 300 K	3.189	3.112
c (Å) at T = 300 K	5.185	4.982
Δ_{cr} (eV)	0.01	-0.169
Δ_{so} (eV)	0.017	0.019
D ₁ (eV)	-3.7	-17.1
D ₂ (eV)	4.5	7.9
D ₃ (eV)	8.2	8.8
D ₄ (eV)	-4.1	-3.9
D ₅ (eV)	4.0	-3.4
D ₆ (eV)	-5.5	-3.4
A ₁	-7.21	-3.86
A ₂	-0.44	-0.25
A ₃	6.68	3.58
A ₄	-3.46	-1.32
A ₅	-3.40	-1.47
A ₆	-4.90	-1.64
$m_{e\parallel}$	0.2	0.32
$m_{e\perp}$	0.2	0.3
C ₁₁ (GPa)	390	369
C ₁₃ (GPa)	145	137
C ₃₃ (GPa)	106	108
C ₄₄ (GPa)	398	373

All parameters were taken from Ref. [15]. These parameters were used to calculate the subband energy and wavefunction by *k*·*p* Hamiltonians [14].

III. RESULTS AND DISCUSSION

Fig. 2(a) shows the measured PL emission spectra of *a*-plane GaN/AlGaIn MQW samples with different well width obtained at room temperature by a pulse laser at 266 nm. It can be clearly seen that the dominant emission peak shifts to lower energy with increasing the well width. This shift is assigned to the reduction of quantum confinement effect. When the quantum well width increases, the conduction and valence subband energy levels move toward the bottom of the wells thus reducing the optical transition energy. Fig. 2(b) shows the calculated spontaneous emission spectra of the *a*-plane GaN/AlGaIn MQWs with the same quantum well widths as in Fig. 2(a). In Fig. 2(c), the experimental PL peak energies of the *a*-plane GaN/AlGaIn MQWs as a function of quantum well width were summarized and compared with the simulated ones. The energies of the simulated results were greater than the experimental results to certain values. This could be due to that the exciton binding energy was not taken into consideration in the simulation model. There have been some works studying the exciton binding energy of GaN/AlGaIn MQWs by measuring PL and photoluminescence excitation (PLE) and values of exciton binding energies ranged from 20 meV to 60 meV [8, 17, 18]. By increasing the quantum well width, the binding energies can be found from 62 to 25 meV by the peak energy separation between simulation and experiment results as shown in Fig. 2(d).

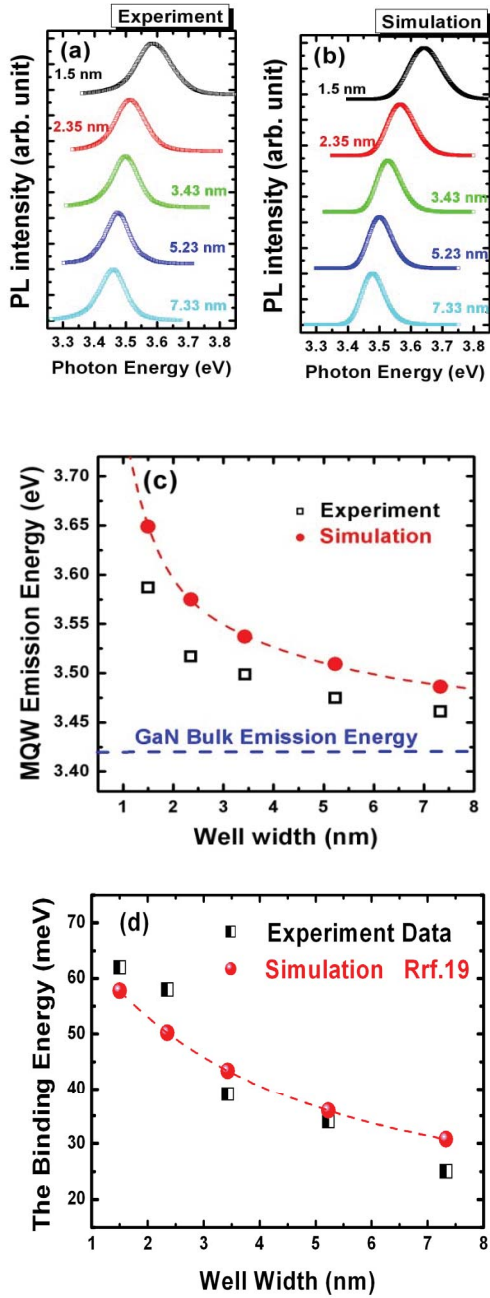


Fig. 2. PL spectra of (a) experimental measurements and (b) simulation results of *a*-plane $\text{Al}_{0.17}\text{Ga}_{0.83}\text{N}$ QWs with quantum well width ranging from 1.5 to 7.33 nm. (c) Experimental and simulated PL peak energy peaks of the *a*-plane MQWs as a function of the quantum well width. (d) Binding energy of the *a*-plane MQWs as a function of the quantum well width.

The binding energy of excitons in the quantum well structure is influenced by the coulomb attraction effect, the effective-mass and the difference in dielectric constants between barriers and wells materials. We considered these effects to calculate the theoretical exciton binding energy by the simple analytical method [19]. The exciton binding energy E_b can be expressed as followed, $E_b = E_0/(1 - 1/2e^{-L_w/2a_x})$. Here E_0 and a_x are the effective Rydberg energy and the effective Bohr radius of the bulk GaN, L_w is the well width. E_0 and a_x are defined according to Ref. [20]. The theoretical

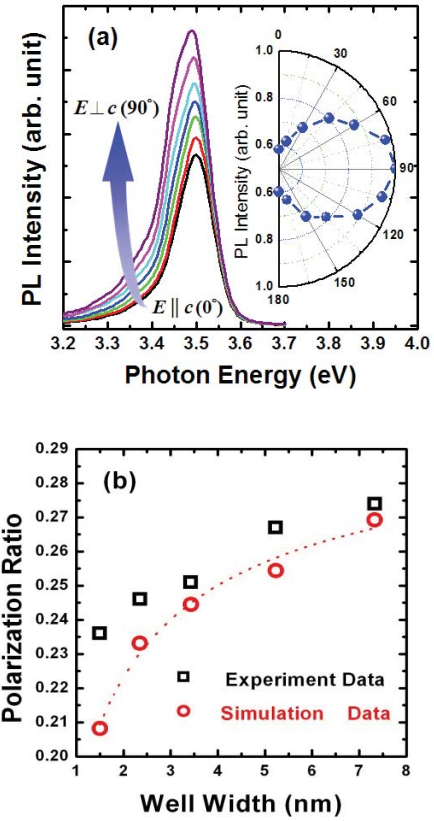


Fig. 3. (a) Light emission polarization characteristics of the *a*-plane GaN/AlGaIn MQWs with a well width of 3.43 nm. (b) DOP of experiment and simulation results of *a*-plane GaN/AlGaIn MQWs as a function of the quantum well width.

exciton binding energy have shown a good agreement with our results, the enhancement of the exciton binding energy in a smaller well can be reasonably explained through the increasing of the quantum confinement effect.

Fig. 3(a) shows the polarization-dependent PL spectra of an *a*-plane GaN/AlGaIn MQW sample with a well width of 3.43 nm. The PL peak energy shifted about 5 meV from $E \perp c$ to $E \parallel c$ polarization directions. The inset shows PL integrated intensity values of *a*-plane GaN/AlGaIn MQWs with polar angle ranging from 0 to 360 degree. Fig. 3(b) displays the experimental and theoretical DOP results of *a*-plane GaN/AlGaIn MQWs as a function of the quantum well width. The simulation results match pretty well to the experimental results and exhibit an increasing trend of DOP values as the quantum well width increases. Slightly lower DOP values in the experimental results could be due to randomly light reflecting and scattering on the rough surface of as-grown GaN/AlGaIn MQW samples.

The DOP values of *a*-plane GaN/AlN MQWs grown on *a*-plane 6H-SiC has been investigated previously by R. Mata *et al.* [21] They presented that the DOP values decreased with increasing the quantum well width due to the effect of quantum confinement and high strain. On the contrast, our results showed that the DOP values of the experimental measurement and theoretical calculation in *a*-plane GaN/AlGaIn MQWs as a function of well width exhibited opposite trends.

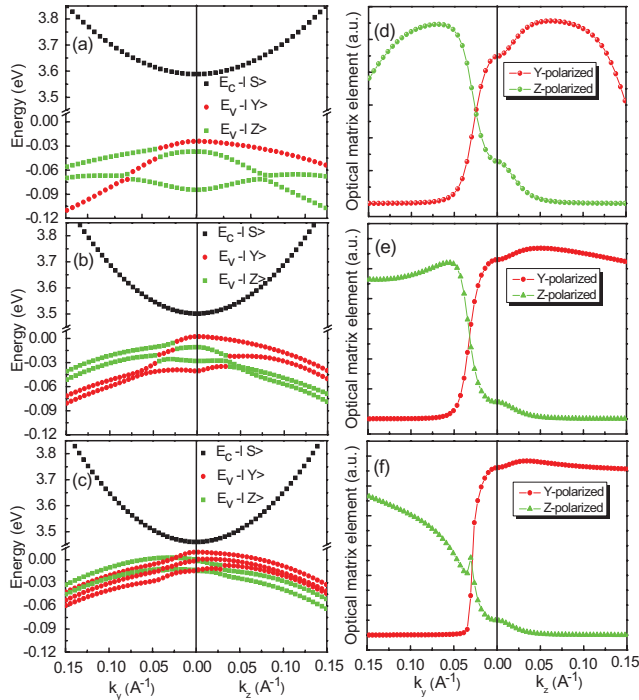


Fig. 4. Dispersion relationships of conduction and valence sub-band energies in a -plane GaN/AlGaIn MQWs along the k_y and k_z directions for quantum well widths of (a) 1.5 nm, (b) 3.43 nm, and (c) 7.33 nm. (d)–(f) Top-most valence sub-band of the polarization-dependent optical matrix element in a -plane GaN/AlGaIn MQWs along the k_y and k_z directions for quantum well width of (d) 1.5 nm, (e) 3.43 nm, and (f) 7.33 nm.

In order to elucidate the mechanism of polarized emissions in a -plane GaN/AlGaIn MQWs with increasing the quantum well width, we analyzed the E – k dispersion relationships of the conduction and valence energy subbands and the mixing of valence subband states in GaN/AlGaIn quantum wells by solving the k · p Hamiltonian and the polarization-dependent optical matrix element, respectively. The strain effects had been taken into account since the GaN/AlGaIn heterostructure was grown on the a -plane thick GaN templates. The strain value of the barrier region is estimated to be larger than the well region.

Fig.4(a)–(c) shows the band structures as functions of the in-plane wave function vector k_y and k_z . The energy differences between other valence subbands in the thicker well width are found to be smaller. Furthermore, the top-most valence subband is mainly occupied by the $|Y\rangle$ -like state, and contributed to the y -polarized light emission. On the other hand, the $|Z\rangle$ -like state moves close to the top-most valence subband with increasing the quantum well width from 1.50 to 7.33 nm; meanwhile, the second and third subband of $|Y\rangle$ -like state are also greatly raised toward the top of the valence subband level.

According to our experimental results, the value of DOP increases with increasing the well width, even if the energy separation between the first $|Y\rangle$ -like and $|Z\rangle$ -like state become small along with the reduction of the confinement effect. To clarify the relationship between polarization light emission and variation of quantum well width, the optical matrix elements of y -polarized ($E_{\perp c}$) and z -polarized ($E_{\parallel c}$)

TABLE II
RATIO OF THE INTEGRATED POLARIZATION-DEPENDENT OPTICAL ELEMENT IN THE TOP-MOST VALENCE SUB-BAND

Well width	1.5 nm	3.43 nm	7.33 nm
f_y/f_z	1.26	1.73	2.00

emission have been analyzed further. Fig.4 (d)–(f) show the optical matrix elements as functions of the in-plane wave function vector k_y and k_z . As we know, the variation of optical matrix elements between y -polarized and z -polarized will affect the value of DOP. Moreover, the actually two-dimensional carrier density in the quantized structure is estimated to be about $1.5 \times 10^{12} \text{ cm}^{-2}$ from the injected carrier density of the PL measurement [22], which is the relatively low carrier injection. The ratio of the integrated polarization-dependent optical matrix element f_y/f_z is shown in table II. Accordingly, we think that the top-most valence subband will dominate the optical transition during polarization-dependent PL measurements, and focus the discussion on the top-most valence subband. Based on the analysis of optical matrix elements, it is worth noting that the y -polarized emission seems to increase with increasing the well width; on the contrary, the z -polarized emission reveals an obvious reduction. The difference between the contribution of y -polarized light and z -polarized light gradually increased, implied the increase of DOP to be possible. Therefore, it is believed that the value of DOP increases with increasing the quantum well width, mainly due to the domination of $|Y\rangle$ -like state contribution.

IV. CONCLUSION

We have investigated the polarized light emission properties on a series of nonpolar GaN/AlGaIn MQWs with various well widths grown on r -plane sapphire substrates. The dominant emission peak shifts to a lower energy with increasing the quantum well width from 3.587 to 3.461 eV due to the reduction of the quantum confinement effect. According to the E – k dispersion relationships of the conduction and valence subband states, the $|Y\rangle$ -like states in the valence band would shift toward to the top-most band with increasing the quantum well width. And the optical matrix element of y -polarized light emission will dominate the optical transition, leading to the increase of DOP value in the thicker well. We have studied the relationship between the band structures and the polarization of light emission in the nonpolar GaN/AlGaIn MQWs, which could be favorable for the further developments of polarized device designs, such as polarized LEDs and polarization-sensitive photodetectors.

ACKNOWLEDGEMENT

The authors would like to acknowledge S. C. Wang and H. C. Kuo at National Chiao Tung University, Hsinchu, Taiwan, for their technical support.

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