Determination of piezoelectric fields in strained GaInN quantum wells using the quantum-confined Stark effect

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We have identified piezoelectric fields in strained GaInN/GaN quantum well *p-i-n* structures using the quantum-confined Stark effect. The photoluminescence peak of the quantum wells showed a blueshift with increasing applied reverse voltages. This blueshift is due to the cancellation of the piezoelectric field by the reverse bias field. We determined that the piezoelectric field points from the growth surface to the substrate and its magnitude is 1.2 MV/cm for $Ga_{0.84}In_{0.16}N$/GaN quantum wells on sapphire substrate. In addition, from the direction of the field, the growth orientation of our nitride epilayers can be determined to be (0001), corresponding to the Ga face. © *1998 American Institute of Physics.* [S0003-6951(98)02338-9]

In recent years, piezoelectric effects in strained quantum well (QW) structures have been frequently discussed. Theoretical and experimental results have shown the existence of piezoelectric fields in GaInAs/GaAs QWs on GaAs(111)[1–3] and the influence of the piezoelectric fields on optical properties in the cases of GaInAs/GaAs QWs[2] and CdS/CdSe superlattices[4] on GaAs(111).

On the other hand, group III nitrides have very large piezoelectric constants, for instance, $e_{31} = -0.57\ \mathrm{C/m^2}$ for InN,[5] -0.22 and $-0.49\ \mathrm{C/m^2}$ for GaN,[5,6] and -0.58 and $-0.6\ \mathrm{C/m^2}$ for AlN.[5,7] Therefore if nitride layers are under biaxial strain, large piezoelectric fields can be generated. In a previous article,[8] theoretical results showed that the induced piezoelectric field in a strained $Ga_{0.87}In_{0.13}N$ layer grown on (0001)-oriented GaN is expected to be 1.1 MV/cm assuming $e_{31} = -0.22\ \mathrm{C/m^2}$. Moreover experimental results[8] showed that the photoluminescence (PL) peak energy of strained $Ga_{0.87}In_{0.13}N$ QWs was redshifted with respect to that of thick $Ga_{0.87}In_{0.13}N$ single layers due to an intrinsic[4] quantum-confined Stark effect[9] (QCSE) caused by the piezoelectric field. These results suggested the existence of a piezoelectric field in the strained GaInN layer. This field significantly affects the band lineup, therefore we should take into account its direction and magnitude for the band engineering in nitride based devices. However, there was no report on the direct observation and determination of the piezoelectric fields in nitride based QWs. In this letter, we determine the piezoelectric fields in strained GaInN QWs by studying the applied voltage dependence of the PL peak energy, the so-called extrinsic QCSE. In addition, the growth orientations of our nitride epilayers are discussed.

In this experiment we used two different substrates, a sapphire(0001) with a low-temperature-deposited AlN buffer layer and a 12 μm thick GaN on sapphire(0001) grown by hydride vapor phase epitaxy (HVPE). The sample structures consist of *n*-GaN (3 μm), GaInN (3 nm)/GaN (6 nm) 5 QWs, *p*-AlGaN (60 nm), and *p*-GaN (120 nm). The two samples on the different substrates were separately grown by metalorganic vapor phase epitaxy (MOVPE). The total undoped region sandwiched by *n* and *p* layers is 51 nm. The carrier concentrations of *n*-GaN, *p*-AlGaN, and *p*-GaN are 2×10^{18}, 2×10^{17}, and $1\times10^{18}\ \mathrm{cm^{-3}}$, respectively, while donor and acceptor concentrations are 2×10^{18} and $5\times10^{19}\ \mathrm{cm^{-3}}$. In this structure, the direction of the built-in electric field is from substrate to growth surface. Using x-ray diffraction measurements, we confirmed that the growth orientation of the nitride epilayers are (0001) or $(000\bar{1})$ and that the GaInN well layers and the *p*-AlGaN layer have the same in-plane *a*-axis lattice constant as the *n*-GaN layer.[10] This indicates that these layers were pseudomorphically grown on the thick underlying GaN, resulting in fully strained layers. Then, taking into account the biaxial stress, we determined that the InN mole fractions in the strained GaInN wells are 16% for the sample on sapphire substrate and 15% for the sample on HVPE grown GaN. We fabricated transparent electrodes for the *p*-side contacts in order to measure PL spectra of the GaInN QWs through the electrodes. PL spectra were taken at room temperature under various applied bias voltages. When the applied voltage was changed from -4 to $+2$ V, we observed that the current in the devices varied from -5 to $+700\ \mu$A. In the case of $+3$ V bias, the current increased to 9 mA. A He–Cd laser with a power of 30 mW and a spot size of 0.3 $\mathrm{mm^2}$ was used as an excitation source.

Figures 1 and 2 show the PL spectra of the GaInN/GaN QWs *p-i-n* structures on sapphire and on HVPE grown GaN under various applied voltages. Multiple peaks seen in the PL spectra must be attributed to interference fringes[11] due to multiple reflection within the air/nitride epilayers/sapphire system. We eliminated this influence by dividing the PL spectra by calculated interference fringes based on the multiple reflection in the Fabry–Pérot étalon. As shown in Figs.

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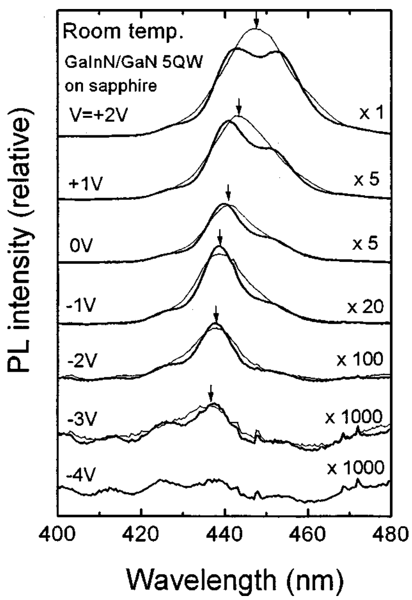

FIG. 1. Room temperature PL spectra of a $Ga_{0.84}In_{0.16}N$/GaN QW *p-i-n* structure on sapphire under various applied voltages. Thick lines represent measured PL spectra and thin lines represent the PL spectra without the influence of interference fringes. Arrows indicate peak positions of the PL spectra.

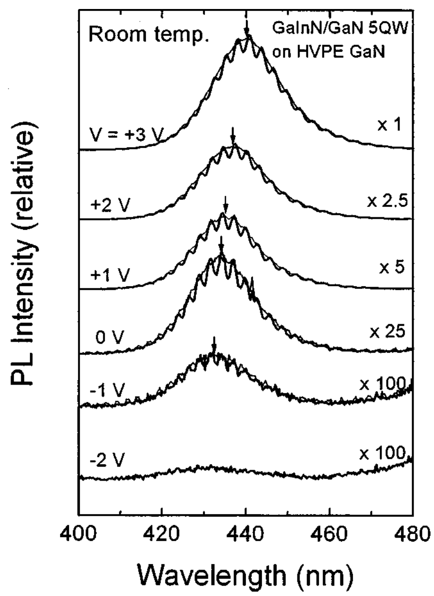

FIG. 2. Room temperature PL spectra of a $Ga_{0.85}In_{0.15}N$/GaN QW *p-i-n* structure on HVPE grown GaN under various applied voltages. Thick lines represent measured PL spectra and thin lines represent the PL spectra without the influence of interference fringes. Arrows indicate peak positions of the PL spectra.

1 and 2, the best fitting results show clear single peaks when we used the refractive index of 2.5,[12] reflectivity from 0.04 to 0.11, and cavity length of 2.6 μm for the sapphire case and 13.4 μm for the HVPE grown GaN case, which are slightly different from our expected values. As a result, we observe a clear blueshift of the PL peak wavelength in the both substrate cases when the reverse applied voltage increased. In the typical case of the QCSE, such as in GaAs/AlGaAs QWs,[9] a redshift is shown with increasing reverse voltages. This is due to an increase of the internal field in the well layer, leading to a smaller effective band gap. Therefore the blueshift in our case should be caused by a decrease of the internal field. This is a cancellation of the piezoelectric field by the reverse bias, similar to the case of GaInAs/GaAs QWs on GaAs(111).[3] When the piezoelectric field is set against the built-in and reverse bias field, the band structure of the GaInN well approaches flatband conditions with increasing reverse bias. Therefore we conclude that the directions of the piezoelectric field in the strained GaInN wells on both substrates are opposite those of the built-in/reverse bias field, which are from the growth surface to the substrate.

In order to estimate the magnitude of the piezoelectric fields, we compared the measured PL peak energies with calculations as a function of the applied voltage. In the calculation, the total internal field (E_{total}) in the well layer is approximated as follows:[13]

$$\begin{aligned} E_{\mathrm{total}} &= E_i - V_{\mathrm{appl}}/(d_u+d_d)+E_{\mathrm{piezo}}, \\ V_{\mathrm{bi}} &= E_i\cdot(d_u+d_d)+E_{\mathrm{piezo}}\cdot NL_w, \end{aligned} \tag{1}$$

where V_{bi}, V_{appl}, E_{piezo}, and E_i represent the built-in potential, the applied voltage, the piezoelectric field, and the internal field in the undoped and depletion regions, respectively. In these equations the positive direction of the electric fields is set from the substrate to the growth surface. The thicknesses of the undoped region, depletion region, the well width, and the number of wells are represented as d_u, d_d, L_w, and N, respectively. The built-in potential (3.3 V) was calculated from the carrier concentrations and the effective mass values. The thicknesses of the undoped region (51 nm) and well width (3 nm) were obtained from x-ray diffraction measurements. The depletion region thickness was calculated from donor and acceptor concentrations, the built-in potential, and the applied voltage. This thickness varied from 89 to 13 nm with the applied voltage from -10 to 3 V. We used the piezoelectric field as a free parameter for fitting to the experimental results. Details after material parameters were described elsewhere.[8] Then we calculated the applied voltage dependence of the lowest transition energy between the conduction band and the valence band in GaInN/GaN QWs with InN mole fractions of 15% and 16% using a multistep potential approximation.[14] In this calculation we did not consider the screening effect of the piezoelectric field by any carrier. Figure 3 shows a comparison between the experiments and the calculations. In the case of a negative applied voltage, our data can be well described assuming a piezoelectric field of -1.2 MV/cm for both $Ga_{0.84}In_{0.16}N$ on sapphire and $Ga_{0.85}In_{0.15}N$ on HVPE grown GaN. Here note that the minus sign of the piezoelectric fields indicates that the direction is from growth surface to substrate, which is consistent with the results described above. For positive applied bias, however, there is a discrepancy as large as 30 meV between the experiments and calculations for a piezoelectric field of -1.2 MV/cm. At present we cannot explain this discrepancy. For a more strict investigation, we need more accurate estimations of the built-in potential and the thickness of the depletion region, and should consider the influence of compositional fluctuation in the GaInN layers.[11,15]

Assuming the piezoelectric constants of linear interpolation of GaN and InN,[5] we expect the theoretical piezoelectric fields of 2.7–2.9 MV/cm in the strained GaInN layer with

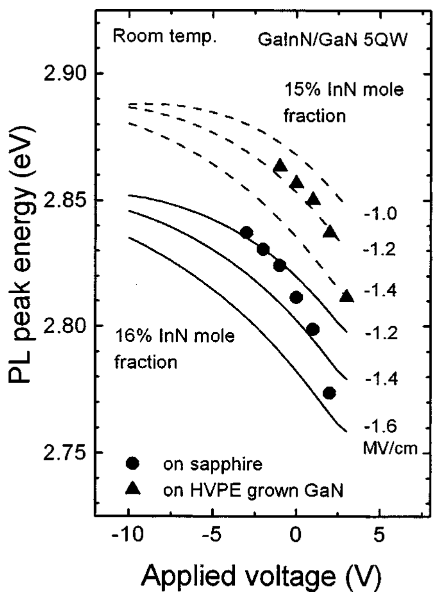

FIG. 3. PL peak energies of a GaInN QW *p-i-n* structure as a function of the applied voltage. Circles and triangles represent the measured PL peak energies on sapphire and on HVPE grown GaN. Solid and dashed lines represent the calculated PL peak energies of $Ga_{0.84}In_{0.16}N$ QWs and $Ga_{0.85}In_{0.15}N$ QWs with the piezoelectric fields from −1.0 to −1.6 MV/cm.

InN mole fraction of 15%–16% using our strain model.[8] These values are two times higher than our values experimentally obtained here. This discrepancy could be attributed to the screening for the piezoelectric fields by free and photogenerated carriers.[8]

In this experiment, PL intensity dramatically decreased with the increase in reverse voltage, i.e., the decreasing internal field in the well layer. In general the transition probability usually increases in this case because of an increase of the overlap integral between the wave function of the electron and that of the hole.[9] However we observed that the photocurrent increased significantly while the PL intensity decreased. This indicates that for increasing reverse bias photogenerated carriers contribute to the current transport rather than to the luminescence, resulting in a decrease of the PL intensity. A reasonable photocurrent sensitivity of 0.05 A/W was found.[16] Further investigations are underway.

By comparing experimentally obtained direction of the piezoelectric field with and the theoretical one, we can conclude on the growth orientation of the nitride heteroepitaxial layers on sapphire. Based on recent results of the sign of piezoelectric constants for group-III nitrides,[5] the orientations of our epilayers on both sapphire and HVPE grown GaN are found to be (0001)—that is the bond starting from Ga to N parallel to the *c* axis points in a positive direction (Ga face). Therefore we conclude that the growth orientations of our nitride epilayers by MOVPE and HVPE are (0001), which is consistent with the results using hemispherically scanned x-ray photoelectron diffraction.[17]

In summary, we observe blueshifts of the PL peak energies in GaInN QWs on both sapphire and HVPE grown GaN with increasing applied reverse voltage. This phenomenon is found to originate in the fact that the applied reverse voltage cancels the internal piezoelectric field, which points from the growth surface to the substrate. From the direction of the piezoelectric field, the growth orientation of our sample by MOVPE and HVPE can be determined to be (0001). We also determined the magnitude of the piezoelectric field to be 1.2 MV/cm in strained $Ga_{0.84}In_{0.16}N$ layers on sapphire. A field of such a direction and a magnitude is expected to strongly affect the electronic and optical properties in heterostructure devices. The effects of strain induced piezoelectric fields should therefore be taken into account for the design and fabrication of group-III nitride based devices.

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