TITLE:
Polarization switching phenomena in semipolar In$_x$Ga$_{1-x}$N/GaN quantum well active layers

AUTHOR(S):
Ueda, M; Funato, M; Kojima, K; Kawakami, Y; Narukawa, Y; Mukai, T

CITATION:
Ueda, M ...[et al]. Polarization switching phenomena in semipolar In$_x$Ga$_{1-x}$N/GaN quantum well active layers. PHYSICAL REVIEW B 2008, 78(23): 233303.

ISSUE DATE:
2008-02

URL:
http://hdl.handle.net/2433/84618

RIGHT:
© 2008 The American Physical Society
Polarization switching phenomena in semipolar In$_{x}$Ga$_{1-x}$N/GaN quantum well active layers

M. Ueda,1 M. Funato,1,* K. Kojima,1 Y. Kawakami,1 Y. Narukawa,1 and T. Mukai2

1Department of Electronic Science and Engineering, Kyoto University, Kyoto 615-8510, Japan
2Nitride Semiconductor Research Laboratory, Nichia Corporation, Tokushima 774-8601, Japan

Received 14 August 2008; revised manuscript received 2 October 2008; published 8 December 2008

We report the observation of optical polarization switching in In$_{x}$Ga$_{1-x}$N/GaN quantum well active layers, using semipolar $\{1122\}$ planes. When the In composition is less than $\sim$30%, the emissions related to the top and second valence bands are polarized along the $\{1100\}$ and perpendicular $\{\bar{1}123\}$ directions, respectively, similar to earlier studies. On the contrary, as the In composition increases above 30%, the polarizations switch, indicating a crossover between the two valence bands. Because the polarization degree is less sensitive to the well width, the observed polarization switch is assigned to the InN deformation potentials.

DOI: 10.1103/PhysRevB.78.233303

A typical nitride-semiconductor-based light emitter consists of c-oriented quantum wells (QWs), where piezoelectric and spontaneous polarizations lower the optical transition probability.1 One way to circumvent this decreased probability is to grow QWs on nonpolar2 or semipolar3,4 planes tilted from the $c$ polarization is expected.8,9 Recently, we have experimentally revealed polarization switching phenomena in semipolar $\{1122\}$ planes, and have fabricated light-emitting diodes (LEDs).6

Unlike the (0001) plane, nonpolar and semipolar planes have low crystal symmetries, which cause optical anisotropy. For example, because the lowest energy transition in GaN is polarized perpendicular to the [0001] direction, polarization is not observed from the [0001] direction, whereas linear polarization is observed from the nonpolar directions. Intermediately, the polarization degree in unstrained, semipolar $\{1122\}$ GaN has been calculated to be 56% (Refs. 10 and 11) and has been experimentally confirmed to be 46% by photoluminescence (PL) and reflectance spectroscopy.5,10 Because the optical anisotropy directly reflects the energy-band structures of emitting layers, critical factors to be investigated in strained-QW-based light emitters are strain and quantum confinement. Their effects have been theoretically studied for arbitrary crystalline orientations of GaN QWs11 and GaN/Al$_{x}$Ga$_{1-x}$N QWs.12 Experimentally, strain effects have been examined for nonpolar $\{1\bar{1}00\}$ (Refs. 14 and 15) and polar (0001) (Refs. 16 and 17) GaN films. Regarding In$_{x}$Ga$_{1-x}$N QWs with relatively low In compositions, the polarization properties have been investigated for semipolar $\{1122\}$ (Ref. 5) and $\{1\bar{1}00\},$18 and nonpolar (1100) (Refs. 19–21) by PL and electroluminescence (EL) spectroscopy. The results consistently showed that the emission is polarized perpendicular to the $c$ axis. In contrast, herein, we revealed polarization switching phenomena in semipolar $\{1122\}$ In$_{x}$Ga$_{1-x}$N/GaN QWs and LEDs through systematic studies on these structures with various well widths and In compositions. Then, the experimental results were analyzed by the $k\cdot p$ approach to gain some insight into the energy-band structures of semipolar or nonpolar In$_{x}$Ga$_{1-x}$N QW.

The QWs and LEDs were fabricated by metalorganic vapor phase epitaxy on $\{1122\}$ GaN bulk substrates. The growth and sample structures are detailed in Refs. 5 and 6.
The polarization properties were consistent with other samples, suggesting the absence of relaxation. As long as In$_{x}$GaN$_{1-x}$ was pseudomorphically grown on GaN, an In composition less than ~30% caused polarization parallel to [1100] ($\rho > 0$), while a composition greater than ~30% switched the polarization direction to [1$\bar{1}$23] ($\rho < 0$).

All the above results can well be interrelated by considering the A and B valence bands.

All the above results can well be interrelated by considering the A and B valence bands. When the In composition was lower than ~30%, the topmost A band was dominated by a $P$ orbit along the [1100] direction, while the second highest B band was dominated by that along the [1$\bar{1}$23] direction. As the In composition increased, these two valence bands approached, and eventually, a crossover occurred, which resulted in the A and B bands being dominated by the [1$\bar{1}$23]-related and [1100]-related states, respectively. Figure 4 is a schematic of this variation in the band alignments. The observed energy separations (Fig. 2) well approximated those between the A and B bands. On the other hand, because the hole population in the A band was inevitably greater than that in the B band, A-band-related emissions were always more intense. As carrier injection increased, the quasi-Fermi level for holes approached the valence band. Consequently, the population in the B band increased with respect to that in the A band, which relatively strengthened the B-band-related emission without remarkably changing the peak energy separation (Fig. 3).

Because carriers were thermally redistributed in the A and B bands under the current experiments at RT, differences in...
the properties of A and B excitons such as thermal stability may influence the relative intensities of polarization spectra acquired for the [1100] and [1123] directions. Therefore, to separately assess the polarization properties of A and B bands, each polarization spectrum was assumed to involve two emission components due to those bands, and was decomposed into two Gaussian curves. Hence, there were totally four Gaussian curves for a pair of polarization spectra. However, because the A-band-related (or B-band-related) component in either polarization spectrum must have the identical peak position and line width, the number of fitting parameters was reduced to eight. Furthermore, from the stronger polarization spectrum, the peak position, line width, and amplitude of the A-band-related emission could be determined without serious errors. This, in turn, contributed to a better fit of the B-band-related parameters, although the much weaker B-band-related emission sometimes caused an uncertainty of at most 20% particularly for QWs with large A-B splitting energies. Using thus determined A and B band components, the polarization degree was evaluated for each band.

Figure 5 displays the well-width dependence of the polarization degrees for the A and B bands. The QWs were grown under the same conditions, and the In composition was 20 ± 2%. The polarization degrees were nearly independent of the well thickness, and ~0.8 for the A band and ~1.0 for the B band. These quantities indicated that both emissions are polarized almost linearly along the perpendicular two directions, strikingly different from bulk GaN. CB stands for the conduction band.

For the same series of the QWs, the A-band polarization degrees were directly evaluated by lowering the measurement temperature to 10 K, where carriers were hardly populated to the B band. Those were 0.83, 0.84, and 0.81 for well widths of 0.8, 1.7, and 5.1 nm, respectively, consistent with Fig. 5. Furthermore, although the large inhomogeneous broadening of PL and EL suggests the presence of localized excitons, the polarization degrees were nearly constant within the spectra, irrespective of the well widths, which indicates that the carrier localization does not affect the polarization properties.

On the other hand, Fig. 6 shows the In-composition dependence of the polarization degrees for the A and B bands in QWs and LEDs with 2–3-nm-thick InGa1−xN. When the In composition was increased from 0 to ~25%, the polarization degree for the A band was gradually increased from ~0.5 to 0.8 and that for the B band was drastically changed from nearly 0 for In=0% (GaN) to about −1.0 for In =10–25%. Further increasing the In composition caused a polarization switch at ~30%. For the In composition above ~30%, the polarization degree for the A (B) band was ~−0.8 (0.9).

Let us discuss the mechanism of the polarization switch, based on the k.p approach. The A and D parameters are generally important to describe QW properties, as A’s express the effective masses, and D’s are the deformation potentials. However, as long as we examined the reported, widely varied A parameters,24 such scattering has a negligible effect on the calculated polarization properties, indicating that, in highly strained InGa1−xN/GaN QWs, the quantum confinement does not affect the valence-band order so significantly as the strain does through the deformation potentials. This finding is consistent with Figs. 5 and 6. Hence, the quantum confinement effect was neglected in the following analysis. Further neglecting the spin-splitting interaction, the 6 × 6 valence-band Hamiltonian can be diagonalized to obtain the eigenenergy for each valence band. The energy separation between the A and B bands at the Γ point in strained InGa1−xN layers with arbitrary orientations can thus be simplified to

$$
E^{X'} - E^{Y'} = \{E_1 - 3E_2 - \sqrt{(E_1 + E_2)^2 + 8(D_0\epsilon_{cr})^2}\}/2,
$$

where $E^{X'}$ ($E^{Y'}$) is the transition energy for the X' (Y') polarization, $E_1 = \Delta_{cr} + D_1(\epsilon_{xx} + \epsilon_{yy})$, $E_2 = D_2(\epsilon_{xx} - \epsilon_{yy})$, $\Delta_{cr}$ is the crystal-field splitting energy, and $\epsilon$ represents strain.
tensor elements.\(^{25}\) \(X'\) and \(Y'\) stand for the two in-plane perpendicular directions, and \(Y' \perp [0001]\). Therefore, \(E^{X'}\) and \(E^{Y'}\) are related to the A or B band. For the (1122) plane, \(X'\) was [1\(\bar{1}\)23], and \(Y'\) was [1\(\bar{1}\)00]. The \((x,y,z)\) orthogonal coordinates were defined with respect to the wurtzite lattice, where \(x\) and \(y\) were in the \(c\) plane, while \(z\) was along the \(c\) axis. Moreover, \(y\) was the rotation axis, that is, \(y\) \([1\ 1\ 0\ 0]\) for (1122) planes. Semipolar planes are characterized by anisotropic strain in the \(c\) plane (\(e_{xy} \neq e_{yz}\)) and the presence of shear strain (\(e_{zz} \neq 0\)), which allow the contributions from \(D_2\) and \(D_6\) and promote band mixing.

Initially we calculated Eq. (1) using the well-accepted physical parameters.\(^{26}\) The \(\text{In}_x\text{Ga}_{1-x}\text{N}\) parameters were derived by the linear interpolation between the GaN and InN parameters, and the strain was calculated assuming the coherently grown. However, this parameter set could not reproduce the polarization switch probably due to the lack of data for the InN deformation potentials, which were substituted derived. Although \(D_1\) and \(D_2\) cannot be determined as they are not involved in Eq. (1), we suggest \(D_1 = D_2 = 0.1\) eV, applying another cubic approximation. The result of this fit is shown as a solid curve in Fig. 2, which agrees reasonably well with the experimental data.

The energy differences of \(E^{X'} - E^{Y'}\) in nonpolar \(\text{In}_x\text{Ga}_{1-x}\text{N}/\text{GaN}\) QWs were reported to be 5, 40, and 60 meV for In compositions of 10, 18, and 23%, respectively,\(^{21}\) which we evaluated from the reported well width and emission wavelength. On the other hand, the energy differences evaluated by Eq. (1) with the parameters in Ref. 26 were 19, 25, and 30 meV for the respective In compositions, while the obtained InN deformation potentials provided a much better fit of 24, 43, and 59 meV, supporting the current analysis. It is interesting to note that neither parameter set predicts polarization switch in nonpolar QWs. Therefore, the determinant of the polarization switching properties in semipolar QWs is the shear strain, \(e_{zz}\), which is absent in nonpolar QWs. Regarding a device application, the present results indicate that cavity mirrors of semipolar laser diodes emitting green or a longer wavelength can be formed by cleavage.

\(^{26}\)funato@kuee.kyoto-u.ac.jp

23. In strained \(\text{In}_x\text{Ga}_{1-x}\text{N}\), the \([X \pm iY]-\)like and \([Z]-\)like hole states are mixed, and therefore, the valence bands are simply denoted as \(A\), \(B\), and \(C\) from the top in this study.