<table>
<thead>
<tr>
<th><strong>Title</strong></th>
<th>Orientation dependence of electronic structure and optical gain of (11N)-oriented III-V-N quantum wells</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Author(s)</strong></td>
<td>Fan, Weijun</td>
</tr>
<tr>
<td><strong>Date</strong></td>
<td>2013</td>
</tr>
<tr>
<td><strong>URL</strong></td>
<td><a href="http://hdl.handle.net/10220/9931">http://hdl.handle.net/10220/9931</a></td>
</tr>
</tbody>
</table>

© 2013 American Institute of Physics. This paper was published in Journal of Applied Physics and is made available as an electronic reprint (preprint) with permission of American Institute of Physics. The paper can be found at the following official DOI: http://dx.doi.org/10.1063/1.4793279. One print or electronic copy may be made for personal use only. Systematic or multiple reproduction, distribution to multiple locations via electronic or other means, duplication of any material in this paper for a fee or for commercial purposes, or modification of the content of the paper is prohibited and is subject to penalties under law.
Orientation dependence of electronic structure and optical gain of (11N)-oriented III-V-N quantum wells

W. J. Fan

Citation: J. Appl. Phys. 113, 083102 (2013); doi: 10.1063/1.4793279
View online: http://dx.doi.org/10.1063/1.4793279
View Table of Contents: http://jap.aip.org/resource/1/JAPIAU/v113/i8
Published by the American Institute of Physics.

Additional information on J. Appl. Phys.
Journal Homepage: http://jap.aip.org/
Journal Information: http://jap.aip.org/about/about_the_journal
Top downloads: http://jap.aip.org/features/most_downloaded
Information for Authors: http://jap.aip.org/authors

ADVERTISMENT

Explore AIP’s open access journal:
- Rapid publication
- Article-level metrics
- Post-publication rating and commenting
Orientation dependence of electronic structure and optical gain of (11N)-oriented III-V-N quantum wells

W. J. Fan

School of Electrical and Electronic Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore, 639798

(Received 14 January 2013; accepted 8 February 2013; published online 25 February 2013)

A ten-band k-p Hamiltonian for III-V-N dilute nitride semiconductor quantum wells (QWs) grown on the (11N)-oriented substrates is presented. The energy dispersion curves, optical transition matrix elements, internal piezoelectric field, and optical gain of InGaAsN/GaAs on the (110), (111), and (11∞)-oriented substrates are investigated including band-anti-crossing, strain, and piezoelectric field effects. The band structures and optical gain are sensitive to the substrate orientation. The fundamental transition energy is the largest for the (111)-oriented QW and the smallest for (11∞)-oriented QW. The absolute values of internal piezoelectric field in the well and barrier layers reach the maximum for the (111)-QW, and zero for the (110) and (11∞)-oriented QWs. There exists an injection current density turning point. When the injection current density is below the turning point, the (111)-oriented QW has the largest peak gain. At the larger injection current density, the (11∞)-oriented QW has the largest peak gain. © 2013 American Institute of Physics. [http://dx.doi.org/10.1063/1.4793279]
where $\epsilon_{ij}$ and $\epsilon'_{ij}$ ($i, j = x, y, z$) are the strain tensors for the (001)- and (11N)-orientations, respectively. $O^T$ is the transpose of the matrix $O$.

We adopt Kane’s 8-band Hamiltonian and band anti-crossing model to form a 10-band Hamiltonian. The 10-band Hamiltonian for any (11N)-orientation epilayer, $H$, can be written as \(^{11-16}\)

$$
H = \begin{bmatrix}
E^{N_0} & c.c. & c.c. & c.c. & c.c. & c.c. & c.c. & c.c. & c.c. & c.c. \\
0 & E^{N_0} & c.c. & c.c. & c.c. & c.c. & c.c. & c.c. & c.c. & c.c. \\
\sqrt{\lambda} V_N & 0 & E^C & c.c. & c.c. & c.c. & c.c. & c.c. & c.c. & c.c. \\
0 & \sqrt{\lambda} V_N & 0 & E^C & c.c. & c.c. & c.c. & c.c. & c.c. & c.c. \\
0 & 0 & \frac{1}{\sqrt{2}} P_+ & 0 & P + Q & c.c. & c.c. & c.c. & c.c. & c.c. \\
0 & 0 & -\sqrt{\frac{2}{3}} P_+ & \frac{1}{\sqrt{6}} P_+ & S^+ & P - Q & c.c. & c.c. & c.c. & c.c. \\
0 & 0 & -\sqrt{\frac{2}{3}} P_+ & 0 & S^+ & P - Q & c.c. & c.c. & c.c. & c.c. \\
0 & 0 & 0 & -\sqrt{\frac{2}{3}} P_+ & S^+ & 0 & -R^* & -S^* & P + Q & c.c. \\
0 & 0 & 0 & 0 & S^+ & \sqrt{2} Q & -\frac{3}{2} S & \frac{3}{2} S & S & P - \Delta & c.c. \\
0 & 0 & -\sqrt{\frac{2}{3}} P_+ & \frac{1}{\sqrt{3}} P_+ & -\sqrt{2} R^* & \frac{3}{2} S^* & \frac{3}{2} S & \frac{3}{2} S & S & 0 & P - \Delta
\end{bmatrix} + VBO, \tag{4}
$$

where the Hamiltonian terms $H$ consist of kinetic terms $H_k$ and strain terms $H_s$ and can be written as

$$
H = H_k + H_s. \tag{5}
$$

The kinetic terms of the Hamiltonian are given by

$$
P_k = -\frac{\hbar^2}{2m_0} \gamma_1 (k_x^2 + k_y^2 + k_z^2),
$$

$$
Q_k = -\frac{\hbar^2}{2m_0} \left\{ \gamma_2 \frac{N^2 - 1}{2 (N^2)} [2(k_x^2 + k_y^2) - 4k_x^2 - 6\sqrt{2}k_x'k'_yN + (k_x^2 + k_y^2 - 2k_x'^2)N^2] \\
+ \gamma_3 \frac{3}{(2 + N^2)} [2(k_x'^2 - k_y'^2) + 2\sqrt{2}k_x'k'_yN(1 - N^2) + (3k_x'^2 + k_y'^2 - 4k_x'^2)N^2] \right\}, \tag{7}
$$

$$
S_k = \frac{\hbar^2}{2m_0(2 + N^2)} \left\{ \sqrt{6} \gamma_2 [6k_x'^2N^2 - i2k'_y(2 + N^2)] + 2\sqrt{3} \gamma_3 [4k_x'k'_y - 2(k'_x + ik'_y)N^2 + (k'_x - ik'_y)N^4] \right\}, \tag{8}
$$

$$
R_k = \frac{\hbar^2 \sqrt{3}}{2m_0(2 + N^2)^2} \left\{ \gamma_2 [2k_x^2 + 2\sqrt{2}N(3k'_x + i2k'_y - \frac{3k'_x N^2}{\sqrt{2}} + ik'_y N^2)] + \gamma_3 [2k'_x(2k'_y + 4k'_x N^2)] \\
+ \gamma_2 [-4k_x'^2 + N^2(k_x'^2 + k_y'^2) + i2k_x'k'_yN^4] + \gamma_3 [-k_x'^2(5N^2 + N^4) + k_y'^2(3N^2 + N^4) + i8k_x'k'_y] \right\}, \tag{9}
$$

$$
P_{ \pm k} = P_0 (k_x' \pm ik_y'),
$$

$$
E^C = E_G + \frac{\hbar^2}{2m_0} \gamma_2 (k_x'^2 + k_y'^2 + k_z'^2),
$$

and

$$
\gamma_c = \frac{1}{m_e} - \frac{E_F}{3} \left( \frac{2}{E_G + \frac{1}{E_G + \Delta}} \right),
$$

\[083102-2\] W. J. Fan  
where $\hbar$ is the reduced Planck constant, $m_e^*$ is the electron effective mass, $m_0$ is the electron mass in free space. $E_G$ is the unstrained band gap. $\Delta$ is the spin-orbit (SO) splitting energy. $\gamma_1$, $\gamma_2$, $\gamma_3$ are not identical to Luttinger parameters ($\gamma_1^L$, $\gamma_2^L$, $\gamma_3^L$) used in the 6-band Hamiltonian, since the conduction band is now treated exactly in the 10-band Hamiltonian and must be subtracted off the original Luttinger parameters. These parameters are called as the modified Luttinger parameters and are related to Luttinger parameters in the following manner:

$$\gamma_1 = \gamma_1^L - \frac{1}{3} \frac{E_P}{E_G}, \quad (13)$$
$$\gamma_2 = \gamma_2^L - \frac{1}{6} \frac{E_P}{E_G}, \quad (14)$$
$$\gamma_3 = \gamma_3^L - \frac{1}{6} \frac{E_P}{E_G}. \quad (15)$$

Note that $P_0$ is the Kane matrix element constant and is normally expressed in term of energy units as

$$E_P = \frac{2m_0}{\hbar^2} P_0^2. \quad (16)$$

$V_{BO}$ describes the valence band edge offset. $x$ is the nitrogen composition. $E_{N0}$ and $V_N$ are the localized nitrogen energy level and the coupling coefficient in the band anti-crossing model, respectively. The above mentioned parameters are layer dependent except the effective mass parameters ($\gamma_1^L$, $\gamma_1$, $\gamma_2$, $\gamma_3$, $E_P$ which are from well material in our calculations). Note that for the strained III-V-N material, the $E_N$ nitrogen level parameter in Ref. 25 is with respect to the valence band maximum (VBM) after strain consideration, with a view to the much weaker shift of $E_N$ with applied pressure. 25 The nitrogen level with respect to the unstrained VBM, $E_{N0}$ is given by

$$E_{N0} = E_N + V_{BO}, \quad (17)$$

$VBM^S$ is the top of strained valence band at $k=0$ point, which can be calculated using the 8-band $H$ at $k=0$ including strain. Note that generally the heavy hole (HH), light hole (LH), and spin-orbit splitting bands are intermixing for the (11N)-oriented $H$, and it is hard to obtain the analytical express of $VBM^S$ unlike the (001)-oriented $H$. The energy origin is taken at the unstrained VBM of the well layer.

For strained material, the Bir-Pikus Hamiltonian must be taken into consideration. The strain terms are similar with the kinetic terms and can be obtained using the following correspondence relations $13-16$:

$$k'_i k'_j \leftrightarrow \varepsilon_{ij} (i, j = x, y, z), \quad (18)$$
$$k'_i \leftrightarrow -\sum_j \varepsilon_{ij} k'_j (i, j = x, y, z), \quad (19)$$

$$\frac{\hbar^2 k'_i}{2m_0} \leftrightarrow a_x, \quad (20)$$
$$\frac{\hbar^2 k'_i}{2m_0} \leftrightarrow -a_x, \quad (21)$$
$$\frac{\hbar^2 k'_i}{2m_0} \leftrightarrow -b, \quad (22)$$
$$\frac{\hbar^2 k'_i}{2m_0} \leftrightarrow -d \frac{1}{2\sqrt{3}}, \quad (23)$$

where $a_x$ and $a_x$ are the hydrostatic deformation potential for conduction and valence band, respectively. $b$ and $d$ are the shear deformation potential. The detailed strain tensors and strained Hamiltonian terms for the [111]-oriented QWs are given in Appendix A.

### III. OPTICAL TRANSITION MATRIX ELEMENTS

The squared optical transition matrix elements, which measure the momentum of the transitions between the hole subbands and the electron subbands, are written as $\varepsilon$

$$Q_\lambda^{n,m} = \frac{2}{m_0} |\langle \Psi_n | \hat{\varepsilon} \cdot \hat{p} | \Psi_m \rangle |^2, \quad i = x', y', z', \quad (24)$$

where $\hat{\varepsilon}$ is the unit vector in the direction of the electric field, $\hat{p}_i$ is the momentum operator, and $\Psi_n$ and $\Psi_m$ are the real electron and hole wave functions, respectively. The real wave function is the product of the envelope wave functions and the Bloch wave functions, which are given in Appendix B.

The expressions for squared optical transition matrix elements in the $x'$, $y'$, and $z'$ directions are given below: $\varepsilon$

$$Q_\lambda^{n,m}_{x'} = \frac{2 P_0^2}{m_0} \left\{ \sum_m \left( -\frac{i}{\sqrt{2}} a^5_{n,m} a^{3*}_{n,m} \right)^2 + \sum_m \frac{i}{\sqrt{6}} a^7_{n,m} a^{3*}_{n,m} + \sum_m \frac{i}{\sqrt{3}} a^{10}_{n,m} a^{3*}_{n,m} \right\}, \quad (25)$$

$$Q_\lambda^{n,m}_{y'} = \frac{2 P_0^2}{m_0} \left\{ \sum_m \left( -\frac{i}{\sqrt{2}} a^6_{n,m} a^{4*}_{n,m} \right)^2 + \sum_m \frac{i}{\sqrt{6}} a^8_{n,m} a^{4*}_{n,m} + \sum_m \frac{i}{\sqrt{3}} a^{10}_{n,m} a^{4*}_{n,m} \right\}, \quad (26)$$

$$Q_\lambda^{n,m}_{z'} = \frac{2 P_0^2}{m_0} \left\{ \sum_m \left( -\frac{i}{\sqrt{2}} a^7_{n,m} a^{4*}_{n,m} \right)^2 + \sum_m \frac{i}{\sqrt{6}} a^8_{n,m} a^{4*}_{n,m} + \sum_m \frac{i}{\sqrt{3}} a^{10}_{n,m} a^{4*}_{n,m} \right\}, \quad (27)$$

---

Downloaded 28 Apr 2013 to 155.69.4.4. This article is copyrighted as indicated in the abstract. Reuse of AIP content is subject to the terms at: http://jap.aip.org/about/rights_and_permissions
\begin{align}
Q^{n,n_i}_{\nu,i} &= \frac{2P_0^2}{m_0} \left\{ \sum_{m} \frac{1}{\sqrt{2}} a_{n,m}^6 a_{n,m}^4 \right\}^2 + \sum_{m} \frac{1}{\sqrt{2}} a_{n,m}^8 a_{n,m}^4 \right\}^2 + \sum_{m} \left( \frac{-1}{\sqrt{3}} a_{n,m}^9 a_{n,m}^{4*} \right) \right\}, \\
Q^{n,n_i}_z &= \frac{2P_0^2}{m_0} \left\{ \sum_{m} i \sqrt{2} a_{n,m}^6 a_{n,m}^4 \right\}^2 + \sum_{m} \sum_{3} \left( \frac{-1}{\sqrt{3}} a_{n,m}^9 a_{n,m}^{4*} \right) \right\}, \\
Q^{n,n_i}_{\nu\nu} &= \frac{2P_0^2}{m_0} \left\{ \sum_{m} i \sqrt{2} a_{n,m}^6 a_{n,m}^4 \right\}^2 + \sum_{m} \sum_{3} \left( \frac{-1}{\sqrt{3}} a_{n,m}^9 a_{n,m}^{4*} \right) \right\}, \\
Q^{n,n_i}_z &= \frac{2P_0^2}{m_0} \left\{ \sum_{m} i \sqrt{2} a_{n,m}^6 a_{n,m}^4 \right\}^2 + \sum_{m} \sum_{3} \left( \frac{-1}{\sqrt{3}} a_{n,m}^9 a_{n,m}^{4*} \right) \right\}, \\
Q^{n,n_i}_{\nu\nu} &= \frac{2P_0^2}{m_0} \left\{ \sum_{m} i \sqrt{2} a_{n,m}^6 a_{n,m}^4 \right\}^2 + \sum_{m} \sum_{3} \left( \frac{-1}{\sqrt{3}} a_{n,m}^9 a_{n,m}^{4*} \right) \right\}, \\
Q^{n,n_i}_z &= \frac{2P_0^2}{m_0} \left\{ \sum_{m} i \sqrt{2} a_{n,m}^6 a_{n,m}^4 \right\}^2 + \sum_{m} \sum_{3} \left( \frac{-1}{\sqrt{3}} a_{n,m}^9 a_{n,m}^{4*} \right) \right\}.
\end{align}

where \(P_0 = (S'|p_x|X') = (S'|p_y|Y') = (S'|p_z|Z')\). Note that the above equations only include the \(S'^{i} \rightarrow X'^{i}, Y'^{i}, Z'^{i}\) transitions. Due to the interaction between valence and conduction bands, \(\Phi_n\) is not a pure conduction states but will have some components contributed from the valence band and vice versa. Therefore, if more accurate results are required, the contribution from the non-conduction band components in \(\Phi_n\) and the non-valence band components in \(\Phi_n\) \((X', Y', Z' \rightarrow S')\) must be considered in the derivation of \(Q^{n,n_i}_i\). So, the additional \(X'^{i}, Y'^{i}, Z' \rightarrow S'\) transition contributions will then be

The last term of \(QA^{n,n_i}_i\) is for \(S'^{i} \rightarrow X'^{i}, Y'^{i}, Z'^{i} \rightarrow S'\) transition, it should be very small and can be ignored for interband transition. The summation of \(Q^{n,n_i}_i\) and \(QA^{n,n_i}_i\), \(Q^{n,n_i}_i\) is the general expression for the transition between any two states, which can be used for not only intersubband but intraband transition also.

IV. PIEZOELECTRIC FIELD IN THE (11N)-ORIENTED ZINC-BLENDE MULTIPLE LAYER SEMICONDUCTORS

Like III-V compound semiconductors, the III-V-N semiconductors are piezoelectric materials. When a stress is applied to the material, the atoms of opposite charge polarity are displaced from their equilibrium positions. The strain-induced piezoelectric polarization will occur. The three components of the strain induced polarization in any layer are given by

\[ P_i = 2\varepsilon_{ij} \epsilon_{jk}, \quad i,j,k = x,y,z, \quad \text{in cyclic order}, \]

where \(\varepsilon_{ij}\) is the piezoelectric coefficient. The strain-induced polarization along the [11N] growth direction is then given by

\[ P^\perp = \frac{-2\varepsilon_{14}}{\sqrt{N^2 + 2}} (N\varepsilon_{xy} + \varepsilon_{yz} + \varepsilon_{xz}), \]

Downloaded 28 Apr 2013 to 155.69.4.4. This article is copyrighted as indicated in the abstract. Reuse of AIP content is subject to the terms at text: http://ajp.aip.org/about/rights_and_permissions
where
\[
\varepsilon_{xy} = \frac{1}{N^2 + 2}[\varepsilon_{zz}' - \varepsilon_{xx}' + \sqrt{2N}\varepsilon_{x}'],
\]
\[
\varepsilon_{yz} = \varepsilon_{xz} = \frac{1}{N^2 + 2}[N(\varepsilon_{zz}' - \varepsilon_{xx}') + (N^2 - 2)\varepsilon_{x'}]/\sqrt{2}.
\]

The polarization induced electric field along the \([11\hat{N}]\) growth direction of the \(j^{th}\) layer is given by\(^{20}\)
\[
F_j = \frac{1}{D} \sum_{k=1}^{n} \left( p_{j}^{k} - p_{j}^{k-1} \right) \frac{L_k}{e_k},
\]
where
\[
\varepsilon = \varepsilon_r\varepsilon_0 \quad \text{and} \quad \varepsilon_r, \varepsilon_0 \quad \text{are the relative dielectric constants}
\]
and absolute permittivity, respectively. \(L_k\) is the thickness of layer \(k\).

V. OPTICAL GAIN AND RADIATIVE CURRENT DENSITY

To avoid the absorption in bandgap error caused by Lorentzian line shape, the optical gain can be written as\(^{21}\)
\[
g(E) = \left[ 1 - \exp \left( \frac{E - \Delta F}{k_B T} \right) \right] \frac{\pi^2 e^2 h^3}{n^2 E^2} R_{sp}(E),
\]
where \(\Delta F = E_f - E_l\) is the quasi-Fermi levels separation and dependent on carrier density. \(E_f\) and \(E_l\) are the electron and hole quasi-Fermi level in the conduction and valence band, respectively. \(k_B\) is the Boltzmann constant, \(T\) is the temperature, \(n\) is the refractive index, \(c\) is the light velocity. The spontaneous emission rate is given by\(^{11,21}\)
\[
R_{sp}(E) = \frac{h e^2 E}{2\pi m_0 a_0 h c^3} \sum_{n,m,n',m'} \int \frac{Q_{nm}^{mn} n m}{4\pi^2 \hbar f_z f_x} \frac{1}{\pi} \times \frac{h/\tau}{(E_h - E_n')^2 + (\hbar/\tau)^2} dk' dk'' = \frac{n^2 E^2}{\hbar^2 \pi^2 c^2} g(E),
\]
where
\[
\begin{array}{c}
\rho_{nm}^{mn} = \text{the squared optical transition matrix elements}, \\
E \text{ is the photon energy}, \\
E_h \text{ is the interband transition energy}, \\
\varepsilon_0 \text{ is the free-space dielectric constant}, \\
\tau \text{ is the intraband relaxation time}, \\
f_z \text{ and } f_x \text{ are the Fermi-Dirac distributions for electrons in the conduction bands and holes in the valence subbands}, \\
\end{array}
\]

The radiative current density, \(J_{rad}\) can be calculated from the spontaneous emission spectrum using\(^{22}\)
\[
J_{rad} = el \int R_{sp}(E) dE,
\]
where \(l\) is the well width.

VI. RESULTS AND DISCUSSIONS

We take \(In_{0.36}Ga_{0.64}As_{0.973}N_{0.027}/GaAs\) QW as an example. The well width and barrier width are taken as 70 and 200 Å, respectively. Some band parameters used are taken from Ref. 23 and listed in Table I. The bowing effect is taken into consideration for the parameters \(E_g\), \(E_{\text{VBO}}\), \(m_e^*\), \(E_h^0\), and \(V_N\) calculations, and their bowing parameters are \(0.477\) eV, \(-0.38\) eV, \(0.0091\), \(0.38\) eV, and \(3.5\) eV, respectively.\(^{23,25}\) The rest parameters of the alloy are obtained by linear interpolation method. Unlike band parameters, the in-plane strain must consider the GaN and InN lattice constants’ contribution, which are \(4.50\) and \(4.98\) Å, respectively.\(^{23}\) The corresponding in-plane strain for the \(In_{0.36}Ga_{0.64}As_{0.973}N_{0.027}\) on GaAs is about -0.02. Note that zinc-blende InN band gap was recently reported only 0.61 eV,\(^{30,31}\) much smaller than the widely used value in Ref. 23. Thanks to band-anti-crossing model,\(^{32}\) the band gap of InN won’t be used and this debate won’t affect the 10-band kp calculation.

The final band line-ups of the \(In_{0.36}Ga_{0.64}As_{0.973}N_{0.027}/GaAs\) QWs grown on the (11N)-oriented substrate with \(N = 0, 1, 3, \infty\) are shown in Fig. 1. (11\infty) is the (001) case. The strain, band anti-crossing and piezoelectric field effects are taken into consideration in the final band line-ups. For the (110) and (001) cases, the piezoelectric field is zero. Note that the Eqs. (4.5,36a-c) in Ref. 34 can be used to calculate the band edges for the (001) case, however, generally the band edges for the non-(001) cases, such as, the (110) and (113) cases have no analytic expressions because of the intermixing of HH, LH, and spin-orbit splitting band at \(k = 0\) point, and have to be numerically calculated using the 8-band strained \(H\) at \(k = 0\). The 8-band strained \(H\) can be easily obtained by removing nitrogen energy terms in Eq. 4.
The \( E^W \) is from Ref. 25, which is with respect to the top of valence band after strain for the strained QWs.

The first 4 electron and the first 6 hole subbands along the \([1'00]\) and \([1'1'0]\) wave vector direction for the \( \text{In}_{0.36}\text{Ga}_{0.64}\text{As}_{0.973}\text{N}_{0.027}/\text{GaAs} \) QWs grown on the \((110), (111), (113), \) and \((001)\) substrates are shown in Fig. 2. The well width is 70 \( \text{Å} \) and the barrier width is 200 \( \text{Å} \). We can see that the energy dispersion curves are obviously dependent on the substrate orientation especially for the valence subbands. The anisotropy effect of valence subbands is strong for the \((110), (113), \) and \((001)\) cases. The anisotropy effect is not found in the \((111)\) case due to its hexagonal symmetry. The electron subbands are basically isotropic because of the isotropy of electron effective mass. For the \((110)\) and \((001)\) cases, the energy curves are two-fold degenerate. However, for the \((111)\) and \((113)\) cases, the two-fold degenerate is broken due to the strain-induced internal electric field which results in the asymmetry QWs.

The squared wavefunctions of the first 4 electron and the first 6 hole energy levels at \( k = 0 \) point are shown in Fig. 3. Due to the internal electric field, the wavefunctions become asymmetry for the \((111)\) and \((113)\) cases. For the \((110)\) case, the LH1 wavefunction becomes abnormal. The reason is that the LH1 strongly coupled with the HH, see the LH1 and HH5 dispersion curves for the \((110)\) case in Fig. 2.

In order to see the anisotropy effect of the valence subbands clearly, the equal-energy contour plots of the first valence subband (HH1) are shown in Fig. 4. We can see that all the patterns have mirror plane symmetry. And, the \((110), (113), \) and \((001)\) cases have the \( C_4 \) rotation symmetry and the \((111)\) case has the \( C_6 \) rotation symmetry. The patterns just reflect the symmetry of \((11N)\)-orientation in real space.

The squared optical transition elements are calculated. The contour plots of the equal squared optical transition element from the first conduction subband \( E_1 \) to the first valence subband (HH1) of the 4 QWs are shown in Fig. 5. Compared to the \((001)\) case, the larger optical transition anisotropy are found in the non-\((001)\) cases, such as the \((110)\) case.

Orientation dependence of the fundamental transition energies from the first conduction subband \( E_1 \) to the first valence subband (HH1) of the 4 QWs are shown in Fig. 6. We find that the \((111)\)-QW has the largest transition energy and the \((001)\)-QW has the smallest transition energy. This consists with the band line-ups in Fig. 1. The strained band gap of the \((001)\)-InGaAsN is the smallest and that of the \((111)\)-QW is the largest. Although there exists the internal electric field in the \((111)\) case, this will cause Stark red-shift, this shift is smaller compared to the strain-induced shift in...
The similar variation trend is observed in the (11N)-InGaAs QWs too in Ref. 9. The strain may cause the piezoelectric field in well and barrier regions for the (11N)-QWs except the (001) and (110) cases. The orientation dependence of the internal strain-induced piezoelectric field in the well layer (a) and barrier layer (b) of the 4 QWs are shown in Fig. 7. We find that (111) case has the largest absolute value of electric field in well and barrier regions. And the field directions in well and barrier are opposite. This variation trend was also reported in the GaN/AlGaN (11N)-oriented QWs19 and InGaAs/GaAs (11N)-oriented QWs.33

Axial approximation is widely used in band structure and optical gain calculation for the (001)-QWs. 34 This approximation assumes that $c L^2/c L^3$ in the $R$ term only, while other terms in Hamiltonian still use $c L^2$ and $c L^3$. The

FIG. 3. The electron and hole squared wavefunctions at $k = 0$ point of the 4 QWs in Fig. 1.

FIG. 4. Equal-energy contour plots of the first valence subband (HH1) of the 4 QWs in Fig. 1. The unit of the energy level in the legend is meV.

FIG. 5. Contour plots of the equal squared optical transition element from the first conduction subband ($E_1$) to the first valence subband (HH1) of the 4 QWs in Fig. 1. The unit of the squared optical transition element in the legend is eV.

FIG. 6. Orientation dependence of the fundamental transition energy from the first conduction subband ($E_1$) to the first valence subband (HH1) of the 4 QWs in Fig. 1.
approximation won’t change the energy levels at $k=0$ point and can greatly reduce the computation time because the double fold integration in density of states and gain calculations can be replaced by a single fold integration. However, this approximation cannot be used in the non-(001) oriented QWs, because it cannot give the correct energy levels at $k=0$ point, results are not shown here. The integration $\int \cdots dk_x' dk_y'$ in Eq. (44) should be integrated in whole $k_x' k_y'$ plane, which is very time-consuming. From Figs. 4 and 5, one can find the energy and optical transition matrix element contour plots show the mirror plane symmetry. Thus, the above mentioned integration can be done within the first quadrant. Using this method, the computation time is significantly reduced. The TE mode and TM mode optical gain spectra at the carrier concentration $n = 2, 4, 6,$ and $8 \times 10^{18} \text{ cm}^{-3}$ of the 4 QWs are calculated and shown in Fig. 8. The temperature is 300 K, and the intraband relaxation time $\tau$ is 0.1 ps. The TE mode gain is dominant because of the compressive strain in the QW. The TE mode peak gain versus radiative current density curves of the 4 QWs are shown in Fig. 9. The transparent radiative current densities are 35.9, 36.6, 38.4, and 39.3 A/cm² for (111), (110), (113), and (001)-oriented QWs, respectively. When $J_{\text{rad}}$ is less than $\sim 52 \text{ A/cm}^2$, the peak gain of (111) > (110) > (113) > (001). When $J_{\text{rad}}$ is larger than $\sim 52 \text{ A/cm}^2$, the peak gain of (111) < (110) < (113) < (001). Note that the four QWs have different fundamental transition energies, only (001)-oriented QW has 1.3 $\mu$m emission wavelength. The nitrogen composition can be adjusted for the QWs to have the same fundamental transition energies. For 1.3 $\mu$m emission wavelength, the nitrogen composition $N = 2.7, 3.0, 3.5,$ and 3.7%.
gain is associated with (111)-oriented QW. When \( J_{\text{rad}} \) is with (001)-oriented QW. These results are similar with those (110)-QWs. There exists an injection current density turning layers are the largest for (111)-QW and zero for (001) and lute values of internal piezoelectric fields in well and barrier layers are the largest for (111)-QW and the smallest for the (001)-QW. The abso-

We find that fundamental transition energy is the largest for \( 1.3 \mu m \) requirement, the rest parameters are unchanged.

The transparent radiative current densities are 32.4, 33.8, and 39.3 A/cm\(^2\) for the (111), (110), (113), and (001)-oriented QWs with emission wavelength of \( \sim 1.3 \mu m \) are shown in Fig. 10. Except the (001) case, the N composition is adjusted to meet \( \sim 1.3 \mu m \) requirement, the rest parameters are unchanged. The transparent radiative current densities are 32.4, 33.8, 37.2, and 39.3 A/cm\(^2\) for the (111), (110), (113), and (001)-oriented QWs with emission wavelength of \( \sim 1.3 \mu m \), respectively. When \( J_{\text{rad}} \) is less than \( \sim 80 \) A/cm\(^2\), the largest peak gain is associated with (111)-oriented QW. When \( J_{\text{rad}} \) is larger than \( \sim 80 \) A/cm\(^2\), the largest peak gain is associated with (001)-oriented QW. These results are similar with those of the InGaAsP QW in Ref. 35, but different with results in Ref. 10 where the (110)-oriented QW has the largest peak gain.

VII. CONCLUSIONS

The 10-band \( k \cdot p \) formulae to calculate band structure and optical gain for the (11N)-oriented QWs are given. The InGaAsN/GaAs (11N)-QWs are investigated including the strain and piezoelectric field effects. The energy dispersion curves and optical gain are strongly orientation dependent. We find that fundamental transition energy is the largest for the (111)-QW and the smallest for the (001)-QW. The absolute values of internal piezoelectric fields in well and barrier layers are the largest for (111)-QW and zero for (001) and (110)-QWs. There exists an injection current density turning point. At the smaller injection current density, the (111)-oriented QW has the largest peak gain. At the larger injection current density, the (001)-oriented QW has the largest peak gain. The injection current density turning points are about 52 and 80 A/cm\(^2\) for the InGaAsN QW with the same N composition of 2.7% and the same emission wavelength of 1.3 \( \mu m \), respectively. The results will be helpful to understand the III-V-N dilute nitride semiconductor (11N)-oriented QW physics and device design.

APPENDIX A: STRAIN TENSOR AND STRAIN HAMILTONIAN TERMS

The strain tensors of the (11N)-oriented III-V-N materials can be derived using the method in Ref. 9. The components of strain tensor for the (11N) orientation are given by

\[
\varepsilon'_{xx} = \varepsilon'_{yy} = \varepsilon_{xx}, \quad (A1)
\]
\[
\varepsilon'_{xy} = \varepsilon_{xz} = 0, \quad (A2)
\]
\[
\varepsilon'_{xz} = \frac{K_1}{2K_2}, \quad (A3)
\]
\[
\varepsilon'_{zz} = \frac{K_3}{K_2}, \quad (A4)
\]

where

\[
K_1 = (C_{11} + 2C_{12})(-C_{11} + C_{12} + 2C_{44})N(N^2 - 1), \quad (A5)
\]
\[
K_2 = 2C_{44}(C_{11} + C_{12} + 2C_{44})
+ [C_{11}(C_{11} + C_{12} + 2C_{44})
- 2C_{12}C_{44} + C_{11}C_{44}N^2]N^2, \quad (A6)
\]
\[
K_3 = -2[C_{44}(C_{11} + 3C_{12} - 2C_{44})
+ C_{11}(C_{11} + C_{12} - 2C_{44})
- 2C_{12}C_{44}N^2]N^2. \quad (A7)
\]

Note that, \( \varepsilon'_{zz} \) is 0 for (110), (111) and (11\infty)-oriented QWs, but generally it is nonzero for the (11N)-QWs. Considering above relations, the strain terms can be simplified as

\[
P_{zz} = -P_0[\varepsilon_{xx}k_z + ik_z\varepsilon_{xx}], \quad (A8)
\]
\[
P_{xx} = -P_0(\varepsilon'_{xz}k_x + i\varepsilon'_{xz}k_z), \quad (A9)
\]
\[
E_{xx}^z = a_z(2\varepsilon'_{xx} + \varepsilon'_{zz}), \quad (A10)
\]
\[
P_z = a_z(2\varepsilon'_{xx} + \varepsilon'_{zz}), \quad (A11)
\]

\[
Q_z = \frac{1}{(2 + N^2)^2} \{b(N^2 - 1)[3\sqrt{2}\varepsilon'_{xx}N + \varepsilon_{xx} - \varepsilon'_{zz}](N^2 - 1)] + d\sqrt{3}\{\sqrt{2}\varepsilon'_{xx}N(1 - N^2) + \varepsilon_{xx} - \varepsilon'_{zz}(2N^2 + 1)]}, \quad (A12)
\]
\[
S_z = \frac{1}{(2 + N^2)^2} \{6(b - d/\sqrt{3})N(N^2 - 1)\varepsilon_{xx} - \varepsilon'_{xx} + [6\sqrt{3}N^2b + (4 - 2N^2 + N^4)d]\varepsilon_{zz}, \quad (A13)
\]
\[ R = -\frac{\sqrt{3}b - d}{(2 + N^2)^2}[3\sqrt{2N} \epsilon' + (N^2 - 1) \epsilon''], \quad (A14) \]

\[ C_{ij} \] is the elastic stiffness constant. \( \epsilon' \) is the in-plane strain and given by
\[ \epsilon' = \frac{a_s - a_f}{a_f}, \quad (A15) \]

\( a_s \) and \( a_f \) are the lattice constants of the substrate and epilayer, respectively.

**APPENDIX B: BASIS FUNCTION AND ENVELOPE WAVE FUNCTIONS**

For the conventional (001)-oriented QW, the basis set in \( U, J > \) representation is widely used, which can diagonalize the spin-orbit Hamiltonian. The basis set used in the \( (x', y', z') \) coordinates are similar and given by

\[ \Phi_N(+) = \left| S \right\rangle \rangle, \quad (B1) \]
\[ \Phi_N(-) = \left| S \right\rangle \langle \langle \left. \right|, \quad (B2) \]
\[ \Phi_e(+) = \left| S \right\rangle \rangle, \quad (B3) \]
\[ \Phi_e(-) = \left| S \right\rangle \langle \langle \left. \right|, \quad (B4) \]

\[ \phi_{3/2, 3/2} = -\frac{i}{\sqrt{2}} \left| (X' + iY') \right\rangle \langle \langle \left. \right|, \quad (B5) \]
\[ \phi_{3/2, -1/2} = -\frac{i}{\sqrt{6}} \left| (X' - iY') \right\rangle \langle \langle \left. \right| + 2Z \right\rangle \langle \langle \left. \right|, \quad (B6) \]
\[ \phi_{1/2, -3/2} = \frac{i}{\sqrt{2}} \left| (X' - iY') \right\rangle \langle \langle \left. \right|, \quad (B7) \]
\[ \phi_{1/2, -1/2} = \frac{i}{\sqrt{3}} \left| (X' + iY') \right\rangle \langle \langle \left. \right| + Z \right\rangle \langle \langle \left. \right|, \quad (B8) \]
\[ \phi_{1/2, -3/2} = \frac{i}{\sqrt{3}} \left| (X' - iY') \right\rangle \langle \langle \left. \right| - Z \right\rangle \langle \langle \left. \right|, \quad (B9) \]

The ten dimensional electron and hole envelope wave function can be expressed as
\[ \Phi_n = \{ \Phi_n^j \}, \quad (j = 1, 2, ..., 10), \quad (B11) \]

where