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Orientation dependence of electronic structure and optical gain of (11N)-oriented III-V-N quantum wells

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Orientation dependence of electronic structure and optical gain of (11N)-oriented III-V-N quantum wells

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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\(\infty\))-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\(\infty\))-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\(\infty\))-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\(\infty\))-oriented QW has the largest peak gain. © 2013 American Institute of Physics. [http://dx.doi.org/10.1063/1.4793279]

I. INTRODUCTION

The dilute nitride semiconductor, InGaAsN, has attracted great attention due to its potential application of 1.3 and 1.55 \(\mu\)m GaAs-based laser diodes used in fiber optical communication system. Most works focus on the (001)-oriented InGaAsN, only a few works investigate the InGaAsN grown on the non-(001)-oriented substrates. Ibanez et al. used photoreflectance and high-resolution x-ray diffraction measurements to investigate the orientation effect on the nitroginc incorporation into the host materials.1 Blanc et al. reported the growth condition and optical properties of GaAsN and InGaAsN/GaAs quantum wells (QWs) grown on the (111)-oriented substrates.2 Miguel-Sanchez et al. investigated the effect of nitrogen on the optical properties of InGaAsN grown on misoriented (111)B GaAs substrates.3 Latkowska et al. reported the micro-photoluminescence of InGaAsN grown on various oriented GaAs substrates.4 Recently, a room-temperature laser emission of InGaAsN/GaAs QW grown on (111)B-GaAs was first reported by Miguel-Sanchez et al.5,6 However, the theoretical work on the orientation effect on the electronic structure and optical gain of the InGaAsN/GaAs QW is still lack in literature.

This paper will present the general formulae of the 10-band k-p Hamiltonian for the strained QW grown on the (11N)-oriented substrates in Sec. II. The squared optical transition matrix elements will be derived in Sec. III. Piezoelectric field in the (11N)-oriented Zinc-blende multiple layer semiconductors will be given in Sec. IV. Optical gain and radiative current density formulae will be given in Sec. V. Results and discussions of the InGaAsN/GaAs (11N)-QWs will be presented in Sec. VI. Conclusions will be given in Sec. VII.

II. 10-BAND k-p HAMILTONIAN FOR (11N)-ORIENTED QWs

We assume that a coordinate system \((x,y,z)\) is for the (001)-oriented QW and a coordinate system \((x',y',z')\) is for the (11N)-oriented QW. The QW growth direction is along the axis \(z\) and \(z'\) for the (001) QW and the (11N) QW, respectively. The (11N)-oriented Hamiltonian can be derived from the (001)-oriented Hamiltonian by using the transformation equations in Ref. 7. Generally, the transformation equations can be described by a rotation matrix, which can be written as7-9

\[
O = \begin{bmatrix}
\cos(\theta) & 1 & \sin(\theta) \\
\sqrt{2} & \sqrt{2} & 0 \\
-\sin(\theta) & 0 & \cos(\theta)
\end{bmatrix},
\]

where \(\theta\) is the angle between axis \(z\) and \(z'\). And, \(\theta = \arctan(\sqrt{2}/N)\). The matix \(O\) rotates the vector from the coordinate system \((x,y,z)\) for the (001)-QW to the coordinate system \((x',y',z')\) for the (11N)-QW. For the wave vector, we have

\[
\begin{bmatrix}
k_x \\
k_y \\
k_z
\end{bmatrix} = O \begin{bmatrix}
k'_{x} \\
k'_{y} \\
k'_{z}
\end{bmatrix},
\]

where \(k_x, k_y, k_z\) and \(k'_{x}, k'_{y}, k'_{z}\) are the wave vectors for the (001)- and (11N)-orientations, respectively.

For the strain tensor, we have

\[
\begin{bmatrix}
\varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\
\varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\
\varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz}
\end{bmatrix} = O \begin{bmatrix}
\varepsilon'_{xx} & \varepsilon'_{xy} & \varepsilon'_{xz} \\
\varepsilon'_{yx} & \varepsilon'_{yy} & \varepsilon'_{yz} \\
\varepsilon'_{zx} & \varepsilon'_{zy} & \varepsilon'_{zz}
\end{bmatrix} O^T,
\]

where \(O\) is the rotation matrix.

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where $\varepsilon_{ij}$ and $\varepsilon_{ij}'(i,j = x, y, z)$ 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:

$$H = H_k + H_c,$$

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

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

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

$$S_k = \frac{\hbar^2}{2m_0(2 + N^2)^2} \left\{ \sqrt{6}(\gamma_2 - \gamma_3)N[2(k_x^2) + k_y^2 - 4k_x^2 + (k_x^2 + k_y^2 - 2k_z^2)N^2 - i2k_yk_N'N^2)] + 2\sqrt{3}\gamma_2 k_y' [6k_y'N^2 - i2k_y(2 + N^2)] + 2\gamma_3 k_y' [4k_y' - 2(k_x' + ik_y')N^2 + (k_x' - i k_y')N^2] \right\},$$

$$R_k = \frac{\hbar^2 \sqrt{3}}{2m_0(2 + N^2)^2} \left\{ (\gamma_2 - \gamma_3)k_y' [2k_x' + 2\sqrt{2}N(3k_x' + i2k_y' - k_N'N^2)\sqrt{2} + i 2k_y'N^2)] + (\gamma_2 + \gamma_3)k_y' [2k_y' + i4k_y'N^2] + \gamma_2 [-4k_y'^2 + N^2(k_x'^2 + k_y'^2) + i2k_y'k_N'^2] + \gamma_3 [-k_y'^2 (5N^2 + N^4) + k_y'^2 (3N^2 + N^4) + i8k_y'k_N'^2] \right\},$$

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

$$E_c = E_G + \frac{\hbar^2}{2m_0} \gamma_c (k_x^2 + k_y^2 + k_z^2),$$

and

$$\gamma_c = \frac{1}{m_e^*} \left( \frac{E_F}{E_G + \Delta} \right).$$
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:

$$\gamma_1 = \gamma_1^L - \frac{1}{3} \frac{E_p}{E_G},$$

$$\gamma_2 = \gamma_2^L - \frac{1}{6} \frac{E_p}{E_G},$$

$$\gamma_3 = \gamma_3^L - \frac{1}{6} \frac{E_p}{E_G}.$$

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

$$E_p = \frac{2m_0}{\hbar^2} P_0^2.$$

$VBO$ describes the valence band edge offset. $x$ is the nitrogen composition. $E^N$ 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 ($\gamma_1$, $\gamma_1^L$, $\gamma_2$, $\gamma_3$, $E_p$ 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. The nitrogen level with respect to the unstrained VBM, $E^N_0$ is given by

$$E^N = E^N_0 + VBM^S,$$

$VBM^S$ 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:

$$k_i' k_j' \leftrightarrow \epsilon_i' \epsilon_j' \quad (i, j = x, y, z),$$

$$\frac{\hbar^2 \epsilon_i'}{2m_0} \leftrightarrow \alpha_z, \label{eq:18}$$

$$\frac{\hbar^2 \gamma_1}{2m_0} \leftrightarrow -\alpha_x, \label{eq:19}$$

$$\frac{\hbar^2 \gamma_2}{2m_0} \leftrightarrow b, \label{eq:20}$$

$$\frac{\hbar^2 \gamma_3}{2m_0} \leftrightarrow \frac{d}{2\sqrt{3}}, \label{eq:21}$$

where $\alpha_x$ and $\alpha_z$ 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:

$$Q_{i,i'}^{n,n'} = \frac{2}{m_0} |\langle \Psi_{n'} | \hat{\epsilon} \cdot \mathbf{p}_i | \Psi_{n} \rangle|^2,$$  \hspace{1cm} (24)

where $\hat{\epsilon}$ is the unit vector in the direction of the electric field, $\mathbf{p}_i$ is the momentum operator, and $\Psi_{n'}$ and $\Psi_{n}$ 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:

\begin{align*}
Q_{x'x}^{n,n'} &= \frac{2P_{2}^2}{m_0} \left\{ \sum_m \left( -\frac{i}{\sqrt{2}} a_{n,m}^6 d_{n,m}^3 \right)^2 + \sum_m \frac{i}{\sqrt{6}} a_{n,m}^7 d_{n,m}^3 \right\}^2 + \sum_m \left( \frac{i}{\sqrt{3}} a_{n,m}^{10} d_{n,m}^3 \right)^2, \label{eq:25} \\
Q_{y'y}^{n,n'} &= \frac{2P_{2}^2}{m_0} \left\{ \sum_m \left( -\frac{i}{\sqrt{2}} a_{n,m}^6 d_{n,m}^3 \right)^2 + \sum_m \frac{i}{\sqrt{6}} a_{n,m}^7 d_{n,m}^3 \right\}^2 + \sum_m \left( \frac{i}{\sqrt{3}} a_{n,m}^{10} d_{n,m}^3 \right)^2, \label{eq:26} \\
Q_{z'z}^{n,n'} &= \frac{2P_{2}^2}{m_0} \left\{ \sum_m \frac{1}{\sqrt{2}} a_{n,m}^6 d_{n,m}^3 \right\}^2 + \sum_m \frac{1}{\sqrt{6}} a_{n,m}^7 d_{n,m}^3 \right\}^2 + \sum_m \frac{1}{\sqrt{3}} a_{n,m}^{10} d_{n,m}^3 \right\}^2, \label{eq:27}
\end{align*}
\[ Q_{v'v}^{i,n} = \frac{2P_0^2}{m_0} \left\{ \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{6s} d_{m,m}^{4s} + \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{8s} d_{m,m}^{4s} + \sum_m \left( -\frac{1}{\sqrt{3}} a_{m,m}^{10s} a_{m,m}^{4s} \right)^2 \right\}, \]  

\[ Q_{z'z}^{i,n} = \frac{2P_0^2}{m_0} \left\{ \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{6s} d_{m,m}^{3s} + \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{8s} d_{m,m}^{3s} + \sum_m \left( -\frac{1}{\sqrt{3}} a_{m,m}^{10s} a_{m,m}^{3s} \right)^2 \right\}, \]  

\[ Q_{z'z}^{n,n} = \frac{2P_0^2}{m_0} \left\{ \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{6s} d_{m,m}^{3s} + \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{8s} d_{m,m}^{3s} + \sum_m \left( -\frac{1}{\sqrt{3}} a_{m,m}^{10s} a_{m,m}^{3s} \right)^2 \right\}, \]  

\[ Q_{z'z}^{n,n} = \frac{2P_0^2}{m_0} \left\{ \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{6s} d_{m,m}^{3s} + \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{8s} d_{m,m}^{3s} + \sum_m \left( -\frac{1}{\sqrt{3}} a_{m,m}^{10s} a_{m,m}^{3s} \right)^2 \right\}, \]  

where \( P_0 = \langle S'|p_x|X' \rangle = \langle S'|p_y|Y' \rangle = \langle S'|p_z|Z' \rangle \). Note that the above equations only include the \( S'^c \rightarrow X'^v, Y'^v, Z'^v \) transitions. Due to the interaction between valence and conduction bands, \( \Phi_{nc} \) 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 \( \Phi_{nc} \) and the non-valence band components in \( \Phi_{nv} \) (\( X'^v, Y'^v, Z'^v \rightarrow S'^v \)) must be considered in the derivation of \( Q_{i,n}^{i,n} \). So, the additional \( X'^v, Y'^v, Z'^v \rightarrow S'^v \) transition contributions will then be

\[ Q_{v'v}^{n,n} = \frac{2P_0^2}{m_0} \left\{ \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{6s} d_{m,m}^{3s} + \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{8s} d_{m,m}^{3s} + \sum_m \left( -\frac{1}{\sqrt{3}} a_{m,m}^{10s} a_{m,m}^{3s} \right)^2 \right\}, \]  

\[ Q_{z'z}^{n,n} = \frac{2P_0^2}{m_0} \left\{ \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{6s} d_{m,m}^{3s} + \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{8s} d_{m,m}^{3s} + \sum_m \left( -\frac{1}{\sqrt{3}} a_{m,m}^{10s} a_{m,m}^{3s} \right)^2 \right\}, \]  

\[ Q_{z'z}^{n,n} = \frac{2P_0^2}{m_0} \left\{ \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{6s} d_{m,m}^{3s} + \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{8s} d_{m,m}^{3s} + \sum_m \left( -\frac{1}{\sqrt{3}} a_{m,m}^{10s} a_{m,m}^{3s} \right)^2 \right\}, \]  

\[ Q_{z'z}^{n,n} = \frac{2P_0^2}{m_0} \left\{ \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{6s} d_{m,m}^{3s} + \sum_m \frac{1}{\sqrt{2}} d_{m,m}^{8s} d_{m,m}^{3s} + \sum_m \left( -\frac{1}{\sqrt{3}} a_{m,m}^{10s} a_{m,m}^{3s} \right)^2 \right\}, \]

The last term of \( QA_{z'z}^{n,n} \) is for \( X'^v, Y'^v, Z'^v \rightarrow S'^v \) transition, it should be very small and can be ignored for interband transition. The summation of \( Q_{i,n}^{i,n} \) and \( QA_{v'v}^{i,n} \), \( QA_{z'z}^{n,n} \) 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 (111)-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

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

where \( e_{ij} \) is the piezoelectric coefficient. The strain-induced polarization along the [111] growth direction is then given by

\[ P_\parallel = -\frac{2\varepsilon_{ij}}{\sqrt{N^2 + 2}} (Ne_{xy} + e_{yz} + e_{zx}), \]
where
\[ e_{xy} = \frac{1}{N^2 + 2} \left[ N' + N + \sqrt{2N} \right], \]
\[ e_{yz} = e_{xz} = \frac{1}{N^2 + 2} \left[ N' - N - \sqrt{2N} \right], \]
\[ (40) \]
The polarization induced electric field along the \([11N]\) growth direction of the \(j^{th}\) layer is given by \(^{20}\)
\[ F_j = e \sum \frac{L_k}{\ell_k} \sum_{k=1}^{N} (\frac{P_{ik}^j}{\ell_k}) \sum_{j=1}^{N} \frac{L_k}{\ell_k}, \]
\[ (42) \]
where \(\varepsilon = \varepsilon_r \varepsilon_0\) and \(\varepsilon_r, \varepsilon_0\) 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 \(^{21}\)
\[ g(E) = \left[ 1 - \exp \left( \frac{E - \Delta F}{k_B T} \right) \right] \frac{\pi^2 c^2 h^3}{n^2 E^2} R_{sp}(E), \]
\[ (43) \]
where \(\Delta F = E_f - E_i\) is the quasi-Fermi levels separation and dependent on carrier density. \(E_f\) and \(E_i\) 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 \(^{11,21}\)
\[ R_{sp}(E) = \frac{\hbar^2 E}{2 \pi m_q^2 h \tau^2} \sum_{\alpha,n} \int \frac{Q_{\alpha,n}^{\alpha,n}}{4 \pi^2} f_i f_e \frac{1}{\pi} \]
\[ \times \frac{\hbar/\tau}{(E_{ch} - E)^2 + (\hbar/\tau)^2} d\kappa', d\kappa', = \frac{n^2 E^2}{\hbar^2 \pi^2 \tau^2} g(E), \]
\[ (44) \]
\(Q_{\alpha,n}^{\alpha,n}\) is the squared optical transition matrix elements, \(E\) is the photon energy, \(E_{ch}\) is the interband transition energy, \(\varepsilon_0\) is the free-space dielectric constant, \(\tau\) is the intraband relaxation time, \(f_i\) and \(f_e\) are the Fermi-Dirac distributions for electrons in the conduction bands and holes in the valence subbands, respectively.

The radiative current density, \(J_{rad}\) can be calculated from the spontaneous emission spectrum using \(^{22}\)
\[ J_{rad} = e l \int R_{sp}(E) dE, \]
\[ (45) \]
where \(l\) is the well width.

VI. RESULTS AND DISCUSSIONS

We take \(\text{In}_{0.36}\text{Ga}_{0.64}\text{As}_{0.97}\text{N}_{0.027}/\text{GaAs}\) 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 \(E_g, VBO, m_e^*, E^\text{av}\), 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. \(^{23}\) 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 \(\text{In}_{0.36}\text{Ga}_{0.64}\text{As}_{0.97}\text{N}_{0.027}\) 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 k-p calculation.

The final band line-ups of the \(\text{In}_{0.36}\text{Ga}_{0.64}\text{As}_{0.97}\text{N}_{0.027}/\text{GaAs}\) 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 [1'10] wavevector direction for the strained QWs grown on the (110), (111), (113), and (001) substrates are shown in Fig. 2. The well width is 70 Å and the barrier width is 200 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 \( c_L^2/C_2 \) 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 $\int \ldots \int \frac{\partial k_x'}{\partial k_x} d\kappa \frac{\partial k_y'}{\partial k_y}$ 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 $8 \times 10^{18}$ cm$^{-3}$ of the 4 QWs are calculated and shown in Fig. 8. The temperature is $300 \, \text{K}$, and the intraband relaxation time $\tau$ is $0.1 \, \text{ps}$. 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 $39.3 \, \text{A/cm}^2$ 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 $1.3 \, \mu\text{m}$ emission wavelength. The nitrogen composition can be adjusted for the QWs to have the same fundamental transition energies. For $1.3 \, \mu\text{m}$ emission wavelength, the nitrogen composition $N = 2.7, 3.0, 3.5,$ and $3.7\%$.
for (001), (113), (110), and (111)-oriented QWs, respectively. The TE mode peak gain versus radiative current density curves of In$_{0.36}$Ga$_{0.64}$AsN/GaAs QWs with emission wavelength of ~1.3 μm are shown in Fig. 10. Except the (001) case, the N composition is adjusted to meet ~1.3 μm 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. The TE mode peak gain for the (113)-oriented QW has the largest peak gain. At the larger injection current density, the (111)-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 μm, 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:

$$\epsilon_{xx}^t = \epsilon_{yy}^t = \epsilon_{zz}^t = 0,$$

$$\epsilon_{xy}^t = \epsilon_{xz}^t = \epsilon_{yz}^t = 0,$$

$$\epsilon_{xx}^t = K_1 \epsilon_{//}^t,$$

$$\epsilon_{zz}^t = K_3 \epsilon_{//}^t,$$

where

$$K_1 = (C_{11} + 2C_{12})(-C_{11} + C_{12} + 2C_{44})N(N^2 - 1),$$

$$K_2 = 2C_{44}(C_{11} + C_{12} + 2C_{44}) + [C_{11}(C_{11} + C_{12} + 2C_{44}) - 2C_{12}C_{44} + C_{11}C_{44}N^2]N^2,$$

$$K_3 = -2[C_{44}(C_{11} - 3C_{12} - 2C_{44}) + C_{11}(C_{11} + C_{12} - 2C_{44}) - 2C_{12}^2C_{44}N^2]N^2.$$

Note that, $\epsilon_{zz}^t$ is 0 for (110), (111) and (11∞)-oriented QWs, but generally it is nonzero for the (11N)-QWs. Considering above relations, the strain terms can be simplified as

$$P_{xx} = -P_0[\epsilon_{xx}^t(k_z^t + ik_x^t) + \epsilon_{xx}^t k_z^t],$$

$$P_{zz} = -P_0[\epsilon_{xx}^t(k_z^t + ik_x^t) + \epsilon_{xx}^t k_z^t],$$

$$E_z^t = a_v(2\epsilon_{xx}^t + \epsilon_{zz}^t),$$

$$P_z = a_v(2\epsilon_{xx}^t + \epsilon_{zz}^t).$$

**VII. CONCLUSIONS**

The 10-band k-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 for the (11N)-oriented QWs are given. The TE mode peak gain versus radiative current density curves of In$_{0.36}$Ga$_{0.64}$AsN/GaAs QWs with emission wavelength of 1.3 μm are shown in Fig. 10. Except the (001) case, the N composition is adjusted to meet ~1.3 μm 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 1.3 μm, respectively. When $J_{rad}$ is less than ~80 A/cm$^2$, the largest peak gain is associated with (111)-oriented QW. When $J_{rad}$ is larger than ~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.
\[ R_c = -\frac{\sqrt{3}b - d}{(2 + N^2)^2} [3\sqrt{2N}c'_{xx} + (N^2 - 1)(c'_{xx} - c'_{zz})], \quad (A14) \]

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

\( a_s \) and \( a_f \) are the lattice constants of the substrate and epi-layer, respectively.

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

For the conventional (001)-oriented QW, the basis set in \( U, J_\sigma \) 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 \(^7\),
\[ \phi_{\sigma}^{(+)} = \left| S_\sigma \uparrow \right\rangle, \quad (B1) \]
\[ \phi_{\sigma}^{(-)} = \left| S_\sigma \downarrow \right\rangle, \quad (B2) \]
\[ \phi_{e}^{(+)} = \left| S' \uparrow \right\rangle, \quad (B3) \]
\[ \phi_{e}^{(-)} = \left| S' \downarrow \right\rangle, \quad (B4) \]
\[ \phi_{v}^{\left( \frac{3}{2}, \frac{3}{2} \right)} = - \frac{i}{\sqrt{2}} \left| (X' + iY') \uparrow \right\rangle, \quad (B5) \]
\[ \phi_{v}^{\left( \frac{3}{2}, \frac{1}{2} \right)} = - \frac{i}{\sqrt{6}} \left| (X' + iY') \downarrow - 2Z' \downarrow \right\rangle, \quad (B6) \]
\[ \phi_{v}^{\left( \frac{3}{2}, -\frac{1}{2} \right)} = \frac{i}{\sqrt{6}} \left| (X' - iY') \uparrow - 2Z' \downarrow \right\rangle, \quad (B7) \]
\[ \phi_{v}^{\left( \frac{3}{2}, -\frac{3}{2} \right)} = \frac{i}{\sqrt{2}} \left| (X' - iY') \uparrow \right\rangle, \quad (B8) \]
\[ \phi_{v}^{\left( \frac{1}{2}, \frac{1}{2} \right)} = \frac{i}{\sqrt{3}} \left| (X' + iY') \uparrow + Z' \downarrow \right\rangle, \quad (B9) \]
\[ \phi_{v}^{\left( \frac{1}{2}, -\frac{1}{2} \right)} = \frac{i}{\sqrt{3}} \left| (X' - iY') \uparrow - Z' \downarrow \right\rangle. \quad (B10) \]

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

where