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Author(s)	Zhu, Yuan-Hui; Yu, Hongyu; Fan, Weijun
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Band structures and optical gain of strained $\text{GaAs}_x\text{P}_{1-x-y}\text{N}_y/\text{GaP}$ quantum wells

Yuan-Hui Zhu, Hong-Yu Yu, and Wei-Jun Fan^{a)}

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

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In the framework of effective mass Hamiltonian of semiconductor quantum well structures and band anticrossing model, we investigated the band structures of fully strained $\text{GaAs}_x\text{P}_{1-x-y}\text{N}_y/\text{GaP}$ quantum wells. The $\text{GaAs}_x\text{P}_{1-x-y}\text{N}_y$ could be widely modified to be direct-band gap or indirect-band gap by changing the mole fraction of As and N in the well layer. We found that an increase in the N mole fraction in the well layer increases the TE mode optical gain very slightly. © 2011 American Institute of Physics. [doi:10.1063/1.3570630]

Interest in the diluted nitride alloys has been greatly motivated due to their unusual fundamental properties and potential applications in optoelectronic devices, such as light-emitting diodes¹ and multijunction high-efficiency solar cells.² It is well known that the incorporation of a few percent of nitrogen into conventional III-V compound semiconductor alloys leads to a strong interaction between the host material conduction band edge and a narrow resonant band formed by the N-related states, and results in a strong conduction band nonparabolicity, an increase in the electron effective mass, a low electron mobility, and the dramatic reduction in the fundamental band gap.³⁻⁶ It is reported that the substitution of only 1% N for As in GaAs reduces the band gap by more than 0.18 eV.^{7,8} The large band gap reductions were also observed in other group III-V-N alloys. And the alloying of GaP with less than 1% GaN changes the nature of band gap from indirect to direct.⁵ Due to the huge band gap reduction, the GaAsPN/GaP quantum well (QW) has been suggested as a promising QW system for the realization of lasing applications on Si substrates since the lattice constant of GaAsPN alloys can be very close to the Si lattice constant. Both tensile and compressive strain can be introduced into the well layer to improve the laser operating characteristics by adjusting the alloy composition in GaAsPN material. Therefore, it is very interesting and useful to investigate the band structures of fully strained GaAsPN/GaP QW and calculate the optical gain for the point of view of both basic research and technological applications.

In this paper, we investigate the band structures of fully strained $\text{GaAs}_x\text{P}_{1-x-y}\text{N}_y/\text{GaP}$ QW which is grown along [001] axis taking into account the band anticrossing (BAC) effect.⁵ We have derived the effective-mass Hamiltonian, the so-called ten-band model,⁹ to calculate the band structures in Γ -valley. The newly formed ten-band Hamiltonian includes two more spin-degenerated diagonal terms into the eight-band Hamiltonian through the following matrix:

$$H = \begin{pmatrix} H_N & \sqrt{y}V_N I & 0 \\ \sqrt{y}V_N I & H_{cc} & H_{cv} \\ 0 & H_{vc} & H_{vv} \end{pmatrix}, \quad (1)$$

where $H_N = E_N I$ is doubly degenerated Hamiltonian, E_N is the energy of the localized states derived from the substitutional N atoms, and I represents second order identity matrix. $H_{cc} = E_c I$ is doubly degenerated Hamiltonian of the lowest conduction band of the host, and H_{vv} is 6×6 effective mass Hamiltonian which includes the spin-orbit coupling within the valence bands. H_{cv} (H_{vc}) represents the mixing between the conduction band and valence bands, which is expressed in the fully eight-band Hamiltonian model.⁹ The adjustable parameter V_N is the coupling between the localized states and the conduction band states. We have neglected the interaction between the localized states and the valence bands, which is consistent with the assumption that the influence of the E_N on valence band energy is minimal and negligible.¹⁰

In this calculation, all the parameters are calculated using a simple linear average between GaAs, GaP at 300 K,¹¹ except the band gap energies and electron effective mass for the QW materials. We have included the bowing parameters as recommended,

$$P(\text{GaAs}_x\text{P}_{1-x-y}) = xp(\text{GaAs}) + (1-x-y)P(\text{GaP}) - b_p x(1-x-y), \quad (2)$$

where b_p represents the bowing factor for electron effective mass $b_m = 0.0086$, while for the band gap in Γ -valley $b_\Gamma = 0.19$ eV and in X valleys $b_x = 0.24$ eV, respectively. The band offsets are calculated based on model-solid theory. The band structure parameters for GaAs, GaP, GaN, and the BAC parameters for GaAsN, GaPN at 300 K are listed in Table I and Table II, respectively.^{11,12}

In Fig. 1, we find a wide range of concentrations for which the $\text{GaAs}_x\text{P}_{1-x-y}\text{N}_y$ layer becomes direct-band gap semiconductor. It is as shown at the right edge of the figure, which corresponds to the “GaAsN-like” case, the lowest conduction band edge is located at the Γ -conduction valley. The dotted line represents the mole fraction relationship of $\text{GaAs}_x\text{P}_{1-x-y}\text{N}_y$ alloy, where the QW layer lattice matches to the barrier layer. With the increasing mole fraction of N, the decreasing lattice constant will introduce a tensile strain, while with the increasing mole fraction of As, the increasing

^{a)} Author to whom correspondence should be addressed. Electronic mail: ewjfan@ntu.edu.sg.

TABLE I. Band structure parameters for GaAs, GaP, and GaN at 300 K (Ref. 11).

Parameter	GaAs	GaP	GaN
a (Å)	5.6533	5.4505	4.5
γ_1	6.98	4.05	2.67
γ_2	2.06	0.49	0.75
γ_3	2.93	1.25	1.10
E_p (eV)	28.8	31.4	25
E_g (eV)	1.4225	2.7779	3.2397
Δ_{SO} (eV)	0.341	0.08	0.017
a_c (eV)	-7.17	-8.2	-2.20
a_v (eV)	1.16 ^a	1.7 ^a	5.20 ^a
b_v (eV)	-2.0	-1.6	-2.2
C_{11} (GPa)	122.1	140.5	293.0
C_{12} (GPa)	56.6	62.03	159.0
VBO (eV)	-0.80	-1.27	-2.64
m_c (m_0)	0.067	0.13	0.15

^aNote that we take a_v positive to define the interband deformation potential constant $a = a_c - a_v$.

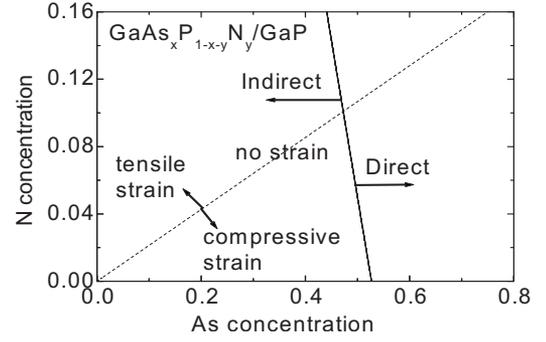
lattice constant will introduce a compressive strain in the QW layer. The induced N elements in the well layer should be larger than the crossover value of 0.1, and makes the band gap of the QW region direct and lattice match to the barrier layer.

We consider a $\text{GaAs}_{0.66}\text{P}_{0.31}\text{N}_{0.03}/\text{GaP}$ type I QW, whose mole fraction parameters in well layer are selected at the lower right corner in the Fig. 1, with a width of 10 nm, and a period of 20 nm. The compressive strain of QW, $e_{xx} = -0.01896$, and the zero energy is set to the top of valence band of unstrained well layer. The lowest electron and hole levels near band gap are shown in Fig. 2. All the energy levels depicted in the figure are twofold degenerate. Due to the strong interaction between conduction bands and nitride levels, and the coupling between conduction bands and valence bands, the lowest energy-wave vector dispersion relation of conduction subbands are nonparabolic. The flattened and downshifted subband E_- is restructured based on the BAC model. The strain effect separates the heavy hole (HH) and light hole subbands. The HH subbands are pushed to the higher energy side and turn out to be the top of valence bands. The effective band gap of this QW is 1.35 eV, equivalent to a cutoff wavelength of about 0.92 μm . Since the main component of E_- subband's wave function is N-related states, which does not contribute to the optical transition, it is expected that the optical transition could be greatly reduced.

The TE mode optical gain spectra are shown in Fig. 3 for $\text{GaAs}_{0.66}\text{P}_{0.34-y}\text{N}_y/\text{GaP}$ QW, $y = 0.03, 0.04, 0.05, \text{ and } 0.06$, respectively. The relationship between spontaneous emission and optical gain is employed here, and the optical gain can be written as

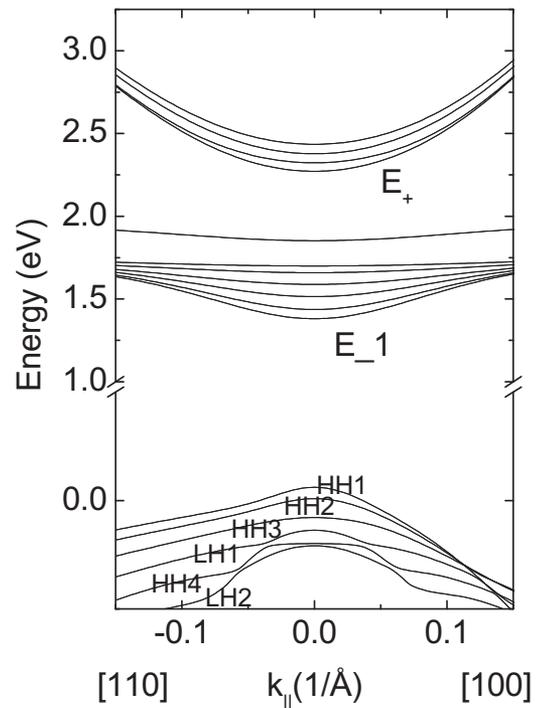
TABLE II. The BAC parameters for GaAsN and GaPN at 300 K (Ref. 12).

Parameter (eV)	GaAsN	GaPN
E^N	1.65	2.18
V	2.7	3.05

FIG. 1. The phase graph of $\text{GaAs}_x\text{P}_{1-x-y}\text{N}_y/\text{GaP}$ QW with relaxed barrier layers.

$$g(E) = \left[1 - \exp\left(\frac{E - \Delta F}{k_B T}\right) \right] \frac{\hbar e^2}{nr\epsilon_0 c m_0^2 l E_{n_c n_v}} \sum \times \int \frac{dk_x dk_y}{4\pi^2} Q^{n_c n_v} f_{n_c} (1 - f_{n_v}) \frac{\hbar / \tau}{(E_{eh} - E)^2 + (\hbar / \tau)^2}, \quad (3)$$

where $\Delta F = E_{fc} - E_{fv}$ is the quasi-Fermi level separation, E is the photon energy, n_r is the refractive index, τ is the intra-band relaxation time, and f_n is the Fermi-Dirac distributions for the electrons in the conduction band and valence band. The quasi-Fermi levels are determined self-consistently from the integration of the two-dimensional density of states in QW and using the charge neutrality condition when the electron and hole density are both the same as the injected carrier density n .¹³ The parameters in our calculations are $n = 6 \times 10^{18} \text{ cm}^{-3}$, $\tau = 0.0658 \text{ ps}$, and $T = 300 \text{ K}$. We can see that the maximum for TE polarized optical gains are basically small and they vary in only 100 cm^{-3} for the calculated nitride mole fraction range. The TE mode optical gain is

FIG. 2. The band structure of a fully strained $\text{GaAs}_{0.66}\text{P}_{0.31}\text{N}_{0.03}/\text{GaP}$ QW with relaxed barrier layers.

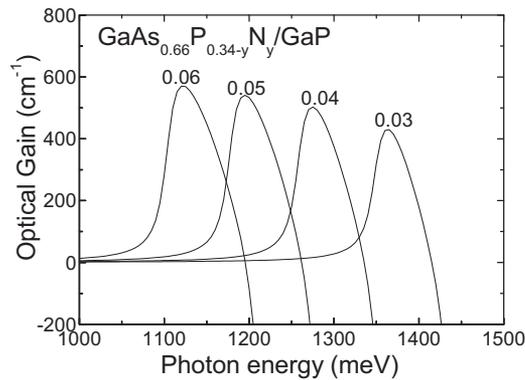


FIG. 3. TE model optical gain for the fully strained $\text{GaAs}_{0.66}\text{P}_{0.34-y}\text{N}_y/\text{GaP}$ QWs.

getting slightly larger as the increasing N mole fraction in the well layer from $y=0.03$ to 0.06 . It can be explained from the reduced compressive strain which lower the conduction electronic subbands. On the other hand, since for a larger nitrogen mole fraction y , an increase in the coupling from the localized N-related states and may significantly lower the overlap of electron and hole wave functions, the optical gain may decrease. The two effects on the optical gain are opposite, the reduced compressive strain effect is slightly higher than the coupling effect from the localized N-related states when increasing N mole fraction.

In this letter, we have given a theoretical model for the band structures for $\text{GaAs}_x\text{P}_{1-x-y}\text{N}_y/\text{GaP}$ QW grown on [001]-oriented substrates. It is found that the HH subbands

are pushed to the top of valence bands because of the compressive strain effect in the well layer. We found that an increase in the N mole fraction in the well layer increases the TE mode gain very slightly because of a decrease in compressive strain effect. It suggests that by doping the nitrogen element into the barrier layer, a decrease in compressive strain may significantly increase the transition probability. Therefore, the compositions at barrier and well layer need to be well understand and carefully designed so that larger optical gain may be obtained in the future.

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