Electronic band structure and optical gain of $\text{Ga}_{\text{NxBiyAs}1-x-y}/\text{GaAs}$ pyramidal quantum dots

Song, Zhi-Gang; Bose, Sumanta; Fan, Wei-Jun; Li, Shu-Shen

2016

Song, Z. G., Bose, S., Fan, W. J., & Li, S. S. (2016). Electronic band structure and optical gain of $\text{Ga}_{\text{NxBiyAs}1-x-y}/\text{GaAs}$ pyramidal quantum dots. *Journal of Applied Physics*, 119(14), 143103-.

<https://hdl.handle.net/10356/80309>

<https://doi.org/10.1063/1.4945700>

© 2016 AIP Publishing LLC. This paper was published in *Journal of Applied Physics* and is made available as an electronic reprint (preprint) with permission of AIP Publishing LLC. The published version is available at: [<http://dx.doi.org/10.1063/1.4945700>]. 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.

Downloaded on 26 Apr 2023 20:49:00 SGT

Electronic band structure and optical gain of $\text{GaN}_x\text{Bi}_y\text{As}_{1-x-y}/\text{GaAs}$ pyramidal quantum dots

Zhi-Gang Song, Sumanta Bose, Wei-Jun Fan, and Shu-Shen Li

Citation: [Journal of Applied Physics](#) **119**, 143103 (2016); doi: 10.1063/1.4945700

View online: <http://dx.doi.org/10.1063/1.4945700>

View Table of Contents: <http://scitation.aip.org/content/aip/journal/jap/119/14?ver=pdfcov>

Published by the [AIP Publishing](#)

Articles you may be interested in

[Intraband optical transition in \$\text{InGaAs}/\text{GaAs}\$ pyramidal quantum dots](#)

J. Appl. Phys. **113**, 064310 (2013); 10.1063/1.4790870

[Analysis of the modified optical properties and band structure of \$\text{GaAs}_{1-x}\text{Sb}_x\$ -capped \$\text{InAs}/\text{GaAs}\$ quantum dots](#)

J. Appl. Phys. **112**, 074311 (2012); 10.1063/1.4755794

[Electronic structure of \$\text{InAs}\$ quantum dots with \$\text{GaAsSb}\$ strain reducing layer: Localization of holes and its effect on the optical properties](#)

Appl. Phys. Lett. **97**, 203107 (2010); 10.1063/1.3517446

[Electronic structure and optical gain saturation of \$\text{InAs}_{1-x}\text{N}_x/\text{GaAs}\$ quantum dots](#)

J. Appl. Phys. **105**, 123705 (2009); 10.1063/1.3143025

[Excitonic properties of strained wurtzite and zinc-blende \$\text{GaN}/\text{Al}_x\text{Ga}_{1-x}\text{N}\$ quantum dots](#)

J. Appl. Phys. **94**, 7178 (2003); 10.1063/1.1623330

A promotional banner for AIP Applied Physics Reviews. On the left is a small image of a book cover titled 'AIP Applied Physics Reviews' showing a diagram of a device. The main part of the banner has a blue background with a bright light source on the right. The text 'NEW Special Topic Sections' is prominently displayed in white. Below this, on an orange background, it says 'NOW ONLINE' in yellow, followed by 'Lithium Niobate Properties and Applications: Reviews of Emerging Trends' in white. The AIP Applied Physics Reviews logo is in the bottom right corner.

NEW Special Topic Sections

NOW ONLINE
Lithium Niobate Properties and Applications:
Reviews of Emerging Trends

AIP Applied Physics
Reviews

Electronic band structure and optical gain of $\text{GaN}_x\text{Bi}_y\text{As}_{1-x-y}/\text{GaAs}$ pyramidal quantum dots

Zhi-Gang Song,^{1,2} Sumanta Bose,^{1,3} Wei-Jun Fan,^{1,3,a)} and Shu-Shen Li²

¹*School of Electrical and Electronic Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore*

²*State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, P.O. Box 912, Beijing 100083, People's Republic of China*

³*NOVITAS, Centre for Micro-/Nano-electronics, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798, Singapore*

(Received 26 January 2016; accepted 28 March 2016; published online 11 April 2016)

The electronic band structure and optical gain of $\text{GaN}_x\text{Bi}_y\text{As}_{1-x-y}/\text{GaAs}$ pyramidal quantum dots (QDs) are investigated using the 16-band $k \cdot p$ model with constant strain. The optical gain is calculated taking both homogeneous and inhomogeneous broadenings into consideration. The effective band gap falls as we increase the composition of nitrogen (N) and bismuth (Bi) and with an appropriate choice of composition we can tune the emission wavelength to span within $1.3 \mu\text{m}$ – $1.55 \mu\text{m}$, for device application in fiber technology. The extent of this red shift is more profound in QDs compared with bulk material due to quantum confinement. Other factors affecting the emission characteristics include virtual crystal, strain profile, band anticrossing (BAC), and valence band anticrossing (VBAC). The strain profile has a profound impact on the electronic structure, specially the valence band of QDs, which can be determined using the composition distribution of wave functions. All these factors eventually affect the optical gain spectrum. With an increase in QD size, we observe a red shift in the emission energy and emergence of secondary peaks owing to transitions or greater energy compared with the fundamental transition. © 2016 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4945700>]

I. INTRODUCTION

Dilute bismide alloys incorporated in GaAs host material have attracted much attention recently.^{1–6} The increased interest results from its unique electronic band structure and potential application in optoelectronic devices in the infrared regime. Unlike dilute nitrogen alloys, for which the band gap mainly decreases due to the coupling of nitrogen resonant state and conduction band (CB),⁷ the band gap of dilute bismide alloys is tuned by the coupling of the bismide resonant state and valence band (VB). The replacement of a small percentage of arsenic by bismuth in GaAs also introduces the resonant energy level as the presence of nitrogen. This resonant energy level couples with the host material's valence band and repulses each other. Therefore, in the presence of large repulsion interaction, the band gap rapidly decreases and offers the possibility of long-wavelength operation of GaAs-based optical devices. Additionally, for the main non-radiative recombination process, a conduction electron and a heavy hole (HH) recombine while exciting a spin-split-off hole from valence band (CHSH). CHSH Auger recombination⁸ could be suppressed by a large splitting between heavy hole and spin-orbital coupling (SO) introduced from the valence band anticrossing (VBAC). This is essential for real device system. Therefore, if nitrogen and bismuth are doped simultaneously in GaAs,^{9,10} the tuning of the electronic structure will be more controllable and CHSH recombination will be inherited.

Both bulk and quantum well of GaBiAs have attracted lot of interest recently. From the experimentalist's aspect, a lot of work has been done on GaBiAs quantum well.^{1–6} Most of them use molecular beam epitaxy followed by related optical characterization of the bandedge.^{11,12} Theoretically, a lot of work^{13,14} has been done since the 12-band model^{15–19} was proposed based on the valence band anticrossing (VBAC) model. However, not much progress has been made on the study of GaBiAs quantum dots (QDs). As a three-dimensional (3D) confinement structure, the self-assembled QDs are composed of several thousand to million atoms. Based on the 10-band $k \cdot p$ band anticrossing (BAC) model for dilute nitrogen and the VBAC model for dilute bismide, we have built a 16-band $k \cdot p$ model to investigate the electronic structure of $\text{GaN}_x\text{Bi}_y\text{As}_{1-x-y}/\text{GaAs}$ QDs. We know that strain plays an essential role in QDs. Doping with nitrogen alone introduces tensile strain, while doping with bismuth alone introduces compressive strain. Therefore, in $\text{GaN}_x\text{Bi}_y\text{As}_{1-x-y}$, the ratio of N and Bi determines the final strain profile: tensile, zero, or compressive. This eventually affects the optical gain spectrum properties.

This paper is organized as follows: The first part is the Introduction followed by the explanation of the theoretical framework of our calculations. We will give a detailed explanation as our Hamiltonian form is different from O'Reilly's model. Section III is the Results and Discussion. We show the variety of the electronic structure of QDs, wave function distribution, band composition, and optical gain under three kinds of strain. Besides, the size scaling is

^{a)}Electronic mail: ewjfan@ntu.edu.sg

also revealed through the red shift of optical gain. Finally, we summarize the contributions of our work.

II. THEORETICAL MODEL

The 10-band $\mathbf{k} \cdot \mathbf{p}$ model used to study the nitrogen-doped QDs is based on the 8-band model extended by introducing the local nitrogen resonant state (additional 2 bands). Similarly, to investigate the bismuth-doped and nitrogen-doped QDs simultaneously, additional bands have to be added in the model to describe and study the effects of bismuth. Unlike the s -like state introduced by dilute nitride, the dilute bismide results in p -like states, which means that six states should be considered with the spin freedom including the SO coupling which is ignored in the O'Reilly 14-band model for dilute bismide-nitride semiconductors. In view of the above consideration, we have constructed a 16-band model to study the $\text{GaN}_x\text{Bi}_y\text{As}_{1-x-y}$ system. The 16-band

Hamiltonian is represented in the Bloch function basis $|S, \uparrow\rangle, |S, \downarrow\rangle, |11, \uparrow\rangle, |10, \uparrow\rangle, |1-1, \uparrow\rangle, |11, \downarrow\rangle, |10, \downarrow\rangle, |1-1, \downarrow\rangle, |S_N, \uparrow\rangle, |S_N, \downarrow\rangle, |11_{Bi}, \uparrow\rangle, |10_{Bi}, \uparrow\rangle, |1-1_{Bi}, \uparrow\rangle, |11_{Bi}, \downarrow\rangle, |10_{Bi}, \downarrow\rangle, |1-1_{Bi}, \downarrow\rangle$ as

$$H_{16} = \begin{pmatrix} H_{10 \times 10} & H_{10 \times 6} \\ H_{6 \times 10} & H_{6 \times 6} \end{pmatrix} + V_0, \quad (1)$$

where $H_{10 \times 10}$ is the 10-band model to describe the nitrogen-doped system, $H_{6 \times 6}$ is the 6-band model to describe the resonant bismuth states, $H_{10 \times 6}$ is the coupling between the valence band and bismuth states, and the V_0 is the confinement potential of the system, which is zero within the QD. As we use the $|10\rangle, |1-1\rangle, |11\rangle$ basis for the p -like states instead of HH, Light hole (LH) and SO, the form of Hamiltonian is different from the O'Reilly's model and can be transformed into it under an unitary transformation. The details of the every element in $H_{10 \times 10}$ are given as follows:

$$H_{10 \times 10} = \begin{pmatrix} E^C & 0 & \frac{i}{\sqrt{2}}P_-^* & iP_z & \frac{i}{\sqrt{2}}P_+^* & 0 & 0 & 0 & V_N & 0 \\ 0 & E^C & 0 & 0 & 0 & \frac{i}{\sqrt{2}}P_-^* & iP_z & \frac{i}{\sqrt{2}}P_+^* & 0 & V_N \\ -\frac{i}{\sqrt{2}}P_- & 0 & HH & S & R & 0 & 0 & 0 & 0 & 0 \\ -iP_z & 0 & S^* & Q - 2\lambda & S & -\sqrt{2}\lambda & 0 & 0 & 0 & 0 \\ -\frac{i}{\sqrt{2}}P_+ & 0 & R^* & S^* & HH - \lambda & 0 & \sqrt{2}\lambda & 0 & 0 & 0 \\ 0 & -\frac{i}{\sqrt{2}}P_- & 0 & -\sqrt{2}\lambda & 0 & HH - \lambda & S & R & 0 & 0 \\ 0 & -iP_z & 0 & 0 & \sqrt{2}\lambda & S^* & Q - 2\lambda & S & 0 & 0 \\ 0 & -\frac{i}{\sqrt{2}}P_+ & 0 & 0 & 0 & R^* & S^* & HH & 0 & 0 \\ V_N & 0 & 0 & 0 & 0 & 0 & 0 & 0 & E^N & 0 \\ 0 & V_N & 0 & 0 & 0 & 0 & 0 & 0 & 0 & E^N \end{pmatrix}, \quad (2)$$

where

$$E^C = E_g + \frac{\hbar^2}{2m_0}\gamma_c(k_x^2 + k_y^2 + k_z^2) + \delta E^{CB}, \quad (3a)$$

$$HH = -\frac{\hbar^2}{2m_0}\left[\frac{L' + M'}{2}(k_x^2 + k_y^2) + M'k_z^2\right] + \delta E^{HH}, \quad (3b)$$

$$Q = -\frac{\hbar^2}{2m_0}\left[M'(k_x^2 + k_y^2) + L'k_z^2\right] + \delta E^Q, \quad (3c)$$

$$S = -\frac{\hbar^2}{2m_0}\left[\frac{1}{\sqrt{2}}N'(k_x + ik_y)k_z\right] + \delta E_{Strain}^S, \quad (3d)$$

$$R = -\frac{\hbar^2}{2m_0}\left[\frac{L' - M'}{2}(k_x^2 - k_y^2) + iN'k_xk_y\right] + \delta E_{Strain}^R, \quad (3e)$$

$$\delta E^{CB} = -\delta E_{VC}^{CB} + \delta E_{Strain}^{CB}, \quad (3f)$$

$$\delta E^{HH} = \delta E_{VC}^{HH} + \delta E_{Strain}^{HH}, \quad (3g)$$

$$\delta E^Q = \delta E_{VC}^Q + \delta E_{Strain}^Q, \quad (3h)$$

$$P_- = p_0(k'_x - ik'_y), \quad (3i)$$

$$P_+ = p_0(k'_x + ik'_y), \quad (3j)$$

$$P_z = p_0k'_z, \quad (3k)$$

$$k'_x = k_x - \epsilon_{xx}k_x - \epsilon_{xy}k_y - \epsilon_{xz}k_z, \quad (3l)$$

$$k'_y = k_y - \epsilon_{yz}k_y - \epsilon_{yy}k_y - \epsilon_{yz}k_z, \quad (3m)$$

$$k'_z = k_z - \epsilon_{xz}k_x - \epsilon_{yz}k_y - \epsilon_{zz}k_z, \quad (3n)$$

$$p_0 = \hbar \sqrt{E_p/2m_0}, \quad (3o)$$

$$V_N = \beta_N \sqrt{x}, \quad (3p)$$

$$\gamma_c = \frac{m_0}{m_c} - \frac{E_p}{3} \left(\frac{2}{E_g} + \frac{1}{E_g + 3\lambda} \right), \quad (3q)$$

$$L' = L - \frac{E_p}{E_g}, \quad (3r)$$

$$M' = M, \quad (3s)$$

$$N' = N - \frac{E_p}{E_g}, \quad (3t)$$

$$\lambda = \Delta_{SO}/3. \quad (3u)$$

The δE_{VC} and δE_{Strain} are contributions from the virtual crystal (VC) and strain factors. The relevant terms will be subsequently explained.

The nitrogen/bismuth composition-dependent terms depending on α_N/α_{Bi} , κ_N/κ_{Bi} , and γ_N/γ_{Bi} describe the VC contributions to the band edges. Other terms corresponding to the strain are added as the VC effect. They vary from the forms given by O'Reilly (14-band model)¹⁵ since our basis is different from the Kane's. Here, we give the details about the VC and strain terms

$$\delta E_{VC}^{CB} = \alpha_N x + \alpha_{Bi} y, \quad (4a)$$

$$\delta E_{VC}^{HH} = \kappa_N x + \kappa_{Bi} y, \quad (4b)$$

$$\delta E_{VC}^Q = \frac{1}{3} (2\kappa_N - \gamma_N) x + \frac{1}{3} (2\kappa_{Bi} - \gamma_{Bi}) y, \quad (4c)$$

$$\delta E_{Strain}^{CB} = a_c (\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}), \quad (4d)$$

$$\delta E_{Strain}^{HH} = \left(a_v + \frac{b}{2} \right) (\epsilon_{xx} + \epsilon_{yy}) + (a_v - b) \epsilon_{zz}, \quad (4e)$$

$$\delta E_{Strain}^Q = (a_v - b) (\epsilon_{xx} + \epsilon_{yy}) + (a_v + 2b) \epsilon_{zz}, \quad (4f)$$

$$\delta E_{Strain}^S = \sqrt{6} (d \epsilon_{xz} - i \epsilon_{yz}), \quad (4g)$$

$$\delta E_{Strain}^R = \frac{3}{2} b (\epsilon_{xx} - \epsilon_{yy}) - i 2 \sqrt{3} d \epsilon_{xy}. \quad (4h)$$

The strain tensor can be calculated as follows:

$$\epsilon_{xx} = \epsilon_{yy} = \frac{a(\text{GaAs}) - a(\text{GaNBiAs})}{a(\text{GaNBiAs})}, \quad (5)$$

$$\epsilon_{zz} = -\frac{2C_{12}}{C_{11}} \epsilon_{xx}, \quad (6)$$

where

$$a(\text{GaNBiAs}) = (1 - x - y)a(\text{GaAs}) + xa(\text{GaN}) + ya(\text{GaBi}). \quad (7)$$

Here, we assume that the non-diagonal terms to be zero and take only the diagonal terms into consideration. Due to the unavailability of the strain parameters of GaBi, we have used the host parameters instead.¹⁷ The coupling matrix $H_{10 \times 6}$ is

$$H_{10 \times 6} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ V_{Bi} & 0 & 0 & 0 & 0 & 0 \\ 0 & V_{Bi} & 0 & 0 & 0 & 0 \\ 0 & 0 & V_{Bi} & 0 & 0 & 0 \\ 0 & 0 & 0 & V_{Bi} & 0 & 0 \\ 0 & 0 & 0 & 0 & V_{Bi} & 0 \\ 0 & 0 & 0 & 0 & 0 & V_{Bi} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad (8)$$

and

$$H_{6 \times 10} = H_{10 \times 6}^\dagger, \quad (9)$$

where

$$V_{Bi} = \beta_{Bi} \sqrt{y}. \quad (10)$$

The last bismuth resonant Hamiltonian term is

$$H_{6 \times 6} = \begin{pmatrix} K & F & G & 0 & 0 & 0 \\ F^* & V2 & F & T & 0 & 0 \\ G^* & F^* & V3 & 0 & -T & 0 \\ 0 & T & 0 & V3 & F & G \\ 0 & 0 & -T & F^* & V2 & F \\ 0 & 0 & 0 & G^* & F^* & K \end{pmatrix}, \quad (11)$$

where

$$K = E_{Bi}^{HH} + \left(a_{Bi} + \frac{b_{Bi}}{2} \right) (\epsilon_{xx} + \epsilon_{yy}) + (a_{Bi} - b_{Bi}) \epsilon_{zz}, \quad (12a)$$

$$V2 = \frac{1}{3} \left(2E_{Bi}^{LH} + E_{Bi}^{SO} \right) + (a_{Bi} - b_{Bi}) (\epsilon_{xx} + \epsilon_{yy}) + (a_{Bi} + 2b_{Bi}) \epsilon_{zz}, \quad (12b)$$

$$V3 = \frac{1}{3} \left(E_{Bi}^{LH} + 2E_{Bi}^{SO} \right) + \left(a_{Bi} + \frac{b_{Bi}}{2} \right) (\epsilon_{xx} + \epsilon_{yy}) + (a_{Bi} - b_{Bi}) \epsilon_{zz}, \quad (12c)$$

$$T = \frac{\sqrt{2}}{3} \left(E_{Bi}^{SO} - E_{Bi}^{LH} \right), \quad (12d)$$

$$F = \sqrt{6} d_{Bi} \epsilon_{xz} - i \sqrt{6} d_{Bi} \epsilon_{yz}, \quad (12e)$$

$$G = \frac{3}{2} b_{Bi} (\epsilon_{xx} - \epsilon_{yy}) - i 2 \sqrt{3} d_{Bi} \epsilon_{xy}. \quad (12f)$$

This concludes the description of the Hamiltonian for the $\text{GaN}_x\text{Bi}_y\text{As}_{1-x-y}$ system and the related parameters as listed in Tables I and II. These parameters are mainly from several works^{15,17} and other GaAs-related papers.²⁰⁻²³ We assume that the QDs are periodically arranged in three dimensions and with the period L_x , L_y , and L_z . We have used the plane waves to expand the basis as follows:

$$\Phi_m = \{\Phi_m^j\} (j = 1, 2, \dots, 16), \quad (13)$$

TABLE I. Parameters of VC, BAC, and VBAC used in calculation of GaN_xBi_yAs_{1-x-y}/GaAs bandstructure taken from Refs. 15, 17, and 19.

Parameter	Bi	N
α (eV)	2.82 ^a	-1.15 ^a
κ (eV)	1.01 ^a	1.36 ^a
γ (eV)	0.55 ^a	-1.53 ^a
β (eV)	1.13 ^b	1.76 ^a
E (eV)	-0.183 ^a	1.706 ^a
Δ_{SO} (eV)	-1.9 ^c	
a_{Bi} (eV)	-1.11 ^b	
b_{Bi} (eV)	-1.71 ^b	
d_{Bi} (eV)	0 ^d	

^aFrom Ref. 15.^bFrom Ref. 17.^cFrom Ref. 19.^dThis parameter is set as 0 as there is no distinct value available in literature.

with

$$\Phi_m^j = \frac{1}{\sqrt{V}} \sum_{n_x, n_y, n_z} a_{m, n_x, n_y, n_z}^j \exp[i(k_{nx}x + k_{ny}y + k_{nz}z)], \quad (14)$$

where $V = L_x L_y L_z$, $k_{nx} = \frac{2\pi n_x}{L_x}$, $k_{ny} = \frac{2\pi n_y}{L_y}$, $k_{nz} = \frac{2\pi n_z}{L_z}$, and n_x , n_y , and n_z are the integer of plane wave numbers. Here, we set the range of these plane wave numbers from -3 to 3. The j is the index of basis.

For GaN_xBi_yAs_{1-x-y}/GaAs pyramidal QDs, the geometry schematic is shown in Fig. 1 with the direction of the pyramid growth along the positive z axis. The doped nitrogen and bismuth atoms are distributed in crystalline throughout the QD. A 3D view of a typical pyramidal QD with the wetting layer is shown in Fig. 2(a), and Fig. 2(b) shows its top view.

The optical gain spectrum with homogeneous broadening is calculated as

$$G(E) = \frac{\pi e^2 \hbar}{m_0^2 \epsilon_0 n_r c E} \sum_{n_c, n_v} \frac{1}{V} |M^{cv}|^2 (f_c + f_v - 1) \frac{1}{\pi} B_{cv}(E - E_{cv}), \quad (15)$$

where E_{cv} is the transition energy and f_c and f_v are the Fermi-Dirac distribution for electrons and holes in CB and VB, respectively. The M^{cv} is the optical transition matrix element and can be calculated as

$$M_i^{cv} = \langle \psi_{n_v, k} | \hat{p}_i | \psi_{n_c, k} \rangle, \quad i = x, y, z, \quad (16)$$

where $\hat{p}_i$ is the momentum operator, and $\psi_{n_v, k}$ ($\psi_{n_c, k}$) is the hole (electron) wave function. An example is given here to show the details of M_i^{cv} calculation

FIG. 1. The geometry schematic of the pyramidal QDs in the side view. The height (H), width ($2H$), and dimensions of the system are an integer multiple of the lattice constant.

$$M_x^{cv} = \frac{p_0}{\sqrt{2}} \sum_{n_x, n_y, n_z} \left(a_{v, n_x, n_y, n_z}^2 + a_{v, n_x, n_y, n_z}^4 \right) a_{c, n_x, n_y, n_z}^{1*} + \left(a_{v, n_x, n_y, n_z}^7 + a_{v, n_x, n_y, n_z}^9 \right) a_{c, n_x, n_y, n_z}^{6*} + \left(a_{c, n_x, n_y, n_z}^{2*} + a_{c, n_x, n_y, n_z}^{4*} \right) a_{v, n_x, n_y, n_z}^1 + \left(a_{c, n_x, n_y, n_z}^{7*} + a_{c, n_x, n_y, n_z}^{9*} \right) a_{v, n_x, n_y, n_z}^6, \quad (17)$$

where $p_0 = \langle S | p_x | X \rangle$. Other terms such as M_y^{cv} and M_z^{cv} can be calculated like M_x^{cv} . Taken the symmetry of x and y directions into consideration, we take the average of M_x^{cv} and M_y^{cv} as the transverse electric (TE) mode and M_z^{cv} as transverse magnetic (TM) mode. Due to this symmetry of QD, the TE mode involves both the HH and LH states, while the TM involves only LH state. Note that the transition of optical gain is primarily due to the CB1-VB1 transition. The hole type (HH or LH) of VB1 determines the mode that gets excited. However, in reality, for our QD systems, the VB1 is mostly HH state for unstrained, compressive strain, and relatively small tensile strain. Therefore, we only show the results of TE mode in our optical transition calculation. All our calculation is done by assuming that the height of the QD is $12H$ except the size effect part.

III. RESULTS AND DISCUSSION

We study the variation in the CB, VB, and band gap under different strain profile types: compressive, *near-zero* (an appropriate choice of N and Bi composition can help us to minimize the strain close to but not equal to zero), and tensile strain. We consider the first 6 conduction band labeled as CB1 to CB6 and the first 6 valence band as VB1 to VB6. Bands beyond this are too far to couple for practical purposes. Figs. 3, 4, and 5 show three cases of GaN_xBi_yAs_{1-x-y}/GaAs pyramidal QDs undergoing positive,

TABLE II. Parameters of GaAs used in calculation are taken from Refs. 20 and 23.

a (nm)	E_p (eV)	E_g (eV)	L	M	N	Δ_{SO} (eV)	a_c (eV)	a_v (eV)	b (eV)	d (eV)
0.565325 ^a	25.5 ^a	1.422 ^b	18.4 ^a	3.77 ^a	19.6 ^a	0.341 ^a	-7.17 ^b	1.16 ^b	-1.7 ^b	-4.55 ^b

^aFrom Ref. 20.^bFrom Ref. 23.

FIG. 2. (a) 3D view and (b) top view of a typical pyramidal QDs structure. Here, we only draw the anions. The purple balls represent the As atoms, blue balls represent the N atoms, and yellow balls represent the Bi atoms. Impurity in the form of N and Bi is distributed uniformly.

near-zero, and negative strain (i.e., tensile, near-zero, and compressive strain). For each case, we have studied the four contributing factors to band edge characteristics—VC, strain, BAC, and VBAC. BAC is induced from doped nitrogen and VBAC is induced from doped bismuth. A stronger BAC lowers the CB1 level further, while a stronger VBAC elevates the VB1 level even further. Under the influence of BAC and VBAC, the band gap decreases rapidly. The other two factors: VC and strain also change the band edge characteristics. For VC, from the theoretical model, we have $\delta E_{VC}^{HH} = \kappa_N x + \kappa_{Bi} y$ and $-\delta E_{VC}^{CB} = -(\alpha_N x + \alpha_{Bi} y)$. Here, we take VB1 band as HH-related term since HH is the dominant hole type

in this band as we can see from the band mixing probability results. Obviously, δE_{VC}^{HH} is positive as the parameters κ_N and κ_{Bi} are both positive. However, the sign of $-\delta E_{VC}^{CB} = -(\alpha_N x + \alpha_{Bi} y)$ is dependent on the choice of the N and Bi composition, i.e., x and y . This is negative for all our three cases studied here. Therefore, in our cases, the CB1 will be lowered, while VB1 will be elevated induced by VC effect. This can explain the variation in the CB1 and VB1 induced by VC in frame (a) of Figs. 3, 4, and 5. Likewise, the variation induced by strain can also be explained in a similar way. The sign of the ϵ_{xx} directly determines the mobility of the CB1 and VB1. As the model says, $\delta E_{strain}^{CB} = a_c(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})$ and $\delta E_{strain}^{HH} = a_v(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})$ (without the b related terms as its magnitude is too small compared with the a_v related terms). Thus, δE_{strain}^{CB} will be positive (negative) while δE_{strain}^{HH} will be of opposite sign when the $\epsilon_{xx} < 0$ ($\epsilon_{xx} > 0$) when a_c is negative and a_v is positive.

Frame (b) of Figs. 3, 4, and 5 shows the band mixing probabilities and energy band structure profile for different strain types occurring from different N and Bi compositions. The conduction band is mainly made of CB state and N state with minimal composition of HH, LH, and SO which come from the coupling between CB and these bands. For different valence bands, the fraction of HH and LH contributions is different. The VBAC couples with the HH (LH) as HH_{Bi} (LH_{Bi}). As a result, the composition of HH_{Bi} is greater than (less than) LH_{Bi} where the composition of HH is greater than (less than) the LH.

Frame (c) of Figs. 3, 4, and 5 shows the contour plot of the charge density (square of the absolute wave function $|\psi|^2$) for the CB1–CB6 and VB1–VB6 bands in QD whose height is $H = 12a$, where a is the lattice constant of the host material. The first two rows in each case represent the charge densities in the x – y plane and the second two rows in the y – z plane. The CB1 is s -like, and CB2 and CB3 are both p -like for the three cases although the strain is different. The s – p splitting is

FIG. 3. For $\text{GaN}_{0.064}\text{Bi}_{0.064}\text{As}_{0.872}/\text{GaAs}$ QDs, $\epsilon_{xx} = +0.005$: (a) The schematic illustration of the VC, strain, BAC, and VBAC. Here, we show their independent influences. (b) The band mixing probabilities and the energy band structure profile. (c) The charge densities (square of the wave function) of the lowest 6 CBs and highest 6 VBs. The first two rows are in the x – y plane and the second two rows are in the y – z plane. (d) The optical gain under four different carrier densities in the order of 10^{18}cm^{-3} . Next, two figures also show the similar results. The different is only the concentration of nitrogen and bismuth doped.

FIG. 4. GaN_{0.016}Bi_{0.027}As_{0.957}/GaAs QDs, $\epsilon_{xx} \simeq 0.00$. (a) Here, the strain hardly affects the band structure of QD as the strain nearly equal to be zero. The C1 and V1 do not change when the strain is introduced. The component of the 12-bands and distribution of wave function are similar to Fig. 3. The peak of optical gain moves to right compared with Fig. 3(d).

defined as $\Delta_{sp} = E_{CB2} - E_{CB1}$. In our cases, the related Δ_{sp} are 95 meV, 62 meV, and 69 meV for Figs. 3, 4, and 5, respectively. The two p -like states are in fact degenerate due to the C_{4v} symmetry instead of C_{2v} in our $\mathbf{k} \cdot \mathbf{p}$ model. The next three bands are different for the different signs of the ϵ_{xx} . The CB4 is s -like while the CB5 and CB6 are d -like when the sign of the ϵ_{xx} is positive. For negative ϵ_{xx} , the CB4 and CB6 are d -like, while the CB5 is p -like. For the valence band in QD with 3D confinement, the band mixing is so strong that they cannot be classified into a single explicit band according to their nodal structure like CB. In our system, not only the host's HH, LH, and SO bands but also the bismuth-related HH, LH, and SO mix together as is evident from frame (b) of Figs. 3, 4, and 5. However, we can classify the bands

according to the highest contributing hole type among HH, LH, and SO. For example, in VB1, the fraction of HH is highest, thus we regard this as an HH band. For the first 6 VBs, HH and LH dominate primarily for all the compositions. Thus far, we have seen the influence of strain on the CB and VB. Here, through the wave function, more insight can be revealed. Since the strain is isotropic in our model, the splitting due to the strain arises first in CB4. The sign of ϵ_{xx} has a profound influence on the wave function characteristics.

Frame (d) of Figs. 3, 4, and 5 shows the optical gain for the TE mode for different carrier densities in the order of 10^{18} cm^{-3} . For a sufficiently high carrier density, we obtain a secondary peak in addition to the primary peak. The position of the peak is determined directly by the effective band gap

FIG. 5. GaN_{0.013}Bi_{0.064}As_{0.923}/GaAs QDs, $\epsilon_{xx} = -0.005$. (a) Here, the compressive strain increases the band gap. The distribution of wave functions has some differences compared with the above two cases for the compressive strain. (d) The peak of optical gain also moves.

(CB1-VB1). Therefore, strain has an influence on the optical gain as it can alter the peak position by altering the effective band gap. The peak broadening due to inhomogeneous effects is considered in our model.

So far, we have investigated the electronic band structure, wave function, and optical gain spectrum for three typical sample of QDs with different kinds of strain. Now, we offer a more general picture of the variation of CB1, VB1, band gap, and strain (ϵ_{xx}) with different combinations of N and Bi compositions as shown in Fig. 6. It displays the variation in CB1 and VB1 for varying compositions, which is mainly affected by the differences in BAC and VBAC. Further, yet another interesting aspect attracts our attention. When we fix the nitrogen composition, the CB1 remains close to the origin level with little change, while the VB1

FIG. 6. (a) and (b) The variation in CB1, VB1, and bandgap with the composition of doped nitrogen and bismuth. (c) The contour of the bandgap and strain with the composition of doped nitrogen and bismuth. As the nitrogen and bismuth are doped uniformly, the composition of the two impurities is discrete. Therefore, the isopotential lines of the strain and bandgap are not continuous.

increases nearly linearly. On the other hand, when we fix the composition of bismuth at low density and vary the composition of nitrogen, both the CB1 and VB1 change. It is of considerable interest to reason why the variation of CB1 is little in first case and the VB1 is relatively large in second case. We can give an explanation in the view of VC and strain for the above scheme. The variation induced by VC is $\delta E_{VC}^{CB} = -\alpha x$ and $\delta E_{VC}^{HH} = \kappa x$ and that induced by strain is $\delta E_{strain}^{CB} = a_c(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})$ and $\delta E_{strain}^{HH} = a_v(\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz})$. From Table II, we know that the sign of α for nitrogen is negative while for bismuth is positive, and the sign of a_c is negative while a_v is positive. Larger bismuth composition means decreasing the δE_{VC}^{CB} and increasing the δE_{strain}^{CB} for a fixed nitrogen composition. These two effects partially cancel the contribution to the CB1, resulting in little variation in CB1. Likewise, greater nitrogen composition means increasing δE_{VC}^{HH} and δE_{strain}^{HH} . These two effects together lift the VB1 even higher when we fix the bismuth composition and vary the nitrogen. Fig. 6(b) illustrates this variation in the band gap. A linear decrement of the band gap occurs at a rate of ~ 36 meV for 1% variation. Compared with the bulk materials,¹⁵ the band gap decrement rate of the in QDs is lesser than that of bulk materials. This can be understood in the view of quantum confinement, as we shall see in the case of size scaling. Here, we do not show the variation of SO as a strong mixing in QDs among HH, LH, and SO. Although we have redefined the band considering their major contributors among HH and LH, but still we cannot point where the SO starts. This is different from the bulk states. The effective band gap of $\text{GaN}_x\text{Bi}_y\text{As}_{1-x-y}/\text{GaAs}$ pyramidal QDs can be tuned by varying the composition of N and Bi, such that the emission wavelength spans the range of $1.3 \mu\text{m}$ – $1.55 \mu\text{m}$, suitable for device applications in fiber technology. Fig. 6(c) shows the contour of the band gap and ϵ_{xx} varying with N and Bi composition. This picture gives a more clear way to decrease the band gap along the zero strain line. This is essential in real experimental systems.

The size of the QD is another important design parameter while considering its optical gain characteristics. Due to 3D confinement, the quantum effect is more obvious with the size decrease in QDs. Comparing the results of the rate of the band gap decrement (81 meV for 0.1% variation) in the $\text{GaBi}_y\text{As}_{1-y}$ system in our case, the quantum confinement slows down the decrement rate. This means that for sufficiently large QDs, the decrement rate will tend to that in bulk material. This phenomenon can be proved from the shift of the peaks. Fig. 7 confirms these predictions. In Fig. 7, we set three different sizes of QD as $H = 12a$, $16a$, and $20a$, where a is the lattice constant of the host material, GaAs in our case. The carrier density is fixed at 6×10^{-3} for all the four cases of Fig. 7 with varying N and Bi compositions. Besides the red shift, another interesting phenomenon about the number of the peak is noteworthy. For the $H = 12a$, there is only 1 peak while for the $H = 16a$ there are 2 peaks, and even 4 peaks for $H = 20a$. Large size of the QDs means smaller subband gap which is more easy to be excited. Different peaks describe different transitions between levels of CB and VB. Thus, we need to determine where the transitions take place. This can be done with the help of the

FIG. 7. The optical gain for different sizes of QDs when the carrier density is fixed ($6 \times 10^{18} \text{ cm}^{-3}$). Four different N and Bi composition combinations are shown here. The shift of the first peak is obvious as the band gap decreases with larger QDs.

location of polarized matrix element. Taking Fig. 7(d) as an example with considering the $H = 16a$ and $20a$, the second peak comes from the transition between CB3 and VB5.

IV. CONCLUSIONS

We have investigated the electronic band structure and optical gain characteristics of $\text{GaN}_x\text{Bi}_y\text{As}_{1-x-y}/\text{GaAs}$ pyramidal quantum dot systems by 16-band $k \cdot p$ model. The band gap is affected from VC, strain, BAC, and VBAC. We obtain clear insights on how these factors influence the electronic structure. Additionally, we give the best line to decrease the band gap along the zero-strain line. This can be used in the device applications in the range of $1.3 \mu\text{m}$ – $1.55 \mu\text{m}$ fiber technology. At the same time, the results of size scaling tell us which transition will be excited more easily. This is very important for lasers amplifiers.

ACKNOWLEDGMENTS

W.-J. Fan would like to acknowledge the support from MOE Tier 1 funding RG 182/14. S.-S.L. would like to acknowledge the support from NSFC No. 61427901.

- ¹G. Vardar, S. W. Paleg, M. V. Warren, M. Kang, S. Jeon, and R. S. Goldman, *Appl. Phys. Lett.* **102**, 042106 (2013).
- ²R. D. Richards, F. Bastiman, C. J. Hunter, D. F. Mendes, A. R. Mohmad, J. S. Roberts, and J. P. R. David, *J. Cryst. Growth* **390**, 120–124 (2014).
- ³F. Bastiman, A. R. B. Mohmad, J. S. Ng, J. P. R. David, and S. J. Sweeney, *J. Cryst. Growth* **338**, 57–61 (2012).
- ⁴M. K. Shakfa, D. Kalincev, X. Lu, S. R. Johnson, D. A. Beaton, T. Tiedje, A. Chernikov, S. Chatterjee, and M. Koch, *J. Appl. Phys.* **114**, 164306 (2013).

- ⁵G. Ciatto, E. C. Young, F. Glas, J. Chen, R. Alonso Mori, and T. Tiedje, *Phys. Rev. B* **78**, 035325 (2008).
- ⁶S. Mazzucato, P. Boonpeng, H. Carrere, D. Lagarde, A. Arnoult, G. Lacoste, T. Zhang, A. Balocchi, T. Amand, X. Marie, and C. Fontaine, *Semicond. Sci. Technol.* **28**, 022001 (2013).
- ⁷J. Wu, W. Walukiewicz, and E. E. Haller, *Phys. Rev. B* **65**, 233210 (2002).
- ⁸S. J. Sweeney, A. R. Adams, M. Silver, E. P. O'Reilly, J. R. Watling, A. B. Walker, and P. J. A. Thijs, *Phys. Status Solidi B* **211**, 525 (1999).
- ⁹S. J. Sweeney and S. R. Jin, *J. Appl. Phys.* **113**, 043110 (2013).
- ¹⁰S. Tixer, S. E. Webster, E. C. Young, T. Tiedje, S. Francoeur, A. Mascarenhas, P. Wei, and F. Schiettekatte, *Appl. Phys. Lett.* **86**, 112113 (2005).
- ¹¹M. Beaudoin, R. B. Lewis, J. J. Andrews, V. B. Yekta, M. M. Shirazi, S. K. O'Leary, and T. Tiedje, *J. Cryst. Growth* **425**, 245–249 (2015).
- ¹²C. Gogineni, N. A. Riordan, S. R. Johnson, X. F. Lu, and T. Tiedje, *Appl. Phys. Lett.* **103**, 041110 (2013).
- ¹³R. Alaya, M. Mbarki, and A. Rebey, *Mater. Sci. Semicond. Process.* **40**, 925–930 (2015).
- ¹⁴M. M. Habchi, A. B. Nasr, A. Rebey, and B. E. Jani, *Infrared Phys. Technol.* **67**, 531–536 (2014).
- ¹⁵C. A. Broderick, M. Usman, and E. P. O'Reilly, *Semicond. Sci. Technol.* **28**, 125025 (2013).
- ¹⁶C. A. Broderick, M. Usman, S. J. Sweeney, and E. P. O'Reilly, *Semicond. Sci. Technol.* **27**, 094011 (2012).
- ¹⁷C. A. Broderick, P. E. Harnedy, P. Ludewig, Z. L. Bushell, K. Volz, R. J. Manning, and E. P. O'Reilly, *Semicond. Sci. Technol.* **30**, 094009 (2015).
- ¹⁸M. Usman, C. A. Broderick, A. Lindsay, and E. P. O'Reilly, *Phys. Rev. B* **84**, 245202 (2011).
- ¹⁹B. Breddermann, A. Baumner, S. W. Koch, P. Ludewig, W. Stolz, K. Volz, J. Hader, J. V. Moloney, C. A. Broderick, and E. P. O'Reilly, *J. Lumin.* **154**, 95–98 (2014).
- ²⁰X. W. Zhang, Y. H. Zhu, and J. B. Xia, *Physics E* **33**, 376–380 (2006).
- ²¹K. Alberi, J. Wu *et al.*, *Phys. Rev. B* **75**, 045203 (2007).
- ²²Y. X. Dang and W. J. Fan, *Phys. Rev. B* **77**, 125334 (2008).
- ²³J. Chen, W. J. Fan, Q. Xu, X. W. Zhang, S. S. Li, and J. B. Xia, *J. Appl. Phys.* **105**, 123705 (2009).